Surface Science Division
Fachverband Oberflächenphysik (O)

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Overview of Invited Talks and Sessions

(lecture rooms HE 101, H 2013, MA 005, MA 041, MA 042, MA 043, A 053, A 060; poster areas Poster B and Poster E)

Invited Talks

O 1.1	Mon	9:30–10:15	HE 101	**Spin LEGOs - Bottom-up Fabrication of Model Magnetic Systems** — •Alexander Ako Khajetoorians
O 9.1	Mon	15:00–15:45	H 2013	**Three dimensional dynamic force spectroscopy at room temperature** — •Shigeki Kawai, Ernst Meyer
O 22.1	Tue	9:30–10:15	HE 101	**Surface science approach to supported metal catalyst preparation - from UHV to metal deposition from solution** — •Martin Sterrer
O 36.1	Wed	9:30–10:15	HE 101	**Exploring the Physics of Graphene with Local Probes** — •Joseph A. Stroscio
O 48.1	Wed	15:00–15:45	HE 101	**Extending the scanning probe toolbox in a molecular playground** — •Ruslan Temirov
O 49.1	Wed	15:45–16:30	HE 101	**Analogies between surface science and electrochemistry** — •Timo Jacob
O 59.1	Thu	9:30–10:15	HE 101	**Electronic transport, Joule-heating, and current-driven dynamics in molecular contacts - theory and simulations** — •Mads Brandbyge, Jing-Tao Lü, Tue Gunst, Per Hedegård
O 70.1	Thu	15:00–15:45	HE 101	**First-principles experiment on electrical conductivity of organic devices with UPS: Charge delocalization, vibration coupling and band-gap states** — •Nobuo Ueno
O 82.1	Fri	9:30–10:15	HE 101	**Nanochemistry with functional molecules - a 2D perspective** — •Willi Auwärter
O 92.1	Fri	13:15–14:00	HE 101	**From surface to interface physics: Hard x-ray photoemission spectroscopy of oxide heterostructures** — •Ralph Claessen

Invited Talks Focussed Session: Frontiers of electronic structure theory: Strong correlations from first principles (jointly with TT)

O 2.1	Mon	10:30–11:00	HE 101	**Non Uniform Polarizability and Coulomb interactions in Compounds and Interfaces** — •George Sawatzky
O 2.6	Mon	12:00–12:30	HE 101	**Actual theoretical trends in angle resolved photoemission: correlation, disorder and temperature effects** — •Ján Minár
O 25.1	Tue	10:30–11:00	HE 101	**Iron Pnicitdes and Chalchogenides: a New Class of Strongly Correlated Electron Systems.** — •Gabriel Kotliar
O 63.1	Thu	10:30–11:00	HE 101	**Random phase approximation and GW for correlated systems** — •Patrick Rinke
O 73.1	Thu	16:00–16:30	HE 101	**Symmetry Breaking and Restoration in Electronic Structure Theory** — •Gustavo Scuseria
O 84.1	Fri	10:30–11:00	HE 101	**Dynamically screened Coulomb interaction and GW self-energy in transition metal compounds** — •Takashi Miyake
O 84.8	Fri	12:30–13:00	HE 101	**Density-functional theory - time to move on?** — •Nicola Marzari

Invited Talks Focussed Session: Functional molecules at surfaces

O 30.2	Tue	10:45–11:15	A 053	**Surface-supported molecular assemblies: insight from scanning tunneling microscopy and photoemission experiments** — •Meike Stöhr
O 30.3	Tue	11:15–11:45	A 053	**How metal surfaces control adsorbate functionality: cooperativity, adatoms, and substrate interactions** — •Felix Hanke
O 44.1	Wed	10:30–11:00	A 053	**Scanning Tunneling Spectroscopy and Atomic Force Microscopy of Functional Molecules on Thin Insulating Films** — •Jascha Repp
O 44.2	Wed	11:00–11:30	A 053	**Conductance switching and quantum interference in molecular junctions** — •Sense Jan van der Molen
O 68.1	Thu	10:30–11:00	A 053	**Frontier Nanoscience: Molecular Superconductors to Molecular Machines** — •SAW WAI Hla
O 68.2	Thu	11:00–11:30	A 053	**Directional motion of a four-wheeled molecule on a metal surface** — •Manfred Parschau
O 68.3	Thu	11:30–12:00	A 053	**Charge transfer dynamics in assemblies of functional molecules** — •Michael Zharnikov

Invited Talks Focussed Session: Coherence and coherent control in nanophotonics and plasmonics

O 40.1	Wed	10:30–11:00	MA 005	**Active control of light propagation in nanophotonic structures** — •Kobus Kuipers
O 40.2	Wed	11:00–11:30	MA 005	**Coherent exciton-plasmon coupling in metal-dye hybrid nanostructures** — •Erich Runge
O 40.3	Wed	11:30–12:00	MA 005	**Control and spectroscopy of plasmonic systems using ultrafast pulse shaping** — •Tobias Brixner, Martin Aeschlimann, Walter Pfeiffer
O 52.1	Wed	16:45–17:15	MA 005	**Spatio-temporal focusing of ultrashort pulses through scattering media** — •Yaron Silberberg
O 52.2	Wed	17:15–17:45	MA 005	**Attosecond control of electrons laser-emitted from a nanoscale metal tip** — •Peter Hommelhoff, Michael Krüger, Markus Schenk, Michael Förster, Georg Wachter, Christoph Lemell, Joachim Burgdörfer
O 52.3	Wed	17:45–18:15	MA 005	**Theory of quantum control of semiconductor quantum dots in complex environments** — Andreas Knorr, •Julia Kabuss, Alexander Carmele, Sverre Theuerholz, Marten Richter

Gaede Prize Talk

O 33.1	Tue	13:30–14:00	HE 101	**Material Design by Atomic Layer Deposition** — •Mato Knez

Invited talks of the joint symposium SYTI

See SYTI for the full program of the symposium.

SYTI 1.1	Tue	9:30–10:00	H 0105	**Search for Majorana fermions in topological insulators** — •Carlo Beenakker
SYTI 1.2	Tue	10:00–10:30	H 0105	**Cooper Pairs in Topological Insulator Bi_2Se_3 Thin Films Induced by Proximity Effect** — •Jinfeng Jia
SYTI 1.3	Tue	10:30–11:00	H 0105	**Gate tunable normal and superconducting transport through a 3D topological insulator** — •Alberto Morpurgo
SYTI 1.4	Tue	11:00–11:30	H 0105	**Weyl Metal States and Surface Fermi Arcs in Iridates** — •Sergey Savrasov
SYTI 1.5	Tue	11:30–12:00	H 0105	**Engineering a Room-Temperature Quantum Spin Hall State in Graphene via Adatom Deposition** — •Marcel Franz

Sessions

O 1.1–1.1	Mon	9:30–10:15	HE 101	**Invited talk (Alexander Ako Khajetoorians)**
O 2.1–2.9	Mon	10:30–13:15	HE 101	**Focussed session: Frontiers of electronic structure theory: Strong correlations from first principles I (jointly with TT)**
O 3.1–3.10	Mon	10:30–13:00	MA 005	**Plasmonics and nanooptics I**
O 4.1–4.10	Mon	10:30–13:00	MA 041	**Graphene I**
O 5.1–5.11	Mon	10:30–13:15	MA 042	**Adsorption on semiconductors, oxides and insulators I**
O 6.1–6.10	Mon	10:30–13:00	MA 043	**Scanning probe methods I**
O 7.1–7.10	Mon	10:30–13:00	A 053	**Metal substrates: Adsorption of organic / bio molecules I**
O 8.1–8.10	Mon	10:30–13:00	A 060	**Electron and spin dynamics**
O 9.1–9.1	Mon	15:00–15:45	H 2013	**Invited talk (Shigeki Kawai)**
O 10.1–10.5	Mon	15:00–17:00	H 0111	**[DS] Focused electron beam induced processing for the fabrication of nanostructures I (focused session, jointly with O – Organizers: Huth, Marbach)**
O 11.1–11.4	Mon	15:00–16:15	H 2032	**[DS] Organic electronics and photovoltaics I (jointly with CPP, HL, O)**
O 12.1–12.13	Mon	16:00–19:15	H 2013	**Surface dynamics**
O 13.1–13.11	Mon	16:00–18:45	MA 005	**Polymeric biomolecular films**
O 14.1–14.12	Mon	16:00–19:00	MA 041	**Adsorption on semiconductors, oxides and insulators II**
O 15.1–15.12	Mon	16:00–19:00	MA 042	**Heterogeneous catalysis I**
O 16.1–16.10	Mon	16:00–18:30	MA 043	**Scanning probe methods II**
O 17.1–17.5	Mon	16:00–17:15	A 053	**Nanotribulogy**
O 18.1–18.6	Mon	16:00–17:30	A 060	**Spin-orbit interaction**
O 19.1–19.6	Mon	17:30–19:00	A 053	**Clean surfaces I**
O 20.1–20.5	Mon	17:45–19:00	A 060	**Theoretical methods I**
O 21.1–21.6	Mon	17:45–19:15	H 1012	**[MA] Joint Session "Topological Insulators I" (jointly with DS, HL, O, TT)**
O 22.1–22.1	Tue	9:30–10:15	HE 101	**Invited talk (Martin Sterrer)**
O 23.1–23.5	Tue	9:30–11:30	H 0111	**[DS] Focused electron beam induced processing for the fabrication of nanostructures II (focused session, jointly with O – Organizers: Huth, Marbach)**
O 24.1–24.7	Tue	9:30–11:15	H 2032	**[DS] Organic electronics and photovoltaics: simulations and optics I (jointly with CPP, HL, O)**
O 25.1–25.9	Tue	10:30–13:00	HE 101	**Focussed session: Frontiers of electronic structure theory: Strong correlations from first principles II (jointly with TT)**
O 26.1–26.10	Tue	10:30–13:00	MA 005	**Plasmonics and nanooptics II**
O 27.1–27.10	Tue	10:30–13:00	MA 041	**Graphene II**
O 28.1–28.11	Tue	10:30–13:15	MA 042	**Heterogeneous catalysis II**
O 29.1–29.10	Tue	10:30–13:00	MA 043	**Metal substrates: Adsorption of organic / bio molecules II**
O 30.1–30.9	Tue	10:30–13:15	A 053	**Focussed session: Functional molecules at surfaces I**
O 31.1–31.10	Tue	10:30–13:00	A 060	**Clean surfaces II**
O 32.1–32.6	Tue	11:30–13:00	H 2032	**[DS] Organic electronics and photovoltaics: simulations and optics II (jointly with CPP, HL, O)**
O 33.1–33.1	Tue	13:30–14:00	HE 101	**Gaede Prize talk (Mato Knez)**
O 34.1–34.60	Tue	18:15–21:45	Poster E	**Poster Session I (Graphene; Plasmonics and nanooptics; Coherence and coherent control in nanophotonics and plasmonics)**
O 35.1–35.148	Tue	18:15–21:45	Poster B	**Poster Session II (Polymeric biomolecular films; Nanostructures; Electronic structure; Spin-orbit interaction; Phase transitions; Surface chemical reactions; Heterogeneous catalysis; Particles and clusters; Surface magnetism; Electron and spin dynamics; Surface dynamics; Methods; Electronic structure theory; Functional molecules)**
O 36.1–36.1	Wed	9:30–10:15	HE 101	**Invited talk (Joseph A. Stroscio)**
O 37.1–37.13	Wed	9:30–13:00	EB 301	**[MA] Joint Session "Topological Insulators II" (jointly with DS, HL, O, TT)**
O 38.1–38.7	Wed	9:30–11:15	H 2032	**[DS] Organic electronics and photovoltaics: electronic properties I (jointly with CPP, HL, O)**
O 39.1–39.11	Wed	10:30–13:15	HE 101	**Focussed session: Frontiers of electronic structure theory: Strong correlations from first principles III (jointly with TT)**

O 40.1–40.6	Wed	10:30–12:45	MA 005	**Focussed session: Coherence and coherent control in nanophotonics and plasmonics I**
O 41.1–41.10	Wed	10:30–13:00	MA 041	**Graphene III**
O 42.1–42.10	Wed	10:30–13:00	MA 042	**Nanostructures at surfaces I**
O 43.1–43.10	Wed	10:30–13:00	MA 043	**Clean surfaces III**
O 44.1–44.10	Wed	10:30–13:30	A 053	**Focussed session: Functional molecules at surfaces II**
O 45.1–45.8	Wed	10:30–12:30	A 060	**Solid / liquid interfaces I**
O 46.1–46.6	Wed	11:30–13:00	H 2032	**[DS] Organic electronics and photovoltaics: electronic properties II (jointly with CPP, HL, O)**
O 47.1–47.8	Wed	11:45–13:45	H 0111	**[DS] Micro- and nanopatterning (jointly with O)**
O 48.1–48.1	Wed	15:00–15:45	HE 101	**Invited talk (Ruslan Temirov)**
O 49.1–49.1	Wed	15:45–16:30	HE 101	**Invited talk (Timo Jacob)**
O 50.1–50.11	Wed	16:00–19:00	BH 243	**[MA] Joint Session "Surface Magnetism I" (jointly with O)**
O 51.1–51.10	Wed	16:45–19:15	HE 101	**Oxides and insulators: Epitaxy and growth**
O 52.1–52.7	Wed	16:45–19:15	MA 005	**Focussed session: Coherence and coherent control in nanophotonics and plasmonics II**
O 53.1–53.7	Wed	16:45–18:30	MA 041	**Graphene IV**
O 54.1–54.10	Wed	16:45–19:15	MA 042	**Nanostructures at surfaces II**
O 55.1–55.10	Wed	16:45–19:15	MA 043	**Theoretical methods II**
O 56.1–56.10	Wed	16:45–19:15	A 053	**Metal substrates: Adsorption of organic / bio molecules III**
O 57.1–57.8	Wed	16:45–18:45	A 060	**Solid / liquid interfaces II**
O 58.1–58.60	Wed	18:15–21:45	Poster B	**Poster Session III (Solid/liquid interfaces; Metals; Semiconductors; Oxides and insulators)**
O 59.1–59.1	Thu	9:30–10:15	HE 101	**Invited talk (Mads Brandbyge)**
O 60.1–60.13	Thu	9:30–13:00	EB 301	**[MA] Joint Session "Surface Magnetism II" (jointly with O)**
O 61.1–61.5	Thu	9:30–13:00	H 0104	**[TT] Focused Session: Charge and Spin Transport through Junctions at the Nanometre Scale**
O 62.1–62.13	Thu	9:30–13:00	BH 334	**[TT] Transport: Graphene 1 (jointly with MA, HL, DY, DS, O)**
O 63.1–63.10	Thu	10:30–13:15	HE 101	**Focussed session: Frontiers of electronic structure theory: Strong correlations from first principles IV (jointly with TT)**
O 64.1–64.10	Thu	10:30–13:00	MA 005	**Plasmonics and nanooptics III**
O 65.1–65.10	Thu	10:30–13:00	MA 041	**Graphene V**
O 66.1–66.10	Thu	10:30–13:00	MA 042	**Nanostructures at surfaces III**
O 67.1–67.9	Thu	10:30–12:45	MA 043	**Metal surfaces: Adsorption of H/O and inorganic molecules**
O 68.1–68.7	Thu	10:30–13:00	A 053	**Focussed session: Functional molecules at surfaces III**
O 69.1–69.5	Thu	10:30–13:00	A 060	**Competition for Gerhard Ertl Young Investigator Award**
O 70.1–70.1	Thu	15:00–15:45	HE 101	**Invited talk (Nobuo Ueno)**
O 71.1–71.4	Thu	15:00–16:45	H 1012	**[MA] Joint Session "Graphen: Spin Transport" (jointly with DS, DY, HL, O, TT)**
O 72.1–72.15	Thu	15:15–19:15	BH 243	**[MA] Joint Session "Surface Magnetism III" (jointly with O)**
O 73.1–73.11	Thu	16:00–19:00	HE 101	**Focussed session: Frontiers of electronic structure theory: Strong correlations from first principles V (jointly with TT)**
O 74.1–74.10	Thu	16:00–18:30	MA 005	**Plasmonics and nanooptics IV**
O 75.1–75.7	Thu	16:00–17:45	MA 041	**Particles and clusters**
O 76.1–76.6	Thu	16:00–17:30	MA 042	**Nanostructures at surfaces IV**
O 77.1–77.6	Thu	16:00–17:30	MA 043	**Electronic structure I**
O 78.1–78.7	Thu	16:00–17:45	A 053	**Metal substrates: Adsorption of organic / bio molecules IV**
O 79.1–79.7	Thu	16:00–17:45	A 060	**Experimental methods**
O 80	Thu	19:30–20:00	HE 101	**General meeting of the Surface Science Division**
O 81	Thu	20:00–21:00	HE 101	**Post deadline session**
O 82.1–82.1	Fri	9:30–10:15	HE 101	**Invited talk (Willi Auwärter)**
O 83.1–83.12	Fri	9:30–12:45	BH 334	**[TT] Transport: Graphene 2 (jointly with MA, HL, DY, DS, O)**
O 84.1–84.8	Fri	10:30–13:00	HE 101	**Focussed session: Frontiers of electronic structure theory: Strong correlations from first principles VI (jointly with TT)**
O 85.1–85.10	Fri	10:30–13:00	MA 005	**Plasmonics and nanooptics V**
O 86.1–86.10	Fri	10:30–13:00	MA 041	**Graphene VI**
O 87.1–87.9	Fri	10:30–12:45	MA 042	**Surface chemical reactions**
O 88.1–88.10	Fri	10:30–13:00	MA 043	**Electronic structure II**
O 89.1–89.10	Fri	10:30–13:00	A 053	**Metal substrates: Adsorption of organic / bio molecules V**

O 90.1–90.8	Fri	10:30–12:30	A 060	**Metals and semiconductors: Epitaxy and growth**
O 91.1–91.67	Fri	11:00–14:00	Poster A	**[MA] Poster II**
O 92.1–92.1	Fri	13:15–14:00	HE 101	**Invited talk (Ralph Claessen)**

Annual General Meeting of the Surface Science Division

Thursday 19:30–20:00 HE 101

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

Post Deadline Session

Post deadline session on Thursday 20:00–21:00 in HE 101, followed by the Surface Science get-together.

O 1: Invited talk (Alexander Ako Khajetoorians)

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

Invited Talk O 1.1 Mon 9:30 HE 101

Spin LEGOs - Bottom-up Fabrication of Model Magnetic Systems — •Alexander Ako Khajetoorians — Institute of Applied Physics, Hamburg University, Hamburg

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 (SAM) with an atom-by-atom bottom-up fabrication to realize complex atomic-scale magnets with tailored properties. As a first such example of this, we demonstrated that it is possible to realize an all-spin based atomic logic gate comprised of coupled Fe atoms [4] on a metallic surface [5]; a demonstration of a fundamental nano-spintronic concept. In this talk, I will address novel developments illustrating advances in the realization of artificially constructed magnetic nanostructures, like complex two-dimensional indirect-exchange based nanomagnets, as well as investigations of the magnetization dynamics of single and coupled spins. [1] R. Wiesendanger, *RMP*, **81**, 1495 (2009); [2] A. J. Heinrich, *et al.* , *Science*, **306**, 466 (2004); [3] A.A. Khajetoorians, *et al.* , *Nature*, **467**, 1084 (2010); [4] A.A. Khajetoorians, *et al.* , *PRL*, **106**, 037205 (2011); [5] A.A. Khajetoorians, *et al.* , *Science*, **332**, 1062 (2011)

O 2: Focussed session: Frontiers of electronic structure theory: Strong correlations from first principles I (jointly with TT)

Time: Monday 10:30–13:15 Location: HE 101

Topical Talk O 2.1 Mon 10:30 HE 101

Non Uniform Polarizability and Coulomb interactions in Compounds and Interfaces — •George Sawatzky — Physics department University of British Columbia 6224 agricultural road Vancouver BC Canada

The polarizability of relatively ionic compounds like the transition metal or rare earths exhibit quite non uniform polarizabilities requiring a full treatment of the non local field effects when studying the the details of especially relatively short range electron -electron interactions. We discuss how this affects the effective on site Coulomb interactions and show that the intermediate range interactions are not monotonically decreasing with distance even for insulating materials. this has important consequences for the use of models like the Hubbard model especially in low dimensional systems. We will use examples of low dimensional systems as well as the Cuprates, Manganites, Fe Pnictides with strongly polarizable anions in this discussion. We suggest that for the Fe Pnictides the Fe-Fe nearest neighbor coulomb interactions can be much smaller than the next nearest neighbor ones and may turn out to be slightly attractive. Similar non local effects are present at surface and interfaces which can lead to band gap closing rather than conventional band bending for semiconductor metal interfaces. In view of this it is rather important to revisit simple on site only based models and to develop first principles approaches taking into account the non uniform polarizability of the systems studied.

O 2.2 Mon 11:00 HE 101

Adatom systems on the silicon 111-surface: Mott or not? — •Philipp Hansmann, Loig Vaugier, and Silke Biermann — Centre de Physique Theorique, Ecole Polytechnique, CNRS-UMR7644, F-91128 Palaiseau, France

For more than a decade now the interest in adsorbate systems on semiconducting substrates has increased due to exotic ground state features among which one finds charge-density waves[1] and even superconductivity[2]. Associated are often surface states with rather small bandwidths and the question about the role of electronic correlations arises naturally. Especially for akaline-metal adatoms on the Si(111) surface such correlations have been claimed to be essential for an explanation of the insulating ground state within a Mott scenario[3]. However, recent experimental findings [4] challange this theory and have reignited the "surface-correlation-controversy". In order to resolve the issue from a state-of-the-art theoretical point of view, the mere solution of an effective many-body problem is only one part of the answer. As long as the interaction parameters for such calculations are not determined in an ab initio way, there cannot be any definitive conclusions. In our work we outline the procedure of the so called constrained random phase approximation to calculate interaction parameters for the semiconductor surface systems in order to promote methods like the merger of density functional- and dynamical mean field theory to be truly ab initio.[1]J.M.Carpinelli et al., Nature 381,398(1996); [2] T. Zhang et al.,Nat.Phys. 6,104(2010); [3]H.H. Weitering et al.,PRL 78,1331(1997); [4]C. Tournier-Colleta et al.,PRB 84,155443(2011)

O 2.3 Mon 11:15 HE 101

Hubbard U and Hund's J from the constrained Random Phase Approximation within a full-potential linearized augmented plane wave approach: trends for 3d and 4d transition metal perovskites — •Loig Vaugier[1], Hong Jiang[2], and Silke Biermann[1] — [1]CPHT, Ecole Polytechnique, Palaiseau, France — [2]College of Chemistry, Peking University, Beijing 100871, China

Determining the Coulomb interactions in real materials presents a serious challenge for first principles approaches. In 2004, a systematic way - called constrained-RPA (cRPA) - of calculating the Hubbard U and Hund's rule J parameters from first-principles has been proposed by Aryasetiawan and coworkers [1]. We have implemented the cRPA method in the framework of the Full Potential Linear Augmented Plane Waves method as implemented in the Wien2k code [2]. Our scheme permits us to calculate the Hubbard interactions in the same basis in which combined LDA+DMFT calculations are performed within the implementation of [3], yielding a fully consistent first-principles scheme. As an application of cRPA, we have calculated Hubbard U's and Hund J's for cubic 3d and 4d transition metal perovskites [4]. In contrast to what is usually assumed, the trend is not necessarily monotonic. Our work emphasizes the dependence of U and J on the choice of the one-electron part of the Hamiltonian.

[1] Aryasetiawan et al. PRB 70, 195104 (2004)
[2] Blaha et al., Wien2k, (2001)
[3] Aichhorn et al., PRB 80, 085101 (2009)
[4] Vaugier, Jiang and Biermann, in preparation

O 2.4 Mon 11:30 HE 101

Strength of the Hubbard *U* at metal and insulator surfaces — •Ersoy Sasioglu, Christoph Friedrich, and Stefan Blügel — Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, 52425 Jülich, Germany

The effective on-site Coulomb interaction (Hubbard *U*) between localized electrons at surfaces of solids is expected to be enhanced since the effective screening volume of the surface is reduced with respect to the bulk. By means of first-principles calculations in conjunction with the constrained random-phase approximation (cRPA) [1] within the full-potential linearized augmented-plane-wave (FLAPW) method [2] we show that this is indeed the case for simple metals and insulators but not necessarily for transition metals and insulators that exhibit pronounced surface states. In the latter case, the screening contribution from surface states as well as the influence of the band narrowing can increase the electron polarization to such an extent that the expected decrease resulting from the reduced effective screening volume is overcompensated. In some cases, the Hubbard *U* parameter is substantially reduced, e.g., by around 30% for the (100) surface of bcc Cr, contrary to the conventional wisdom. We show a systematic study for prototype materials including transition-metal surfaces.
[1] E. Şaşıoğlu, C. Friedrich, and S. Blügel, PRB **83**, 121101(R) (2011).
[2] http://www.flapw.de

O 2.5 Mon 11:45 HE 101

Multi-orbital Kondo physics of Co in Cu hosts — •Tim Wehling[1], Brigitte Surer[2], Matthias Troyer[2], Philipp Werner[2], Andreas Läuchli[3], Aljoscha Wilhelm[1], and Alexander Lichtenstein[1] — [1]1. Institut für Theoretische Physik, Universität Hamburg, D-20355 Hamburg, Germany — [2]Theoretische Physik, ETH Zurich, Wolfgang-Pauli-Strasse 27, 8093 Zürich, Switzerland — [3]Institut für Theoretische Physik, Universität Innsbruck, Technikerstrasse 25/2, A-6020 Innsbruck, Austria

We investigate the electronic structure of cobalt atoms on a copper surface and in a copper host by combining density functional calculations with a numerically exact continuous-time quantum Monte Carlo treatment of the five-orbital impurity problem. In both cases we find low energy resonances in the density of states of all five Co d-orbitals. The corresponding self-energies indicate the formation of a Fermi liquid state at low temperatures. Our calculations yield the characteristic energy scale – the Kondo temperature – for both systems in good agreement with experiments. We quantify the charge fluctuations in both geometries and suggest that Co in Cu must be described by an Anderson impurity model rather than by a model assuming frozen impurity valency at low energies. We show that fluctuations of the orbital degrees of freedom are crucial for explaining the Kondo temperatures obtained in our calculations and measured in experiments.

Topical Talk O 2.6 Mon 12:00 HE 101

Actual theoretical trends in angle resolved photoemission: correlation, disorder and temperature effects — •Ján Minár — Universität München, Department Chemie, Butenandtstr. 5-13, D-81377 München, Germany

The fully self-consistent combination of local spin-density approximation (LSDA) and dynamical mean field theory (DMFT) provide a powerful tool to treat correlations beyond plain LSDA. The KKR or multiple scattering approach implemented on this basis allows among others to deal with alloy and surface systems as well as to study various spectroscopic properties on equal footing [1]. The latter feature is of particular interest because a direct comparison with experimental data reveal the impact of correlation effects unambiguously as matrix element, surface and temperature effects are included [2]. Here, we present a generalisation of the state of the art description of the photoemission process, the so-called one-step-model of photoemission that describes the photoemission process in a coherent way. To illustrate the applicability of this formalism several examples of ARPES calculations from simple transition metals (Fe, Co), transition metal oxides (NiO, VO$_2$) as well as from complex disordered alloys (Ni$_x$Pd$_{1-x}$, GaMnAs, SrTiO$_3$/La$_x$Sr$_{1-x}$MnO$_3$) will be presented [3].

[1] J. Minár, J. Phys.: Cond. Mat. (Topical Review) **23**, 253201 (2011).

[2] H. Ebert,D. Ködderitzsch and J. Minár, Rep. Prog. Phys. **74**, 096501 (2011).

[3] A. Gray et al., J. Minar et al., Nature materials **10**, 759 (2011); J. S. Barriga et al., Phys. Rev. B **82**, 104414 (2010)

O 2.7 Mon 12:30 HE 101

Valence-band correlations and core hole effects in the x-ray absorption and magnetic circular dichroism spectra — •Ondřej Šipr[1], Stephan Borek[2], Angelika Chassé[2], Hubert Ebert[3], and Jan Minár[3] — [1]Institute of Physics AS CR v.v.i., Praha, Czech Republic — [2]Institut für Physik, Martin-Luther-University Halle-Wittenberg, Germany — [3]Department Chemie, Universität München, Germany

A quantitative description of the x-ray absorption spectra (XAS) and x-ray circular magnetic dichroism spectra (XMCD) should account for correlations between valence electrons in the initial state and for a core hole in the final state. We employ the local spin density approximation (LSDA) plus dynamical mean field theory (DMFT) formalism to describe the correlations between the d electrons and the linear-response theory within the time-dependent density-functional-theory (TDDFT) to describe the core hole. The most important effects beyond the LSDA are thus included and yet the scheme is computationally tractable.

The impact of many-body effects on XAS and XMCD is assessed by investigating $L_{2,3}$-edge spectra of $3d$ transition metals. We find that the LSDA+DMFT alone improves the LSDA results, in particular concerning the asymmetry of the L_3 white line. To get more accurate results, particularly concerning the ratio of the intensities of the L_3 and L_2 peaks, the dynamic aspects of the core hole have to be included via the TDDFT linear response framework. Similar conclusions follow also from our study of Heusler alloys (Cu$_2$MnAl).

The work was supported by projects SFB 762 and P108/11/0853.

O 2.8 Mon 12:45 HE 101

Progress and problems of DFT+DMFT approach — •Alexander Lichtenstein — Institute of Theoretical Physics, University of Hamburg, 20355 Hamburg

Effects of strong electron correlations in real materials can be described within the QMC, GW or DFT+DMFT methods. We discuss recent progress of realistic Dynamical Mean Field Theory of complex systems including oxides and magnetic nanomaterials. Possible future directions to overcome standard problems of the DFT+DMFT scheme and to include non-local correlation effects will be reviewed.

O 2.9 Mon 13:00 HE 101

GW+EDMFT simulation of the U-V Hubbard model — •Thomas Ayral[1], Silke Biermann[2], and Philipp Werner[1] — [1]Theoretische Physik, ETH Zurich, 8093 Zürich, Switzerland — [2]Centre de Physique Théorique, Ecole Polytechnique, CNRS-UMR7644, 91128 Palaiseau, France

We study the extended Hubbard model with on-site and nearest-neighbor repulsion on a square lattice within a GW+EDMFT scheme at finite temperature and half-filling. This technique combines the successful description of screening effects due to non-local interactions within Hedin's GW approximation with the dynamical mean field description of strong local interactions. We analyze the role of the frequency-dependence of the local interactions in the formation of the charge-ordered phase and show that non-local contributions to the self-energies generated via the GW approximation have a substantial impact on the local observables and on the phase diagram, depending on the interaction parameters. Our work thus has implications for electronic structure techniques based on Hedin's GW approximation in that it demonstrates a local many-body vertex to be sufficient for fully self-consistent GW calculations.

O 3: Plasmonics and nanooptics I

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

O 3.1 Mon 10:30 MA 005

SHG imaging of gold nanocones in focused beams of different polarisations. — •Philipp Reichenbach[1], Dominik Gollmer[2], Monika Fleischer[2], Dieter Kern[2], and Lukas Eng[1] — [1]Institut für Angewandte Photophysik, Technische Universität Dresden, George-Bähr-Straße 1, 01069 Dresden — [2]Institut für Angewandte Physik, Eberhard Karls Universität Tübingen, Auf der Morgenstelle 10, 72076 Tübingen

Nanostructures with sharp tips provide strong dipolar second-harmonic (SHG) light sources due to the combination of extreme field enhancement and breaking the centro-symmetry. We present second-harmonic measurements at gold nano-cones that are illuminated by a radially polarized, focused femtosecond beam at 800 nm in order to excite the tip. Nevertheless, we observe second-harmonic radiation emission either from the tip or from the cones's bottom edges, depending on the cone size and surrounding medium. This behavior can be readily explained through numerical calculations of the field enhancement at the tip apex and the bottom face of the cones.

Furthermore, our measurements with a radially polarized focused beam are compared to measurements with linear or azimuthal polarization. Thus, the z-component of the electric field exciting the cone tip can be purposely switched on and off. Hence, we are able to clearly discriminate between SHG emission from the bottom edges and from the tip apex.

O 3.2 Mon 10:45 MA 005

Enhancement of non-linear effects using nano-wires — •Woyten Tielesch[1], Mathieu Gentile[1], Mario Hentschel[2], Harald Giessen[2], and Manfred Fiebig[3] — [1]HISKP, Universität Bonn, Germany — [2]4. Physikalisches Institut and Research Center SCoPE, Universität Stuttgart, Germany — [3]Departement of Materials, ETH Zürich, Switzerland

Gold nano-wires are artificial sub-wavelength materials with tailored optical properties. Experimental and theoretical investigations show amplified local fields on the nanoscale. In a non-linear material this makes nano-wires act as an optical catalyst. We present a method using such a catalyst to enhance non-linear functionality of a given material.

Our sample consists of fields of regularly spaced gold nano-wires on a Cr_2O_3 substrate. Cr_2O_3 shows second-harmonic generation (SHG) for incident light peaked around 1.05 eV and has been intensively characterized for reference. Accordingly, the wires have linear resonances between 0.9 eV and 1.5 eV. In our experiment we use amplified 120 fs laser pulses to investigate the influence of the wires on the SHG spectrum of the substrate. Fundamental wavelengths from 0.8 eV to 1.1 eV are used.

A significant modification of SHG due to the wires is observed. We demonstrate that the spectral profile of the SHG signal is strongly correlated to the linear spectrum of the wires. In addition, we show that a strong signal occurs in a direction where the bare substrate shows no signal at all, a fact still requiring theoretical explanation.

O 3.3 Mon 11:00 MA 005

Adiabatic nanofocusing of ultrashort light pulses. — •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, Germany — [2]Photonic System Laboratory, School of EECS, Seoul, Korea — [3]Center for Subwavelength Optics and Department of Physics and Astronomy, Seoul, Korea

We demonstrate the use of a novel ultrasharp and ultrasmooth single-crystalline gold taper for adiabatic nanofocusing of few-cycle light pulses. We show that the grating-induced launching of spectrally broadband surface plasmon polariton wavepackets onto the shaft of such a taper generates isolated, point-like light spots with 10 femtosecond duration and sub-10-nm diameter at its very apex. This nanofocusing is so efficient that nano-localized electric fields exceeding the atomic field are reached with conventional high-repetition rate laser oscillators. Strong optical nonlinearities are induced at the tip end and we use here the resulting second harmonic to fully characterize the time structure of the localized electric field in frequency-resolved interferometric autocorrelation measurements. The conclusions drawn from our experiments are beautifully confirmed by numerical simulation based on the finite-difference time-domain (FDTD) method. Our results strongly suggest that these nanometer-sized ultrashort, light spots will enable new experiments probing the dynamics of optical excitations of individual metallic, semiconducting and magnetic nanostructures.

O 3.4 Mon 11:15 MA 005

Trapping light in random ZnO nanorod arrays - Localization of light in space and time — •Manfred Mascheck[1], Slawa Schmidt[1], Martin Silies[1], David Leipold[2], Erich Runge[2], Takashi Yatsui[3], Kokoro Kitamura[3], Motoichi Ohtsu[3] und Christoph Lienau[1] — [1]Carl-von-Ossietzky-Universität, Oldenburg — [2]Technische Universität Ilmenau — [3]University of Tokyo

A random array of ZnO nanorods is used to directly visualize the weak localization of light in space and time. In an ultrafast second harmonic microscope pairs of 6-fs laser pulses at variable delay are focused to the diffraction limit onto the ZnO nanorod array in a dispersion-balanced set-up. The generated SH emission is collected in reflection geometry and detected as a function of the spatial position of the laser focus as well as for the delay between the pulses. Pronounced spatial intensity fluctuations of the SH due to multiple random scattering within the array and a distinct modification of the correlated time structure of the local electric field are observed as predicted for the localization of light. By using the one parameter scaling theory the histogram of the intensity values gives evidence for being near the transition between weak- and strong localisation.

O 3.5 Mon 11:30 MA 005

Revealing nonlinear plasmon-photon interactions using k-space spectroscopy — •Jan Heckmann, Nicolai B. Grosse, and Ulrike Woggon — Institut für Optik und Atomare Physik, Technische Universität Berlin

Surface plasmon (SP) excitation in metal-dielectric structures is exemplified by an enhanced local electromagnetic field, which boosts nonlinear effects. Since the first demonstration of SP-related second-harmonic generation (SHG) by Simon et al., understanding the microscopic origin of the nonlinearity has remained an active research topic.

We propose that all permutations of plasmon (p) and photon (f) are allowed in the second-order nonlinear process of SHG (which can generate either p or f), and that each process can be identified by its own requirement for nonlinear k-vector-matching. Hence, the type of nonlinear interaction can be identified by resolving the SHG intensity as a function of exit angle, while the fundamental excitation angle is varied. To test this hypothesis, we built a k-space spectrograph that analysed SHG from a thin metal film in the Kretschmann geometry which was driven by femtosecond-pulsed laser light.

Our experimental results show that for excitation angles in the vicinity of the SHG peak, there is an off-diagonal component which is consistent with the signature of the pp-f interaction. This is in contrast to the purely photonic ff-f interaction which lies on the diagonal. Hence, in plasmon SHG, two plasmons at the fundamental frequency are annhiliated to create a second-harmonic photon.

O 3.6 Mon 11:45 MA 005

Non - Linear Optical Imaging of Gold Nano - Cones with a Parabolic Mirror Microscope — •Anke Horneber[1], Dai Zhang[1], Monika Fleischer[2], Kai Braun[1], Dieter P. Kern[2], and Alfred J. Meixner[1] — [1]Institute of Physical Chemistry,Eberhard Karls University Tübingen, Germany — [2]Institute for Applied Physics, Eberhard Karls University Tübingen, Germany

Governed by the lightning rod effect and localized surface plasmon resonances, linear optical properties of metallic nanoantennas have been widely investigated [1]. In our latest work, we have combined a femtosecond erbium fibre laser (774 nm) with a home-built parabolic mirror (NA 0.998) assisted confocal optical microscope [2] to investigate the non-linear optical effects from nano structures of different materials, and geometries. Due to the intensely confined electric field at the tip apex and its centrosymmetry breaking geometry, single gold nano-cone showed dramatic non-linear optical properties, which depend sensitively on the polarization condition. Combined with numerical simulation, we will demonstrate and analyse systematically the non-linear optical imaging of individual gold nano-cones.

[1] M. Fleischer, C. Stanciu, F. Stade, J. Stadler, K. Braun, A. Heeren, M. Haeffner, D. P. Kern and A. J. Meixner, Appl. Phys. Lett. 93 (2008) 111114. [2] J. Stadler, C. Stanciu, C. Stupperich, and A. J. Meixner, Opt. Lett. 33 (2008) 681.

O 3.7 Mon 12:00 MA 005

Towards Synthesis and Investigation of Surface Plasmon Polariton Lasers — •Günter Kewes[1], Andreas Ott[1,2], Yan Lu[1,2], Matthias Ballauff[1,2], and Oliver Benson[1] — [1]Humboldt Universität Berlin — [2]Helmholtz Zentrum Berlin

Surface plasmons attract a lot of research interests because of their wide range of applications in nanophotonics, but the field is gathering for an active element, e.g. a surface plasmon polariton laser (spaser) [1]. Coherent amplification of radiation through excitation of surface plasmons in dye-doped Au-SiO2 core-shell nanoparticles is investigated to synthesize a spaser. Spherical and rod-like Au nanoparticles with tuneable plasmon resonances are covered with a silica shell by a modified Stöbe method. A suitable dye (according to the surface plasmon excitation) is incorporated to generate a gain medium that compensates for the absorption loss in the metal [2]. The emission of the nanoparticles is observed through a home-built confocal microscope with single molecule sensitivity where the nanoparticles can be identified and manipulated by an atomic force microscope at the same time [3].

References: [1] M. A. Noginov, et al., Nature 460, 1110 (2009). [2] W. Ni, et al., J. Am. Chem. Soc. 132, 4806 (2010). [3] S. Schietinger, et al., Nano Lett. 9, 1694 (2009).

O 3.8 Mon 12:15 MA 005

Optical Nanoantennas for Ultrafast Spectroscopy of Single 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 signals are reduced further when single nanoobjects such as quantum dots, molecules, or nanoparticles are the systems of interest. Considering the example of a mechanically oscillating single gold nanodisc, we demonstrate how such a weak nonlinear response can be enhanced by one order of magnitude using an optical nanoantenna. Our numerical model explains all experimantally observed effects of the antenna. Furthermore it allows us to perform optimization studies to obtain more effective antenna structures to reach higher enhancement factors. Finally we give an outlook on our work on enhancing the nonlinear response of colloidal quantum dots.

O 3.9 Mon 12:30 MA 005

Nanoscale heat flux for hyperbolic materials — •Svend-Age Biehs and Maria Tschikin — Institut für Physik, Carl von Ossietzky Universität Oldenburg, D-26111 Oldenburg

We consider the radiative heat flux between two hyperbolic media for distances much smaller than the thermal wavelength. Based on a generalization of the heat flux expression derived by Polder and van Hove for anisotropic media we study the influence of so called hyperbolic modes by using a Maxwell-Garnett effective medium description for the material properties. In particular, we will show that these modes give a maximal transmission over a broad band of frequencies and for large lateral wave vectors due to photon tunneling. We demonstrate that the heat flux associated with these modes can be very close to the fundamental limit derived by P. Ben-Abdallah and K. Joulain at the nanoscale. Hence, hyperbolic materials can be considered as very good candidates for realizing a black body in the near-field regime.

O 3.10 Mon 12:45 MA 005

Präparation und Anordnung von Goldnanopartikeln zur Untersuchung von nichtlinearen optischen Prozessen — •Valerie Mondes[1], Antonia Menski[1], Matthias Buchholz[1], Matthias Kling[2], Christina Graf[1], Jürgen Plenge[1] und Eckart Rühl[1] — [1]Freie Universität Berlin, Institut für Chemie und Biochemie, Physikalische und Theoretische Chemie, Takustr. 3, 14195 Berlin — [2]Max-Planck Institut für Quantenoptik, Hans-Kopfermann-Str. 1, 85748 Garching

Geordnete Strukturen von metallischen Nanopartikeln können hohe plasmonische Feldverstärkungseffekte bei der Anregung durch Femtosekundenlaserstrahlung aufweisen. Sie sind daher ideale Systeme zur Untersuchung von nichtlinearen optischen Prozessen. Alternativ zu den oft verwendeten lithographisch hergestellten Strukturen wurden in dieser Arbeit Goldnanopartikel mit Methoden der Kolloidchemie hergestellt und durch induzierte Selbstorganisation auf Saphirträgern in Monolagen angeordnet. Die Form und Größe der Nanopartikel wurde variiert und Nanostrukturen aus kugel-, würfel- bzw. prismenförmigen Goldnanopartikeln aufgebaut. Die Strukturen wurden mittels Transmissions- und Rasterelektronenmikroskopie charakterisiert.

Die in Monolagen angeordneten Goldnanopartikel wurden mit Femtosekundenlaserstrahlung ($\lambda = 804$ nm, $\tau = 80$ fs) angeregt. Die Zwei-Photonen-Photolumineszenz und Frequenzvervielfachung an den Nanostrukturen wurden genutzt, um plasmonische Feldverstärkungseffekte für Strukturen mit unterschiedlichen Geometrien zu charakterisieren.

O 4: Graphene I

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

O 4.1 Mon 10:30 MA 041

Photoemission Microspectroscopy of Single Layer Graphene on Iridium. — •Christian Witt, Jan Vanis, Michael Horn-von Hoegen, and Frank-J. Meyer zu Heringdorf — University Duisburg-Essen, Faculty of Physics and CeNiDE, Lotharstrasse 1, 47048 Duisburg

Graphene is one of the most investigated materials in modern physics. Especially the differences of the band structure of free standing Graphene and Graphene grown on a substrate is of great interest. A standard method to grow single layer Graphene is chemical vapor deposition using Ethene as a carbon source and heated Iridium crystals as substrate and catalyst. We combined photoemission electron microscopy with various illumination sources to investigate the morphology and band structure of Graphene on Iridium. In our experiments, under illumination with a Helium discharge lamp (photon energy of 21.2 eV) we find the well known energy bands of Graphene. In contrast, under illumination with 200 nm femtosecond laser pulses (photon energy of 6.2 eV) we find a significant density of states at the Γ point.

O 4.2 Mon 10:45 MA 041

Local Gating of an Ir(111) Surface Resonance by Graphene Islands — •Simon Johannes Altenburg[1], Jörg Kröger[2], Tim Wehling[3], Burkhard Sachs[3], Alexander Lichtenstein[3], and Richard Berndt[1] — [1]Institut für Experimentelle und Angewandte Physik, Christian-Albrechts-Universität zu Kiel, D-24098 Kiel, Germany — [2]Institut für Physik, Technische Universität Ilmenau, D-98693 Ilmenau, Germany — [3]I. Institut für Theoretische Physik, Universität Hamburg, D-20355 Hamburg, Germany

The infuence of graphene islands on the electronic structure of the Ir(111) surface is investigated. Scanning tunneling spectroscopy (STS) indicates the presence of a two-dimensional electron gas with a binding energy of $-160\,\mathrm{meV}$ and an effective mass of $-0.18\,\mathrm{m_e}$ underneath single-layer graphene on the Ir(111) surface. Density functional calculations reveal that the STS features are predominantly due to a hole-like surface resonance of the Ir(111) substrate. Nanometer-sized graphene islands act as local gates, which shift and confine the surface resonance. Funding by the Deutsche Forschungsgemeinschaft via SPP 1459 and SFB 668, the Schleswig-Holstein-Fonds as well as computer time at HLRN are acknowledged.

O 4.3 Mon 11:00 MA 041

Direct observation of electron confinement in epitaxial graphene nanoislands — Soo-Hyon Phark[1], Jerome Borme[1,2], •Augusto Leon Vanegas[1], Marco Corbetta[1], Dirk Sander[1], and Jürgen Kirschner[1] — [1]Max Planck Institute of Microstructure Physics, Weingerg 2, 06120 Halle, Germany — [2]International Iberian Nanotechnology laboratory, Avenida Mestre Jose Veiga, 4715-310 Braga, Portugal

A central question for the future applications of graphene is how the substrate and the lateral confinement of a graphene island affect the electronic properties. In this work we have used scanning tunneling spectroscopy to measure the differential conductance dI/dV of the graphene nanoisland deposited on Ir(111)[1]. The dI/dV maps show a spatial modulation, which depends on energy. We ascribe this spatial modulation of the local density of states to quantum confinement. An analysis of the energy dependence of these modulations gives a linear dispersion relation, $E = E_0 \pm \hbar v_F|\vec{k}|$ with $E_0 = -90 \pm 20$ meV and a Fermi velocity $v_F = (6.0 \pm 0.4) \times 10^5\ m/s$. These findings are discussed in view of recently publish data [2,3].

[1] Soo-Hyon Phark, et al., ACS Nano, 2011, 5 (10), pp 8162-8166.
[2] S. Rusponi, et al., Phys. Rev. Lett. 105 (2010) 246803.
[3] M. Kralj et al., Phys. Rev. B 84, 075427 (2007).

O 4.4 Mon 11:15 MA 041

Wave function mapping of graphene quantum dots with soft confinement — •Dinesh Subramaniam[1], Florian Libisch[2], Yan Li[3], Christian Pauly[1], Viktor Geringer[1], Raphel Reiter[2], Torge Mashoff[1], Marcus Liebmann[1], Joachim Burgdörfer[2], Carsten Busse[4], Thomas Michely[4], Riccardo Mazzarello[3], and Markus Morgenstern[1] — [1]II. Physikalisches Insitut B and JARA-FIT, RWTH Aachen University, D-52074 Aachen, Germany — [2]Institute for Theoretical Physics, Vienna University of Technology, A-1040 Vienna, Austria — [3]Institute for Theoretical Solid State Physics and JARA-FIT, RWTH Aachen University, D-52074 Aachen, Germany — [4]II. Physikalisches Institut, Universität zu Köln, Zülpicherstr. 77, D-50937 Köln, Germany

Using low-temperature scanning tunneling spectroscopy, we map the local density of states of graphene quantum dots (QDs) supported on Ir(111). Due to a band gap in the projected Ir band structure around the graphene K point, the electronic properties of the QDs are dominantly graphene-like. Indeed, we compare the results favorably with tight binding calculations on the honeycomb lattice based on parameters derived from density functional theory. We find that the interaction with the substrate towards the edge of the island softly opens a gap in the Dirac cone, which implies soft-wall confinement. Interestingly, this confinement is required for highly symmetric wave functions. Further influences of the substrate are given by the known moire potential and a 10 % penetration of an Ir surface resonance into the graphene layer.

O 4.5 Mon 11:30 MA 041

Adsorption effects on the electronic and magnetic properties of nanosized Graphene structures on the Ir(111) Surface — •Yan Li[1], Dinesh Subramaniam[1], Nicolae Atodiresei[2], Predrag Lazic[3], Vasile Caciuc[2], Marcus Liebmann[1], Marco Pratzer[1], Christian Pauly[1], Alexander Georgi[1], Riccardo Mazzarello[1], Stefan Blugel[2], and Markus Morgenstern[1] — [1]RWTH Aachen, Aachen, Germany — [2]Forschungszentrum Jülich, Jülich, Germany — [3]MIT, Massachusetts, USA

We have studied the structural, electronic and magnetic properties of graphene nanoribbons and flakes grown on the Ir(111) surface by *ab initio* simulations and low-temperature scanning tunneling spectroscopy. The calculated formation energy and the experimental STM images indicate that in zigzag terminated flakes each C atom at the edge is saturated by one hydrogen atom. Due to the interplay between a) the strong interaction between Ir atoms and C atoms at the edge and b) the lattice mismatch, a superstructure consisting of alternating regions of strongly bound, *sp3*-hybridized C atoms and weakly bound, *sp2*-hybridized C atoms is formed at the edge. As a result of the interaction with the surface, no magnetic edge state near the Fermi level exists in the supported ribbon: this conclusion is corroborated by both calculation and experiments. We also studied theoretically the electronic structure of unsaturated nanoribbons on the same surface. No magnetic edge state was obtained in this system either.

O 4.6 Mon 11:45 MA 041

SPA-LEED study of strain state of single layer graphene on Ir(111): hysteretic behaviour of lattice parameter and wrinkle formation — •C. Klein[1], H. Hattab[1], A. T. N'Diaye[2], D. Wall[1], G. Jnawali[1], J. Coraux[3], C. Busse[2], R. van Gastel[4], B. Poelsema[4], T. Michely[2], F.-J. Meyer zu Heringdorf[1], and M. Horn-von Hoegen[1] — [1]Department of Physics, Universität Duisburg-Essen — [2]II. Physikalisches Institut, Universität zu Köln — [3]Institut Néel, CNRS-UJF, Grenoble Cedex 9, France — [4]Physics of Interfaces and Nanomaterials, MESA+ Institute for Nanotechnology, University of Twente, Enschede, The Netherlands

Employing high resolution low energy electron diffraction (SPA-LEED) the lattice parameter of single layer graphene on Ir(111), prepared by thermal decomposition of ethylene at 1530 K, was studied. We analyzed the strain state and the wrinkle formation kinetics as function of temperature. Using the moiré spot separation as a magnifying mechanism for the difference in the lattice parameters between Ir and graphene, we achieved an unrivalled relative precision of ca. 0.1 pm for the graphene lattice parameter. Our data reveals a characteristic hysteresis of the graphene lattice parameter which is explained by the interplay of reversible wrinkle formation and film strain. We show that epitaxial graphene on Ir(111) always exhibits residual compressive strain at room temperature, and provide important guidelines for strategies to avoid wrinkling.

Hattab et. al., Nano Letters (under revision, Nov. 2011)

O 4.7 Mon 12:00 MA 041

Morphology-dependent corrugation of Graphene/Ir(111): An XSW study — •Sven Runte[1], Chi Võ Văn[2], Johann Coraux[2], Jörg Zegenhagen[3], Thomas Michely[1], and Carsten Busse[1] — [1]II. Phys. Inst., Universität zu Köln, Germany — [2]Institut Néel, Grenoble, France — [3]European Synchrotron Radiation Facility, Grenoble, France

Graphene grown on metal substrates often shows a superperiodic moiré structure due to the lattice mismatch. In the resulting large unit cells varying local registries between the carbon and the metal atoms are found, leading to a local variation of the respective bond strength. Hence the graphene layer is not flat but significantly corrugated [1].

We performed X-ray Standing Wave (XSW) measurements for graphene/Ir(111) using (111)- and (222)-crystal reflections to determine the height distribution of the carbon atoms. We show that the peak-to-peak corrugation for a fully closed film is 1 Å and about half this value for small graphene flakes. This can be rationalized by postulating different strain states resulting from the cool-down from high growth temperatures and different thermal expansion coefficients of graphene and its substrate. These measurements also clarify the open question of the real shape of the corrugated layer from scanning probe experiments [2,3]. Finally, the influence of intercalated atoms and metal clusters on graphene's corrugation is shown.

[1] C. Busse *et al.*, Phys. Rev. Lett. **107**, 036101 (2011).
[2] A. T. N'Diaye *et al.*, New J. Phys. **10**, 043033 (2008).
[3] Z. Sun *et al.*, Phys. Rev. B **83**, 081415 (2011).

O 4.8 Mon 12:15 MA 041

Minigap isotropy and broken chiral symmetry in graphene with periodic corrugation — •Jaime Sánchez-Barriga, A. Varykhalov, D. Marchenko, M. R. Scholz, and O. Rader — Helmholtz-Zentrum Berlin

The chirality of charge carriers in graphene determines its peculiar scattering properties and in particular the avoided backscattering, predicted to be observable as the closing of minigaps in periodically corrugated graphene. By angle-resolved photoemission we show that the corrugated graphene layer that forms on Ir(111) exhibits isotropic minigaps which close nowhere in k-space, as expected for non-chiral particles. Artificially introducing an extra periodic superpotential by deposition of clusters with different compositions confirms the minigap isotropy indicating that the origin of this behavior is directly connected to the breaking of the chiral symmetry in the system.

O 4.9 Mon 12:30 MA 041

Extrinsic spin-orbit splitting in graphene on Ir(111) adjustable by interface chirality — •Dmitry Marchenko, J. Sánchez-Barriga, M. R. Scholz, O. Rader, and A. Varykhalov — Helmholtz-Zentrum Berlin

By means of spin- and angle-resolved photoemission we reveal a giant Rashba-type spin-orbit splitting in the π-band of graphene grown on Ir(111). We demonstrate that the magnitude of the splitting depends on the strength of the chemical interaction between graphene and iridium and can be regulated through the mutual rotational displacement of the graphene layer and the Ir(111) substrate.

O 4.10 Mon 12:45 MA 041

Ion Beam induced Defects in Graphene — •Sebastian Standop[1], Georgia Lewes-Malandrakis[1], Charlotte Herbig[1], Ossi Lehtinen[2], Arkady V. Krasheninnikov[2], Thomas Michely[1], and Carsten Busse[1] — [1]II. Physikalisches Instiut, Universität zu Köln — [2]Materials Physics Division, University of Helsinki, Finland

We explore ion irradiation as a tool to intentionally create defects in graphene. Defects not only alter graphene's structure, but were predicted to significanty affect its electronic properties [1]. Ion irradiation of graphene grown epitaxially on Ir(111) was conducted at room temperature with 1-15 keV noble gas ions (He, Ne, Ar, Xe) at an angle of 75° with respect to the surface normal. While for low energies and light ions only single holes or the absence of defect patterns are observed, for ion energies beyond a few keV and heavier ions pronounced damage patterns in great variety are observed as surface damage in scanning tunneling microscopy. These patterns consist of sequences of holes in graphene, some of them decorated by bright protrusions, with a maximum length exceeding 40 nm. We interpret the holes as to result from multiple scattering of the ions in between graphene and the Ir(111) surface. The protrusions are assumed to show Ir adatoms under the graphene layer created by the energy deposition of the ion to the substrate. Our interpretation is supported by corresponding molecular dynamics simulations of ion impacts in conjunction with ab initio density function theory calculations as well as annealing studies performed *in situ.* [1] M. M. Ugeda et al., PRL 104, 096804 (2010)

O 5: Adsorption on semiconductors, oxides and insulators I

Time: Monday 10:30–13:15 Location: MA 042

O 5.1 Mon 10:30 MA 042

Tailoring Hybrid States at Inorganic/Organic Interfaces: Pyridine/ZnO(10-10) — •Oliver T. Hofmann, Yong Xu, Patrick Rinke und Matthias Scheffler — FHI, Berlin

Hybrid inorganic/organic systems (HIOS) have opened up new opportunities for the development of optoelectronics due to their potential of achieving synergy beyond simply combining the best features of two distinct material classes. Even new physics and thus added value could be achieved if new quantum mechanical states occur at the interface, provided their energetic position is readily controllable. Theory and experiment indicate that such states can be found for a pyridine monolayer adsorbed on the transparent conductive oxide ZnO. We employ density functional theory, augmented with the electron-density dependent vdW-TS scheme, to investigate the nature of these states and the factors governing their energetic position. We find that conventional semi-local functionals give the wrong ordering of the pyridine orbitals and underestimate the bond strength between adsorbate and substrate, favoring an incorrect morphology. Both issues are ameliorated by incorporating exact exchange. The hybrid states, found approximately 1eV above the valence band edge and within the conduction band, originate from the ZnO conduction band and the pyridine LUMO. The large adsorption-induced interface dipole responsible for the energetic alignment is attributed to strong charge rearrangement within the subsystems. Having identified the interaction mechanism, we propose tailoring the energetic position of the interface state by controlling the interface dipole, e.g. by pre-covering ZnO with small molecules.

O 5.2 Mon 10:45 MA 042

DFT study of the interaction of hydrogen with stepped ZnO surfaces — •Jakub Goclon and Bernd Meyer — Interdisziplinäres Zentrum für Molekulare Materialien und Computer-Chemie-Centrum, Universität Erlangen-Nürnberg

The nature of the interaction of hydrogen with ZnO surfaces, which is a very important process in heterogeneous catalysis, is still mostly unresolved. While our previous study [1] was devoted to hydrogen adsorption on the ideal ZnO(10$\bar{1}$0) surface in comparison with experimental observations [2], we will present here results on hydrogen interaction with stepped surfaces. The steps were represented by (10$\bar{1}$1) and (20$\bar{2}$1) crystal cuts, considering both Zn and O terminations.

Using DFT calculations in combination with a thermodynamic analysis we have calculated the relative stability of various structural models representing surface steps as function of hydrogen and water chemical potentials. Different surface coverages of hydrogen on O and Zn sites formed by homolytic, heterolytic, and mixed types of adsorption were considered. Based on the phase diagrams from our thermodynamic analysis we find that at low hydrogen chemical potential only OH groups are present, while with increasing hydrogen partial pressure heterolytic adsorption becomes more favorable. For the O-terminated steps the onset of zinc hydroxide formation, which was found to be a stable configuration on the flat ZnO(10$\bar{1}$0) surface, is observed.

[1] J. Goclon, B. Meyer, *in preparation*

[2] Y. Wang, B. Meyer, X. Yin, M. Kunat, D. Langenberg, F. Traeger, A. Birkner, Ch. Wöll, *Phys. Rev. Lett.* 95 (2005) 266104

O 5.3 Mon 11:00 MA 042

Theoretical Investigations of the Interface between Copper and Zinc Oxide — •Björn Hiller and Jörg Behler — Lehrstuhl für Theoretische Chemie, Universitätsstraße 150, 44801 Bochum, Germany

Heterogeneous catalysis is used in many industrial processes for production of main base chemicals. For instance, in methanol synthesis copper clusters on on a zinc oxide support are used. Although this process is of great importance, the microscopic structure of the catalytic system is not known.

In experiments it has been found, that there are strong interactions between the copper particles and the support as the copper entrenches into zinc oxide. A theoretical treatment of interface systems is elaborate due to differences in cell dimensions of the subsystems. This leads to either very large calculations or an artificial stress in the system. Furthermore the entrenching increases the number of possible interfaces which have to be investigated in order to fully understand the system.

To identify the most stable interfaces we need to obtain reliable geometries. For this we suggest an approach that finds possible matching cells and also fully relaxed geometries. Using this technique we present energies for interfaces between low-index copper surfaces and ZnO(10$\bar{1}$0) and ZnO(11$\bar{2}$0), respectively.

O 5.4 Mon 11:15 MA 042

New mechanism for work-function tuning: ZnO surfaces modified by a strong organic electron acceptor — •Yong Xu[1], Oliver T. Hofmann[1], Patrick Rinke[1], Matthias Scheffler[1], Raphael Schlesinger[2], Norbert Koch[2], and Antje Vollmer[3] — [1]Fritz Haber Institute Berlin — [2]Humboldt-Universität zu Berlin — [3]Helmholtz-Zentrum Berlin

A key task for optimizing optoelectronic devices comprising hybrid inorganic/organic systems is to control the energy level alignment at interfaces. The use of interlayers provides a pathway to solve this challenge. To demonstrate the concept we investigated the polar surfaces of ZnO, modified by the prototypical organic electron acceptor 2,3,5,6-tetrafluoro-7,7,8,8-tetracyanoquinodimethane (F4TCNQ) theoretically and experimentally. DFT-PBE ΔSCF calculations of the O 1s surface core-level shifts combined with XPS measurements suggest that ZnO(000-1)/ZnO(0001) are H/OH covered. Depositing F4TCNQ on these surfaces considerably increases the work function that is shown to be insensitive to the doping level. F4TCNQ on ZnO(0001) exhibits an extraordinary high work function due to the appearance of upright adsorption. The PBE+vdW results are in line with the UPS data that shows work-function increases up to 1.4/2.8 eV on ZnO(000-1)/ZnO(0001). In contrast to F4TCNQ on metals, where pronounced bidirectional charge transfer occurs, the charge transfer to F4TCNQ is small, pinning the LUMO close to the Fermi level. The polarization of the system, caused by strong charge rearrangement within the adsorbate, is the main mechanism for the large work-function increase.

O 5.5 Mon 11:30 MA 042

Adsorption and laserinduced desorption of CO on a rutile(110)-surface — •Hendrik Spieker and Thorsten Klüner — Theoretical Chemistry, Carl von Ossietzky Universität, PO Box 2503, 26111 Oldenburg

The CO/TiO$_2$-system – being a model system for surface chemistry – is experimentally as well as theoretically of very high interest. To understand and compute the interaction of a CO molecule with titanium dioxide a Ti$_9$O$_{18}$Mg$_7{}^{14+}$-cluster, which is embedded within a finite point charge field, is used to approximate the rutile(110)-surface. [1] Thus, we are now able to calculate the first two-dimensional potential energy surfaces representing the ground state and the first excited state of the CO molecule on MP2-level which are corrected for the basis set superposition error. Applying wave packet propagation methods to these potential surfaces yields a quantum state resolved description of laserinduced desorption of CO from the rutile(110)-surface and reveals a completely new, mixed desorption mechanism. Dependent on the angle between the surface normal and the CO bond axis, a transition from a MGR- to an Antoniewicz-like desorption can be observed. In addition, a negative correlation between the rotational and translational degrees of freedom of the CO molecule was found. Finally, this leads to a desorption probability of the CO molecule in accordance with the expected value for metal oxides like TiO$_2$.

[1] M. Mehring, T. Klüner, *Chem. Phys. Lett.* **513**, 212 (2011).

O 5.6 Mon 11:45 MA 042

Adsorption of amino acids on the TiO$_2$ (110) surface — •Ralf Tonner — Fachbereich Chemie, Philipps-Universität Marburg, Germany

The optimal adsorption modes for amino acids glycine and proline on the ideal TiO$_2$(110) surface have been investigated using density functional theory (PBE) applying periodic boundary conditions (VASP). Binding modes with anionic acid moieties bridging two titanium atoms after transferring a proton to the surface are the most stable configurations for both molecules investigated similar to previous results for carboxylic acids. In contrast to the latter, amino acids can form hydrogen bonds via the amino group towards the surface-bound proton which provide an additional stabilization of 15-20 kJ mol^{-1}.

Calculations of vibrational frequencies complement the adsorption study and provide guidance for future experimental investigations. Dispersion effects can influence the relative stabilities of adsorption modes considerably.

O 5.7 Mon 12:00 MA 042

The adsorption of H2O on TiO2-(110) investigated by Helium Atom Scattering — •Niklas Osterloh[1] and Franziska Traeger[2] — [1]Physical Chemistry 1, Ruhr-University Bochum, Germany — [2]Institute for Business Engineering, University of Applied Science Gelsenkirchen, Germany

Previously reported experimental and theoretical studies disagree on, whether or not water on a defect free rutile TiO2(110)-surface adsorbs dissociative. The experimental results showed almost no dissociative behavior, but theoretical studies predicted exactly the opposite. [1,2] To clarify this question, we investigated water on rutile(110) by helium atom scattering (HAS), a most surface sensitive and non-destructive method, as well as by thermal desorption spectroscopy (TDS). The angular distributions of the helium atoms clearly show a (1x1) superstructure for temperatures between 130 and 300 K. While a fully dissociated layer was ruled out by previous studies [3], this symmetry rules out any half-dissociated layer. Neither the angular distribution nor the curves of specular intensity versus temperature showed any indications for a phase transition. In this talk we will present and discuss this results.

[1] Diebold, U., The surface science of titanium dioxide. Surface Science Reports, 2003. 48: p. 53-229 [2] Pang, C.L., R. Lindsay, and G. Thornton, Chemical reactions on rutile TiO2(110). Chemical Society Reviews, 2008. 37(10): p. 2328-2353 [3] Henderson, M.A., An HREELS and TPD study of water on TiO2(110): The extent of molecular versus dissociative adsorption. Surface Science, 1996. 355(1-3): p. 151-166

O 5.8 Mon 12:15 MA 042

Ab initio calculations on the adsorption of water on rutile (110) — •Jan Mitschker and Thorsten Klüner — Theoretical Chemistry, Carl von Ossietzky Universität Oldenburg, PO Box 2503, 26111 Oldenburg

Despite its apparent simplicity, the adsorption and photoreaction of water on surfaces is still a very challenging task. However, a fundamental understanding of the interaction is of great importance for a systematic surface modification. Furthermore, many substrates reveal interesting photochemical properties. As an example system, H_2O on titanium dioxide has attracted a great deal of attention, especially, because of its ability to split water under light irradiation. Though many theoretical and experimental studies have been performed, there is no satisfying agreement on how the process actually takes place. We address this problem by combining highly accurate *ab initio* potential energy surfaces (obtained on MP2 and CASPT2 level) with an explicit quantum dynamical treatment of the reaction in all relevant degrees of freedom. Such a procedure is indispensable to account for the quantum mechanical character of reactions involving hydrogen. The rutile(110) surface is modeled by a TiO_2 cluster embedded in a finite point charge field. The dynamics after an electronic excitation is simulated within the jumping wave packet model. In our talk, we present first results for the adsorption on the rutile(110) surface.

O 5.9 Mon 12:30 MA 042

Cu induced morphology changes at Pb/Si (111) interface: separation of "5x5"-Cu structure into individual domains. — •Pavel Shukrynau[1,2], Pingo Mutombo[2], Lars Smykalla[1], Vladimir Chab[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

The adsorption of small amount of Cu onto Pb covered Si (111-7x7 surface was studied with the variable temperature scanning tunnelling microscopy and spectroscopy. We observe many small clusters that appear on flat surface of 1x1-Pb islands upon RT deposition of copper. The behaviour of the clusters indicates that they are anchored to the underlying silicon substrate. Following temperature treatment fastens chemical reaction and transforms the clusters into shallow depressions of variable shape and size. Tunnelling spectra taken over the depressions suggest the formation of the copper silicides. Moreover, new objects having pronounced hexagonal form appear on rt3xrt3R30-Pb surface upon annealing. The filled and the empty state STM images of the hexagons differ strongly giving the evidence of an electronic effect. The hexagons are coalesced with the increase of Cu concentration and/or with the temperature rise. Detailed analysis of such agglomerate reveals hexagonal-like symmetry of pseudo-5x5 Cu structure. We suppose, that hexagonal objects are, possibly, individual "5x5"-Cu domains surrounded by the border made of Pb atoms.

O 5.10 Mon 12:45 MA 042

Reflectance anisotropy spectroscopy of clean and adsorbate-covered Si(111) surfaces: comparison of experiment and hybrid density functional theory — Soumya Banerjee, Sofia Giorgi, John F. McGilp, and •Charles H. Patterson — School of Physics, Trinity College Dublin, Dublin 2, Ireland.

Reflectance anisotropy (RA) at surfaces of cubic semiconductors provides a means of probing the electronic structure and optical transitions of their outermost atomic layers. We present experimental data and hybrid density functional theory (DFT) calculations for RA spectra of the clean Si(111)-2x1, Si(111)-3x1-Ag and Si(111)-5x2-Au surfaces. We test several structural models for the metal adsorbate covered surfaces as their exact structures are not known. Models which consist of linear regions of pi-bonded Si in honeycombs, which are separated by metal-rich rows give good agreement with experimental RA data. The exchange functional in these hybrid DFT calculations is adjusted so that the bulk Si band gap agrees with the experimental band gap. There is no need for a 'scissors' shift of the conduction band in these calculations.

O 5.11 Mon 13:00 MA 042

Interaction of Ta with Si (100) surface: Intermixing at the interface. — •Pavel Shukrynau[1,2], Pingo Mutombo[2], Lars Smykalla[1], 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.

The adsorption of small amounts of tantalum on Si (100)-2x1 reconstructed surface was investigated systematically using scanning tunneling microscopy/spectroscopy combined with first-principles density functional calculations. We found that the room temperature deposition of Ta on to Si (100)-2x1 surface followed by moderate annealing results in the formation of the short nanochains running perpendicular to the silicon dimer rows of the substrate. The chains are sporadically distributed over the surface and their density is metal coverage dependent. Filled and empty state images of the chains differ strongly giving the existence of covalent bonds within a particular chain. Careful analysis of these images allowed us to build up several structural models. Simulating the STM images on the base of these models and consequently comparing them with experiment, one of the proposed geometries is confirmed to match best the Ta chains. Tunneling spectra taken over each individual protrusion within a chain reveal small energy gap, showing semiconductor-like behavior of constituent atoms.

O 6: Scanning probe methods I

Time: Monday 10:30–13:00 Location: MA 043

O 6.1 Mon 10:30 MA 043

Combined ion and electron sputtering for STM tip cleaning — •David Hellmann, Ludwig Worbes, Hanna Fedderwitz, Nils Könne, Konstantin Kloppstech, and Achim Kittel — EHF, Physik, Fak. 5, Carl von Ossietzky Universität Oldenburg, Carl-von-Ossietzky-Straße 9-11, 26129 Oldenburg

In STM applications, atomic resolution of a surface reconstruction close to the ground state is considered as an indicator for a clean STM tip and sample surface. Diverse cleaning procedures are suggested in literature for both, tip and samples [1]. In practice not all of them seem to work reliably. Especially removing carbon residues from tips without reducing their sharpness can be challenging. In our experience using a combination of oxygen and electron sputtering yields good and, of equal importance, reproducible results. For this we employ a commercial ion gun and a home made minituarised electron source, respectivly [2]. Here we report about the results of a systematic investigation focused on this combined treatment. Literature: [1] C. J. Chen, Introduction to Scanning Tunneling Microscopy, 2nd ed. (Oxford University Press, Oxford, 2008). [2] D. Hellmann, L. Worbes and A. Kittel, Rev. Sci. Instrum., 82 (2011)

O 6.2 Mon 10:45 MA 043

Ultra compact 4-tip STM/AFM for electrical measurements at the nanoscale — •Vasily Cherepanov, Stefan Korte, Marcus Blab, Evgeny Zubkov, Hubertus Junker, Peter Coenen, and Bert Voigtländer — Peter Grünberg Institut (PGI-3), Forschungszentrum Jülich, 52425 Jülich, Germany, and JARA-Fundamentals of Future Information Technology

A new type of ultra miniature nano drive was specially developed to serve as an SPM coarse positioning unit. This Koala Drive makes the scanning probe microscopy design ultra compact and leads accordingly to a high mechanical stability. We use the Koala-drive to build a compact 4-tip STM/AFM where four independent scanning units are integrated on a diameter of 50 mm. Here we present the design of the microscope and show several measurement examples to demonstrate the device performance, such as four point measurements on silicide nanowires and graphene samples.

O 6.3 Mon 11:00 MA 043

Development of a Scanning Tunneling Microscope for Measurements down to 15 mK — •Maximilian Assig, Fabian Zinser, Markus Etzkorn, Christian R. Ast, and Klaus Kern — Max-Planck-Institut für Festkörperforschung,

The investigation of novel physical phenomena implies the design and the construction of new instruments and measurement techniques, which can overcome experimental limitations and open new areas in measurement accuracy. Scanning Tunneling Microscopy (STM) is a technique for probing the electronic structure of single adsorbed atoms, molecules and nanostructures at surfaces with atomic resolution. In this contribution we present the realization of a scanning tunneling microscope (STM) operating at temperatures of 15 mK which is accomplished by attaching the STM to a dilution refrigerator. We can apply high magnetic fields up to 14 T perpendicular and 0.5 T parallel to the sample surface. An ultra high vacuum (UHV) preparation chamber is attached to the cryostat allowing *in situ* preparation of the samples to be investigated. The electronic resolution of our STM was verified by taking tunneling spectra between a superconducting Aluminum tip and a Cu(111) surface at the base temperature of the cryostat. From fits to the BCS theory of superconductivity we were able to extract an upper limit for the effective temperature of the electrons which is $T_{\text{eff}} = 87 \pm 3\,\text{mK}$ for our best measurement. This corresponds to an energy resolution of $\Delta E = 3.5 \text{k}_\text{b}\text{T} = 26 \pm 1\,\mu\text{eV}$.

O 6.4 Mon 11:15 MA 043

Spatial variations of heat transfer at nanoscales investigated by Near-field Scanning Thermal Microscopy (NSThM) — •Ludwig Worbes, David Hellmann, Hanna Fedderwitz, Nils Könne, Konstantin Kloppstech und Achim Kittel — EHF/EPKOS, Institut für Physik, Universität Oldenburg

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 a 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 spatial resolution.

This heat flux can be mediated by different mechanisms: A possible transport mechanism is thermal near field radiation especially relevant for small distances. A strong enhancement of near field heat flux by thin and electrical high resistive layers or adsorbed molecules is predicted by theory [2]. Another possibility is phononic or electronic heat transport through adsorbed molecules forming a molecular junction between sample and probe. We present measurements performed on Au(111) surfaces to discuss the influence of adsorbates.

[1] Uli F. Wischnath et al., Rev. Sci. Instrum. 79, 073708 (2008)
[2]A.I. Volotkitin, B. N. J. Persson, Rev. Mod. Phys. 79, 1291 (2007)

O 6.5 Mon 11:30 MA 043

Next generation SPM control system extends the range of applications in surface science — •Alessandro Pioda — SPECS Surface Nano Analysis GmbH

Novel scanning probe microscopy techniques, modes of operation, and advances in microscope hardware are pushing the boundary for signal resolution and flexibility in SPM measurements. Here we present a new state of the art SPM control system, which improves signal precision, resolution, bandwidth and noise performance by about one order of magnitude compared to current generation controllers. The controller incorporates the performance of expensive dedicated instruments in a compact modular multichannel package. In combination with the well proven and flexible Nanonis SPM control software, this next generation controller is the ideal platform for the most demanding microscopy, spectroscopy and transport measurements tasks, opening the door to a larger range of applications compared to current systems. Furthermore, the flexible and easily configurable user interface of the controller and the large number of measurement channels allows its operation as a high performance DC and AC source and measurement interface with ppm precision and multiple lock-in amplifiers, opening new perspectives for materials research.

O 6.6 Mon 11:45 MA 043

Determination of the electron-phonon coupling in ultra-thin Pb films with STM — •Tobias Märkl[1], Michael Schackert[1], Martin Hölzer[2], Sergey Ostanin[2], Arthur Ernst[2], and Wulf Wulfhekel[1] — [1]KIT, Karlsruhe — [2]MPI, Halle

The typical quantity to characterize the electron-phonon coupling of a material is the energy-dependent Éliashberg function $\alpha^2F(\omega)$ determining the superconducting properties of the material. It can be determined with tunneling spectroscopy in the superconducting state and inversion of the Éliashberg equations or directly using inelastic tunneling spectroscopy (ITS) in the normal state.

We used scanning tunneling microscopy (STM) at 1K in UHV to locally measure inelastic tunneling spectra of thin Pb films on Cu(100) and CuN/Cu(100) to determine $\alpha^2F(\omega)$ as function of the local Pb thickness. The films were prepared in situ with varying thickness up to 25 atomic layers and were in the normal state due to the proximity effect. We find a good agreement of the obtained Éliashberg function with ab initio calculations for bulk lead.

O 6.7 Mon 12:00 MA 043

Scanning tunneling microscopy of Ni layers on W(110) — •Johannes Schöneberg, Alexander Weismann, and Richard Berndt — Institut für Experimentelle und Angewandte Physik der Universität Kiel Leibnizstr. 19 D-24118 Kiel

The growth and electronic properties of one to seven monolayers of Ni grown on W(110) were investigated with a low-temperature scanning tunneling microscope. The features in dI/dV spectra from these layers are distinctly different. We analyze the data experimental in terms of bulk band structure calculations. Financial support through SFB 668 is acknowledged.

O 6.8 Mon 12:15 MA 043

Single Molecule and Single Atom Sensors for Atomic Resolution Imaging of Chemically Complex Surfaces — •Georgy Kichin[1,2], Christian Weiss[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

To image the inner structure of molecules have always been the challenge for the surface science. Recently we have demonstrated that this task can be solved with a low-temperature scanning tunneling microscope (STM) if molecular hydrogen or deuterium is condensed in the junction [1,2,3]. In this contribution we will demonstrate that individual Xe atom, single CO and CH_4 molecules adsorbed at the tip apex of the STM produce similar resolution as achieved with hydrogen [4]. This result supports our earlier claim that a single molecule adsorbed at the STM tip can act as a nanoscale force sensor / signal transducer.

[1] R. Temirov et al. *New J. Phys.*,**10**, 053012, (2008)
[2] C. Weiss et al. *Phys. Rev. Lett.*, **105**, 086103, (2010)
[3] C. Weiss et al. *J. Am. Chem. Soc.*, **132**, 11864, (2010)
[4] G. Kichin et al. *J. Am. Chem. Soc.*, **133**, 16847, (2011)

O 6.9 Mon 12:30 MA 043

Electron transport studies through a single octanethiol

molecule — •René Heimbuch, Avijit Kumar, Hairong Wu, Bene Poelsema, and Harold Zandvliet — Physics of Interfaces and Nanomaterials, MESA+ Institute for Nanotechnology, University of Twente, the Netherlands

Single molecules, used as functional electronic components define the field of molecular electronics. These molecules need to be contacted via electrodes to the macroscopic world. Previously, a single octanenthiol molecule was trapped between an STM tip and a substrate and the conductance was measured. In our work, we study the full transport through a single octanethiol molecule bridging the gap between the STM tip and the substrate. Control over the switching behavior of the molecule has been achieved through careful tuning of the electrodes' interspace and voltage. For an electric field exceeding $4-6\cdot 10^9$ V/m, the switch can be turned "ON". Once trapped, we also measure an increase in the conductance of the molecule upon compression. This method is used to investigate the transport properties of the molecule as function of temperature.

O 6.10 Mon 12:45 MA 043

Atomic Forces and Energy Dissipation of a Bi-Stable Molecular Junction — •Christian Lotze[1], Martina Corso[1], Katharina Franke[1], Felix von Oppen[2], and Nacho Pascual[1] — [1]Inst. f. Experimentalphysik FU Berlin — [2]Inst. f. theoretische Physik FU Berlin

Tuning Fork based dynamic STM/AFM is a well established method combining the advantages of scanning tunneling and dynamic force microscopy. Using tuning forks with high stiffness, stable measurements with small amplitudes, below 1 Å can be performed. In this way, conductance and frequency shift measurements of molecular junction 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 to the properties of the junction. These lead, for example, to conductance fluctuations, telegraph noise and the possibility to switch the electrical transport through the junction.

In this presentation, we characterize a model bi-stable molecular system using dynamic force spectroscopy. The effect of current-induced stochastic fluctuations of conductance are correlated with fluctuations in force. In our experiment we identified the last from both, frequency shifts and energy dissipation measurements, picturing a regime in which electrical transport and mechanical motion are coupled.

[1] N. Fournier *et. al*, PhysRevB 84, 035435 (2011),

[2] L. Gross *et. al*, Science 324, 1428 (2009)

O 7: Metal substrates: Adsorption of organic / bio molecules I

Time: Monday 10:30–13:00 Location: A 053

O 7.1 Mon 10:30 A 053

Order or disorder? The adsorption of NTCDA on Ag(111) investigated by VT-STM — •Holger Wetzstein[1,2], Sebastian Fiedler[1,2], Jeremias Weinrich[1,2], Martin Winnerlein[1,2], Achim Schöll[1,2], and Friedrich Reinert[1,2] — [1]Physikalisches Institut, Experimentelle Physik VII und Wilhelm Conrad Röntgen Research Center for Complex Material Systems (RCCM), Universität Würzburg, D-97074 Würzburg — [2]Gemeinschaftslabor für Nanoanalytik, Karlsruher Institut für Technologie KIT, D-76021 Karlsruhe

The adsorption of organic molecules on single crystalline substrates results in a wealth of structural arrangements. This polymorphism is due to the interplay between lateral and vertical interactions and strongly depends on coverage, temperature and preparation. We investigated the adsorption of NTCDA on Ag(111) surfaces at different temperatures with the help of variable temperature scanning tunneling microscopy and low energy electron diffraction to analyze the structural and electronic properties. This systems shows various adsorbate superstructures and a particularly interesting reversible order-disordering transition upon cooling, so called inverse melting. While some thermodynamic parameters of this transition have already been derived, the driving force for this ordering phenomenon as well as the geometric arrangement of the molecules in the disordered phase has not yet been accessed. Our STM data shows various ordered and disordered structural phases at different temperatures. By correlating our new results with already existing data we intend to shed light on the mechanism involved in the ordering of organic molecules on metal substrates.

O 7.2 Mon 10:45 A 053

Observing Structural Phase Dynamics and Molecular Aggregation in Real Time: Dispersive NEXAFS Applied to Organic Films — •Markus Scholz[1,2], Christoph Sauer[1,2], Michael Wiessner[1,2], Holger Wetzstein[1,2], Achim Schöll[1,2], and Friedrich Reinert[1,2] — [1]Physikalisches Institut, Experimentelle Physik VII und Wilhelm Conrad Röntgen Research Center for Complex Material Systems (RCCM), Universität Würzburg, D-97074 Würzburg — [2]Gemeinschaftslabor für Nanoanalytik, Karlsruher Institut für Technologie KIT, D-76021 Karlsruhe

We present a novel experimental approach which allows following structural and electronic changes in organic films by quick near edge X-ray absorption fine-structure spectroscopy (QNEXAFS). This technique utilizes the energy-dispersive mode of the BESSY UE52-PGM beamline and allows NEXAFS with about one second time resolution. We show the potential of the method on the example of thin films of the organic molecule 1,4,5,8-naphthalene-tetracarboxylicacid-dianhydride (NTCDA). The time-evolution of the NEXAFS signal recorded at different temperatures allows distinguishing between different processes that are involved in the reorganization of the film. Moreover, since the technique also monitors spectroscopic details we are able to study the interplay between film morphology, molecular orientation, and intermolecular interaction in real time. In a meta-stable phase we observe aggregated molecules that exhibit coherent coupling. The signature change of the vibronic progression and of the peak width allow us to quantify the coherent length of the electronic excitation.

O 7.3 Mon 11:00 A 053

Ultrathin heterostructures and mixed layers of the organic semiconductors NTCDA and PTCDA on Ag(111) — •Gregor Öhl, Carolin R. Braatz, and Peter Jakob — Philipps-Universität, Marburg, Germany

Heterostructures as well as mixed layers of the organic semiconductors PTCDA and NTCDA have been grown on Ag(111) and their thermal evolution (temperature range 80 - 550 K) investigated *in situ* using FT-IRAS, SPA-LEED and TDS. Specifically, the influence of the long range order within the first monolayer on the stacking and the thermal evolution of the heterolayers will be discussed. The high spectral resolution of IRAS thereby allows a clear discrimination of the two molecular species and of the various phases of the layered NTCDA/PTCDA system. Effects such as orientational changes, lateral ordering, dewetting and interlayer exchange become accessible this way. Depending on the stacking order of the PTCDA and NTCDA layers and on the amount of deposited material, the relevance of the individual processes is found to vary substantially. For the mixed PTCDA/NTCDA monolayers on Ag(111), results on the thermal evolution are presented.

O 7.4 Mon 11:15 A 053

Dissecting an organic-metal bond by molecular manipulation — •Christian Wagner, Norman Fournier, Christian Weiss, Ruslan Temirov, and F. Stefan Tautz — Peter Grünberg Institut (PGI-3), Forschungszentrum Jülich, 52425 Jülich, Germany and JARA-Fundamentals of Future Information Technology

Scanning probe microscopy with a dynamic AFM has been able to answer some fundamental questions of surface science, like the force necessary to move an atom[1]. Recently, we demonstrated the gradual removal of a single 3,4,9,10-perylenetetracarboxylic-dianhydride (PTCDA) molecule from Ag(111) using a dynamic AFM [2]. The continuous force gradient measurement allowed the structural control over the junction. Here, we show how to extract details of the molecule-surface bonding (physisorption, chemisorption, bonding via functional groups) from such an experiment. The importance of a full-fledged simulation of the lifting -including tip oscillation- is emphasized. We point out the necessity of, and fundamental problems related to, a curved tip trajectory. We study PTCDA on Au(111) and Ag(111) and find qualitatively and quantitatively different binding potentials and adsorption energies. The data represents a good benchmark for existing and future ab-initio calculations on these systems. Our method

should be applicable to various substrate-adsorbate systems and hence has the potential to answer many open questions in the field.
[1] M. Ternes et al., *Science* **319**, 1066 (2008)
[2] N. Fournier et al., *Phys. Rev. B* **84**, 035435 (2011)

O 7.5 Mon 11:30 A 053

Force-controlled lifting of molecular wires — •Norman Fournier[1,2], Christian Wagner[1,2], Christian Weiss[1,2], Ruslan Temirov[1,2], and F. Stefan Tautz[1,2] — [1]Peter Grünberg Institut (PGI-3), Forschungszentrum Jülich, 52425 Jülich, Germany — [2]JARA-Fundamentals of Future Information Technology

Understanding of the charge transport on a single-molecule level is vital for the future success of molecular electronics. Often, however, this understanding is hindered by the lack of data obtained under well-controlled experimental conditions. Recently, we have shown that a low-temperature dynamic atomic force microscope (AFM) can be used to perform well-controlled and tunable single molecule transport studies [1]. In this experiment a single 3,4,9,10-perylene-tetracarboxylicacid-dianhydride (PTCDA) molecule is lifted from a metal surface, while the stiffness of the junction is recorded along with the conductivity. Here, we compare lifting of PTCDA from Au(111) and from Ag(111), i.e., two situations where PTCDA is either connected to gold or to silver electrodes. We find clear differences in the conductivity and the stiffness in both cases that we attribute to the different character of the molecule-metal bond.
[1] N. Fournier et al. *Phys. Rev. B* **84**, 035435 (2011)

O 7.6 Mon 11:45 A 053

Importance of electron correlations for π-conjugated organic molecules on metal substrates — •Christoph Sauer[1,2], Florian Bruckner[1,2], Holger Wetzstein[1,2], Sina Gusenleitner[1,2], Achim Schöll[1,2], and Friedrich Reinert[1,2] — [1]Physikalisches Institut, Experimentelle Physik VII und Wilhelm Conrad Röntgen Research Center for Complex Material Systems (RCCM), Universität Würzburg, D-97074 Würzburg — [2]Gemeinschaftslabor für Nanoanalytik, Karlsruher Institut für Technologie KIT, D-76021 Karlsruhe

We demonstrate that electron correlations play an important role for the energy balance when the adsorption of π-conjugated molecules on metal substrates leads to charge transfer into the former lowest unoccupied molecular orbital (LUMO). By annealing an organic heterostructure of tin-phthalocyanine (SnPc) on top of a Ag(111) surface precovered with one monolayer (ML) of 3,4,9,10-perylene-tetracarboxylic-dianhydride (PTCDA) we produce a pure ML of SnPc on Ag(111). Therefore our high resolution photoemission spectroscopy (PES) analysis proves that the adsorption of SnPc is energetically favoured over PTCDA on Ag(111). We identify that this behavior is a consequence of a smaller Coulomb repulsion (U_C) between the electron in the former LUMO and the electrons in the other molecular orbitals for SnPc. The difference in U_C for SnPc and PTCDA is demonstraded by a comparison of PES and inverse PES data from multilayer and ML samples and values in the order of 1 eV are found. Hence U_C is not negligible for the adsorption energy balance.

O 7.7 Mon 12:00 A 053

Modification of the PTCDA/Ag(111) interaction by the formation of a hetero-organic interface with CuPc — •Benjamin Stadtmüller[1,2], Tomoki Sueyoshi[1,2], Serguei Soubatch[1,2], F. Stefan Tautz[1,2], and Christian Kumpf[1,2] — [1]Peter Grünberg Insitut (PGI-3), Forschungszentrum Jülich, Germany — [2]Jülich-Aachen Research Alliance - Fundamentals of Future Information Technology

In recent years the adsorption of large organic molecules on noble metal surfaces has been studied in great detail. One key aspect in these studies was the characterization of the interaction between the organic adsorbates and the metal substrate. Based on these studies we have now started to investigate hetero-organic systems consisting of more than one molecular species. Here we present a X-Ray Standing Waves (XSW) and photoelectron spectroscopy (UPS) study of the adsorption behavior of CuPc on one closed layer of PTCDA on Ag(111). The CuPc molecules adsorb on top of the closed PTCDA layer and form a disordered CuPc layer at submonolayer coverages and room temperature, which condenses into the commensurate 'stacked bilayer'-structure upon cooling below 160K. XSW reveals an adsorption height of CuPc on PTCDA which is significantly smaller than the sum of the van der Waals radii of the atomic species. Even more interestingly, for this system the vertical adsorption geometry of the underlying PTCDA molecule changes: The molecular backbone is pushed towards the silver surface. Furthermore, UPS experiments reveal a shift of the PTCDA F-LUMO. These results clearly indicate a modified interaction between PTCDA and the silver surface by the adsorption of CuPc.

O 7.8 Mon 12:15 A 053

Electronic and geometric structure of organic overlayers from angle-resolved UPS and DFT calculations — •Matus Milko[1], Sophia Huppmann[2,3], Markus Scholz[2,3], Wiessner Michael[2,3], Achim Schöll[2,3], Friedrich Reinert[2,3], and Peter Puschnig[1] — [1]Chair of Atomistic Modelling and Design of Materials, Montanuniversität Leoben, Austria — [2]Experimentelle Physik VII und Wilhelm Conrad Roentgen Research Center for Complex Material Systems, Universität Würzburg, Germany — [3]Gemeinschaftslabor für Nanoanalytik, Karlsruher Institut für Technologie KIT, Germany

We present a combined experimental and theoretical study on the electronic and geometric structure of metal-free phthalocyanine (H_2Pc) and copper phtalocyanine (CuPc) adsorbed on Au(110). Experimentally, mono-layers of the molecules were analyzed by low energy electron diffraction (LEED) revealing ordered superstructures. Then, angular resolved photoelectron spectroscopy (ARPES) was employed to examine the valence electronic structure. Theoretically, we computed the electronic structure within the framework of density functional theory corrected for many body effects which leads to correct ordering of orbitals. Moreover, using ARPES orbital maps of the highest occupied molecular orbitals in reciprocal space were obtained which we could directly compare to our *ab initio* results. We demonstrate, how one can extract information about the azimuthal orientation of the molecules on the substrate by this approach. Thus in combination with LEED we can provide a complete two-dimensional structure determination.

O 7.9 Mon 12:30 A 053

Low Temperature Scanning Tunneling Microscopy Study of Co-Phthalocyanine Molecules on Au (111) and Graphene/Ir (111) — •Samuel Bouvron, Philipp Erler, Stefan Ambrus, Udo Dehm, David Heese, Elizabeta Ćavar, and Mikhail Fonin — Fachbereich Physik, Universität Konstanz

Metal-phthalocyanines have attracted substantial attention due to their possible applications in molecular electronic devices. Since it may affect the electronic structure and magnetic properties of the molecule, the interaction between a molecule and a substrate is of crucial importance. Furthermore, the adsorption behavior of molecules on surfaces is decisive in a bottom up approach to build molecular electronics. For a better understanding of the interaction between Cobalt-Phthalocyanine molecules (CoPc) and surfaces, we investigated CoPc molecules deposited on Au (111) and Graphene/Ir (111) at different coverages by means of low-temperature scanning tunneling microscopy (STM) and near-edge xray absorption spectroscopy (NEXAFS). The possible use of the graphene layer to decouple the CoPc molecule from a metallic substrate will be discussed.

O 7.10 Mon 12:45 A 053

Naphthalocyanine on Au(100) _ adsorption and structural formation at submonolayer coverage — •Patrick Mehring, Axel Beimborn, Tobias Lühr, and Carsten Westphal — Technische Universität Dortmund, Experimentelle Physik 1, Germany

The formation of metal-free naphthalocyanine (H2Nc) structures on Au(100) is investigated by means of room temperature scanning tunneling microscopy at submonolayer coverage. The molecules adsorb with their plane parallel to the surface and arrange in two types of ordered domain structures. A striped phase with an orientation perpendicular to the ridge of the Au(100)_hex reconstruction and a densely packed phase with an unequal distribution along the high-symmetry surface directions is found. In the densely packed domains only one configuration of H2Nc is observed. Subsequent annealing induces a phase transformation of the adlayer. The number and size of H2Nc domains arranged in the striped phase decreases and the molecular sequence within the densely packed domain structure is changed.

O 8: Electron and spin dynamics

Time: Monday 10:30–13:00 Location: A 060

O 8.1 Mon 10:30 A 060

Empty topological surface state on Bi$_2$Se$_3$ — •Daniel Niesner[1], Sergey Eremeev[2], Evgueni Chulkov[3], and Thomas Fauster[1] — [1]Universität Erlangen, Lehrstuhl für Festkörperphysik, Staudtstr. 7, 91058 Erlangen, Germany — [2]Tomsk State University, pr. Lenina 36, 634050 Tomsk, Russia — [3]Donostia International Physics Center (DIPC), and CFM, Centro Mixto CSIC-UPV/EHU, Departamento de Física de Materiales, UPV/EHU, 20080 San Sebastián, Spain

Topological insulators are characterized by spin-polarized, linearly dispersing surface states that arise from a symmetry inversion of the bulk bands at band gap edges. In case of Bi$_2$Se$_3$ the Fermi surface is formed by a single Dirac-cone at the $\overline{\Gamma}$-point.

Using laser-based photoemission with 6.2 eV photon energy we find the Dirac-point 0.3 eV below the Fermi energy.

In mono- and bichromatic two-photon photoemission we find a second linearly dispersing band 1.4 eV above the Fermi level with a group velocity of $5 \cdot 10^5 \frac{\mathrm{m}}{\mathrm{s}}$. Lifetimes amount to ≈ 74 fs. Circular dichroism indicates a high degree of spin polarization.

These data are in good agreement with DFT calculations showing a topologically protected surface state 1.5 eV above Fermi level. The calculations compare favorably with the other empty electronic states found in the two-photon photoemission experiments.

O 8.2 Mon 10:45 A 060

The role of the excitation pathway in the photoinduced melting of the CDW in $1T$-TiSe$_2$ — •Gerald Rohde, Stefan Hellmann, Timm Rohwer, Christian Sohrt, Ankatrin Stange, Kerstin Hanff, Lutz Kipp, Michael Bauer, and Kai Rossnagel — Institut für Experimentelle und Angewandte Physik der Christian-Albrechts-Universität zu Kiel

Charge-density waves (CDWs) are broken-symmetry states of low-dimensional solids that are brought about by strong electron-phonon or electron-electron interaction. In a time-resolved XUV ARPES study we recently showed that the long-range order associated with the CDW phase in the transition metal dichalcogenide $1T$-TiSe$_2$ can be destroyed within less than 30 fs after intense illumination with a 800 nm light pulse [1]. In this contribution we present complementary data recorded at pulsed 400 nm excitation. Surprisingly we find that for the short-wavelength excitation the CDW collapse is considerably slowed down. Our time-resolved ARPES data show furthermore that the initiating absorption processes take place at well separated locations in electron momentum space for the two different wavelengths. Possible scenarios that consider the effect of the absorption pathway on the phase transition dynamics will be discussed.

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

O 8.3 Mon 11:00 A 060

Electronic lifetimes in a Bi quantum well with Rashba spin-splitting — •Svenja Vollmar, Andreas Ruffing, Sebastian Jakobs, Alexander Baral, Mirko Cinchetti, Stefan Mathias, Martin Aeschlimann, and Hans Christian Schneider — University of Kaiserslautern

2-photon photoemission spectroscopy and ab-initio calculations suggest that a part of the band structure of a Bi monolayer (quantum well) on a Cu(111) substrate is well described [1] by a simple Rashba Hamiltonian, which includes the effects of the spin-orbit interaction together with an asymmetric confinement potential of a quantum-well. The understanding of the consequences of the Rashba spin-split electronic bands on the electronic spin dynamics is of general importance for spin transport and diffusion lengths in such systems.

Using a combination of 1-photon and 2-photon photoemission spectroscopy, we determine the energy and momentum dependent electronic lifetimes in the Bi quantum well, and find a plateau around the intersection of the Rashba bands. To understand this characteristic energy and momentum dependence, we calculate the electronic lifetime due to carrier-carrier scattering in a simple model of a 2D electron gas including a Rashba interaction with effective Rashba parameters derived from experiment. We reproduce the observed plateau in the lifetimes using this model, and explain this behavior by a change of available scattering phase space for electrons below and above the intersection of the Rashba bands.

[1] S. Mathias et al., Phys. Rev. Lett. 104, 066802 (2010)

O 8.4 Mon 11:15 A 060

Ultrafast melting of a charge-density wave in the Peierls insulator Rb:TaS$_2$ — •Kerstin Hanff, Stefan Hellmann, Timm Rohwer, Michael Bauer, Lutz Kipp, and Kai Rossnagel — Institute of Experimental and Applied Physics, University of Kiel, 24098 Kiel, Germany

Ultra-short high-harmonic pulses enable us to study ultrafast dynamics of condensed matter systems on femto- and picosecond time scales. In particular, they allow us to identify the nature and strength of interactions between various degrees of freedom in complex materials, in which typically two or more of the lattice, charge, spin and orbital degrees of freedom are strongly coupled. Our recent studies focused on the investigation of electronically driven charge-density waves employing time- and angle-resolved photoelectron spectroscopy. Here, we present the ultrafast dynamics of a lattice driven CDW system. Rb adsorption on 1T–TaS$_2$ serves as a model system revealing a pronounced metal-to-insulator transition. Induced by a charge transfer, this intercalation process leads to a structural change into a commensurate CDW phase. Upon strong photoexcitation by an optical pump pulse the electronic gap closes and the Peierls insulator Rb:TaS$_2$ undergoes a transition into a transient metallic state. We are able to distinguish different time scales during the excitation and relaxation processes, which indicate the influence of the electronic and lattice systems.

O 8.5 Mon 11:30 A 060

Singlet fission and efficient electron transfer from the "dark" multi-exciton state in pentacene — Wai-Lun Chan[1], •Manuel Ligges[1,2], Askat Jailaubekov[1], Loren Kaake[1], Luis Miaja-Avila[1], and Xiaoyang Zhu[1] — [1]Department of Chemistry & Biochemistry, University of Texas, Austin, TX 78712, USA — [2]Fakultät für Physik, Universität Duisburg-Essen, 78756 Duisburg

Singlet fission refers to the creation of two or more electron-hole pairs from the absorption of a single photon in organic chromophores. This process holds great promise in the field of photovoltaics, because it may lead to power conversion efficiencies exceeding the theoretical limit for single junction solar cells, the so called Shockely-Queisser limit [1]. One of the key challenges in the implementation of singlet fission is the efficient extraction of charge carriers. Using time-resolved two-photon photoemission on the model system pentacene/C$_{60}$, we show that the process of singlet fission is accompanied by efficient electron transfer from a multi-electron intermediate state, previously been referred to as the " dark " multi-exciton state [2]. In addition, we show that - contrary to common belief - singlet fission in pentacene cannot be described in terms of simple rate models but involves coherent coupling between the initially excited singlet exciton and the intermediate multi-exciton state.

[1] W. Shockley & H. J. Queisser, J. Appl. Phys. **32**, 510 (1961)
[2] P. M. Zimmerman et al., Nature Chem. **2**, 648 (2010)

O 8.6 Mon 11:45 A 060

The role of intermediate states in two-photon photoemission from Si(001) — •Henning Husser and Eckhard Pehlke — Institut für Theoretische Physik und Astrophysik, Universität Kiel, Germany

Two-photon photoemission (2PPE) spectra contain detailed information about the unoccupied states [1], and time resolved 2PPE can reveal the dynamics. We have developed a non-perturbational approach to calculate photocurrents by time-dependent simulations and applied it to the calculation of normal-emission photocurrents from Si(001). Here we focus on the analysis of 2PPE Si(001) normal emission spectra from the simulations in the light of the expression known from perturbation theory. The intermediate states occurring in this expression are linked to both the initial state and to the final state by matrix elements. Intermediate states can become prominent in the spectra if they couple strongly to the initial states or the final states. Variation of the polarization of the light wave can be used to tune the matrix elements via the respective selection rules. Resonances in the emission intensity for a fixed initial state as a function of photon energy can be assigned to intermediate states. This will be used to derive information about the intermediate states in case of normal-emission 2PPE from Si(001). In particular the role of surface resonances, as reported by Fauster et al. [2], will be investigated.

[1] W. Schattke et al., Phys. Rev. B 78, 15534 (2008).

[2] T. Fauster et al., Verhandl. DPG (VI) 46, 1/490 (2011).

O 8.7 Mon 12:00 A 060

Orbital Symmetry Dependent Electron Transfer through Molecules Assembled on Metal Substrates — •Florian Blobner[1], Pedro Coto[2], Francesco Allegretti[1], Michel Bockstedte[2], Oscar Rubio-Pons[2], Haobin Wang[3], David Allara[4], Michael Zharnikov[5], Michael Thoss[2], and Peter Feulner[1] — [1]Physik-Department E20, Technische Universität München, 85748 Garching, Germany — [2]Institut für Theoretische Physik und Interdisziplinäres Zentrum für Molekulare Materialien, Friedrich-Alexander-Universität Erlangen-Nürnberg, 91058 Erlangen, Germany — [3]Department of Chemistry and Biochemistry, MSC 3C, New Mexico State University, Las Cruces, 88003 New Mexico, USA — [4]Departments of Chemistry and Material Science, Pennsylvania State University, 16802 Pennsylvania, USA — [5]Angewandte Physikalische Chemie, Universität Heidelberg, 69120 Heidelberg, Germany

Femtosecond charge transfer dynamics in self-assembled monolayers of cyano-terminated ethane-thiolate on gold substrates was investigated with the core hole clock method. Electrons from the nitrogen K-shell are state-selectively excited into the two symmetry-split π^* orbitals of the cyano end group with x-ray photons of well-defined polarization. The charge transfer times from these temporarily occupied orbitals to the metal substrate differ significantly. Theoretical calculations show that these two π^* orbitals extend differently onto the alkane backbone and the anchoring sulfur atom, thus causing the observed dependence of the electron transfer dynamics on the symmetry of the orbital.

O 8.8 Mon 12:15 A 060

Trapping of image-potential resonances on free-electron-like metal surface — •Ulrich Höfer[1,2], Matthias Winter[1], Eugene V. Chulkov[2], and Pedro M. Echenique[2] — [1]Fachbereich Physik, Philipps-Universität Marburg, Germany — [2]Donostia International Physics Center (DIPC), San Sebastián, Spain

Image-potential states have been studied by two-photon photoemission (2PPE) for the surface of Al(100) where the whole series is energetically degenerate with free-electron-like bulk states. In contrast to expectations, the series of resonances is not smeared out to one broad structure as a result of a strong coupling to the bulk continuum. Instead, the first resonance (n=1) is found to be suppressed and the resonances with quantum numbers n=2,3,4,5 are resolved as individual peaks in the time-resolved spectra. Both effects are suggested to be a consequence of resonance trapping [1].

Here, we combine the multiple scattering approach to describe surface states with an open quantum system formalism that properly takes into account strong coupling of resonances to a continuum. The theory is able to quantitatively describe trapping of adjacent surface resonances for simple metals.

[1] M. Winter, E. V. Chulkov, U. Höfer, PRL **107**, 236801 (2011)

O 8.9 Mon 12:30 A 060

Time-resolved 2PPE study on NiO(001) thin films — •Mario Kiel, Stephan Grosser, and Wolf Widdra — Martin-Luther-Universität Halle-Wittenberg, 06120 Halle, Germany

The electronic structure of unoccupied states within ultra-thin films of the transition metal nickel oxide has been investigated by time-resolved two-photon photoemission (2PPE) in combination with scanning tunneling spectroscopy (STS). The thin films have been prepared under UHV conditions by molecular beam epitaxy in an oxygen atmosphere on a Ag(001) substrate at room temperature.

For the NiO bilayer a series of image-potential states has been identified. From time-resolved data lifetimes of 30, 50, and 120 fs have been determined for the n=1–3 image state, respectively. The observed binding energies can be well described on the basis of the dielectric properties of NiO. For the bilayer the permittivity is already close to the bulk like. Besides the image-potential states unoccupied Ni 3d states can be identified for the NiO bilayer as well as for thicker films in the 2PPE spectra. These states exhibit layer-dependent energy shifts which will be compared with layer-resolved STS data in the range from 2 to 8 monlolayers NiO. Additionally, 2PPE features from occupied NiO states have been identified due to their characteristic energy shift upon photon energy variation.

O 8.10 Mon 12:45 A 060

Hot carrier relaxation in HOPG probed at the H-point by means of time-resolved XUV photoemission — •Ankatrin Stange, Christian Sohrt, Timm Rohwer, Stefan Hellmann, Gerald Rohde, Kerstin Hanff, Lutz Kipp, Kai Rossnagel, and Michael Bauer — Institut für Experimentelle und Angewandte Physik, Universität Kiel, 24118 Kiel, Germany

Time- and angle-resolved XUV photoelectron spectroscopy (tr-ARPES) is applied to study the relaxation dynamics of excited hot carriers in HOPG and graphene. The XUV probe used in the experiment allows us to record electronic structure transients at large momentum values so that in particular the boundary of the first Brillouin zone becomes accessible. In the case of HOPG this capability provides a most direct access to the momentum region relevant for optical excitation and subsequent relaxation of the hot carriers. The results are discussed with respect to other time-resolved experiments which in the past were restricted to probes in the visible/NUV regime.

O 9: Invited talk (Shigeki Kawai)

Time: Monday 15:00–15:45 Location: H 2013

Invited Talk O 9.1 Mon 15:00 H 2013

Three dimensional dynamic force spectroscopy at room temperature — •Shigeki Kawai and Ernst Meyer — Klingelbergstrasse 82, CH-4056 Basel

Measurement of force and potential above the surface is of crucial importance to investigate the adsorption and friction on a surface at atomic-scale. Such information can be extracted via the frequency shift of an oscillating cantilever in dynamic force spectroscopy (DFS). Since the first site-dependent measurement of the force in 2001, this technique rapidly evolved, and is now used for high-resolution three-dimensional force mapping mainly at low temperature where the thermal drift is negligibly small.

Here we realized 3D-DFS measurements even at room temperature (RT). The thermal drift as a critical issue in the measurement at RT was precisely excluded by an atom-tracked tip-positioning, which was activated each before the distance dependence measurement. Then, high-density and high*resolution 3D force field was measured on ionic crystal surfaces and self-assembled molecule. A detailed contact mechanism such as deformations of the surface and tip and movement of the molecule was studied.

O 10: [DS] Focused electron beam induced processing for the fabrication of nanostructures I (focused session, jointly with O – Organizers: Huth, Marbach)

Time: Monday 15:00–17:00 Location: H 0111

Invited Talk O 10.1 Mon 15:00 H 0111

Focused electron beam lithography in the 1-10 nanometer range. — •Cornelis Wouter Hagen — Delft University of Technology, Charged particle Optics Group, Lorentzweg 1, 2628CJ Delft, The Netherlands

What if one would like to make something really small, for instance something consisting of only a few thousand atoms, then how would one do it? And what if one would also like to have control over its final shape and its composition? How could that be achieved? The answer is: with focused electron beam induced processing (FEBIP), because an electron beam can be focused down to a tiny sub-nanometer spot. When such a beam is scanned over a substrate with an adsorbed monolayer of precursor molecules, the molecules are dissociated. Only at the positions where the electron beam has been, solid fragments are left behind at the surface, forming a high-resolution pattern. I will review what we have learned about this process, focusing on the superb resolution, and the fundamentals of the dissociation process. To turn FEBIP into a user-friendly lithography technique, dedicated instruments will have to be developed. I will sketch the route that we envision towards such instrumentation.

Topical Talk O 10.2 Mon 15:30 H 0111

Fabrication of 1 nm thick Carbon Nanomembranes using FEBIP — •Armin Gölzhäuser — Universität Bielefeld, Bielefeld, Germany

We employ a combination of molecular self-assembly and focused electron beam induced processing (FEBIP) to fabricate only 1 nm thick, but mechanically stable carbon nanomembranes (CNM). Self-Assembled Monolayers (SAMs) of amphiphilic biphenylthiols are formed on gold surfaces and then exposed to electron beams that lead to a C-H cleavage. The dehydrogenation is followed by a lateral cross-linking between neighboring molecules [1]. The resulting two-dimensional film can be released from the surface, forming a mechanically stable CNM with the thickness of the original monolayer, i.e. 1 nm [2]. We have developed procedures for the handling of CNMs, i.e. to transfer them onto arbitrary surfaces and to prepare them as free-standing films. It will be shown that free-standing CNMs can be used as supports for transmission electrons microscopy [3]. Free-standing CNMs also can act as substrates for a FEBIP fabrication of very small metal clusters [4].

[1] A. Turchanin et al. Langmuir 25, 7342 (2009).
[2] A. Turchanin et al. Adv. Mater. 21, 1233 (2009).
[3] C.T. Nottbohm et al. Ultramicroscopy 108, 885 (2008).
[4] W.F. van Dorp et al. Nanotechnology 22, 115303 (2011).

Topical Talk O 10.3 Mon 16:00 H 0111

Towards a microscopic understanding of the electron beam induced deposition of tungsten — •Harald Jeschke, Kaliappan Muthukumar, Ingo Opahle, Juan Shen, and Roser Valentí — Institut für Theoretische Physik, Goethe-Universität Frankfurt, 60438 Frankfurt am Main, Germany

We present two density functional theory investigations into the electron beam induced deposition with tungsten hexacarbonyl $W(CO)_6$ as precursors. For the initial adsorption of the precursor on SiO_2 substrates, we consider two different surface models, a fully hydroxylated and a partially hydroxylated SiO_2 surface, corresponding to substrates under different experimental conditions and leading to physisorption and chemisorption, respectively. On the partially hydroxylated surface, we find a spontaneous dissociation of the precursor molecule with chemisorption of $W(CO)_5$ and removal of one of the CO ligands [1]. Other precursors like $MeCpPtMe_3$ and $Co_2(CO)_8$ are discussed. We also investigate the nature of the granular deposits with varying compositions of tungsten, carbon and oxygen that are produced in the EBID process. We employ an evolutionary algorithm to predict the crystal structures starting from a series of chemical compositions known from experiment. We approximate the amorphous structures by reasonably large unit cells that can accommodate local structural environments that resemble the true amorphous structure. Our predicted structures show an insulator to metal transition close to the experimental composition at which this transition is actually observed.

[1] K. Muthukumar *et al.*, Phys. Rev. B **84**, 205442 (2011).

O 10.4 Mon 16:30 H 0111

Proximity Effects in Focused Electron Beam- Induced Processing on Ultra-thin Membranes — Marie-Madeleine Walz, Florian Vollnhals, Florian Rietzler, Michael Schirmer, 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

A fundamental challenge in lithographic and microscopic techniques employing focused electron beams are so-called proximity effects due to backscattering in the sample or forward scattering in an already formed deposit. In this work, we apply a method which allows for visualizing processes on the substrate surface triggered by an electron beam. The resulting defects are decorated by iron deposits formed by decomposition of, e.g., $Fe(CO)_5$ and the corresponding technique is denoted as electron beam induced surface activation (EBISA). Applying this technique for the deposition of nanostructures has the advantage that no forward scattering in an already formed deposit occurs [1,2]. Conventional wisdom holds that by using thin membranes proximity effects can be effectively reduced. We demonstrate that, contrary to the expectation, proximity effects on a 200 nm SiN-membrane are even larger than on the respective bulk substrate. A peculiar charging effect is suggested to play a key role in this unexpected phenomenon.

This work is supported by the DFG through grant MA 4246/1-2.

[1] Walz et al., Angew.Chem.Int.Ed.49 (2010) 4669, [2] Walz et al., PCCP, 13 (2011) 17333.

O 10.5 Mon 16:45 H 0111

Binary Pt-Si Nanostructures Prepared by Focused Electron-Beam-Induced Deposition — •Marcel Winhold[1], Christian Schwalb[1], Fabrizio Porrati[1], Roland Sachser[1], Achilleas S. Frangakis[2], Britta Kämpken[3], Andreas Terfort[3], Norbert Auner[3], and Michael Huth[1] — [1]Physikalisches Institut, Goethe-Universität, Max-von-Laue-Str.1, 60438 Frankfurt am Main — [2]Institut für Biophysik, Goethe-Universität, Max-von-Laue Str. 1, 60438 Frankfurt am Main — [3]Institut für Anorganische und Analytische Chemie, Goethe-Universität, Max-von-Laue Str. 7, 60438 Frankfurt am Main

Binary systems of Pt-Si were prepared by focused electron-beam-induced deposition (FEBID) using the two precursors trimethyl(methylcyclopentadienyl)platinum(IV) ($MeCpPt(Me)_3$) and neopentasilane ($Si(SiH_3)_4$) simultaneously. By this new approach for the preparation of binary systems with FEBID, we can vary the relative flux of the two precursors during deposition. We analyzed the binary composites of platinum and silicon by means of energy dispersive X-ray spectroscopy, atomic force microscopy, electrical transport measurements, and transmission electron microscopy. The results show strong evidence for the formation of an amorphous, metastable Pt_2Si_3 phase, leading to a maximum in the conductivity for a Si:Pt ratio of 3:2.[1] Furthermore the influence of post-treatment by electron irradiation as well as annealing on samples with Si:Pt ratios of 3:2 and 1:1 will be presented.

O 11: [DS] Organic electronics and photovoltaics I (jointly with CPP, HL, O)

Time: Monday 15:00–16:15 Location: H 2032

Invited Talk O 11.1 Mon 15:00 H 2032

Three-dimensional hybrid organic/inorganic heterojunctions based on rolled-up nanomembranes — •Carlos Cesar Bof Bufon[1], Dominic J. Thurmer[1], Christoph Deneke[1], and Oliver G. Schmidt[1,2] — [1]Institute for Integrative Nanosciences, IFW Dresden, Helmholtzstrasse 20, 01069 Dresden, Germany — [2]Material Systems for Nanoelectronics, Chemnitz University of Technology, Reichenhainerstrasse 70, 09107 Chemnitz, Germany

In this work we present a method based on self-released strained nanomembranes (metallic and/or semiconducting) for electrically contact single molecular layers [1]. During release of the nanomembrane, the strain relaxation gives rise to a self-rolling process in which the membrane bonds back to substrate top surface where the thin organic layer was previously deposited. By this means, we are able to fabricate semiconductor-molecule-semiconductor heterojunctions. In this last case, the type of doping and its concentration can be independently and precisely set for each electrode in order to tune the device electronic properties. Such a novel hybrid devices was observed to display completely different electric characteristics which are not expected or possible to be demonstrated by using their elements separately. In addition, the strained nanomembrane based electrodes provide a soft and robust contact on top of the organic film. Furthermore, applying the self-rolling phenomenon, we achieve an approach that is fully integrative on a chip, and several components can be fabricated in parallel using well-established semiconductor processing technologies. [1] Bufon,C.C.B., Nano Lett.11,3727(2011)

O 11.2 Mon 15:30 H 2032

Transport properties of hybrid organic/ferromagnetic metal heterojunctions based on strained nanomembranes — •Maria Esperanza Navarro Fuentes, Carlos Cesar Bof Bufon, Daniel Grimm, and Oliver G Schmidt — Institute for Integrative Nanosciences, IFW-Dresden, Helmholtz Strasse 20, 01069 Dresden, Germany

In this work we investigated the transport properties of organic/inorganic hybrid heterojunctions formed by rolled-up nanomembranes. This method allowed us to create soft metallic contacts on self-assembled monolayers (SAM) of phosphonic acids. As previously reported, the metal/SAM contact can be accomplished regardless the presence of pinholes in the thin organic layer [1]. By comparing the field-emission plots of hybrid heterojunctions formed by the combination of noble and ferromagnetic metals we were able to evaluate the influence of the interfacial oxide layer in transport properties of such heterojunctions. Moreover, the evaluation of the current-voltage curves allow us to clearly distinguish whether the tunneling behaviour is due to the native oxide of the ferromagnet or to the SAM layer behaving as an ultra-thin insulating material. In this particular case, the capability of understanding the nature of the organic/inorganic interface and their influence on the transport properties is an essential step in the creation organic spin valves.

[1] Bufon, C.C.B. et.al.; Nano Lett., 2011, 11 (9), 3727.

O 11.3 Mon 15:45 H 2032

Contact property tailoring by SAM treatment of the Au/P3HT interface — Shahidul Alam, •Torsten Balster, and Veit Wagner — School of Engineering and Science,Jacobs University Bremen, Campus Ring 1, 28759 Bremen

The properties of the contact between the organic semiconductor and the metal not only influence the injection behaviour and limit the switching speed of an organic field effect transistor, they also determine the rectification in a Schottky diode. In this study, vertical Au/P3HT/Au structures on PET foils has been prepared and investigated by means of I-V measurements.

Due to the asymmetry in the deposition of the top and bottom metal electrode the devices showed diode, i.e. rectifying behaviour. To change the contact properties, especially the barrier heights self-assembled monolayers by 1-hexanethiol and nonafluoro-1-hexanethiol on top of the bottom electrode have been prepared prior to the P3HT and top electrode deposition.

The overall current density was reduced in comparison to the untreated sample due to the tunneling barrier introduced. However, the rectification ratio of the 1-hexanethiol has been increased by more than a factor of 2. The influence of the SAMs on the barrier height was analyzed using the Fowler-Nordheim tunneling model.

O 11.4 Mon 16:00 H 2032

Organic Field Effect Transistor Studies on Contact Phenomena and Charge Carrier Injection in Bottom Contact Devices — •Christopher Keil, Dominik Klaus, and Derck Schlettwein — Justus-Liebig-Universität Gießen, Institut für Angewandte Physik, Heinrich-Buff-Ring 16, D-35392, Gießen.

Thin films of the perfluorinated phthalocyanine $F_{16}PcCu$ were prepared under high vacuum conditions. As substrate a SiO_2 insulating layer on a Si gate was chosen. Different metal contacts were evaporated as bottom contacts before the organic layer deposition. Organic thin film transistors of the molecular semiconductors were thereby achieved. The electrical contact behaviour of the organic semiconductor to electrodes of different metals (Au, Ag, Al) was investigated. The contact characteristics and the formation of an injection barrier will be discussed. Modelling of transistor characteristics and charge carrier injection are shown and their influence on the calculation of the intrinsic charge carrier mobility in the semiconductor channel is shown.

O 12: Surface dynamics

Time: Monday 16:00–19:15 Location: H 2013

O 12.1 Mon 16:00 H 2013

Density driven solidification of a 2D molecule gas on a bulk insulator: Co-Salen on NiO(001) — •Josef Grenz, Alexander Schwarz, and Roland Wiesendanger — Institute of Applied Physics, University of Hamburg, Jungiusstr. 11, 20355 Hamburg

Co-Salen is a planar metal-organic Schiff base complex and known for its oxygen affinity and tendency to pair in dimers. Previous atomic force microscopy studies in UHV have shown, that this molecule initially adsorbs on NaCl(001) as monomers and with increasing coverage exhibts a bimodal island growth with dimers as building blocks [1,2]. However, on NiO(001), which also crystallizes in the rocksalt structure, for low coverages (< 1 ML) no growth can be detected, only step edge decoration. After complete decoration, diffusing molecules can be observed on flat terraces using $z(t)$-spectroscopy on a fixed (x, y)-position: Whenever a molecule passes underneath the tip, its z-position is adjusted accordingly. Increasing the amount of deposited molecules leads to more frequent adjustments events. If the density of molecules becomes large enough, diffusion stops. High resolution AFM measurements at low temperatures reveal the formation of an amorphous monolayer consisting of monomers. After this density driven solidification of a molecule gas layer-by-layer step flow growth sets in.

[1] S. Fremy, *et al.*, Nanotechnology **20**, 405608 (2009).

[2] K. Lämmle, *et al.*, Nano Lett. **10**, 2965 (2010).

O 12.2 Mon 16:15 H 2013

Signatures of non-adiabaticity in the scattering of O_2 at Ag(111)? — •Itziar Goikoetxea[1,2], Jörg Meyer[1], J. Inaki Juaristi[2], Maite Alducin[2], and Karsten Reuter[1] — [1]Technische Universität München, Germany — [2]Centro de Física de Materiales, San Sebastián, Spain

We study the scattering of O_2 at Ag(111) using molecular dynamics techniques based on a six-dimensional first-principles adiabatic potential energy surface (PES). In preceding work [1] we had shown that the measured extremely low initial sticking coefficient at this surface can be rationalized by late and large energy barriers of 1.2 eV and an extremely narrow entrance channel leading to dissociation. Unfortunately, these adiabatic PES characteristics render the sticking a rather insensitive quantity with respect to an at times conjectured spin or charge non-adiabaticity in the O_2-Ag(111) interaction. We therefore now turn to the regime where the latter is brief and focus on the O_2 scattering properties. Intriguingly, the adiabatic simulations reproduce both in-plane and out-of-plane scattering data [2] even to the level of distinct features. These features have been interpreted as indications for two distinct scattering regions: a smooth surface region above the chemisorption well at large distances from the surface, and a more corrugated surface region at closer distances [2]. We qualify these interpretations and the underlying low-dimensional model conceptions based on our high-dimensional first-principles simulations.

[1] I. Goikoetxea *et al.*, *accepted at* New J. Phys.

[2] A. Raukema et *et al.* J. Chem. Phys. **103**, 6217 (1995).

O 12.3 Mon 16:30 H 2013

Time-resolved laser-induced desorption of atomic Deuterium and Hydrogen from HOPG — •Robert Frigge and Helmut Zacharias — Physikalisches Institut, Universität Münster, Germany

Formation processes of molecular hydrogen upon radiation of adsorbed atoms on graphitic dust particles play an important role in the interstellar circuit of matter. However, the conversion process is still not fully understood yet.

Atomic hydrogen desorption from HOPG is examined after surface excitation with fs-laser pulses at $\lambda = 400$ nm. Desorbed neutral H atoms are ionized using (2+1) REMPI via the $2s \leftarrow 1s$ 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 addressed with different adsorption potentials, depending upon the

neighboring H atom position on the graphene lattice [2,3]. 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 about 700 fs with a coverage dependent variation. This correlation time indicates short lifetimes of the excited electrons and supports a calculation in the DIMET model.
[1]R. Frigge et al., Phy. Rev. Lett., **104**, 256102 (2010)
[2]L. Jeloaica, V. Sidis, Chem. Phys. Lett., **300** 157 - 162 (1999)
[3]L. Hornekær et al., Phy. Rev. Lett., **97**, 186102 (2006)

O 12.4 Mon 16:45 H 2013

Non-adiabatic Effects in the Reaction of Chlorine Molecules with Potassium — •Felix Becker, David Krix, and Hermann Nienhaus — University of Duisburg-Essen and CeNIDE, Germany

The energy released in an exothermic chemical reaction of a gas molecule with a metal surface may be dissipated adiabatically by the creation of phonons or non-adiabatically by excitation of the electronic system. In the past, non-adiabatic effects in the reaction of Cl$_2$ with K were studied by exoelectron emission and chemiluminescence measurements only.

Here, we present XPS and chemicurrent data detecting low-energy holes as well as photons generated by the chlorination of potassium. Two kinds of large-area Schottky diodes were used as hot charge carrier detectors. The first were formed by direct deposition of K on H-terminated *p*-Si(111), the second had an intermediate silver layer between K and Si. For thin metal layers hot holes could be measured. They travel ballistically through the metal film and traverse the Schottky barrier if the kinetic energy is larger than the barrier height (typ. 0.4 eV). Chemiluminescence photons can be distinguished from hot holes by varying the metal film thickness as the mean free path (mfp) of the photons exceeds the mfp of hot holes. The metal film thickness dependent reverse currents strongly indicate that the presence of a rough silver film enhances the chemiluminescence during the reaction.

O 12.5 Mon 17:00 H 2013

Beating the heat atomistically: Watching phonons cool down during O$_2$ dissociation on Pd(100) — •Jörg Meyer and Karsten Reuter — Technische Universität München, Germany

Energy conversion at interfaces is at the center of the rapidly growing field of basic energy science. One particular example is the conversion of chemical energy into heat which comes as an unavoidable by-product of all exothermic elementary reaction steps in heterogeneous catalysis. While engineers routinely deal with important consequences on a macroscopic scale based on well-known continuum theories and empirically determined effective parameters, an atomistic understanding is very limited at best. Aiming at multiscale modeling, our novel QM/Me approach extends the power of embedding techniques to metallic systems. A huge atomistically described bath can thus be included in *ab initio* molecular dynamics simulations of chemical reactions at catalyst surfaces. Applied to O$_2$ dissociation on Pd(100) as a representative showcase system, for which electron-hole pair excitations are unlikely to act as dominant primary energy dissipation channel [1], we quantify concomitant phonon excitations based on a newly developed projection scheme. Thanks to the phononic details implicitly incorporated in the bath, we obtain a high resolution for individual modes over the entire surface Brillouin zone. We can thus unravel the role of surface phonons as well as question the validity of the harmonic approximation for the solid during the dynamics – commonly employed in model Hamiltonians – from an unprecedented first-principles perspective.
[1] J. Meyer and K. Reuter, New J. Phys. **13**, 085010 (2011)

O 12.6 Mon 17:15 H 2013

Dynamics of Vibrational Modes of Pb Adsorbate Layers on Si(111): Mode Conversion and De-Excitation — •Annika Kalus, Simone Wall, Sung Sakong, Tim Frigge, Anja Hanisch-Blicharski, Peter Kratzer, Martin Kammler, and Michael Horn-von Hoegen — Universität Duisburg-Essen

Ultrafast time resolved reflection high energy electron diffraction was used to study the vibrational dynamics of adsorbate layers upon excitation with a fs laser pulse in a pump probe setup. We employed the Debye-Waller effect $I = I_0 \exp(-\langle(\boldsymbol{uk})^2\rangle)$ to follow the temporal evolution of the vibrational amplitude $\boldsymbol{u}$ of the adsorbate atoms. The SIC($\sqrt{3} \times \sqrt{3}$) reconstruction of Pb on Si(111) was used as model system and excited by 50 fs, 800 nm laserpulses at a fluence of 4 mJ/cm^2. We observe two time constants of 100 ps and 3 ns for the vibrational de-excitation. With the $\boldsymbol{k}$ dependence of the Debye-Waller effect we identified the fast decay as a mode with a dominant parallel amplitude while the slow mode exhibits a dominant vertical amplitude. Both time constants can be explained with classical molecular dynamics simulations. The electronic and phononic band structures of the substrate plus adsorbate layer were calculated using density functional theory. The hot electrons created by the laser pulse initially excite solely optical phonons. These parallel modes convert on a 100 ps time scale to modes perpendicular to the surface that dissipate their energy into the Si substrate on a ns time scale. This surprisingly long lifetime is explained by the small overlap between the low-energy vertical Pb modes with an energy of 2 - 4 meV and the Si acoustic phonons.

O 12.7 Mon 17:30 H 2013

Phonon density of states of ultra-thin europium films from in-situ 151Eu nuclear inelastic scattering — •Olga Bauder[1], Marthe Kaufholz[2], Marchin Zajac[3], and Svetoslav Stankov[1,2] — [1]Laboratory for Applications of Synchrotron Radiation, KIT, Germany — [2]Institute for Synchrotron Radiation, KIT, Germany — [3]European Synchrotron Radiation Facility, Grenoble, France

It is well known that in thin films atoms vibrate in a manner significantly different as compared to the bulk. This is attributed to the broken translation symmetry and consequently to the reduced coordination of the surface atoms. For 3d metals these anomalies were investigated both theoretically and experimentally for the Fe(110) surface. However, there are no studies for the surfaces of 4f metals reported so far. We have investigated the phonon DOS of epitaxial ultra-thin Eu metallic films by in-situ nuclear inelastic scattering on 151Eu. The results reveal striking deviations of the phonon spectra of 1.1 nm thick film compared to that of bulk Eu. By reducing the film thickness, a systematic hardening, instead of softening of the phonon DOS is detected. * S.S. acknowledges the support by the Helmholtz Association for establishing a Helmholtz-University Young Investigator Group ”Interplay between structure and dynamics in epitaxial rare earth nanostructures” (VH-NG-625).

O 12.8 Mon 17:45 H 2013

Watching It Freeze: Peierls Distortion of the In/Si(111) Surface — •Simone Wall[1], Boris Krenzer[1], Stefan Wippermann[2], Simone Sanna[2], Friedrich Klasing[1], Anja Hanisch-Blicharski[1], Martin Kammler[1], Wolf Gero Schmidt[2], and Michael Horn-von Hoegen[1] — [1]University of Duisburg-Essen and CeNIDE, Duisburg, Germany — [2]Paderborn University, Paderborn, Germany

TR-RHEED was employed to investigate the dynamics of the Peierls-instability-driven phase transition on the (8x2) In/Si(111) surface. Far below the critical temperature of 90K, the (8x2)-(4x1) phase transition is electronically driven through weak excitation with a fs-laser pulse and results in a long-lasting super-cooled excited (4x1) phase. This metastable situation far away from equilibrium is only accessible through the excitation by the fs-laser pulse. A thermal excitation of the phase transition due to laser induced heating was experimentally excluded. The recovery of the (8x2) ground state on a timescale of 500 ps is triggered by adsorbates that act as nucleation seeds - the same way that super-cooled water in a bottle freezes upon the insertion of seeds. With increasing density of adsorbates the recovery to the groundstate proceeds much faster. Density functional theory calculations reveal the microscopic scenario of the phase transition, which occurs one-dimensionally along the Indium chains. The surface unit cells fall back into their ground state one at a time, like a row of falling dominoes. The phase front propagates at about 800 m/s, comparable to the speed of sound.

O 12.9 Mon 18:00 H 2013

Probing diffusion of single nanoparticles at water/oil interfaces with fluorescence correlation spectroscopy — Dapeng Wang, Hans-Jürgen Butt, and •Kaloian Koynov — Max Planck Institute for Polymer Research, Mainz, Germany

A good understanding of the dynamics and self organization of nanometer-sized objects, e.g., molecules, macromolecules and nanoparticles (NPs) at immiscible liquid/liquid interfaces is not only of fundamental interest for the soft mater physics and cell biology, but is also very important for a number of technological applications in material synthesis, pharmacy, microfluidics and nanotechnology. Here, we show that the fluorescence correlation spectroscopy (FCS), a method based on measuring the fluctuations of the fluorescent light intensity caused by the diffusion of fluorescent species through a very small observation volume, is very well suited for studies of NPs diffusion on liquid/liquid interfaces as it offers the possibility to monitor fast diffusing, nanometer size objects at extremely low surface coverage. We used FCS to study the diffusion of fluorescent semiconductor nanoparticles (quantum dots) on planar water/oil interfaces. The effects of several important parameters, i.e. the particles size, their surface functionalization (hydrophobic/hydrophilic) and the oil phase viscosity were systematically explored. Most notably, a significant slow-down of nanoparticle diffusion at the water/oil interface was observed. The effect was most evident when the viscosities of both liquid phases were similar, i.e. at the water/decane interface.

O 12.10 Mon 18:15 H 2013

Heat Transport from Self Organised Ge Nano-Structures to Si(001) Substrate — •Tim Frigge, Anja Hanisch-Blicharski, Simone Wall, Annika Kalus, Martin Kammler, and Michael Horn-von Hoegen — University of Duisburg-Essen and CENIDE, Duisburg, Germany

We used ultrafast time-resolved reflection high energy electron diffraction to investigate the heat transport from nanoscale Ge clusters to a Si(001) substrate. From the transient cooling behaviour upon fs-laser excitation the thermal properties of these nanostructures could be determined without further calibration. On Si(001) Ge grows in a Stranski-Krastanov mode and can be used for self organisation of nanostructures. Island formation occurs at a critical coverage of 3 monolayers with metastable hut-clusters of a width of 25nm and a height of 2.5nm. Further Ge deposition results in the formation of 50 nm wide dome-clusters with a height of 6nm. Both cluster-types exhibit atomically flat side facets, are mono-crystalline, epitaxial, defect-free, and have a uniform size distribution. The interface between the Ge-islands and the Si(001)-substrate is abrupt. At a base temperature of 25K and a transient heating by 100K, caused by the fs laser pump-pulse, different cooling rates for both clusters were determined. Hut-clusters cool in 50ps while dome-clusters cool three times slower in 150ps. A comparison with the theoretically expected thermal boundary conductance of the diffuse mismatch model (DMM) for two-dimensional uniform Ge layers shows that the cooling rate of the nano scale islands is reduced by more than a factor two!

O 12.11 Mon 18:30 H 2013

Ultrafast Electron Dynamics in the Topological Insulator Material Bi_2Se_3 — •Patrick Kirchmann[1,2], Jonathan Sobota[2,3,4], Shuolong Yang[2,3,4], James Analytis[2,3], Yulin Chen[2,3,4], Ian Fisher[2,3], and Zhi-Xun Shen[2,3,4] — [1]Fritz Haber Institute of the Max Planck Society, Department of Physical Chemistry, Faradayweg 4-6, D-14195 Berlin, Germany — [2]Stanford Institute for Materials and Energy Sciences, SLAC National Accelerator Laboratory, 2575 Sand Hill Road, Menlo Park, CA 94025, USA — [3]Geballe Laboratory for Advanced Materials, Department of Applied Physics, Stanford University, Stanford, CA 94305, USA — [4]Department of Physics, Stanford University, Stanford, CA 94305, USA

Using femtosecond time- and angle-resolved photoemission spectroscopy, we investigated the non-equilibrium electron dynamics of the topological insulator Bi_2Se_3. We studied p-type Bi_2Se_3, in which the metallic Dirac surface state and bulk conduction bands are unoccupied. Optical excitation leads to a meta-stable population at the bulk conduction band edge, which feeds a population of the surface state persisting for > 10 ps. This unusually long-lived population of a metallic Dirac surface state with spin texture may present a channel in which to drive transient spin-polarized currents.

O 12.12 Mon 18:45 H 2013

Two-photon photoemission studies Germanium(100) - Binding energies, lifetimes and dispersion of the surface states — •Jens Kopprasch[1,2], Kristof Zielke[1,2], Cornelius Gahl[1,2], Christian Eickhoff[1,2], Jörg Schäfer[3], and Martin Weinelt[1,2] — [1]Max-Born-Institut, Max-Born-Straße 2a, 12489 Berlin, Germany — [2]Freie Universität Berlin, Fachbereich Physik, Arnimallee 14, 14195 Berlin, Germany — [3]Universitat Würzburg, Fakultät für Physik und Astronomie, Am Hubland, 97074 Würzburg, Germany

Germanium(Ge) has the same crystal structure as silicon (diamond-like) but opposite to Si the band gap is much smaller (0.67 eV at 300 K) and has a local minimum at the Γ-point. This difference in band structure leads to a growing interest of Ge in semiconductor industry, where it is used for solar cells, high-power transistors, infrared optics and x-ray detectors.

The surface reconstruction on Ge(100) is also comparable to Si(100). This leads to the so-called dangling-bond states D_{up} and D_{down}. By using two-photon-photoemission (2PPE) spectroscopy we observed both surface states and could identify the first image-potential state n=1. Binding energies, lifetimes and dispersion of these states will be presented. Measurements at 90K within a range of $k_{\|} = \pm 0.5 \AA^{-1}$ and a maximum time delay of 50ps show the conduction band minimum and a number of transitions among the bulk bands. We will present this measurements and discuss their origin and the concomitant carrier dynamics.

O 12.13 Mon 19:00 H 2013

Excitonic features in image-potential resonances on Si(100) probed by two-photon photoemission — •Martin Weinelt[1,2], Christian Eickhoff[1,2], and Cornelius Gahl[1,2] — [1]Max-Born-Institut, Max-Born-Straße 2a, 12489 Berlin, Germany — [2]Freie Universität Berlin, Fachbereich Physik, Arnimallee 14, 14195 Berlin, Germany

Electronic transitions into unoccupied image-potential resonances $n = 1$ and $n = 2$ on silicon(100) were studied with angle-resolved femtosecond pump-probe photoelectron spectroscopy. Off-resonant excitation out of valence bands unveils the typical behavior of electrons trapped in the image-potential in front of a surface, characterized by a well-defined binding energy [1] and an effective mass of 1. However, tuning the excitation energy of the pump-pulse across the resonance between the occupied dangling-bond D_{up} and unoccupied $n = 1, 2$ surface states reveals excitonic features, both in the dispersion and the binding energy of the probed state. As photoemission probes the population of specific states, resonant excitation out of the discrete D_{up} surface state implies the formation of a surface exciton population on a femtosecond timescale.

[1] P. M. Echenique and J. B. Pendry, J. Phys. C **11**, 2065 (1978)

O 13: Polymeric biomolecular films

Time: Monday 16:00–18:45 Location: MA 005

O 13.1 Mon 16:00 MA 005

Photoelectron Diffraction on SnPc/Ag(111) — •Michael Greif, Luca Castiglioni, Jürg Osterwalder, and Matthias Hengsberger — Physik Institut, University of Zurich, Winterthurerstrasse 190, 8057 Zurich

Photoelectron diffraction is a method to monitor the atomic structure of surfaces. From the emitter site in the sample the photoelectron propagates as wave that is then coherently scattered by the neighboring atoms. The directly emitted and the scattered waves create interference fringes in the detector plane. By scanning all emission directions on top of the sample with the detector, a 2-D data set is recorded that gives structural information about the examined system.

In the presented work we investigated Tin-Phthalocyanine molecules (SnPc) on a Ag(111) surface with X-Ray photoelectron diffraction (XPD) and UV photoelectron diffraction (UPD). SnPc shows a well ordered wetting layer growth on a Ag(111) surface. Hence core levels of the Sn-Atom in the center of the molecule serve as well defined emitter sites for photoelectron diffraction experiments.

The diffraction patterns correspond to the structural environment around the Sn-Atoms. Comparing our measurements with simulations using single scattering calculations (SSC), we see indications of the conformational change that the SnPc molecules undergo upon adsorption. Additionally our measurements show the azimuthal orientation of the molecules with respect to the Ag(111) surface. Due to a higher probability of backscattering for low energy electrons, the UPD patterns also show contributions of the substrate structure.

O 13.2 Mon 16:15 MA 005

Core-energy level energy difference between the surface and bulk regions of organic semiconductor films — •Hiroyuki Yoshida[1,2], Eisuke Ito[3], Masahiko Hara[3], Naoki Sato[1], Thomas Ules[4], and Michel G. Ramsey[4] — [1]Institute for Chemical Research, Kyoto University, Uji, Kyoto 611-0011 JAPAN —

[2]PRESTO, Japan Science and Technology Agency (JST), 4-1-8 Honcho Kawaguchi, Saitama 332-0012, Japan — [3]Flucto-Order Functions Research Team, RIKEN-HYU Collaboration Research Center, RIKEN Advanced Science Institute, 2-1 Wako, Hirosawa, Saitama 351-0198, Japan — [4]Institute of Physics,Karl-Franzens University Graz, A-8010 Austria

There has been an argument whether the energy level determined by PES is difference between the surface and bulk regions for decades. The reason was that no appropriate experimental method has been available to distinguish the energy levels between the surface and bulk of materials.

We have recently developed a novel analytical method of the core level energies with depth resolution; X-ray photoemission spectra (XPS) are measured at multiple detection angles and the energy profiles are precisely analyzed using target factor analysis.

By applying this method to organic semiconductor thin films, we found that the core-levels of the first surface layer are different from those of the bulk by about 0.3 eV. The origin is also discussed from the systematical study on different organic materials.

O 13.3 Mon 16:30 MA 005

X-ray reflectivity measurements of lipid membranes at the water/oil interface — •Annika Elsen[1], Lars Joergensen[2], Klaas Loger[1], Benjamin Runge[1], Oliver H. Seeck[3], Beate Klösgen[2], Olaf M. Magnussen[1], and Bridget M. Murphy[1] — [1]Institute for Experimental and Applied Physics, CAU, Kiel, Germany — [2]MEMPHYS, Department of Physics, Chemistry and Pharmacy, SDU, Odense, Denmark — [3]PETRA III, DESY, Hamburg, Germany

For a better understanding of the function of biological membranes the arrangement of the lipids in the bilayer as well as the structural integration of the proteins, providing the functions of the membrane, has to be known. In a first attempt a biological membrane can be modelled with phosphocholine monolayers at the water/oil interface. Unfortunately the application of structure-sensitive techniques on membranes in such environment is limited. However, with X-ray diffraction techniques it is possible to obtain structural information on the membrane at the liquid/liquid interface on a submolecular scale. Here, we present X-ray reflectivity measurements of 1,2-dipalmitoyl-sn-glycero-3-phosphocholine (DPPC) and 1-palmitoyl-2-oleoyl-sn-glycero-3-phosphocholine (POPC) monolayers at the water/perfluorohexane interface, the latter with different bulk concentrations, carried out at the new liquid interface scattering apparatus (LISA) at the beamline P08 (PETRA III, DESY). Preliminary results of the vertical monolayer structure at the interface will be presented, giving information on the arrangement of the lipids.

O 13.4 Mon 16:45 MA 005

Interaction of noble gas atoms and aromatic molecules with Au substrates: dispersion-corrected DFT calculations — •Uwe Friedel and Axel Gross — Institute of Theoretical Chemistry, Ulm University, D-89069 Ulm/Germany

Dispersion-corrected density functional theory calculations provide a computationally efficient method to evaluate the adsorption properties of atoms and molecules that are bound via van der Waals forces to surfaces. We have used this approach to address the interaction of noble gas atoms and aromatic molecules with metal surfaces. First, the reliability of this approach has been validated by comparing it with high-quality quantum chemical calculations for small finite reference systems. The calculated adsorption energies are in good agreement with available experimental data. The relevance of our results with respect to the interpretation of images obtained with the scanning tunneling hydrogen microscope [1] are discussed.

[1] S. Tautz *et al.*, Direct Imaging of Intermolecular Bonds in Scanning Tunneling Microscopy, *J. Am. Chem. Soc.* **2010**, *132*, 11864-11865

O 13.5 Mon 17:00 MA 005

Controlling on-surface polymerization by hierarchical and substrate-directed growth — •Leif Lafferentz[1], Volker Eberhardt[2], Carlo Dri[3], Christina Africh[3], Giovanni Comelli[3], Friedrich Esch[3], Stefan Hecht[2], and Leonhard Grill[1] — [1]Fritz-Haber-Institut der MPG, Berlin, Germany — [2]Department of Chemistry, Humboldt-Universität zu Berlin, Berlin, Germany — [3]IOM-CNR Laboratorio TASC, Basovizza-Trieste, Italy

The on-surface synthesis of oligomers under ultra-high vacuum conditions has been intensely studied in the last years [1,2] as such processes allow the formation of stable covalently bound molecular structures on surfaces. However, so far all experiments relied on a one-step polymerization, which limits the control of the process and leads to rather simple architectures. Another issue that needs to be addressed is the reduction of defects, because covalent linking processes are typically irreversible and therefore lack a capability for self-repair. We present experiments that address these issues by employing a sequential connecting process, which achieves greater control of the network formation and reduces the number of defects. This novel approach opens the possibility for the formation of more sophisticated structures.

[1] Grill, L. et al. Nat. Nanotechnol. 2, 687-691 (2007)

[2] Gourdon, A. Angew. Chem.-Int. Edit. 47, 6950-6953 (2008)

O 13.6 Mon 17:15 MA 005

Bis(terpyridine) adsorption on graphite and graphene: Theoretical studies — •Daniela Künzel and Axel Gross — Institute of Theoretical Chemistry, Ulm University, D-89069 Ulm/Germany

Bis(terpyridines) (BTPs) form various self-assembled monolayer structures on different surfaces such as graphite or graphene [1]. Their adsorption properties and the structure formation are of interest from a fundamental point of view and for possible applications. The ordered adsorption process is governed by strong van der Waals interactions between the BTP molecule and the surface and by weak intermolecular hydrogen bonds. Using dispersion-corrected DFT, the surface-adsorbate interaction of isolated molecules can be described accurately [2].

Interesting effects on the structure formation can occur when the surface shows periodic lateral variations on a larger scale in its properties. As an example, force field results addressing the BTP adsorption on a buckled graphene adlayer on Ru(0001) will be presented [3].

[1] C. Meier, D. Künzel *et al.*, *J. Phys. Chem. C* **2010**, *114*, 1268.

[2] D. Künzel, K. Tonigold, J. Kucera, M. Roos, H. Hoster, R.J. Behm, A. Groß *ChemPhysChem* **2011**, *12*, 2242.

[3] M. Roos, D. Künzel, B. Uhl, H. Huang, O.B. Alves, H. Hoster, A. Groß, R.J. Behm *J. Am. Chem. Soc.* **2011**, *133*, 9208.

O 13.7 Mon 17:30 MA 005

Structure-property relation in oligoethylene glycol terminated alkanethiol monolayers under electron irradiation as applied to specific and non-specific protein adsorption — •Yekkoni L. Jeyachandran and Michael Zharnikov — Angewandte Physikalische Chemie, Universität Heidelberg, 69120 Heidelberg, Germany

We investigated the possibility to use electron irradiation for the controlled modification of the protein-repelling and protein-affinity properties of oligoethylene glycol (OEG) terminated alkanethiol (AT) monolayers. The modifications were induced either directly by electron irradiation or in combination with the successive exchange reaction with the molecular substituents bearing special anchor group for protein adsorption. The direct irradiation treatment allowed for controlled non-specific adsorption of proteins, whereas the irradiation-promoted exchange reaction (IPER) enabled their controlled specific adsorption. Combining these two approaches with lithography, we fabricated both non-specific and specific protein patterns of various shapes, including gradient ones, on different length scales. The specific protein adsorption relied on well-known biotin-avidin interaction, utilising biotinylated-OEG-AT molecules as the substituents in IPER. Potential applications of gradient protein patterns for cell adhesion and mobility analyses, as well as novel strategies for multi-protein patterning by a combination of direct writing and IPER will be discussed.

O 13.8 Mon 17:45 MA 005

Biocompatible Nanomembranes based on PEGylation of Cross-Linked Self-Assembled Monolayers — •Nikolaus Meyerbröker[1], Zi-An Li[2], Wolfgang Eck[1], and Michael Zharnikov[1] — [1]Angewandte Physikalische Chemie, 69120 Heidelberg, Germany — [2]Fakultät für Physik und Center forNanoIntegration, Universität Duisburg-Essen, 47048 Duisburg, Germany

Self-assembled monolayers (SAMs) represent an efficient means to modify the properties of surfaces by covering them with an uniform monomolecular layer. Because of weak intermolecular interactions, SAMs cannot exist without a substrate as support. However, if these films consist of an aromatic framework, they can be laterally cross-linked by electron irradiation and persist as a freestanding membrane after the removal from the substrate. If, additionally, nitro-substituted aromatic molecules are used, they can be not only cross-linked by the irradiation but also reduced to reactive amines which can serve as binding sites for further species. As such species we used poly(ethylene glycols), which made the resulting bilayer protein-repelling. Using this approach, we prepared an ultrathin, mechanically stable and protein-repelling membrane which can be used as highly transparent support in transmission electron microscopy (TEM). Whereas the low Z character and ultimate thinness (ca. 5 nm) of this support guarantees high imaging quality, protein-repelling ensures the lack of protein denaturing, which extend the possibilities of TEM experiments in their applications to sensitive biological targets.

O 13.9 Mon 18:00 MA 005

Mechanical Metamaterials — •Tiemo Bückmann[1], Nicolas Stenger[1], Michael Thiel[2], Christoph Eberl[3], Tobias Kennerknecht[3], and Martin Wegener[1,2,4] — [1]Institut für Angewandte Physik and DFG-Center for Functional Nanostructures (CFN), Karlsruhe Institute of Technology(KIT), 76131 Karlsruhe, Germany — [2]Nanoscribe GmbH, 76344 Eggenstein-Leopoldshafen, Germany — [3]Institute for Applied Materials, Karlsruhe Institute of Technology(KIT), 76344 Eggenstein-Leopoldshafen, Germany — [4]Institut für Nanotechnologie (INT), Karlsruhe Institute of Technology(KIT),76344 Eggenstein-Leopoldshafen, Germany

Auxetic materials attract attention due to their mechanical properties for over 100 years. These advanced materials with negative Poisson's ratio have recently gained special interest. State-of-the-art fabrication techniques allow for greater design freedom and systematic investigation.We consider the characteristics and the design of structured polymeric materials with the aim to create three-dimensional (3D) mechanical metamaterials with negative Poisson's ratios. 3D models of different structures are simulated with finite-element methods using the software package Comsol Multiphysics. Samples of relevant geometries with sizes between tens of micrometers and 0.3 millimeters are fabricated using direct laser writing (DLW). Arbitrary 3D manufacturing offered by DLW allows for tuning the Poisson's ratio of the material. The fabricated mechanical metamaterials are well structured, show a high degree of translational symmetry, and maintain fidelity to the blueprint over the extent of the entire structure.

O 13.10 Mon 18:15 MA 005

Reaction mechanism of debromination on coinage metals — •Jonas Björk[1], Felix Hanke[2], and Sven Stafström[1] — [1]Linköping University, Sweden — [2]University of Liverpool, UK

Covalent bonded molecular networks can be formed through self-assembly on various surfaces. A successful approach has been to use molecular building blocks with specific hydrogen atoms replaced by bromine atoms. The bromine atoms can split-off, allowing covalent coupling between the un-saturated carbon atoms. However, despite the experimental success in the field, there is a lack of theoretical understanding of covalent self-assembly. In particular, a coherent picture is lacking for the temperature dependence of the debromination reaction and the adsorption properties of reactants and products.

Here, we present a theoretical study of the debromination on the close-packed (111)-facets of coinage metals, commonly used in covalent self-assembly. Within the framework of van der Waals density-functional theory, and using bromobenzene as model component for the debromination, the catalytic activities of the Au, Ag and Cu surfaces are compared. It is found that the reactions are described by similar mechanisms on all surfaces, in that the C-Br dissociation follows an almost identical path and that there are no radical products. The reaction proceeds easiest on the Cu(111) surface, while it is associated with the largest energy barrier on Au(111). Finally, the consequences of the energy barriers on the temperature dependence for each surface will be discussed.

O 13.11 Mon 18:30 MA 005

Molecular polymerisation on a stepped surface — •Alex Saywell[1], Jutta Schwarz[2], Stefan Hecht[2], and Leonhard Grill[1] — [1]Department of Physical Chemistry, Fritz-Haber-Institute of the Max-Planck Society, Berlin, Germany — [2]Department of Chemistry, Humboldt University, Berlin, Germany

On-surface reactions have the potential to provide new synthetic routes for the production of novel molecular species. In such reactions the surface is likely to play a more complex role than simply functioning as a flat, inert support. Step edges and defect sites of catalytic surfaces are considered as 'active sites' for chemical reactions.[1] Probing a surface with atomic resolution allows site specific information to be obtained about the structure and location of these active sites.[2]

Here we investigate the influence of the step edges of the Au(10,7,7) surface on a model chemical system, with respect to the catalytic activity of the step edges and the adsorption geometry of monomer units and polymer chains. Low temperature UHV-STM provides the spatial resolution to identify catalytic sites and facilitates the characterisation of molecular structures. Our results demonstrate that the Au(10,7,7) surface possesses catalytically active sites, and that the local geometrical structure of these sites plays an important role in the on-surface chemistry. The step edges also provide a template for highly orientated polymers formed via the on-surface reaction.

[1] Taylor, H.S. *Proc. R. Soc. London Ser. A* **108**, 105-111 (1925).

[2] Vang, R.T. *et al. Chem. Soc. Rev.* **37**, 2191 (2008).

O 14: Adsorption on semiconductors, oxides and insulators II

Time: Monday 16:00–19:00 Location: MA 041

O 14.1 Mon 16:00 MA 041

Gold adsorption on pristine and defective ceria films — •Yi Pan, Niklas Nilius, and Hans-Joachim Freund — Fritz-Haber-Institut der MPG, Faradayweg 4-6, 14195 Berlin, Germany

Scanning tunnelling microscopy and spectroscopy have been employed to study the adsorption of individual Au adatoms on well defined CeO2(111) films grown on Ru(0001). In correspondence with recent DFT calculations, the Au adatoms can be stabilized in two charge states on the oxide surface, giving rise to the appearance of features with different size and bias-dependent contrast in the STM. The relative abundance of the two species sensitively depends on the reduction state of the surface, i.e. on the density of oxygen vacancies. This interrelation suggests that an exchange of electrons between the adatoms and the Ce 4f states is responsible for the bi-modal charge distribution. Moreover, the Au charge state can be switched reversibly via electron injection from the STM tip, providing insight into the nature of the participating Au electronic states.

O 14.2 Mon 16:15 MA 041

Nucleation, growth and shape of Au clusters on CeO_2 (111) — •Hans Hermann Pieper and Michael Reichling — Universität Osnabrück, Germany

Gold nano-clusters of variable size on CeO_2 (111) are investigated by non-contact atomic force microscopy (NC-AFM) and Kelvin probe force microscopy (KPFM). The cluster size and nucleation behaviour is controlled by means of sample temperature during deposition and post-deposition annealing. The exact cluster shape is revealed by Kelvin compensated NC-AFM and measurements in the constant height mode, thus eliminating tip convolution effects and image distortion due to electrostatic forces.

Furthermore, we establish a relation between the KPFM contrast and the cluster size and demonstrate charging of individual clusters to an equivalent of a few electrons.

O 14.3 Mon 16:30 MA 041

Adsorption of Metalophthalocyanines on thin CoO(111) films on Ir(100) — •Tobias Schmitt, Martina Reuschl, Carsten Tröppner, Lutz Hammer, and M.Alexander Schneider — LS f. Festkörperphysik, Uni. Erlangen, Germany

Cobalt oxide is technologically relevant as a low-temperature catalyst for carbon monoxide oxidation and is often used as a substrate for other oxidic and metallic catalysts. Also of particular interest is the functionalisation of catalytic surfaces by functional organic molecules or the preparation of molecular layers for organic electronics. For these applications an understanding of the interaction of large molecules with the cobalt oxide surface is needed.

On Ir(100) thin films of cobalt oxide can be grown in a variety of structures and surface terminations[1,2] that allow a systematic study with surface science methods in UHV. We investigated the adsorption of large metallophthalocyanine molecules by low-temperature scanning tunneling microscopy. As an example we identified different adsorption geometries of iron-(II)-phthalocyanine on the CoO(111)-c(10x2)-phase on Ir(100). It appears that the most favourable adsorption geometry leads to a maximisation of the interaction of the carbon pi-system with the oxygen atoms at the surface and hence the interaction of the central metal ion of the molecule with the substrate is less important.

[1] M. Gubo, et al., Phys. Rev. B 83, 075435 (2011) [2] W. Meyer, et al., Phys. Rev. Lett. 101, 016103 (2008)

O 14.4 Mon 16:45 MA 041

Adsorbate-induced reconstructions of the polar NiO(111) surface — •Christina Ebensperger and Bernd Meyer — Interdisziplinäres Zentrum für Molekulare Materialien und Computer-Chemie-Centrum, Universität Erlangen-Nürnberg

Bulk-truncated structures of polar surfaces are intrinsically unstable and especially susceptible to reconstructions and reactions with adsorbates. Indeed, our DFT+U calculations show that the adsorption of small molecules (H_2, O_2, H_2O, CO, CO_2) on NiO(111) alters the surface structure considerably. Phase diagrams of the energetically most stable surface reconstructions depending on temperature and pressure conditions exhibit a wide variety of configurations with different degree of surface hydroxylation and carbonate formation. An adsorbate free (2×2)-O-octopolar structure, a fully hydroxylated (1×1)-OH surface and tridentate carbonate complexes including O surface atoms are energetically most favorable. Interestingly, in many cases the transformation between different stable phases does not only involve adsorption or desorption of molecules and the rearrangement of Ni and O surface atoms, but also requires mass transport/diffusion of NiO units. NEB calculations for reaction barriers of subprocesses of transformations between surface structures explain the observed high thermal stability of surface carbonates and hydroxyl groups.

[1] C. Ebensperger, B. Meyer, *phys. stat. sol. (b)* 248 (2011) 2229

O 14.5 Mon 17:00 MA 041

Tuning the growth geometry of metal ad-particles by doping the oxide support — •Niklas Nilius, Xiang Shao, and Hans-Joachim Freund — Fritz-Haber-Institut der Max-Planck-Gesellschaft, Faradayweg 4-6, D-14195 Berlin, Germany

Doping is a versatile yet little examined approach to tailor the physical and chemical properties of oxide thin films. By means of scanning tunnelling microscopy, we demonstrate that small amounts of Mo embedded in a CaO matrix change the growth behaviour of gold. While 3D deposits are formed on the pristine oxide, strictly 2D growth prevails on the doped films. The crossover in particle shape is driven by charge transfer processes from the Mo d-states into the Au islands. The negatively charged gold exhibits a larger adhesion and therefore tends to wet the oxide surface. The Mo d-states that are responsible for the electron exchange are identified inside the CaO band gap via tunnelling spectroscopy. The impact of the Mo dopants on the Au growth is suppressed by Li co-doping, which provides traps for the Mo electrons in the CaO film.

O 14.6 Mon 17:15 MA 041

LEED I(V) analysis of oxygen physisorption on the rumpled NaCl(100) surface — Anne Möller, Stephan Härtel, •Jochen Vogt, and Helmut Weiss — Chemisches Institut der Universität Magdeburg, Universitätsplatz 2, 39106 Magdeburg, Germany

Among the diatomic molecules, O_2 is unique due to its magnetic properties in the gas phase and in the bulk[1]. The structure of O_2 adsorbed on the NaCl(100) surface is of interest in many respects, e. g. for studies of the surface aligned photochemistry of O_2. We have characterized the physisorption of O_2 using low-energy electron diffraction (LEED) with primary electron currents in the nA range and electron energies above 70 eV. No signs of electron beam induced charging of the NaCl surface were perceptible even at cryogenic temperatures. A saturated 2D phase O_2-p(1×1)/NaCl(100) was prepared at temperatures below 31 K. LEED diffraction spot intensities were recorded as a function of electron energy. The subsequent determination of the adsorbate structure based on a full-dynamical LEED-I(V) analysis reveals that O_2 is bound on top of the Na^+ cations. The rumpling of the NaCl(100) surface [2] appears to be unaffected by the adsorbed O_2, consistent with its very weak interaction with the substrate. The details of the adsorbate structure will be discussed and compared with the results of model calculations.

[1] Y. A. Freiman, H. J. Jodl, Phys. Rep. **401** (2004), 1
[2] J. Vogt, H. Weiss, Surf. Sci. **491** (2001), 155

O 14.7 Mon 17:30 MA 041

Optical spectroscopy of PTCDA molecules on a KCl (100) surface in the limit of ultralow densities — •A. Paulheim, M. Müller, C. Marquardt, and M. Sokolowski — Institute for Chemistry, University of Bonn

We use fluorescence spectroscopy as a tool to study aggregation and structural site transitions of molecules in the limit of isolated entities on surface. For this purpose submonolayers of PTCDA were vacuum deposited on thin epitaxial KCl films grown on the Ag(100) surface. The structural and optical properties were investigated by SPA-LEED and by fluorescence(FL) and FL excitation spectroscopy, respectively. For the limit of isolated molecules (1% ML coverage), we observed an irreversible transition in the FL spectra, if the intensity of the exciting light is increased by an additional focussing optics. The FL spectra of this novel phase is blue shifted with respect to that of the original phase by 130 cm^{-1} and the vibronic modes exhibit a smaller FWHM due to reduced inhomogeneous site broadening. In addition, we analysed the polarization of the emitted light and were able to determine the azimuthal orientation of the molecules with respect to the substrate. In both phases, the original and the novel phase, the molecules show the same orientation. So far, the origin of the blue shift is unknown. A possible reason may be photo-induced diffusion of the molecules to surface step sites. This demonstrates that photo-induced heating in combination with FL spectroscopy can be used as a technique for studying the diffusion of molecules on surfaces and the optical properties of molecules depending on the respective adsorption sites.

O 14.8 Mon 17:45 MA 041

NEXAFS/XPS Study of Azobenzene adsorbed on metal oxide structure — •Michael Naboka, Alexei Nefedov, and Christof Wöll — Karlsruher Institute of Technologies

In recent years, molecular switches have attracted considerable attention because of the high potential application in electronic and photonic devices. The molecular switches enable the storage of information on a molecular level, and may find a numerous application in nanotechnology, and molecular electronics. The integration of molecular switches with inorganic surfaces has recently become a hot topic as it can give rise to novel hybrid materials in which the properties of the two components are mutually affected or even enhanced in a reversible fashion. One of the candidates for such a molecular switch can be azobenzene, a chemical compound composed of two phenyl rings linked by a N=N double bond. Hear we present some results of the NEXAFS/XPS study of the Azobenzene molecule adsorbed on metal oxide surfaces.

O 14.9 Mon 18:00 MA 041

Adsorption Properties of a Thin Vitreous Silica Film on Ru(0001) — •Leonid Lichtenstein, Christin Büchner, Stefanie Stuckenholz, Markus Heyde, and Hans-Joachim Freund — Fritz-Haber-Institut der Max-Planck-Gesellschaft, Faradayweg 4-6, 14195 Berlin, Germany

Silica is a technologically very important material. Particularly, it is widely used as a support for metal nanoparticles in catalysis. However, neither the exact atomic structure nor the precise adsorption properties of the silica substrate are well known. Therefore, our goal is to study the adsorption of metal particles on a well defined thin film of vitreous silica by using low temperature dynamic force microscopy (DFM, also known as nc-AFM) in combination with scanning tunneling microscopy (STM) in ultra-high vacuum.

Recently, we resolved the atomic structure of a vitreous silica film on Ru(0001) [1]. Our results showed good agreement with the postulated glass model from Zachariasen [2] and diffraction experiments on silica glass [3,4]. Herein, we use this film as a template for the adsorption of metal single atoms and nanoparticles. Studying the exact adsorption geometry provides insight into the catalytic properties of this combined sample system.

[1] L. Lichtenstein *et al.*, Angew. Chem. Int. Ed., **in press** (2011), DOI: 10.1002/anie.201107097
[2] W. H. Zachariasen, J. Am. Chem. Soc. **54**, 3841 (1932)
[3] R. L. Mozzi *et al.*, J. Appl. Crystallogr. **2**, 164 (1969)
[4] D. I. Grimley *et al.*, J. Non-Cryst. Solids **119**, 49 (1990)

O 14.10 Mon 18:15 MA 041

Submonolayers of Au/Pd on the hematite (0001) and magnetite (111) surfaces — •Adam Kiejna, Tomasz Pabisiak, and Tomasz Ossowski — Institute of Experimental Physics, University of Wrocław, plac M. Borna 9, Wrocław, Poland

Ultra-thin films and nanostructures formed by noble metals on oxide surfaces exhibit enhanced catalytic activity for the CO oxidation. Iron oxide-based catalysts are superior to other oxides, at least for several reactions. 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 Au/Pd atoms on two stable iron-oxide surfaces: hematite (0001) and a magnetite (111). For each surface, adsorption on two terminations has been studied: one terminated with iron and the other with oxygen. Both Au and Pd bind strongly to hematite and magnetite surfaces and induce large changes in their geometry. DFT and DFT+U provide qualitatively similar surface geometries but they differ much in the prediction of the surface energetics and the electronic and magnetic properties of the oxides. Pd binds stronger than Au both to hematite and magnetite surfaces and the Au/Pd bonding to the O-terminated surface is distinctly stronger than that to the Fe-terminated one. For hematite, the DFT+U bonding is by 0.3-0.6 eV weaker than DFT on the Fe-terminated surface and about 2 eV stronger on the O-terminated one. For magnetite, in each case, DFT+U gives stronger bonding than DFT. The differences between DFT and DFT+U results are discussed based on the calculated electronic structure.

O 14.11 Mon 18:30 MA 041

The relevance of surface defects for the adsorption of pyrrole on GaAs(001)-c(4x4) surfaces — •Thomas Bruhn[1], Bjørn-Ove Fimland[3], Michael Kneissl[1], Norbert Esser[1,2], and Patrick Vogt[1] — [1]TU Berlin, Institut für Festkörperphysik, Hardenbergstr.36, 10623 Berlin, Germany — [2]Leibniz-Institut für Analytische Wissenschaften, ISAS e.V., Berlin, Albert-Einstein-Str.9, 12489 Berlin, Germany — [3]NTNU, NO-7491 Trondheim, Norway

The basic principles that determine the adsorption mechanisms of organic materials on solid surfaces are still not sufficiently understood and represent a key issue for recent semiconductor research. In our work we have investigated the adsorption of the aromatic molecule pyrrole (C4H4NH) on the GaAs(001)-$c(4 \times 4)$ reconstruction. The samples were prepared under UHV conditions and the adsorption process was monitored in-situ with a reflectance anisotropy spectroscopy (RAS) setup operating from 1.5 to 8 eV. At sub-monolayer coverage, single adsorbed pyrrole molecules were investigated by scanning tunneling microscopy (STM), scanning tunneling spectroscopy (STS) and photoelectron spectroscopy (XPS). Our results reveal that pyrrole predominantly physisorbs on As-rich $c(4 \times 4)$ reconstruction and essentially retains its initial electronic structure. Additional, however, we could identify a significant amount of molecules which are chemisorbed at surface defects. Our results demonstrate that the occurence of surface defects plays an important role for the reactivity of the As-rich GaAs $c(4 \times 4)$ surface to the adsorption of pyrrole.

O 14.12 Mon 18:45 MA 041

Adsorption of Au atoms on the h-BN/Rh(111) nanomesh — •Hans Peter Koch, Robert Laskowski, and Peter Blaha — Institute of Material Chemistry, Unversity of Technology, Getreidemarkt 9/165-TC, A-1060 Vienna, Austria

The h-BN/Rh(111) nanomesh [1] consists of a highly corrugated single layer of h-BN on a Rh(111) surface. Due to the lattice mismatch a nanostructure with a periodicity of 3.2 nm is formed. In this nanostructure BN forms "pores" of about 2 nm, which are separated by "wires", where BN is 0.1 - 0.2 nm further away from the transition metal than in the "pores". The "pores" of the nanomesh show the extraordinary ability to trap molecules and metallic clusters - forming well-ordered arrays and prohibiting aggregation.

We have theoretically studied the adsorption of Au atoms on bulk h-BN and on various models of the h-BN/Rh(111) nanomesh. While Au binds only weakly to bulk h-BN and h-BN/Rh(111) at the "wire" configurations, the underlying Rh atoms in the "pores" modify considerably the electronic structure of h-BN and Au adsorbs strongly on top of the B atoms. The adsorption is accompanied by a strong outward relaxation of the B atoms and a significantly charging of the Au atoms [2].

Furthermore, we will present first results of the adsorption of small Au[n] clusters (n=2-4) in the "pores". Their adsorption properties show similar trends as observed for single Au atoms.

[1] M. Corso et al., Science 303: 217 (2004)
[2] HP. Koch et al., Phys. Rev. B in print

O 15: Heterogeneous catalysis I

Time: Monday 16:00–19:00 Location: MA 042

O 15.1 Mon 16:00 MA 042

Flow Reactor Investigations of the Ethylene Epoxide Oxide Formation over Ag(111) — •Regina Wyrwich[1], Sebastian Böcklein[1], Sebastian Günther[2], and Joost Wintterlin[1] — [1]Ludwig-Maximilians-Universität, München, Germany — [2]Technische Universität München, Germany

The partial oxidation of ethylene to form ethylene epoxide (EtO) over Ag catalysts is a large scale catalytic process in chemical industry. Although intensive studies have been performed in the last decades the mechanism of the reaction is still not clear. Surface science experiments are hardly possible because of the extremely low reaction probability of the ethylene molecules, an example of the "pressure gap" problem. To overcome this problem we used a specially designed flow reactor in which experiments on single crystals up to atmospheric pressure could be realized. Product gas analysis was performed by quadrupole mass spectrometry (QMS). Because of the low reaction probability the QMS data are strongly affected by errors and cross sensitivities, but we show that by a careful analysis EtO formation on a Ag(111) single crystal surface can be unambiguously detected. An initial annealing step to 600 °C reproducibly led to an active state of the sample. Quantitative data on the pressure, temperature and gas composition dependence of the activity and selectivity were obtained. Indications of a participation of oxygen atoms in the near-surface bulk of the Ag sample were found. We also report on experiments in which Ag samples were promoted by Cs, an important component of the industrial EtO catalyst.

O 15.2 Mon 16:15 MA 042

Oxygen dissociation on pristine and doped CaO films — •Yi Cui, Niklas Nilius, and Hans-Joachim Freund — Fritz-Haber-Institut der Max-Planck-Gesellschaft, Faradayweg 4-6, D-14195 Berlin, Germany

Dissociation of O2 is often the initial step for oxidation reactions on supported metal catalysts. As the dissociation cross section is low on the surface of many wide-gap oxides, we have tried to improve the performance by inserting impurity ions that act as electron donors. For this purpose, Mo-doped CaO films have been prepared and analyzed with respect to their O2 adsorption behavior, using scanning tunneling microscopy. Whereas at room temperature, both the pristine and doped films spontaneously dissociate oxygen, intact O2 molecules are detected on pristine CaO upon exposure at 100 K. These molecules can be split in a controlled manner by electron injection from the STM tip. On the doped films, on the other hand, oxygen dissociation takes place at any temperature, suggesting that a spontaneous electron transfer from the Mo dopants into the anti-bonding oxygen orbitals triggers the decay of the molecule.

O 15.3 Mon 16:30 MA 042

CO oxidation reaction on mesoporous Au/TiO_2 model catalysts - a kinetic and spectroscopic study — •Matthias Roos[1], Dominique Böcking[2], Kwabena Offeh Gyimah[1], Gabriela Kucerova[1], Joachim Bansmann[1], Nicola Hüsing[2,3], and R. Jürgen Behm[1] — [1]Institute of Surface Chemistry and Catalysis, Ulm University, D-89069 Ulm, Germany — [2]Institute of Inorganic Chemistry II, Ulm University, D-89069 Ulm, Germany — [3]Materials Chemistry, Paris-Lodron University, A-5020 Salzburg, Austria

Ultrathin mesoporous Au/TiO_2 layers of about 150 nm thickness, can be considered as a close-to-realistic model system for realistic Au/TiO_2 catalysts. Their catalytic properties towards the CO oxidation reaction were studied using two different types of reactors, which have been developed for kinetic measurements on low surface area model catalysts. A locally resolving and differentially pumped mass spectrometer was used to determine reaction parameters like reaction orders and the activation energy of the samples [1,2]. In order to measure absolute

reaction rates, a micro flow tube reactor was developed, based on the design by K. Wong et al. [3], which was optimized for the CO oxidation on mesoporous Au/TiO_2 film samples. Furthermore, infra red spectroscopic measurements were performed to investigate the accumulation of stable carbon based species on the sample surface, such as surface carbonates, as potential origin for the observed deactivation.
[1] M. Roos et al., *J. Chem. Phys.* 133, **2010**, 94504.
[2] M. Roos et al., *Beilstein J. Nanotechnol.* 2, **2011**, 593.
[3] K. Wong et al., *Faraday Discuss.* 105, **1996**, 237.

O 15.4 Mon 16:45 MA 042

Chemical-to-electric energy conversion in reactions of oxygen and hydrogen molecules on Pt surface. — •Ievgen Nedrygailov, Jan Philipp Meyburg, Eckart Hasselbrink, and Detlef Diesing — Fakultät für Chemie, Universität Duisburg-Essen, D-45117 Essen, Germany

A number of scientific and technological challenges motivate the study of energy transfer to the electronic degrees of freedom in the course of exothermic chemical reactions on catalyst surfaces. However, the energy flow in the single steps of a reaction is incompletely understood. In the present study, we use planar metal-oxide-semiconductor (MOS) Pt-SiO_2-n-Si diodes for the detection of electronic excitations associated with the reactive interaction of hydrogen and oxygen molecules on Pt surfaces. We show experimental results for the chemically induced currents in the mentioned diodes while the Pt top electrode is exposed to H_2, O_2 and hydrogen−oxygen mixture in different molar ratios. Experiments were carried out for initial temperature of the diodes ranging from 298 to 500 K. Chemical heating of the diodes up to 900 K was observed for pressures of 10 mbar. The mechanisms of chemically induced currents generated and detected in our MOS diodes are discussed.

O 15.5 Mon 17:00 MA 042

Chemical Waves and Rate Oscillations in the H2 + O2 Reaction on a Bimetallic Rh(111)/Ni Catalyst — •Tim Smolinsky[1], Florian Lovis[1], Andrea Locatelli[2], Miguel Niño[2,3], and Ronald Imbihl[1] — [1]Institut für Physikalische Chemie und Elektrochemie, Leibniz-Universität Hannover, Callinstr. 3-3a, D-30167 Hannover, Germany — [2]Sincrotrone Trieste, S.C.p.A., S.S. 14, km 163.5 in Area Science Park, 34012 Basovizza, Trieste, Italy — [3]Instituto Madrileño de Esudios Avanzados IMDEA Nanociencia, Cantoblanco 28049, Madrid, Spain

The H2 + O2 reaction on a Rh(111) surface alloyed with Ni was studied in the 10-6 - 10-4 mbar range using photoemission electron microscopy (PEEM), low energy electron microscopy (LEEM) and its spectroscopic variant (SPELEEM) as main analytical methods. The Rh(111)/Ni surface was prepared by decomposing Ni(CO)4 on the Rh(111) surface resulting in an alloy with about 25% Ni in the topmost layers. The original bistable system Rh(111)/O2 + H2 is transformed into an excitable system through the addition of Ni. Chemical wave patterns involving target patterns, pulse trains and rotating spirals can be observed. These spatiotemporal patterns were accompanied by rate oscillations observed with mass-spectrometry. Under reaction conditions three-dimensional NiO particles form on the surface ranging from less than 1 μm up to 50 μm in size. The size of these particles depends on the total pressure. A preliminarily excitation/oscillation mechanism is proposed based on the reversible segregation of Ni to the surface thus modifying the catalytic properties of the Rh/Ni surface.

O 15.6 Mon 17:15 MA 042

First-principles kinetic Monte Carlo simulations of CO oxidation at Pd(100): Surface oxide or metal? Both! — •Max J. Hoffmann[1], Matthias Scheffler[2], and Karsten Reuter[1] — [1]TU München, Germany — [2]Fritz-Haber-Institut, Berlin, Germany

CO oxidation at Palladium model catalysts is an evergreen in the quest to establish an atomic-scale understanding of heterogeneous catalytic processes and the relation between atomistic structure and catalytic activity. Notwithstanding and despite numerous experiments, the character of the active surface above Pd(100) under ambient reaction conditions remains heavily debated [1]. The pristine metal surface, a thin surface oxide layer, and bulk palladium oxide have each been suggested to be present and responsible for the catalytic activity.

Contributing to this we perform first-principles kinetic Monte Carlo (1p-kMC) simulations for each of these phases as a function of temperature and partial pressures. Next to obtaining their inherent catalytic activities at steady-state, we can use the determined surface coverages to infer on the stability ranges of the different phases. Intriguingly, this indicates an overlap of the stability regimes of pristine and oxidized Pd(100), which could be underlying the experimentally observed bistability switching between different reaction kinetics.[2]

[1] Gao *et al.*, J. Phys. Chem. C, **114**, 6874 (2010).
[2] Frenken *et al.*, Topics Catal. **36**, 43 (2005).

O 15.7 Mon 17:30 MA 042

The electrochemical promotion of ethylene oxidation at bimetallic Pt-Ag/YSZ catalyst — •Arafat Toghan[1], Rosa Arrigo[2], Axel Knop-Gericke[2], Robert Schlögl[2], and Ronald Imbihl[1] — [1]Institut für Physikalische Chemie und Elektrochemie, Universität Hannover, Callinstrasse 3-3a, D-30167 Hannover, Germany — [2]Fritz-Haber-Insititut der Max-Planck Gesellschaft, Abteilung Anorganische Chemie, Faradayweg 4-6, D-14195 Berlin, Germany

The electrochemical promotion of the C2H4 + O2 reaction at bimetallic Pt/Ag catalyst interfaced to yttrium stabilized zirconia (YSZ) has been studied at high pressure (close to 1 mbar) using X-ray photoelectron spectroscopy (XPS) at BESSY as in situ method to identify the relevant surface species. Setting the working electrode at positive potential of 2V causes a relative rate increase in the CO2 production up to 120%; the electrocatalytic promotion effect (EPOC) is non-Faradaic (Lambda= 2.18). An EPOC effect is only observed at high p(C2H4)/p(O2) ratios when a carbonaceous CHx layers builds up inhibiting O2 adsorption. Only at low p(C2H4) the application of an electric potential causes a decrease in the carbon signal associated with a growth of the O1s signal at 529.3 eV [1-2]. The latter species can be assigned to an electrochemically generated oxygen spillover species at Ag sites. [1] A. Toghan, L. M. Rösken, R. Imbihl, ChemPhysChem 2010, 11, 1452-1459. [2] A. Toghan, L. M. Rösken, R. Imbihl, Phys. Chem. Chem. Phys. 2010, 12, 9811-9815.

O 15.8 Mon 17:45 MA 042

Interaction of H_2O with ceria and Pt/ceria model catalysts — •Y. Lykhach[1], G. N. Vayssilov[2], M. Happel[1], N. Tsud[3], H. A. Aleksandrov[2], T. Skála[4], V. Johánek[3], P. St. Petkov[2], K. C. Prince[4], V Matolín[3], K. M. Neyman[5,6], and J. Libuda[1] — [1]FAU Erlangen-Nürnberg, Germany — [2]University of Sofia, Bulgaria — [3]Charles University in Prague, Czech Republic — [4]Sincrotron Trieste, Italy — [5]Universitat de Barcelona, Spain — [6]ICREA, Barcelona, Spain

The interaction of H_2O with ceria-based catalysts plays an important role in hydrogen production via reforming. Still, we are lacking detailed understanding of the water surface chemistry on pure and metal-loaded ceria. We have performed a comprehensive investigation of water adsorption and dissociation on stoichiometric CeO_2(111), partially reduced $CeO_2 - x$, and Pt/CeO_2(111) films on Cu(111), combining high resolution photoelectron spectroscopy (HR-PES), resonant PES, infrared absorption spectroscopy (IRAS), and density functional theory (DFT). Identification of OH-derived spectral signatures and chemisorbed water on ceria turned out to be difficult, both in HR-PES or IRAS. Despite strong signals from OH/H_2O in O 1s core level spectra upon annealing to 500 K, no corresponding vibrational bands were detected on both CeO_2 and $CeO_2 - x$ films above 200 K. DFT suggest that these experimental findings result from strong hydrogen bond between OH and neighboring oxygen anions and strong bending of OH group. Dissociation and spillover on Pt/CeO_2(111) is monitored by RPES via the Ce oxidation state as a function of temperature.

O 15.9 Mon 18:00 MA 042

When atomic-scale resolution is not enough: Spatial effects in *in-situ* model catalyst studies — •Sebastian Matera[1,2] and Karsten Reuter[1] — [1]TU München — [2]Fritz-Haber-Institut der MPG

A central goal in *in-situ* studies of defined model catalysts has been to obtain (at best) equally 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. 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]. We consider two limiting cases for flow geometries in modern *in-situ* reaction chambers: i) the gas approaches the single crystal from the side, ii) the flow direction is perpendicular to the surface. Using the CO oxidation at RuO_2(110) as a showcase we obtain a strong coupling between surface chemistry and mass, heat and momentum transfer. This generates substantial variation in gas-phase pressures and temperature between the inlet and the catalyst surface.

In particular for case i) we obtain large lateral changes in surface composition across the catalyst surface. This prevents the aspired direct relation between measured activity and defined catalyst structure, and therewith underscores the importance of carefully designed reactor geometries in *in-situ* studies. [1] S. Matera and K. Reuter, Catal. Lett. **133**, 156 (2009); Phys. Rev. B **82**, 085446 (2010).

O 15.10 Mon 18:15 MA 042

Dynamic distribution patterns of ultrathin VOx films on Rh(111) during the O2+CH3OH reaction. — •Martin Hesse and Ronald Imbihl — Institut für Physikalische Chemie und Elektrochemie, Leibniz-Universität Hannover, Callinstr. 3a, 30167 Hannover, Germany

Vanadium oxides play an important role as catalysts in partial oxidation of hydrocarbons. As a model system for VOx based catalysts we studied the behavior of ultrathin VOx films on a Rh(111) surface in the O2+CH3OH reaction. VOx catalyzes the production of formaldehyde. The reaction was investigated in the 10-4 - 10-5 mbar range with photoemission electron microscopy (PEEM) as a spatial resolving method. We observed that at $T > 600°C$ the distribution of VOx on Rh(111) is no longer homogeneous but a stationary macroscopic concentration pattern developed consisting of parallel stripes of VOx surrounded by bare Rh(111) surface. In analogy to the patterns formed in the O2 + H2 reaction on Rh(111)/VOx we interpret the patterns as being due to reactive phase separation[1]. The dependence of the rate of formaldehyde production on the distribution pattern of vanadium oxide on Rh(111) was studied.

[1] F. Lovis et. al, J. Phys. Chem. C 115, 2011, 19141

O 15.11 Mon 18:30 MA 042

Structural Investigation of the $(7\times\sqrt{3})$rect Oxygen Phase on Ag(111) — •Martin Ehrensperger[1], Miguel À. Niño[2], Tevfik O. Menteş[2], Andrea Locatelli[2], Sebastian Böcklein[1], Wolfgang Moritz[1], Sebastian Günther[3], and Joost Wintterlin[1] — [1]Ludwig-Maximilians-Universität München, Germany — [2]Sincrotrone Trieste S.C.p.A., Italy — [3]Technische Universität München, Germany

We have investigated the structure of the $(7\times\sqrt{3})$rect oxygen phase on the Ag(111) surface by means of a low-energy electron diffraction (LEED)-I/V analysis. Further techniques were scanning tunneling microscopy, x-ray photoelectron spectroscopy (XPS), and low-energy electron microscopy. Three rotational domains are observed on a completely covered substrate surface. The symmetry is Pm with a mirror plane parallel to the $<\bar{1}\bar{1}2>$ substrate directions. According to XPS the structure contains about one monolayer of an oxygen species that is closely related to the so-called "electrophilic" oxygen. Following the literature this oxygen species is the active species for the partial oxidation of ethylene to give ethylene oxide over Ag catalysts. Structures were tested containing adsorbed O atoms on the unchanged Ag(111) surface, possible reconstructions of the surface, surface oxide type structures and structures derived from bulk silver oxides. Relative integral intensities suggest a thickness of at least two layers of Ag atoms. All models deduced from variations of known structures of the entire Ag-O system or comparable surface oxygen systems of other metals can be excluded.

O 15.12 Mon 18:45 MA 042

From atoms to eddies: a novel general approach to chemical reaction engineering — •Matteo Maestri[1,2], Alberto Cuoci[1], Sebastian Matera[2], and Karsten Reuter[2] — [1]Politecnico di Milano, Italy — [2]TU München, Germany

The identification of the dominant reaction mechanism is a center piece in the quest towards an atomic-scale understanding of a catalytic process. Inherently, this mechanism is a multiscale property and its identification requires efficient and general tools that properly integrate a detailed (first-principles) description of the surface catalytic chemistry and the macroscale flow structures in the reactor. To this end we recently introduced the new solver CatalyticFOAM [1]. By exploiting the operator splitting technique, it allows for the solution of Navier-Stokes equations even for complex reacting flow profiles at surfaces. Here, we now extend its functionality to also explicitly account for site heterogeneity and the detailed surface chemical distributions in the microkinetic description of the surface reactivity. Relying on the assumption of a quasi-instantaneous adaption of the reactive chemistry to changes in the fluid properties above the surface [2] allows us to efficiently integrate corresponding kinetic Monte Carlo based microkinetics through an interpolation technique. We demonstrate our approach using the CO oxidation on $RuO_2(110)$ for different reactor configurations and fluid dynamics conditions. [1] M. Maestri and A. Cuoci, CatalyticFOAM, www.catalyticfoam.polimi.it; [2] S. Matera and K. Reuter, Phys. Rev. B 82, 085446 (2010).

O 16: Scanning probe methods II

Time: Monday 16:00–18:30 Location: MA 043

O 16.1 Mon 16:00 MA 043

ncAFM Force Spectroscopy of Long Range Tip Sample Interaction using FIM Characterized Tip — •Jens Falter[1], Daniel-Alexander Braun[1], Gernot Langewisch[1], Hendrik Hölscher[3], Harald Fuchs[1], and André Schirmeisen[2] — [1]Center for Nanotechnology (CeNTech) and Institute of Physics, University of Muenster (WWU) — [2]Institute of Applied Physics (IAP), Justus-Liebig-University Giessen — [3]Karlsruher Institute for Technology (KIT), Karlsruhe

Beyond imaging, non contact Atomic Force Microscopy (ncAFM) measures interaction forces between the sample surface atoms and the probing tip with atomic precision. Nevertheless, the full interaction geometry is often unknown because of the unknown tip structure. A comparison with theory to understand the underlying contrast mechanism therefore is often not possible. The implementation of the qplus sensor [1] allows combining ncAFM with the Field Ion Microscope (FIM)[2] which provides the tip structure with atomic precision. Here we present ncAFM force spectroscopy experiments with a FIM-characterized tip. Combining these microscopy techniques, the tip structure can be determined and compared with analytical models based on the given tip geometry. A comparison of our distance and voltage dependent force curves with theoretical models is in excellent agreement for the electrostatic force interactions while the van der Waals contribution is underestimated by the models. Furthermore, our approach provides a quantitative value for the absolute distance. [1] F.J. Giessibl, Appl. Phys. Lett. 76, 1470 (2000) [2] E.W. Müller, Z. Physik 131, 136 (1951)

O 16.2 Mon 16:15 MA 043

Development of a Diamond-based Scanning Probe Spin Sensor with sub-nm Spatial Resolution — •Eike Oliver Schäfer-Nolte[1,2], Friedemann Reinhard[2], Markus Ternes[1], Jörg Wrachtrup[2], and Klaus Kern[1] — [1]Max-Planck Institut für Festkörperforschung, Stuttgart, Germany — [2]3. Physikalisches Institut, Universität Stuttgart, Germany

The detection of single spins with high spatial resolution is a longstanding challenge in physics. The nitrogen-vacancy (NV) center in diamond is one of the few solid-state systems where the spin state can be optically measured [1]. By attaching a nanodiamond containing this "probe spin" to the tip of an atomic force microscope a controlled coupling between the NV and nearby spins on the sample can be achieved, allowing an indirect observation of these spins via the fluorescence signal from the NV [2]. This approach provides an unprecedented sensitivity by exploiting the quantum nature of the NV spin, enabling coherent manipulation by pulsed detection schemes well known from EPR- and NMR-spectroscopy. In this case the sensitivity is limited by the coherence time of the NV, which exceeds 1ms in pure diamond [3]. This corresponds to an energy resolution on the order of kHz.

We report on our efforts developing such a Scanning Probe Spin Sensor and present details of the experimental setup along with first experimental data.

References: [1] F. Jelezko, Phys. Stat. Sol. (a) 203, 3207 (2006) [2] J.M. Taylor, Nature Physics 4, 810 (2008) [3] G. Balasubramanian, Nature Materials 8, 383 (2009)

O 16.3 Mon 16:30 MA 043

Magnetoresistive Tunnelling Structures with Magnetostrictive Electrodes as Sensors for Atomic Force Microscopy — •Tobias Meier[1], Ali Tavassolizadeh[2], Dirk Meyners[2], and Hendrik Hölscher[1] — [1]Institute of Microstructure Technology, Karlsruhe Institute of Technology, D-76021 Karlsruhe, Germany — [2]Inorganic Functional Materials, Christian-Albrechts-Universität zu Kiel, D-24118 Kiel, Germany

We introduce a new approach on self-sensing cantilevers for the atomic force microscopy using magnetoresistive tunnelling structures (TMR-Sensors). As the resistance of a tunnelling barrier between two ferromagnetic electrodes strongly depends on the magnetisation of the electrodes material, one can measure the orientation of the magnetisation of the electrodes by measuring the resistance of the tunnelling barrier. Combining such a layer system with magnetostrictive materials, one can change the magnetisation of one electrode by applying mechanical strain and stress to the electrode and therefore change the resistance of the tunnelling barrier. Such TMR-Sensors show huge gauge-factors and can be integrated on an atomic force cantilever to measure its deflection.

O 16.4 Mon 16:45 MA 043

Revealing the angular symmetry of chemical bonds by atomic force microscopy — •Joachim Welker and Franz J. Giessibl — Faculty of Experimental and Applied Physics, University of Regensburg, Universitätsstraße 31, 93053 Regensburg

The angular symmetry of chemical bonds determines the structure of condensed matter from the atomic to the macroscopic scale. Angular dependence is characteristic of covalent bonding, which occurs in organic molecules aswell as bulk solids. Here, we have measured the angular dependence of chemical bonding forces between two atomic bonding partners: a carbon monoxide molecule that is adsorbed to a copper surface and the front atom of the metallic tip of a combined scanning tunneling microscope (STM) and atomic force microscope (AFM). We present tomographic maps of force and current as a function of distance that reveal the emergence of strongly directional chemical bonds and a conductive channel as tip and sample approach. The force maps show pronounced single, dual or triple minima depending on the directional preferences of the bonds that develop, while tunneling currents maps show a single dip for all three tip conditions.

O 16.5 Mon 17:00 MA 043

Molecular ordering and local work function of pentacene on ioniccrystalline surfaces — •Julia Neff[1], Jan Götzen[1,2], Peter Milde[3], and Regina Hoffmann-Vogel[1] — [1]Karlsruher Institut für Technologie, Physikalisches Institut, 76131 Karlsruhe, Germany — [2]Mechanical Engineering and Materials Science, Yale University, CT 06511, USA — [3]Institut für Angewandte Photophysik, Technische Universität Dresden, 01069 Dresden, Germany

The electronic properties of molecular thin films are closely related to their structural order. Therefore a precise control of the molecular packing and the crystalline orientation of semiconducting organic molecules like pentacene is of vital interest for the optimization of organic electronic devices. The growth of pentacene on KCl(001) and KBr(001) at submonolayer coverage was studied by dynamic scanning force microscopy. Pentacene was found to arrange in islands with an upright configuration on these bulk insulators. Molecularly resolved images of the islands show two different types of patterns that appear to switch repeatedly. In both patterns defects, such as a molecular vacancy and domain boundaries, were observed. Insight into the electronic structure is gained by Kelvin probe force microscopy. The measured charge densities show differences of about 1V between bare substrate regions and pentacene islands.

O 16.6 Mon 17:15 MA 043

Probing defects with the Phantom Force — •Alfred Weymouth, Thorsten Wutscher, and Franz Giessibl — Universität Regensburg, Regensburg, Germany.

Simultaneous force and tunneling microscopy (AFM and STM, respectively) offer complementary information that can be used to probe local phenomena. Typically, this is done by assuming the two channels represent independently the electronic and atomic structure (e.g. [1]). We have recently demonstrated that it is possible to dominate AFM data by locally altering the attractive electrostatic force between tip and sample via the tunneling current and sample resistivity [2]. While the AFM data can no longer be assumed to be decoupled from the STM data, this opens the possibility of using simultaneous AFM and STM data to probe local surface conductivity. Here we demonstrate that we can probe conductance changes over a defect on the H-terminated Si(100) surface.

[1] G.H. Enevoldsen et al., Phys. Rev. Lett., **102**, 136103 (2009).

[2] A.J. Weymouth et al., Phys. Rev. Lett., **106**, 226801 (2011).

O 16.7 Mon 17:30 MA 043

Superlubric sliding of metallic nanoparticles: The influence of contact area and crystallinity — •Dirk Dietzel[1,2], Tristan Mönninghoff[1], Michael Feldmann[1,2], Udo D. Schwarz[3], and Andre Schirmeisen[1,2] — [1]Institute of Applied Physics, University of Giessen — [2]Institute of Physics & Center for Nanotechnology, University of Muenster — [3]Dep. of Mech. Eng., Yale University, USA

The precise analysis of contact area dependence of nanoscale friction is a long standing problem in nanotribology. Currently, interest is especially spurred by the assumption that the scaling of friction with contact area might be a unique fingerprint to identify superlubric sliding. Superlubricity, or also termed structural lubricity, originates from the lattice mismatch at the interface of two atomically flat surfaces, and predicts a decrease of shear stress with contact area, and thus a sublinear contact area dependence of friction. To measure the interfacial friction we have manipulated metallic nanoparticles of different size on atomically flat surfaces by contact mode AFM techniques[1]. Our results confirm the sublinear scaling of friction with contact area. Moreover, we could identify different scaling factors for amorphous and crystalline particles. The experiments have been accompanied by numerical simulations of friction of Au and Sb particles on HOPG, which have indicated that not only contact area and crystallinity are important, but also the precise shape of the nanoparticle is crucial for friction. The good agreement between experiment and simulation enables us to quantitatively predict nanoscale friction from fundamental atomic quantities. [1]Dietzel et al., Phys. Rev. Lett. 101, 125505 (2008)

O 16.8 Mon 17:45 MA 043

Hidden Atomic Resolution - Investigation of a Complex Oxide Material with 2D Force Spectroscopy — •Christin Büchner, Leonid Lichtenstein, Stefanie Stuckenholz, Markus Heyde, and Hans-Joachim Freund — Fritz-Haber-Institut der Max-Planck-Gesellschaft, Faradayweg 4-6, 14195 Berlin, Germany

For the first time, a model system of an amorphous oxide network has been prepared. A double layer film of silicon dioxide was grown on a Ru(0001) support, exhibiting a complex network of differently sized ring units [1]. This atomically flat system was investigated using frequency-modulated dynamic force microscopy (FM-DFM). Under very stable imaging conditions (UHV, low temperature), we performed two-dimensional (2D) force spectroscopy mapping. Measuring Δf(z)-curves up to very short distances to the surface, a significant variation in the contrast generating shift can be observed. The repulsive regime exhibits a significantly higher corrugations than the attractive branch. This method gives insight into the contrast formation of DFM and may be employed for different systems, where achieving atomic resolution is challenging. High resolution scanning probe microscopy images of a thin vitreous silica film will be presented together with 2D force spectroscopy data. The force mapping results will be discussed together with a general consideration of characteristic Δf(z)-curves.

[1] Lichtenstein et al., Angew. Chem. IE. doi: 10.1002

O 16.9 Mon 18:00 MA 043

A pick-and-place technique for the assembly of integrated quantum optical hybrid devices — •Andreas W. Schell, Günter Kewes, Janik Wolters, Tim Schröder, Thomas Aichele, and Oliver Benson — Nanooptik, Humboldt-Universität zu Berlin, Deutschland

Combining pre-selected nanoparticles with nano-or microstructures produced in a top down process is an important but challenging step in the production of hybrid devices for nano-optics. Here, a pick-and-place technique for the controlled bottom up assembly of integrated quantum optical devices based on atomic force microscopy combined with optical confocal microscopy is introduced [1]. This technique allows for the placement of nanoparticles on nearly arbitrarily shaped samples. By coupling nitrogen vacancy defect centers in diamond nanocrystals, which are capable of emitting single photons, to photonic and plasmonic structures like photonic crystals, photonic crystal fibers or nanoantennas using this pick-and-place technique, hybrid quantum optical elemements are produced.

[1] A.W. Schell et al., Rev. Sci. Instrum. 82, 073709 (2011).

O 16.10 Mon 18:15 MA 043

Scanning Microwave Microscopy Mapping of Semiconducting and Dielectric Components in CMOS Logic devices

— •Matthias A. Fenner[1], Thomas Schweinböck[2], and Jesper Witteborn[2] — [1]Agilent Technologies, Lyoner Str. 20, 60528 Frankfurt, Germany — [2]Infineon Technologies AG, Am Campeon 12, 85579 Neubiberg, Germany

We report Scanning Microwave Microscopy (SMM) investigations of CMOS logic devices. SMM combines Atomic Force Microscopy (AFM) and a microwave Vector Network Analyzer to map the microwave signal reflected from the tip sample junction. The reflected signal depends on the impedance of the junction [1]. Varying dielectric and semiconducting material properties lead to modified impedances and can thus be detected. Applying a low frequency AC bias between tip and sample leads to modulation of the semiconductor space charge region and the reflected signal [2]. Both signals can be acquired simultaneously.

Cross sections of 90-nm technology node CMOS logic devices have been prepared and investigated using SMM to map dielectric properties and dopant density.

[1] Huber, H.P., et al., Review of Scientific Instruments, 2010. 81(11), p. 113701-9. [2] Smoliner, J., et al., Journal of Applied Physics, 2010. 108(6), p. 064315-7.

O 17: Nanotribulogy

Time: Monday 16:00–17:15 Location: A 053

O 17.1 Mon 16:00 A 053

Imaging and energy dissipation mechanisms on metallic and insulating surfaces studied with AFM in pendulum geometry — •Markus Langer, Marcin Kisiel, Urs Gysin, and Ernst Meyer — Department of Physics, University of Basel, Klingelbergstrasse 82, CH-4056, Switzerland

In pendulum geometry the Cantilever is oscillating perpendicular to the sample surface. This opens the possibility to use ultra sensitive cantilever with spring constants of mN/m with a force sensitivity of $10aN/\sqrt{Hz}$. For surface characterisation of mixed materials its useful to image the surface topography first. Calculations show that in pendulum geometry the contrast mechanism is influenced by two types of forces - the axial force and the lateral force gradient. This is confirmed experimentally. To study the electronic contribution in detail, it is necessary to compensate the electrostatic force present due to contact potential difference between the cantilever tip and the sample surface. We used frequency modulated - Kelvin Probe Force Microscopy (fm-KPFM) to compensate the contact potential.

We can distinguish between metallic and insulating surfaces an determine the electronic contribution to the energy dissipation. This effect is enhanced, if we gently functionalize the probe, by covering the tip apex with an insulator or metal.

The measurements are performed on Cu(100) substrate with $0.6ML$ coverage of NaCl. All experiments are done under UHV and cryogenic conditions (77K).

O 17.2 Mon 16:15 A 053

Spin friction observed on the atomic scale — •Boris Wolter[1], Yasuo Yoshida[1], Kirsten von Bergmann[1], André Kubetzka[1], Saw-Wai Hla[2], and Roland Wiesendanger[1] — [1]Institut für Angewandte Physik, Universität Hamburg — [2]Nanoscale and Quantum Phenomena Institute, Ohio University, Athens, Ohio

We present a combined experimental and theoretical study of frictional phenomena occurring when a single magnetic atom is moved over a magnetic surface with the help of a spin-polarized scanning tunnelling microscope tip [1]. By monitoring the spin-resolved atom manipulation traces and comparing them with the results of Monte-Carlo simulations, we are able to reveal the characteristic friction force variations resulting from the occurrence of 'spin friction'.

[1] D. Serrate et al., Nature Nanotechnology 5, 350-353 (2010)

O 17.3 Mon 16:30 A 053

Evolution of nanocrystalline iron surfaces with grain level roughness under sliding contact loads — •Pedro A. Romero, Tommi T. Järvi, and Michael Moseler — Fraunhofer-Institut für Werkstoffmechanik IWM, Wöhlerstraße 11, 79108 Freiburg, Deutschland

Iron systems like steel alloys are one of the main industrial materials in our technological society. Various iron based technologies could benefit from a more fundamental understanding of the nanoscale mechanisms dictating friction and wear in order to improve product performance, efficiency and lifetime. Here, we communicate results from large scale atomistic simulations of nanocrystalline iron systems encompassing hundreds of nanograins and millions of atoms. The constructed model captures the sliding induced plasticity and heating responsible for friction at the contacting interfaces. Controlled pressure simulations will bring forth distinct mechanisms dictating friction and wear in nanocrystalline iron surfaces such as the nucleation and arrest of dislocations at grain boundaries, grain growth, rotation and elongation, as well as grain boundary annealing and motion. The simulations will demonstrate that pure iron nanocrystalline systems prefer to coarsen interface grains while iron-carbon systems prefer to develop an amorphous boundary layer in order to mediate the sliding induced plastic deformation.

O 17.4 Mon 16:45 A 053

Direction dependence of friction for commensurate and moderately incommensurate surfaces — •Michael Wolloch[1,2], Peter Mohn[1], Josef Redinger[1], and András Vernes[1,2] — [1]CMS, Institute of Applied Physics, Vienna University of Technology, Gußhausstraße 25-25a, 1040 Vienna, Austria — [2]Austrian Center of Competence for Tribology, Viktor-Kaplan-Strasse 2, 2700 Wiener Neustadt, Austria

We present results from our calculations of quasi-static sliding of two atomically flat surfaces in dry, wearless contact using the Density Functional Theory package *VASP*. The main focus of our work was to determine to which extent commensurability of the surfaces and the sliding direction effects the friction force. The examined systems include commensurable fcc (111) Aluminium slabs and moderately incommensurate surfaces like bcc (110) Titanium on hcp (001) Titanium. A model consistent with stick-slip friction was devised to calculate the friction forces along sliding paths of up to $1\mu m$ on a quantum mechanical basis. To map all forces and energies for rigid and relaxed atomic positions the top slab was scanned over the bottom one on a properly fine grid, which covers the entire unit cell. In this manner, it is shown that the mean friction force depends on the sliding direction and that due to relaxations incommensurate paths may result, counter-intuitively, in higher friction then commensurate ones.

O 17.5 Mon 17:00 A 053

Suppression of electronic friction on Nb-films below the critical temperature — •Marcin Kisiel[1], Enrico Gnecco[2], Urs Gysin[1], Laurent Marot[1], Simon Rast[1], and Ernst Meyer[1] — [1]University of Basel, Klingelbergstr.82 4056 Basel, Switzerland — [2]IMDEA Nanoscience, Campus Universitario de Cantoblanco, Facultad de Ciencias Módulo C-IX, 28049 Madrid, Spain

The origins of non-contact friction are investigated by highly sensitive force microscopy in the pendulum geometry. In this mode probe is suspended perpendicularly to the sample and the tip's vibrational motion is parallel to the surface. In the pendulum geometry very soft (k~mN/m) and therefore sensitive cantilevers can be used avoiding snapping into the contact due to high longitudinal stiffness. The friction forces acting on a sharp probe tip oscillating below 3nm distances from 140nm thick Nb surface have been measured. Measurements reveal a reduction of dissipation in the superconducting state compared to the normal state by a factor 3. Therefore, electronic friction is found to be the dominant dissipation mechanism with power losses of 80ueV/cycle at separations of 0-3nm. Measurement across the critical temperature of Nb film shows that the character of transition is smooth reflecting the increasing normal electron population which are giving rise to the electronic induced friction. A good agreement with the BCS theory has been found in the drop of friction coefficient, as predicted by the theory[1].

1. B. N. J. Persson, Solid State Communications 115, 145 (2000)

O 18: Spin-orbit interaction

Time: Monday 16:00–17:30 Location: A 060

O 18.1 Mon 16:00 A 060

Detection of the spin-orbit splitting at the β–Bi/Si(111)-$\sqrt{3}\times\sqrt{3}$ surface by scanning tunneling spectroscopy — •Patrick Reissner, Paolo Sessi, and Matthias Bode — Physikalisches Institut, Experimentelle Physik II, Universität Würzburg, Am Hubland, D-97074 Würzburg, Germany

The $\sqrt{3}\times\sqrt{3}$ reconstruction formed by the adsorption of Bi on the Si(111) surface has been recently reported to show a giant Rashba-Bychkov (RB) effect. Photoemission studies have highlighted its complex band structure consisting of multiple spin split bands with nontrivial spin texture [1]. Nevertheless a microscopic characterization is still missing. Here, we report on a combined STM/STS study of Bi/Si(111) performed at cryogenic temperature. We show how it is possible, by means of STS, to locally detect the strength of the RB-splitting. Concerning occupied states, our results are in agreement with previously reported experiments. For unoccupied states, not accessible by standard photoemission techniques, we also observe spectroscopic features that are assigned to RB spin split states. Finally, by taking advantage of the high spatial resolution of STM, the influence of defects on the local density of states is discussed.

[1] K. Sakamoto *et al.*, PRL **103** , 156801 (2009)

O 18.2 Mon 16:15 A 060

Tl/Si(111) - Rotation of the Rashba spin perpendicular to the surface - The unoccupied electronic structure — •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

Tl/Si(111) exhibits an occupied Rashba-split surface state with a peculiar spin structure in reciprocal space [1]. Along the $\bar{\Gamma}\bar{K}$ direction of the hexagonal two-dimensional surface Brillouin zone the spin polarization is rotating from the normal Rashba direction to the direction perpendicular to the surface. This is due to a spin frustration at the $\bar{K}$ point and can be simply understood as a consequence of the 2D symmetry of the hexagonal system. Our spin-resolved inverse photoemission study reveals an unoccupied spin-orbit split surface state along $\bar{\Gamma}\bar{K}$ with the same out-of-plane rotation of the spin polarization. Remarkably, at the $\bar{K}$ point the two spin components are split in energy by more than 0.5 eV, whereas the lower surface band approaches the Fermi level. This gives rise to a nearly complete spin polarization at E_F. As the out-of-plane spin polarization is always negative for $\bar{K}$ and positive for $\bar{K}'$, interesting transport properties can be expected. Our results are supported and discussed on the basis of calculations within the LDA and the GW approximation including spin-orbit coupling.

[1] K. Sakamoto et al., Phys. Rev. Lett. **102**, 096805 (2009)

O 18.3 Mon 16:30 A 060

Manipulating the Rashba-type spin splitting of Pb quantum well states through interface engineering and the substrate charge density — •Bartosz Slomski[1,2], Gabriel Landolt[1,2], Jürg Osterwalder[2], and J. Hugo Dil[1,2] — [1]Swiss Light Source, Paul Scherrer Institut, CH-5232 Villigen PSI, Switzerland — [2]Physik-Institut, Universität Zürich, CH-8057 Zürich, Switzerland

Using spin and angle resolved photoemission spectroscopy we show how the Rashba-type spin splitting in Pb quantum well states [1] can be controlled either by changing the metal-substrate interface or the donor concentration of the n-type Si(111) substrate. Replacing the wetting layer from Pb to Bi reduces the Rashba constant by 50% [2], whereas an increase of the donor concentration by a factor of 20 enhances the constant by almost 50%. Both findings are explained in terms of a modified charge distribution close to the Pb nuclei [3] mediated by the metal-substrate interfaces. Especially the dependency of the Rashba constant on the substrate charge density opens the possibility to manipulate the Rashba effect through an external gate voltage and thus to realize a spin-based field effect transistor as proposed by Datta and Das [4].

[1] J.H. Dil, et al. Phys. Rev. Lett. 101, 266802 (2008)
[2] B. Slomski, et al. PRB 84, 193406 (2011)
[3] G. Bihlmayer, et al. Surf. Sci. 600, 3888 (2006)
[4] S. Datta, et al. Appl. Phys. Lett. 56, 7 (1990)

O 18.4 Mon 16:45 A 060

Quasi-two-dimensional electron gas under in-plane magnetic field and gate electric field in the presence of Rashba and Dresselhaus spin-orbit interactions — •Enver Nakhmedov[1,2], Oktay Alekperov[2], and Reinhold Oppermann[1] — [1]Institut für Theoretische Physik, Universität Würzburg, Am Hubland, 97074 Würzburg, Germany — [2]Institute of Physics, Azerbaijan National Academy of Sciences,H. Cavid str. 33, AZ1143 Baku, Azerbaijan

Interplay of Rashba- and Dresselhaus spin-orpit interactions with the orbital and Zeeman effects of an in-plane magnetic field and gate electric field is studied in a quasi-two-dimenstional electron gas with finite thickness. It is shown that subsidiary valleys arise in the energy-momentum spectrum under particular values of the SO coupling constants, the magnetic field and the Lande factor, which may display a negative differential conductivity and the Gunn effect. Anticrossing and gaps yield multiple extrema in the energy spectrum, indicating in the ballistic conductance as pulsed projections on the energy plateaus.

We show that out-of-plane equilibrium spin current appears under in-plane magnetic field. In the absence of the magnetic field, the average values of the in-plane components of the spin current are shown to coincide with the well-known results obtained for a strictly 2D electron gas, revealing a cubic dependence on the SO coupling constants. In-plane magnetic field contribute new terms to the in-plane components of the spin-current too. The out-of-plane component of the spin current vanishes completely with the magnetic field, and depends quadratically or linearly on the SO coupling constants.

O 18.5 Mon 17:00 A 060

Empty bulk state with a Rashba-type spin-polarization observed on Au(111) — •Sune N. P. Wissing, Anna Zumbülte, Christian Eibl, Anke B. Schmidt, and Markus Donath — Physikalisches Institut, Westfälische Wilhelms-Universität Münster, Germany

Recently, we demonstrated the potential of spin- and angle-resolved inverse photoemission for investigating Rashba phenomena by following the well-known Rashba-split surface state of Au(111) beyond the Fermi level.

Here, we report on the first measurements of a Rashba-type spin polarization in unoccupied bulk states on Au(111). We observe a downward-dispersing spectral feature with strong spin polarization. This feature is attributed to a transition between sp-like bulk states. We will discuss the origin of the observed spin polarization, also in view of recent theoretical and experimental results concerning Rashba splitting in bulk states [1,2].

[1] A. Kimura *et al.*: Phys. Rev. Lett. **105**, 076804 (2010)
[2] E. E. Krasovskii and E. V. Chulkov: Phys. Rev. B **83**, 155401 (2011)

O 18.6 Mon 17:15 A 060

Three-Dimensional Spin Rotations at the Fermi Surface of the Metallic Surface System Au/Ge(111) — •Philipp Höpfner[1], Jörg Schäfer[1], Andrzej Fleszar[2], Jan Hugo Dil[3,4], Bartosz Slomski[3,4], Werner Hanke[2] und Ralph Claessen[1] — [1]Experimentelle Physik 4, Universität Würzburg — [2]Theoretische Physik 1, Universität Würzburg — [3]Swiss Light Source, Villigen PSI, Switzerland — [4]Physik-Institut, Universität Zürich, Switzerland

Adatom-induced ($\sqrt{3}\times\sqrt{3}$)-reconstructions at semiconductor surfaces have attracted significant scientific interest in the past. This is due to the manifold of intriguing low-dimensional properties contained therein, ranging from correlated Mott-Hubbard physics to superconducting surface states. Moreover, as a result of space inversion symmetry-breaking at the solid-vacuum interface, a Rashba-type spin-orbit coupling may lead to a lift of the spin degeneracy in the surface states. A significant spin-splitting in metallic surface states at a semiconductor surface would offer the perspective to manipulate spins electronically.

Here, we present a fully three-dimensional analysis of the spin-properties in the metallic surface system Au/Ge(111) by both spin-resolved photoelectron spectroscopy and advanced density-functional modeling. Contrary to a conventional Rashba situation, the spin texture exhibits strong out-of-plane spin components following a three-fold symmetry. Moreover, the observation of additional radial spin components shows the complexity of the spin-orbit interaction in

Au/Ge(111), and reveals an interplay with Dresselhaus-like spin-orbit effects as a result of the crystalline anisotropies.

O 19: Clean surfaces I

Time: Monday 17:30–19:00 Location: A 053

O 19.1 Mon 17:30 A 053

Electron coincidence studies from S-overlayers on Cu(100) and Ni(100) — •Changhui Li[1], Swapnil Patil[1], Zheng Wei[1], Lucie Behnke[1], Frank O. Schumann[1], Gianluca di Filippo[2], Giovanni Stefani[2], and Jürgen Kirschner[1] — [1]Max-Planck-Institut für Mikrostrukturphysik, Weinberg 2, 06120Halle — [2]Dipartimento di Fisica, Università Roma Tre,Rome, Italy

In a previous double photoemission study of a Cu(100) surface we proved that the Auger process proceeds via a single step rather than a two-step process. The evidence was the emergence of a diagonal line in the 2D-Energy spectrum in the coincidence experiment [1]. In related coincidence measurements on atomic targets diagonal lines in the 2D-Energy distributions are reported in the literature. In order to bridge the gap between solids and atomic targets we prepared S-layers on a solid surface. We exposed a Cu(100), a oxygen passivated Cu(100) and a Ni(100) surface to H_2S gas. This caused the formation of S overlayers with nominal coverages of 0.25, 0.48 and 0.5 ML. We excited these structures with circular polarized light. The photon energy was adjusted such that the S 2p photoelectron and related Auger electron were both in the energy window of our coincidence spectrometer. We do not find a continuous energy sharing between photoelectron and Auger electron. Furthermore, we did not observe a helicity dependence of the coincidence and singles spectra. This means that the Auger emission from S proceeds via a two-step process.

[1] G. van Riessen, Z. Wei, R. S Dhaka, C. Winkler, F.O. Schumann, and J. Kirschner, J. Phys.: Condens. Matter 22, 092201 (2010).

O 19.2 Mon 17:45 A 053

Electronic Surface Properties of Transparent Conducting Oxides from First Principles: In_2O_3, SnO_2, and ZnO — •Benjamin Höffling[1,2], Sebastian Küfner[1,2], and Friedhelm Bechstedt[1,2] — [1]Institut für Festkörpertheorie und -optik, Friedrich-Schiller-Universität,Max-Wien-Platz 1, 07743 Jena,Germany — [2]European Theoretical Spectroscopy Facility (ETSF)

Transparent Conducting Oxides (TCOs) are important for their usage as transparent electrodes in optoelectric and photovoltaic devices as well as transparent electronics. The surface properties of these materials are therefore of great interest for future technical applications. Electronic parameters like the ionization energy, the electron affinity and the work function can be used for electronic band alignment with other semiconducting materials. The possible existence of electronic surface states in the fundamental band gap and the influence of dangling bonds play a crucial role for the efficiency of charge carrier separation in photovoltaic applications. Yet all of these key parameters are still controversially discussed in literature. We employ Density Functional Theory and most modern Quasiparticle Theory to predict electron affinity, ionization potential, surface energy and surface band structures for different surface orientations and terminations of the TCOs In_2O_3, SnO_2 and ZnO. The results are compared with experimental observations and interpreted with regard to possible applications in optoelectric devices.

O 19.3 Mon 18:00 A 053

Bulk and Surface Characterization of In2O3(001) Single Crystals — •Daniel Hagleitner[1], Manfred Menhart[1], Peter Jacobson[1], Sara Blomberg[2], Karina Schulte[2], Edvin Lundgren[2], Frank Kubel[3], Christoph Puls[3], Andreas Limbeck[3], Herbert Hutter[3], Lynn Boatner[4], Michael Schmid[1], and Ulrike Diebold[1] — [1]Institute of Applied Physics, TU Wien, Austria — [2]Division of Synchrotron Radiation Research, Lund University, Sweden — [3]Institute of Chemical Technologies and Analytics, TU Wien, Austria — [4]Materials Science and Technology Division, Oak Ridge National Laboratory, USA

Indium oxide, In2O3, has drawn increased attention from researchers over recent years. When doped with SnO2, the material is commonly referred to as Indium Tin Oxide (ITO), which is the prototypical Transparent Conducting Oxide (TCO). ITO combines high optical transparency in the visible range with a conductivity approaching that of a metal. Despite the technological importance of ITO, surprisingly little is known about its surface properties or those of pure indium oxide. We will present STM, STS, PES, LEIS and XRD results of high-quality single crystals grown by the flux method. In particular, we will discuss atomically-resolved STM images of the In2O3(001) single crystal surface depending on the surface preparation (reduced/oxidized/hydrogenated) conditions. PES and STS data show a significant difference of the electronic structure (surface states, band bending) depending on the surface preparation.

O 19.4 Mon 18:15 A 053

***SnO_2*: Band Structure Measurements by ARPES and Determination of Resistivity and Carrier Concentration** — •Stephan Machulik[1], Valentina Scherer[1], Christoph Janowitz[1], Helmut Dwelk[1], Alicia Krapf[1], Klaus Irmscher[2], and Recardo Manzke[1] — [1]Humboldt-Universität zu Berlin, Institut für Physik, Newtonstr. 15, Berlin, Germany — [2]Leibniz-Institut für Kristallzüchtung, Max-Born-Str. 2, Berlin, Germany

So far the experimental band structure of SnO_2 has only been measured on thin films or the surface of crystals prepared by sputtering [1]. These methods however lead to oxygen deficient and reconstructed surfaces. For the cleaved surfaces of single crystals, investigated by us, a higher resolution for the band structure measurements was obtained, due to less surface imperfections. By comparing our results with HSE hybrid functional band structure calculations good agreement has been found [2]. Prior to the angular resolved photoemission (ARPES) measurements the resistivity (ρ) and the carrier concentration (n) was determined by van der Pauw measurements.

[1] M. Batzil and U. Diebold, Progress in Surface Sience 79 (2005) 47-154

[2] J. B. Varley, A. Janotti, and C. G. Van de Walle, Physical Review B 81, 245216 (2010)

O 19.5 Mon 18:30 A 053

Ab-initio study of tin dioxide surfaces: stability and electronic structure — •Sebastian Küfner[1], Andre Schleife[2,1], Benjamin Höffling[1], and Friedhelm Bechstedt[1] — [1]Institut für Festkörpertheorie und -optik, Friedrich-Schiller-Universität, Max-Wien-Platz 1, D-07743 Jena, Germany — [2]Department of Physics, University of California, Santa Barbara, California 93106-9530, USA

SnO_2 as an transparent conducting oxide is an interesting material for application in transparent circuits, photovoltaic or optoelectronic devices. However, the electronic structures as well as the relative stability of different orientations and terminations of SnO_2 surfaces are not well known.

We apply the density functional theory to calculate the total energies and the atomic geometries of the low-index surfaces (001), (100), (110), (111) of rutile SnO_2. From a comparison to the quasiparticle bulk band structure we conclude that the results of the approximate LDA-$\frac{1}{2}$ scheme are sufficiently accurate while they can be obtained at significantly lower computational cost. Therefore, the LDA-$\frac{1}{2}$ method is used to calculate the surface band structures.

Calculating the surface free energy depending on the oxygen chemical potential, we find the oxygen-terminated (100) and (110) surfaces to be most stable, in accordance with experiments and other ab-initio results. We show that the insulating character is conserved for the surfaces (except for the tin terminated (110) one) even though surface states appear in the fundamental band gap. Furthermore, we obtain the ionization energies and electron affinities.

O 19.6 Mon 18:45 A 053

k-space microscopy with synchrotron radiation on Ag and Bi_2Te_3 — •Marten Patt, Vitaliy Feyer, Lukasz Plucinski, Carsten Wiemann, and Claus Michael Schneider — PGI-6, Forschungszentrum Jülich GmbH, Jülich, Germany

Momentum resolved photoelectron detection combined with an imaging energy filter gives access to a robust bandstructure imaging of the full k-space with comparatively short acquisition times. With our

NanoESCA installation at the *Nanospectroscopy Beamline* at the synchrotron *ELETTRA* (Italy)[1] we combine this method with a microspot refocused synchrotron beam, which provides a defined excitation region (ca. 10 μm). The complete angular distribution of the excited electrons at one kinetic energy is measured parallel in one acquisition with an angular resolution $< 0{,}09$ Å^{-1}.
We present results of the well-known Ag (001) single crystal Fermi surface as well as of $\mathrm{Bi_2Te_3}$, which belongs to a new class of materials: the topological insulators [2]. Clear Dirac cone features are visible. Furthermore, we discuss the possibility of future time-resolved measurements due to the efficiency of this method.
[1] http://www.elettra.trieste.it/beamlines/NASP
[2] J.E. Moore, Nature (London) 464, 194 (2010)

O 20: Theoretical methods I

Time: Monday 17:45–19:00 Location: A 060

O 20.1 Mon 17:45 A 060

Can we replace a metallic support for an ultra-thin insulating film using a perfect conductor model? — •Ivan Scivetti and Mats Persson — Surface Science Research Centre, the University of Liverpool, Liverpool L69 3BX, UK

The study of atoms and molecules deposited on ultra-thin, insulating films supported by metal substrates is an emerging and exciting area of research, in which Density Functional Theory (DFT) could play a key role. In fact, further understanding of these systems could lead to creation and design of novel functionalized nanostructures or molecular devices for electronics, photovoltaics, information storage and processing, catalysis and chemical sensors [1].

However, DFT simulations of these systems are very challenging, since charging plays in many cases an important role [2]. Therefore, there is a need to develop simplified computational schemes.

In this work we assume that the metallic support can be replaced by a perfect conductor model without having to consider the metal electrons explicitly, which would enable us to handle different charge states and reduce the computational time. To this end, we have developed a novel DFT approach, providing appropriate expressions for the total energy and forces. To evaluate the quality and the range of this approximation, we show preliminary results for adsorbates over an insulating film in different charge states.

[1] Mohn, F et. al., Phys. Rev. Letter 105, 266102 (2010).
[2] Jascha Repp, et al., Science 305, 493 (2004).

O 20.2 Mon 18:00 A 060

juRS - Massively Parallel Real-Space DFT Calculations — •Paul Baumeister, Daniel Wortmann, and Stefan Blügel — Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, D-52425 Jülich Germany

We present a new DFT tool developed in Jülich that combines equidistant real-space grids and the Projector Augmented Wave (PAW) method. The code is explicitly designed for the structural relaxation of systems consisting of several thousand atoms with very flexible boundary conditions. The real-space treatment of wave functions, densities and potentials enable a simple, efficient and strong parallelization with respect to communication and load balancing. Besides the parallel computation of k-points, we employ a domain decomposition to the real-space cell and a parallelization over eigenvalues (bands). Hence, we exploit the local character of the Kohn-Sham equation and approximate the kinetic energy operator with a localized high-order finite difference stencil. The extremely sparse Hamiltonian favours iterative diagonalization schemes. We will discuss the difficulties due the interplay of wave function convergence and density convergence. Further, we will demonstrate the efficiency of the parallelization on massively parallel supercomputer architectures such as IBM's BlueGene which support cartesian nearest neighbor communication on the hardware level.

O 20.3 Mon 18:15 A 060

Implementation of screened hybrid density functionals for periodic systems with numerical atomic orbitals:Basis function fitting and integral screening — •Honghui Shang and Jinlong Yang — University of Science and Technology of China, Hefei, China

In hybrid functional calculations of the electronic structure, evaluation of the Hartree-Fock exchange (HFX) is currently the computational bottleneck. Although the scaling with system size can be linear when numerical atomic orbitals (NAOs) are used, the computation of HFX carries a large prefactor. The development of efficient algorithms that reduce the prefactor therefore becomes crucial. In this work, an efficient $O(N)$ implementation of screened hybrid density functionals is presented for periodic systems. NAOs of valence electrons are fitted with gaussian type orbitals (GTOs), which can be used for an analytical evaluation of the electron repulsion integrals (ERIs) that are the building blocks of HFX. The strict locality of the NAOs is employed for an efficient two-electron integral screening technique. In this way, the prefactor of HFX is significantly reduced while retaining the $O(N)$ scaling. This hybrid scheme, denoted as NAO2GTO, is implemented in the SIESTA package. We have tested our method for a variety of systems ranging from molecules to solids. When the DZP basis set is used, good agreement with results obtained from plane wave packages is reached. Our implementation, for the first time, enables screened hybrid functional calculations using NAOs for non-trivial periodic systems.
*present addess: Fritz-Haber-Institut der MPG, Berlin

O 20.4 Mon 18:30 A 060

A linear-scaling DFT+U study of Friedel oscillations and localization in very dilute Gallium Manganese Arsenide — •David D. O'Regan[1,2], Nicholas D. M. Hine[1,3], Mike C. Payne[1], and Arash A. Mostofi[3] — [1]Cavendish Laboratory, University of Cambridge. — [2]Theory and Simulation of Materials, École Polytechnique Fédérale de Lausanne. — [3]The Thomas Young Centre and the Department of Materials, Imperial College London.

We tackle the long-standing difficulties of large system size and strong electronic correlation simultaneously in this work, demonstrating a linear-scaling DFT+U method [1]. Our implementation within the ONETEP code [2] allows for full local orbital optimization and thus systematic variational convergence, and we demonstrate scaling up to 7,000 atoms. Our method furthermore allows for nonorthogonal projectors [3], which may be self-consistently optimized [4].

The ferromagnetic interaction between distant localized magnetic moments in the prototypical dilute magnetic semiconductor (Ga,Mn)As is mediated by defect-induced holes, whose long-ranged character is critical. We present DFT+U calculations of 1,728 atom super-cells of (Ga,Mn)As, accessing the very dilute (0.1%) limit. We analyze the localization and symmetry of the hole density, and characterize its long-range Friedel oscillations.

[1] O'Regan, Hine, Payne and Mostofi, *submit.* (2011), *arXiv*:1111.5943.
[2] Hine et. al. *Comp. Phys. Commun.,* **180**, 1041 (2009).
[3] O'Regan, Payne and Mostofi, *PRB* **83**, 245124 (2011).
[4] O'Regan, Hine, Payne and Mostofi, *PRB* **82**, 081102(R) (2010).

O 20.5 Mon 18:45 A 060

Analysis and elimination of the linearization error within the FLAPW method — •Gregor Michalicek, Markus Betzinger, Christoph Friedrich, 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 (FLAPW) method is widely considered to be one of the most accurate electronic structure methods for solids, providing the density functional answer to high precision. Within the atom-centered muffin-tin (MT) spheres, its basis consists of solutions to the radial scalar-relativistic Dirac equation evaluated at a predefined energy parameter and – as is characteristic of linearized methods – also includes their first energy derivatives to allow for variations around the energy parameter. In some cases, however, the flexibility of the basis is insufficient, and the remaining *linearization error* noticeably affects calculated physical quantities, e.g., equilibrium lattice constants and band gaps. Then, the results may also depend on parameters that are not convergence parameters, such as the MT radii and the energy parameters. To remove the dependence and improve the numerical precision, we analyze in detail how the basis can be extended in a systematic manner by adding local orbitals, defined with either energy parameters at higher energies or second-order energy derivatives. Furthermore, improving the MT part of the basis in this way leads to a faster basis-set convergence so that the resulting basis yields a higher precision than the popular APW+lo method at equal basis-set sizes.

O 21: [MA] Joint Session "Topological Insulators I" (jointly with DS, HL, O, TT)

Time: Monday 17:45–19:15 Location: H 1012

O 21.1 Mon 17:45 H 1012

Atom-specific spin mapping and buried topological states in a homological series of topological insulators — Sergey V. Eremeev[1,2], Gabriel Landolt[3,4], Tatiana V. Menshchikova[1,2], Bartosz Slomski[3,4], Yury M. Koroteev[1,2], Ziya S. Aliev[5], Mahammad B. Babanly[5], •Jürgen Henk[6], Arthur Ernst[6], Luc Patthey[4], Andreas Eich[7], Alexander A. Khajetoorians[7], Julian Hagemeister[7], Oswald Pietzsch[7], Jens Wiebe[7], Roland Wiesendanger[7], Pedro M. Echenique[2], Stepan S. Tsirkin[1,2], Imamaddin R. Amiraslanov[8], J. Hugo Dil[3,4], and Evgueni V. Chulkov[2] — [1]Tomsk State University, Russian Federation — [2]Donostia International Physics Center, San Sebastián, Spain — [3]Universität Zürich, Switzerland — [4]Paul-Scherrer-Institut, Villigen, Switzerland — [5]Baku State University, Azerbaijan — [6]Max-Planck-Institut für Mikrostrukturphysik, Halle, Germany — [7]Universität Hamburg, Germany — [8]Azerbaijan National Academy of Science, Baku, Azerbaijan

By *ab-initio* calculations and spin-resolved photoemission experiments we demonstrate that a homological series of topological insulators—the binary chalcogenides Bi_2Te_3, Bi_2Se_3, and Sb_2Te_3 with the addition of a group IV element—can be tuned in such a way that ideal and isolated Dirac cones are located within the topological transport regime [1]. These compounds exhibit exotic buried topological states strongly protected against surface perturbations and with complex spin textures.

[1] S. V. Eremeev *et al*, Nature Comm. (2011), in press.

O 21.2 Mon 18:00 H 1012

In-plane anisotropy of Fe atoms on $Bi_2Se_3(111)$ — J. Honolka[1], A. A. Khajetoorians[2], V. Sessi[3], T. O. Wehling[4], S. Stepanow[1], J. Mi[5], B. B. Iversen[5], •T. Schlenk[2], J. Wiebe[2], N. Brookes[3], A. I. Lichtenstein[4], P. Hofmann[5], K. Kern[1], and R. Wiesendanger[2] — [1]Max-Planck-Institut für Festkörperforschung, Heisenbergstrasse 1, 70569 Stuttgart, Germany — [2]Institute for Applied Physics, Universität Hamburg, D-20355 Hamburg, Germany — [3]ESRF, Grenoble, France — [4]1. Institut für Theoretische Physik I, Universität Hamburg, D-20355 Hamburg, Germany — [5]Interdisciplinary Nanoscience Center, Aarhus University, Denmark

Topological insulators exhibit a linearly dispersing gapless topological surface state where both the spin and momentum degrees of freedom are locked. The topological nature of this state results in interesting effects such as suppression of back-scattering. Recently, the robustness of these surface states against magnetic order has been investigated intensively. Here, we explore the magnetic properties of single Fe adatoms on the Bi_2Se_3 surface, in the coverage range $< 1\%$, with combined non-local x-ray magnetic circular dichroism techniques and local low temperature scanning tunneling spectroscopy. We show that the Fe adatoms relax into the surface and exhibit a magnetic easy axis within the surface-plane, contrary to recent reports. Futhermore, we show how *ab-initio* approaches can give a reorientation of the easy axis from out-of-plane to in-plane when considering the interplay of Coulomb interactions, spin orbit coupling, and dynamic hybridization effects.

O 21.3 Mon 18:15 H 1012

Ab initio study of Rashba splitting of 2DEG at the surfaces of topological insulators — Sergey V. Eremeev[1,2], •Maia G. Vergniory[3,4], Tatiana V. Menshchikova[2], and Evgueni V. Chulkov[4,5,6] — [1]Institue of Strength and Materials Science, Tomsk, Russia — [2]Tomsk State University, Tomsk, Russia — [3]Max Planck Institute of Microstructure Physics, Halle, Germany — [4]Donostia International Physics Center, Donostia, Spain — [5]Departamento de Fisica de Materiales UPV/EHU, Donostia, Spain — [6]Centro de Fisica de Materiales CFM-MPC and Centro Mixto CSIC-UPV/EHU, Donostia, Spain

The surface of three dimensional topological insulators (TI) holds a metallic surface state (SS) with Dirac dispersion. Recently it has been demonstrated by using Angle Resolved Photoemission Spectroscopy (ARPES) that besides de Dirac cone 2D electron gas (2DEG) arise at the surface of Bi2Se3 and Bi2Te3 after a few hours of exposition in vacuum or upon deposition of atoms. In this work by means of DFT ab initio calculations we present a new interpretation for the driving mechanism of the simultaneous formation and evolution of the parabolic and M-shaped 2D electron gas (2DEG) bands at the surface of Topological Insulators. As it has been probed in previous publications [7,8] it might be due to an expansion of the van der Waals spacing produced by impurities intercalation. We will show the effect of these expansions on the spatial relocalization of the Dirac cone and we will compare our results with some experimental data for different binary and ternary compounds.

O 21.4 Mon 18:30 H 1012

Reactive chemical doping of the Bi_2Se_3 topological insulator — •Hadj Mohamed Benia, Chengtian Lin, Klaus Kern, and Christian R. Ast — Max-Planck-Institut für Festkörperforschung, 70569 Stuttgart, Germany

We studied the evolution of the surface electronic structure of the topological insulator Bi_2Se_3 as a function of water vapor exposure using angle resolved photoemission spectroscopy. We find that a surface reaction with water induces a band bending, which shifts the Dirac point deep into the occupied states and creates quantum well states with a strong Rashba-type splitting. The surface is thus not chemically inert, but the topological state remains protected. The band bending is traced back to Se-abstraction leaving positively charged vacancies at the surface. Due to the presence of water vapor, a similar effect takes place when Bi_2Se_3 crystals are left in vacuum or cleaved in air, which likely explains the aging effect observed in the Bi_2Se_3 band structure.

O 21.5 Mon 18:45 H 1012

Unoccupied electronic states of topological insulators — •Christian Langenkämper[1], Anna Zumbülte[1], Sune N. P. Wissing[1], Anke B. Schmidt[1], Markus Donath[1], Peter Krüger[2], Richard C. Hatch[3], Philip Hofmann[3], Kenta Kuroda[4], Koji Miyamoto[5], and Akio Kimura[4] — [1]Physikalisches Institut, Westfälische Wilhelms-Universität Münster, Germany — [2]Institut für Festkörpertheorie, Westfälische Wilhelms-Universität Münster, Germany — [3]Department of Physics and Astronomy, Aarhus University, Denmark — [4]Graduate School of Science, Hiroshima University, Japan — [5]Hiroshima Synchrotron Radiation Center, Hiroshima University, Japan

We report on the first investigation of the unoccupied electronic states of materials which are currently discussed in the context of topological insulators: $Bi_2Se_3(111)$, Sb(111) and $TlBiSe_2(111)$. First, different preparation methods (sputter-annealing, cleaving with scotch-tape) will be compared with regard to the surface quality of the samples, i.e. crystallographic order and chemical composition. Second, spin-resolved inverse-photoemission data will be presented. The experimental requirements concerning energy and momentum resolution will be addressed. Our first results show predominantly bulk-derived features with only small spin asymmetries. The experimental data will be discussed along with theoretical calculations for the unoccupied states.

O 21.6 Mon 19:00 H 1012

Quantization of conduction and valence band states through adsorption of nonmagnetic impurities on Bi_2Se_3 — •Marco Bianchi[1], Richard Hatch[1], Zakaria Abd El-Fattah[3], Jianli Mi[2], Bo Brummerstedt Iversen[2], and Philip Hofmann[1] — [1]Department of Physics and Astronomy, Interdisciplinary Nanoscience Center, Aarhus University, 8000 Aarhus C, Denmark — [2]Departamento de Física de Materiales CSIC-UPV/EHU-Materials Physics Center, E-20018 Donostia-San Sebastián, Spain —

[3]Center for Materials Crystallography, Department of Chemistry, Interdisciplinary Nanoscience Center, Aarhus University, 8000 Aarhus C, Denmark

Angle-resolved photoemission (ARPES) can give detailed information on the surface electronic structure of materials. Here we present an ARPES study of the adsorption-induced changes in the electronic structure of the topological insulator $Bi_2Se_3(111)$. Exposure to CO results in strong shifts of the features observed by ARPES. The spectral changes can be explained by a simultaneous confinement of the bulk conduction band and valence band states. This is only possible because of the unusual bulk electronic structure of Bi_2Se_3. The valence band quantization leads to spectral features which resemble those of a band gap opening at the Dirac point. Similar effects are observed when Rb is adsorbed on the surface. In this case up to seven quantum well states are found in the valence band, both above and below the Dirac point.

O 22: Invited talk (Martin Sterrer)

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

Invited Talk O 22.1 Tue 9:30 HE 101

Surface science approach to supported metal catalyst preparation - from UHV to metal deposition from solution — •Martin Sterrer — Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, Germany

Oxide-supported metal nanoparticles represent an important class of heterogeneous catalysts. Their catalytic activity depends on various parameters such as nanoparticle size, morphology, or nature of the support. Surface science studies of metal nanoparticles grown on single-crystalline oxide supports contributed substantially to the understanding of the physical and chemical properties of these systems and with the availability of spectroscopic methods that allow for in situ studies at elevated pressure, even reactivity studies under realistic pressure conditions are possible. Maximizing the abundance of active sites for catalysis is the primary goal and is achieved by choosing appropriate preparation conditions. While UHV model systems are typically prepared by physical vapor deposition of the metal onto clean oxide surfaces, in most preparation procedures used for powder catalysts the precursor for the metal nanoparticle is a metal salt dissolved in an aqueous solution and the important adsorption process occurs at the solid-liquid interface. In this contribution, I will present results of our surface science approach to supported metal catalyst preparation utilizing thin single crystalline oxide films as substrates. I will discuss the influence of hydroxyl groups on Au and Pd nucleation and sintering on MgO(001) films and present first results for the deposition of Pd from aqueous $PdCl_2$ solutions on $Fe_3O_4(111)$ films.

O 23: [DS] Focused electron beam induced processing for the fabrication of nanostructures II (focused session, jointly with O – Organizers: Huth, Marbach)

Time: Tuesday 9:30–11:30 Location: H 0111

Invited Talk O 23.1 Tue 9:30 H 0111

Free electrons for building nanodevices — •Ivo Utke — Empa, Swiss Federal Laboratories for Materials Science and Technology, Thun, Switzerland

Finely focused electron beams in scanning electron microscopes are routinely used to visualize small nanometer-sized objects. But add chemistry and they give you materials and structures for exciting physics to do at the nanometer scale! When functional gas molecules (metal-carbonyls, siloxanes, biphenyls, etc.) are injected into an electron microscope chamber held at a pressure of 1e-6 mbar or lower, they form adsorbed layers on many substrates. Focused electron beams can interact with these molecular layers, triggering surface reactions that can be used to locally etch or deposit, or to induce intermolecular reactions between the adsorbed molecules. All of these focused electron beam induced processes (FEBIP) can be performed on almost any kind of substrate [1]. This presentation will cover the fundamentals of FEBIP and give a state of the art overview on exciting nanodevices realized in the fields nanoelectronics, nanomechanics, nanophotonics, and nano(bio)sensors. Special attention will be given to FEBIP with two molecules involved, which led to the development of high performance magnetic sensors [2] having applications in bead detection.

[1] I. Utke, A. Gölzhäuser, Angew. Chem. Int. Ed. 2010, 49, 9328.
[2] L. Bernau et al., Angew. Chem. Int. Ed. 2010, 49, 8880.

Topical Talk O 23.2 Tue 10:00 H 0111

From electronic correlations to strain sensing: Nanongranular metals and their applications — •Christian Schwalb, Marcel Winhold, Fabrizio Porrati, Roland Sachser, and Michael Huth — Physikalisches Institut, Goethe-Universität, Max-von-Laue-Str.1, 60438 Frankfurt am Main

Granular metals are artificial materials that consist of a conducting phase of metallic nanoparticles embedded in a carbon-rich dielectric matrix. The charge transport in such systems is dominated by tunneling between neighboring metallic nanoparticles, a process that is strongly influenced by correlation effects, such as the Coulomb blockade in the limit of weak inter-grain coupling. Additionally the tunneling coupling in these materials has an intrinsically exponential dependence on the inter-grain distance.

In this work, we present a practical application for these fundamental processes. Using focused electron-beam-induced deposition (FEBID) we can create strain-sensing elements based on nanogranular metals. The gauge factor for these sensing elements depends on their conductivity that can be altered by electron-beam irradiation leading to a change in the sensitivity that can be attributed to a persistent change of the dielectric carbon matrix. Due to the high resolution of the FEBID process strain-sensing elements with dimensions below 20 nm are feasible, therefore enabling, e.g., the fabrication of nano-cantilevers for ultra-fast AFM applications.

Topical Talk O 23.3 Tue 10:30 H 0111

Tailored cobalt nanostructures by FEBID — •José M. de Teresa[1,2], Rosa Córdoba[2], Luis Serrano-Ramón[1,2], Amalio Fernández-Pacheco[1,2], and Ricardo Ibarra[1,2] — [1]Instituto de Ciencia de Materiales de Aragón, Universidad de Zaragoza-CSIC, Spain — [2]Laboratorio de Microscopías Avanzadas, Instituto de Nanociencia de Aragón, Universidad de Zaragoza, Spain

Focused-electron-beam-induced-deposition (FEBID) using Co2(CO)8 gas precursor allows the direct writing of cobalt-based magnetic structures [1]. We first grew high-purity cobalt structures with FEBID using high beam currents [2, 3]. The coercive field of these structures can be controlled via the shape anisotropy [4], and single-domain behavior can be observed [5]. Interestingly, the domain-wall propagation field can be lower than the domain-wall nucleation field, with potential magnetic applications [6]. The spin polarization of these cobalt deposits is large enough for its use in Spin Electronics [7]. We have recently achieved the growth of narrow high-cobalt-content nanowires (30 nm) and Hall sensors (100 nm), opening the route for the growth of cobalt structures tailored at the nanoscale [8].

[1] I. Utke et al., J. Vac. Sci. Technol. B 26 (2008) 1197 [2] A. Fernández-Pacheco et al, J.Phys. D: Appl. Phys. 42 (2009) 055005 [3] R. Córdoba et al., Nanoscale Res. Lett. 6 (2011) 592 [4] A. Fernández-Pacheco et al, Nanotechnology 20 (2009) 475704 [5] M. Jafaar et al., Nanoscale Res. Lett. 6 (2011) 407 [6] A. Fernández-Pacheco et al, Appl. Phys. Lett. 94 (2009) 192509 [7] S. Sangiao et al., Solid State Commun. 151 (2011) 37 [8] L. Serrano-Ramón et al., ACSnano 5 (2011) 7781

O 23.4 Tue 11:00 H 0111

Structural, electrical and magnetic properties of CoPt-C al-

loys prepared by focused electron-beam induced deposition — •Fabrizio Porrati[1], Evgenyia Begun[1], Marcel Winhold[1], Roland Sachser[1], Achilleas Frangakis[2], and Michael Huth[1] — [1]Physikalisches Institut, Goethe Universität, Frankfurt am Main — [2]Institut für Biophysik, Goethe Universität, Frankfurt am Main

CoPt-C binary alloys have been fabricated by focused electron beam-induced deposition with the simultaneous use of the $Co_2(CO)_8$ and $(CH_3)_3CH_3C_5H_4Pt$ precursor gases. The alloys are made of CoPt nanoparticles embedded in a carbonaceous matrix. TEM investigations show that as-grown samples are in an amorphous phase. By means of a post-growth low-energy electron irradiation treatment the CoPt nanoparticles transform into face-centred tetragonal $L1_0$ CoPt nanocrystallites. In pararrel, the system undergoes a transition from a superparamagnetic to a ferromagnetic state at room temperature. By variation of the post-growth electron irradiation time the electrical- and magneto-transport properties of the alloy can be continuously tuned.

O 23.5 Tue 11:15 H 0111

Electron Beam Induced Surface Activation of Oxide Surfaces for Nanofabrication — •Florian Vollnhals[1], Tom Woolcot[2], Steffen Seiler[1], Marie-Madeleine Walz[1], Hans-Peter Steinrück[1], Geoff Thornton[2], and Hubertus Marbach[1] — [1]Lehrstuhl für Physikalische Chemie II and Interdisciplinary Center for Molecular Materials (ICMM), Friedrich-Alexander-Universität Erlangen-Nürnberg, Egerlandstr. 3, 91058 Erlangen — [2]London Centre for Nanotechnology and Department of Chemistry, University College London, 17-19 Gordon Street, London WC1H 0AH, UK

The controlled fabrication of structures on the nanoscale is a major challenge in science and engineering. Direct-write techniques like Electron Beam Induced Deposition (EBID) were shown to be suitable tools in this context. Recently, Electron Beam Induced Surface Activation (EBISA) has been introduced as a new focused electron beam technique. In EBISA, a surface, e.g. SiO_2, is irradiated by a focused electron beam, resulting in an activation of the exposed area. The activated area can then react and decompose precursor gases like iron pentacarbonyl, $Fe(CO)_5$. This leads to a primary deposit, which continues to grow autocatalytically as long as $Fe(CO)_5$ is supplied, resulting in pure (>90%at.), crystalline iron nanostructures.[1] We expand the use of this concept by exploring EBISA to produce metallic nanostructures on $TiO_2(110)$ in UHV; atomistic insight into the process is obtained via Scanning Tunneling Microscopy (STM) and chemical insight via Auger Electron Specroscopy (AES). Supported by the DFG (MA4246/1-2).

[1] M.-M. Walz et al., Angew. Chem. Int. Ed. 49 (2010), 4669

O 24: [DS] Organic electronics and photovoltaics: simulations and optics I (jointly with CPP, HL, O)

Time: Tuesday 9:30–11:15 Location: H 2032

O 24.1 Tue 9:30 H 2032

Excited states of terminally dicyanovinyl-substituted oligothiophenes and C_{60}: Frenkel vs. charge-transfer excitons — •Björn Baumeier[1], Denis Andrienko[1], and Michael Rohlfing[2] — [1]Max Planck Institute for Polymer Research, Ackermannweg 10, 55128 Mainz, Germany — [2]Department of Physics, University of Osnabrück, Barbarastr. 7, 49076 Osnabrück, Germany

Excited states of terminally dicyanovinyl-substituted oligothiophenes (DCV*n*T) and C_{60}, a donor-acceptor combination used in state-of-the-art small-molecule-based organic photovoltaic devices, are studied using *ab initio* many-body Green's functions theory within the *GW* approximation and the Bethe-Salpeter equation. Calculations including resonant-antiresonant transition coupling and dynamical screening for DCV*n*T monomers yield excitation energies in excellent agreement with spectroscopic data. More importantly, it is possible with this approach to explicitly treat excited states in model dimers of DCV*n*T and C_{60}. This in particular allows to gain nanoscale insight into the relative energies of local (Frenkel) and charge-transfer excitations, which influence the charge generation in devices.

We will present results for model systems of DCV4T:C_{60} and DCV5T:C_{60} and will analyze the dependence of the relative excitations on, e.g., the arrangement of donor and acceptor molecules in the dimer and the length of the donor, as well as discuss the consequences for performance in organic photovoltaic devices.

O 24.2 Tue 9:45 H 2032

Microscopic simulations of charge transport in disordered organic semiconductors — •Denis Andrienko, Bjoern Baumeier, Falk May, Manuel Schrader, and Victor Ruehle — Max Planck Institute for Polymer Research, Mainz, Germany

Charge carrier dynamics in an organic semiconductor can often be described in terms of charge hopping between localized states. The hopping rates depend on electronic coupling elements, reorganization energies, and driving forces, which vary as a function of position and orientation of the molecules. The exact evaluation of these contributions in a molecular assembly is computationally prohibitive. Various, often semi-empirical, approximations are employed instead. In this work, we review some of these approaches and introduce a software toolkit which implements them.[1] The purpose of the toolkit is to simplify the workflow for charge transport simulations, provide a uniform error-control for the methods, flexible platform for their development, and eventually allow in silico pre-screening of organic semiconductors for specific applications. All implemented methods are illustrated by studying charge transport in amorphous films of tris(8-hydroxyquine)aluminium, a common organic semiconductor.

[1] V. Rühle, A. Lukyanov, F. May, M. Schrader, T. Vehoff, J. Kirkpatrick, B. Baumeier, D. Andrienko, J. Chem. Theory Comput., 7, 3335 (2011)

O 24.3 Tue 10:00 H 2032

Migration of singlet excitons in thin films of oligothiophene molecules — •Jens Ludwig, Susanne Hintschich, Hannah Ziehlke, Karl Leo, and Moritz Riede — Institut für Angewandte Photophysik, Technische Universität Dresden, 01069 Dresden, Germany

In organic materials, such as thin amorphous films of oligothiophenes, localized singlet excitons constitute the primary photoexcitations. Via Förster Resonant Energy Transfer (FRET) they migrate between different molecular sites, represented by an inhomogeneously broadened density of states (DOS).

Dispersive exciton migration in thin films of dicyano-substituted terthiophenes is probed by time resolved spectroscopy using a streak camera and simulated with a Monte-Carlo program based on thermally activated hopping of excitons. The time-resolved spectral relaxation and its temperature dependence, as well as the energy dependent decay curves are consistently described within this picture. Side chains appended to the backbone of the oligothiophenes impact the morphology and average intermolecular distance and hence significantly influence the efficiency of exciton migration. In this presentation, oligothiophene derivates with different side chains are compared regarding their exciton dynamics in thin films. We also consider energy transfer to C_{60} in blend layers with the terthiophene derivatives, leading to a very fast quenching of luminescence from the terthiophene molecules.

O 24.4 Tue 10:15 H 2032

Vibrational Davydov-splittings in oriented organic semiconductor crystals: polarization-dependent measurements versus theoretical calculations — •Tobias Breuer[1], Mali Celik[2], Peter Jakob[3], Ralf Tonner[2], and Gregor Witte[1] — [1]AG Molekulare Festkörperphysik — [2]AG Theoretische Oberflächenchemie — [3]AG Oberflächenphysik, Philipps-Universität Marburg, D-35032 Marburg

Vibrational properties of highly ordered crystalline perfluoropentacene (PFP) films epitaxially grown on KCl(100) and NaF(100) substrates have been studied by means of transmission infrared spectroscopy and density functional theory. The different molecular orientations adopted by PFP on both substrates (standing vs. lying) and their epitaxial ordering [1] enable precise polarization-resolved measurements along individual crystallographic directions and thus allow an unambiguous experimental determination of the polarizations of the IR modes. Computations of the vibrational spectra beyond the single-molecule approximation were employed at the periodic dispersion-corrected density functional level (PBE-D2PBC) and compared to non-periodic calculations (PBE/def2-TZVPP). Thereby, a comparison between experiment and different theoretical models was enabled. A microscopic explanation for the experimentally observed Davydov splitting of some modes and the IR-inactivity of others was derived, based on the mutual coupling of the dynamical dipole moments of the two molecules within the unit cell.

[1] T. Breuer et al., Phys. Rev. B 83, 155428 (2011).

O 24.5 Tue 10:30 H 2032

XPS investigation of charge transfer complexes with strong donor / acceptor molecules: composites and interfaces — •Sebastian Stolz, Eric Mankel, Julia Maibach, Thomas Mayer, and Wolfram Jaegermann — Technische Universität Darmstadt, Materials Science Institute, Surface Science Division, Petersenstraße 32, 64287 Darmstadt, Germany

Organic charge transfer complexes like TTF-TCNQ have raised interest due to their electronic and optical properties being highly sensitive to small variations of the molecular constituents. In this manner, the electrical properties of TTF-TCNQ and its derivates vary significantly, and hence different applications for organic electronic devices are imaginable. Thin film layers of DBTTF-TCNQ were prepared in UHV and inert atmospheres respectively to avoid contamination. Preparation methods used were (1) evaporation of solution grown crystals, (2) drop casting under Ar atmosphere, and (3) co-evaporation of the individual molecules with varying donor / acceptor ratios. Additionally, DBTTF was deposited stepwise onto a clean TCNQ substrate in order to investigate the reaction mechanism. The resulting thin films were analyzed by in-situ photoemission spectroscopy, partially carried out at the U49/2 beamline at Bessy II. The stoichiometric ratio of donor and acceptor molecules was determined and the formation of the CT-complex was confirmed for all samples. In case of a stoichiometric ratio unequal to 1:1, the spectra show a mixture of the CT-complex and neutral excess molecules. Finally, the experimentally determined spectra were compared to DFT-calculations.

O 24.6 Tue 10:45 H 2032

A new differential reflectance spectroscopy method with enhanced sensitivity — •Harald Zaglmayr, Lidong Sun, and Peter Zeppenfeld — Institute of Experimental Physics, Johannes Kepler Univeristät, Linz, Austria

Differential reflectance spectroscopy (DRS), measures the normalized difference of the reflectance of the bare and adsorbate covered surface, respectively. The technique possesses enhanced surface sensitivity and is thus widely used for the in-situ study of organic thin film growth [1,2]. The signal to noise ratio of the obtained spectra, which determines the sensitivity of the method, strongly depends on the stability of the light source. Here, we introduce a new method to overcome the influence of the instability of the light source by normalizing the spectrum of the reflected beam with that of the incident beam, which are measured simultaneously. Our approach shows a drastic improvement of the signal to noise ratio of the DR spectra. The new instrument has been successfully applied to monitor the in-situ growth of alpha-sexithiophene (α-6T) and cobalt-tetramethoxyphenylporphyrin (Co-TMPP) on the Cu(110)-(2x1)O reconstructed surface. The details of the technical realization and the scientific results concerning the organic thin film growth will be reported in this contribution.

[1] R.Forker, T.Fritz; Phys. Chem. Chem. Phys., 2009, 11, 2142-2155

[2] U.Heinemeyer *et al.*; Phys. Rev. Lett., 2001, 104, 257401

O 24.7 Tue 11:00 H 2032

Interface Effects on the Glass Transition in Thin Polystyrene Films studied with High Temperature Single Molecule Fluorescence Microscopy — •Dominik Wöll[1], Bente Flier[2], Moritz Baier[2], Klaus Müllen[3], Stefan Mecking[2], and Andreas Zumbusch[2] — [1]Zukunftskolleg, Universität Konstanz, Germany — [2]Fachbereich Chemie, Universität Konstanz, Germany — [3]Max-Planck-Institut für Polymerforschung Mainz, Germany

The glass transition is a ubiquitous phenomenon in many materials. Despite its high importance and considerable research efforts, a full understanding of this property is still lacking. In thin polymer films, interfaces complicate things as they alter the glass transition in their vicinity. Experimental approaches to study the influence of interfaces on dynamics in polymers are thus very challenging. In our contribution, we present single molecule fluorescence spectroscopy as a new method to investigate such interfacial effects on the glass transition of polymers. We measured the translational diffusion coefficients of single perylene diimide molecules in thin polystyrene films up to temperatures of 150 °C and analyzed their distributions. These distributions and the number of mobile molecules depend strongly on film thickness. They can be modeled with Monte Carlo random walk simulations assuming a reduced glass transition temperature and an increased residence probability of dye molecules at the polymer surface.

O 25: Focussed session: Frontiers of electronic structure theory: Strong correlations from first principles II (jointly with TT)

Time: Tuesday 10:30–13:00 Location: HE 101

Topical Talk O 25.1 Tue 10:30 HE 101

Iron Pnicitdes and Chalchogenides: a New Class of Strongly Correlated Electron Systems. — •Gabriel Kotliar — Rutgers University Piscataway NJ

The discovery of superconductivity in the iron pnictides and chalchogenides took the scientific community by surprise. Since then many tools have been applied to these systems, and many competing physical pictures have been proposed.

In this talk will argue that compounds in this family should be thought as Hund's metals, a new class of strongly correlated materials where the correlations are controlled by the strength of the Hund's rule coupling J rather than by the Hubbard U. While correlations in these materials are strong, their physical properties are strikingly different from that of transition metal oxides.

In support of this picture we will present several LDA+DMFT studies for various observables stressing the role of various spectroscopies such as optical conductivity, photoemission and inelastic neutron scattering.

O 25.2 Tue 11:00 HE 101

Dynamical screening of the large local magnetic moment in Fe-based superconductors — •Alessandro Toschi[1], Ryotaro Arita[2], Philipp Hansmann[1,3], Shiro Sakai[1,3], Giorgio Sangiovanni[1], and Karsten Held[1] — [1]Institute of Solid State Physics, Vienna University of Technology (Austria) — [2]Department of Applied Physics, University of Tokyo (Japan) — [3]Ècole Polytechnique, Palaiseau Cedex (France)

Electronic correlation plays a subtle role in Fe-based superconductors. In fact, due to the presence of several moderately correlated bands close to the Fermi level, one observes the formation of a large local magnetic moment driven by the Hund's exchange interaction, which takes place, however, in a mainly metallic background ("Hund's metal"[1]). This physical scenario, as it is shown by our LDA+DMFT calculations[2,3], provides the key to understand the discrepancies observed between experimental estimates of the magnetic moment in the magnetically ordered phase and those obtained via standard LSDA calculations. The magnitude of the discrepancy observed in different compounds would be hence related to the efficacy of the metallic screening, which is decreasing when going from the 1111 (e.g., LaFeAsO) to the 122 class, and eventually to the 11 materials (e.g., FeTe).

[1] K. Haule and G. Kotliar, New J. Phys. **11**, 025021 (2009).

[2] P. Hansmann, R. Arita, A. Toschi, S. Sakai, G. Sangiovanni, and K. Held, Phys. Rev. Lett. **104**, 197002 (2010).

[3] A. Toschi, R. Arita, P. Hansmann, G. Sangiovanni, and K. Held, *in preparation.*

O 25.3 Tue 11:15 HE 101

Iron under extreme conditions: the impact of electronic correlations — •Leonid Pourovskii — CPHT-Ecole Polytechnique, Palaiseau, France — IFM, Linköping university, Linköping, Sweden

We have applied a fully self-consistent full-potential ab initio dynamical mean-filed theory approach to study the impact of electronic correlations on electronic, elastic, and magnetic properties of iron at both moderate and high pressures and temperatures. Our simulations have established the existence of an electronic topological transition in the hcp phase of iron at pressures of about 30-40 GPa, with new hole pockets appearing in the Fermi surface with decreasing volume and leading to anomalies in the Debye sound velocity, lattice parameters c/a ratio and Mössbauer central shift. These anomalies are indeed observed in our experiments. With our calculations extended to pressures and temperatures expected for the Earth deep core we find that the fcc and hcp phases remain in the Fermi liquid regime, while the bcc phase is an incoherent *bad* metal as evidenced by a significant non-Fermi liquid life-time broadening of low-energy electronic states and a large entropic contribution to the electronic free energy. Our calculations also suggest that all three likely crystal structure of iron and iron-rich alloys in the Earth inner core, the hcp, the face centered cubic (fcc), and the body centered cubic (bcc), have sufficiently high magnetic susceptibility to stabilize the geodynamo. The strongest effect is predicted for the bcc Fe, which at the Earth core conditions is still characterized by a Curie-Weiss behavior of the magnetic susceptibility corresponding to a local magnetic moment 1.5 Bohr magnetons.

O 25.4 Tue 11:30 HE 101

Local Density Approximation for Gutzwiller wavefunctions. A SIESTA implementation and a case study: double-exchange magnetism in bulk iron. — •Giovanni Borghi[1], Michele Fabrizio[2,3], and Erio Tosatti[2,3] — [1]Theory and Simulation of Materials, EPFL, Lausanne, Switzerland — [2]SISSA, Trieste, Italy — [3]ICTP, Trieste, Italy

By means of the constrained-search formulation of Density Functional Theory [1], the Kohn-Sham auxiliary system of non-interacting electrons can be generalized to a system of particles that are coupled through local Hubbard-type interactions, and whose ground-state wavefunction is computed within Gutzwiller Variational Method. The resulting Gutzwiller Density Functional is a natural extension of DFT+U functionals, with an additional set of many body parameters that have to be optimized together with the density. Among these, a band-mass renormalization parameter à la Landau accounts for the reduced mobility of correlated particles and their suppressed kinetic energy. We show how the increased flexibility of the Gutzwiller Density Functional can be exploited to better understand the origin of magnetism in transition metals. A comparison of total energies of the paramagnetic and ferromagnetic phases of iron suggests the double-exchange rather than the Stoner mechanism as an explanation of magnetic ordering in this system [2].

[1] M. Levy, Proc. Natl. Acad. Sci. USA **76**, 6062 (1979); E. Lieb, Int. J. Quantum Chem. **24**, 243 (1983).

[2] GB, M. Fabrizio and E. Tosatti, *in preparation.*

O 25.5 Tue 11:45 HE 101

***T*-matrix approach for electron-magnon interactions in ferromagnetic materials** — •Mathias C.T.D. Müller, Christoph Friedrich, Ersoy Sasioglu, and Stefan Blügel — Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, 52425 Jülich, Germany

Recent ARPES experiments [1,2] indicate that the scattering between electrons and magnons taking place in systems with localized d and f orbitals leads to a pronounced renormalization of the electron band dispersion, creating a *kink* near the Fermi energy very similar to the renormalization due to electron-phonon coupling. In order to describe this renormalization from first principles we use the T-matrix formalism, which describes the correlated motion of an electron-hole pair of opposite spins in terms of ladder diagrams. The multiple scattering gives rise to collective spin excitations [3]. Through emitting and absorption of these magnons, the energy of an electron propagating through a spin-polarized system gets renormalized. Our implementation of the corresponding self-energy correction $\Sigma = -iGT$ is based on the all-electron full-potential linearized augmented-plane-wave (FLAPW) method `FLEUR` [4] combined with Wannier functions [5]. We present first results for elementary ferromagnets.

[1] J. Schäfer *et al.*, Phys. Rev. Lett. **92**, 097205 (2004).

[2] A. Hofmann *et al.*, Phys. Rev. Lett. **102**, 187204 (2009).

[3] E. Şaşıoğlu *et al.*, Phys. Rev. B **81**, 054434 (2010).

[4] www.flapw.de

[5] F. Freimuth *et al.*, Phys. Rev. B **78**, 035120 (2008).

O 25.6 Tue 12:00 HE 101

The magnetism in $\mathrm{LaCoO_3}$ from the perspective of the dynamical mean field theory. — •Vlastimil Křápek and Jan Kuneš — Institute of Physics, Academy of Sciences of the Czech Republic, Cukrovarnická 10, 16253 Praha 6, Czech Republic

Despite numerous studies the character of the high-temperature magnetism in insulating $\mathrm{LaCoO_3}$ is still controversial. Two candidates for the origin of the high-temperature Curie-Weiss response have been considered in literature: the intermediate spin state (IS, S=1) [1] and the high spin state (HS, S=2) [2]. We use the dynamical mean field approximation combined with the local density approximation (LDA+DMFT) to study $\mathrm{LaCoO_3}$. We discuss the meaning of IS and HS states in the presence of change fluctuations due to the covalency Co-O bonds and conclude that HS is the dominant magnetic state for all realistic interaction parameters.

[1] M. A. Korotin *et al.*, Phys. Rev. B **54**, 5309 (1996).

[2] P. M. Raccah and J. B. Goodenough, Phys. Rev. **155**, 932 (1967).

O 25.7 Tue 12:15 HE 101

Pressure driven half-metallic ferromagnetism and magnetic moment collapse in $\mathrm{LaMnO_3}$: a hybrid functional study — •Jiangang He and Cesare Franchini — University of Vienna, Faculty of Physics and Center for Computational Materials Science, A-1090 Vienna, Austria

The application of hydrostatic pressure to the antiferromagnetic and insulating e_g perovskite $\mathrm{LaMnO_3}$ induces an electronic structure transition towards a metallic state at $\approx$ 34 GPa, and a progressive quenching of the underlying Jahn-Teller structural distortions [1,2]. By means of the Heyd, Scuseria, and Ernzerhof (HSE) screened hybrid functional approach we outline the evolution of the structural, electronic, and magnetic properties of $\mathrm{LaMnO_3}$ in the pressure range $0 - 140$ GPa. Beside providing an atomistic understanding of the observed insulator-to-metal transition we predict the formation of a transport half-metal ferromagnetic cubic phase at elevated pressure ($>$ 80 GPa), associated with a high-spin ($S = 2$, 3.7 μ_B) to low-spin ($S = 1$, 1.7 μ_B) magnetic moment collapse, and characterized by a significantly large spin polarization ($I \approx 80 - 90\%$). Our results open up the possibility of realizing colossal magnetoresistance behaviours in a stoichiometric manganite.

References:

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M. Baldini *et al.* Phys. Rev. Lett. **106**, 066402 (2011).

[2] G. Trimarchi and N. Binggeli, Phys. Rev. B **71**, 035101 (2005);
A. Yamasaki *et al.* Phys. Rev. Lett. **96**, 166401 (2006).

O 25.8 Tue 12:30 HE 101

Electronic properties of $\mathrm{RbO_2}$ from DFT+DMFT calculations — •Roman Kovacik and Claude Ederer — School of Physics, Trinity College Dublin, Ireland

Recently, p-electron magnetism has received great attention as alternative option for spintronic applications. The "p-magnetism" is often defect-induced and systematic studies are hampered by poor reproducibility and wide spread in experimental data. It is therefore desirable to study intrinsic p-magnetism in pure bulk materials. We present results of a combined density functional theory + dynamical mean field theory (DFT+DMFT) study for $\mathrm{RbO_2}$, an insulating antiferromagnet where magnetic properties arise from partially filled oxygen p orbitals. For the high-symmetry tetragonal structure, we calculate the Hamiltonian in the basis of maximally localized Wannier functions [1] with antibonding π^* character, which is then solved within DMFT using a continuous-time quantum Monte Carlo solver [2]. We construct a metal-insulator phase diagram as function of temperature and Hubbard interaction parameters U and J. For realistic values of U and J, we find that $\mathrm{RbO_2}$ is a paramagnetic insulator at room temperature. We also find indications for orbital order at low temperatures ($T \approx 30$ K) in agreement with our previous DFT study [3]. Furthermore, we discuss differences between the realistic Hamiltonian and the one based on the semicircle density of states.

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[2] E. Gull, A. J. Millis, *et al.*, Rev. Mod. Phys. 83, 349 (2011).

[3] R. Kováčik and C. Ederer, Phys. Rev. B 80, 140411(R) (2009).

O 25.9 Tue 12:45 HE 101

Crystalline and Magnetic Anisotropy of the 3d Transition-Metal Oxides — •Andreas Schrön[1,3], Claudia Rödl[1,2,3], and Friedhelm Bechstedt[1,3] — [1]Institut für Festkörpertheorie und -optik, Friedrich-Schiller-Universität Jena, Max-Wien-Platz 1, 07743

Jena, Germany — [2]Laboratoire des Solides Irradiés, Ecole Polytechnique, CNRS, CEA-DSM, 91128 Palaiseau, France — [3]ETSF

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 the investigation of the crystalline anisotropy of MnO and NiO, which is solely driven by exchange striction along the unique symmetry axis in the [111] direction, while the magnetic anisotropy may be explained in terms of magnetic dipole interactions. In the TMOs FeO and CoO, however, orbital ordering and spin-orbit interaction play an additional, yet crucial role for both crystalline and magnetic anisotropy. Investigation of the latter materials is a demanding task both experimentally and theoretically.

We present our density-functional theory (DFT) study of the crystalline and magnetic anisotropy of the 3d TMOs. For the proper treatment of exchange and correlation (XC) we apply the generalized gradient approximation (GGA) to DFT within the parametrization of Perdew, Burke, and Ernzerhof (PBE). The on-site Coulomb interaction is corrected with an effective interaction U according to Dudarev's approximation (GGA+U).

O 26: Plasmonics and nanooptics II

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

O 26.1 Tue 10:30 MA 005

Evolutionary optimization of plasmonic nano antennas — •Thorsten Feichtner, Oleg Selig, Markus Kiunke, and Bert Hecht — 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

Various aspects of light-matter interaction can be optimized by means of plasmonic nanoantennas. This includes excited-state lifetime of antenna-based super emitters as well as spectral and directional aspects of the emitted light. So far the design of elementary nano-antennas was inspired by radio-frequency (rf-) technology.

However, at optical frequencies material properties and experimental settings need to be re-considered, so alternative antenna designs can optimize certain aspects of light-matter interaction. In order to find such optimized designs we use a checkerboard-type array of gold cubes. We show that evolutionary optimization can be used to find unexpected antenna geometries that optimize a desired quantity, such as the near-field intensity enhancement, yielding a performance that surpasses that of a conventional rf-based optical antenna design and demonstrate, that this system can be used to achieve more complex functionalities, such as a rotation of the polarization from far field to near field by 90° while maintaining a 1000-fold intensity enhancement. Additionally we identify a new but simple structure combining split ring and dipolar antenna features resulting in enhanced near fields compared to the known dipolar nano antennas.

O 26.2 Tue 10:45 MA 005

Polarizing Beam Splitter - A new approach based on transformation optics — •Jonathan Mueller[1] and Martin Wegener[1,2] — [1]Institut für Angewandte Physik and DFG-Center for Functional Nanostructures (CFN), Karlsruhe Institute of Technology (KIT), 76128 Karlsruhe, Germany — [2]Institut für Nanotechnologie, Karlsruhe Institute of Technology (KIT), 76021 Karlsruhe, Germany

Standard optical elements (*e.g.* lenses, prisms) are mostly designed of piecewise homogeneous and isotropic dielectrics. However, in theory one has far more possibilities to influence electromagnetic waves, namely all the components of the permittivity and permeability tensors. In the past few years, on the one hand, new microfabrication methods allowed for new freedom in controlling the optical parameters using so called artificial metamaterials. On the other hand, the theory of transformation optics has given a somewhat intuitive approach for the design of such structures. In our work, we focus on purely dielectric structures in a non-resonant and therefore non-lossy regime.

A polarizing beam splitter is chosen as the object of study since the use of transformation optics in this case provides some features that may be of interest for applications. Namely, the deviation angle does not vary as a function of tilts or shifts of the structure with respect to the incoming beam. Finite element simulations of a full metamaterial structure have been carried out and a practical method for the fabrication of the device using direct laser writing is proposed.

O 26.3 Tue 11:00 MA 005

Optical Force Stamping Lithography — •Spas Nedev, Alexander S. Urban, Andrey A. Lutich, and Jochen Feldmann — Ludwig-Maximilians-Universität München

Optical lithography techniques are widely used for fabrication of nanoscale devices. The ability to fabricate such structures with arbitrary size and shape is essential for their wide applications in optoelectronics, biological and medical sciences. The conventional far-field lithography is a diffraction limited technique which is not suitable for structures with lateral feature size beyond the diffraction limit. Some far-field lithography techniques can go beyond this limit, but they do not allow arbitrary pattern formation. Scanning near-field optical microscopy techniques can also be used for nanostructure production beyond the diffraction limit. However, they are characterized by low throughput, due to their scanning nature and pose restriction for maximal structure size.

Here we introduce a new optical lithography technique, optical force stamping lithography (OFSL) [1]. This approach employs optical forces on single nanoparticles in multiple focused Gaussian beams produced by a spatial light modulator. The so formed optical stamp provides rapid immobilization of single nanoparticles onto a substrate with positioning accuracy well beyond the diffraction limit. OFSL is not restricted to nanoparticle type or substrate. We believe that these evident advantages of the optical force stamping lithography will make it a standard tool for fabrication on nanodevices.

[1] Nano Lett., 2011, 11 (11), pp 5066-5070

O 26.4 Tue 11:15 MA 005

Electrically connected resonant optical antenna — •Jord C. Prangsma[1], Martin Kamp[2], Johannes Kern[1], Alexander Knapp[1], and Bert Hecht[1] — [1]Experimental Physics 5, University of Würzburg, Germany — [2]Technical Physics, University of Würzburg, Germany

Interaction of quasi-static electric fields and localized plasmon resonances is of interest for various applications such as plasmon-enhanced optoelectronics and photovoltaics, electro-optical switching as well as nonlinear optics. Two-wire optical antennas provide an ideal platform for such applications since the antenna arms may in principle be used as dc electrical leads. However, when attaching electrical leads care must be taken in order to maintain the favourable resonant near-field intensity enhancement afforded by two-wire optical antennas.

Here, we propose a design that allows us to electrically connect two-wire optical antennas with hardly any effect on its bonding-mode resonance. The design provides a perfect spatial overlap between the near-field intensity enhancement region and the quasi-static electric field which is produced by applying a voltage to the connecting leads, essential for a large interaction between both in the gap region. Besides numerical studies of the structures optical response we demonstrate the fabrication of connected optical antennas on glass substrates and characterize their optical properties which are in line with the simulations. The design opens new avenues for realizing electro-plasmonic interfaces for applications in quantum optics and nonlinear optics.

O 26.5 Tue 11:30 MA 005

Fabrication of highly ordered nanostructures by controlling the local near fields of gold nanoparticles — •Frank Hubenthal[1], Sören Maag[1], Abdul Jamali[2], Bernd Witzigmann[2], Thomas Baumert[3], and Frank Träger[1] — [1]Experimental Physics I, Clusters and Nanostructures, Institute of Physics and CINSaT, University of Kassel — [2]Computational Electronics and Photonics and CINSaT, University of Kassel — [3]Experimental Physics III, Femtosecond Spectroscopy and Ultrafast Laser Control, Institute of Physics and CINSaT, University of Kassel

Generation of highly ordered nanostructures with dimensions well below the diffraction limit in a parallel process is a great challenge in modern nanotechnology. One possibility to achieve this goal is irradiation of spherical or triangular gold nanoparticles with laser light and exploit the local near fields, which are strongly influenced by the excitation of surface plasmons. In our experiments spherical and triangular gold nanoparticles supported on fused silica were irradiated with laser light with a pulse duration of 35 fs and a central wavelength of 790 nm. The irradiation causes a strongly localized ablation of the fused silica surface and nanostructures with dimensions well below the diffraction limit are generated. Finally, we present first studies applying two pulses with different polarisation directions, with the aim to generate complex but predetermined nanostructures. In addition, varying the time delay between the two pulses permits to estimate the nanoparticle ablation time, by investigating the generated structures as a function of time delay.

O 26.6 Tue 11:45 MA 005

Quantitative measurement of scattering and absorption cross-sections of individual nano-objects — •Martin Husnik[1], Stefan Linden[2,3], Richard Diehl[4], Jens Niegemann[4], Kurt Busch[4,5], and Martin Wegener[1,3] — [1]Institut für Angewandte Physik and DFG-Center for Functional Nanostructures (CFN), Karlsruhe Institute of Technology (KIT), 76128 Karlsruhe, Germany — [2]Physikalisches Institut, Universität Bonn, 53115 Bonn, Germany — [3]Institut für Nanotechnologie, Karlsruhe Institute of Technology (KIT), 76344 Eggenstein-Leopoldshafen, Germany — [4]Institut für Theoretische Festkörperphysik and DFG-Center for Functional Nanostructures (CFN), Karlsruhe Institute of Technology (KIT), 76128 Karlsruhe, Germany — [5]Institut für Physik, Humboldt-Universität zu Berlin, and Max-Born-Institut, 12489 Berlin, Germany

The physics and applications of nanostructures are a rapidly growing field of research in photonics. Determining the scattering and absorption cross-sections of individual particles quantitatively would significantly increase the understanding of the optical properties of nanoparticles.

Here, we combine a previously developed spatial modulation technique with a polarization-sensitive common-path interferometer. This enables the simultaneous measurement of both the absolute scattering and absorption cross-sections of single particles. Example spectra of individual straight antennas, split-ring resonators, and intermediates will be presented and compared with numerical calculations based on a Discontinuous Galerkin Time-Domain (DGTD) approach.

O 26.7 Tue 12:00 MA 005

Bottom-up Synthesis of Bowtie Nanoantenna Arrays for SERS Imaging and Spectroscopy — •Paul Kühler, Thomas Becker, Enrico Da Como, Theobald Lohmüller, and Jochen Feldmann — FB Physik, Ludwig Maximilian Universität, München

We present a novel high-throughput strategy for the bottom-up synthesis of large arrays of strongly coupled plasmonic nanostructures as reliable substrates for surface enhanced Raman scattering (SERS) imaging and spectroscopy.

We demonstrate the synthesis of billions of bowtie-shaped gold nanoantennas on a single solid substrate by using a refined combination of colloid lithography and plasma processing. With this approach, we are able to precisely control the tip-to-tip distance and the shape of the triangular gold nanoantennas for various particle sizes on a length scale well below 30 nm. We demonstrate the broad applicability of these nanostructures for SERS spectroscopy by confocal Raman imaging of graphene monolayers and substrate supported membranes. In addition to experimental studies, we have done numerical modeling to investigate the influence of shape and interparticle distance of realistic particle geometries on the propagation of SERS enhancement at the nanoantenna junctions.

This approach is a favorable alternative to current state-of-the-art fabrication technology for generating SERS active substrates over a large surface area and with high accuracy.

O 26.8 Tue 12:15 MA 005

Highly doped ZnO films with tailored plasma frequency grown by atomic-layer deposition for three-dimensional infrared metamaterials — •Andreas Frölich[1,2,3] and Martin Wegener[1,2,3] — [1]Institut für Angewandte Physik, Karlsruhe Institute of Technology (KIT), 76128 Karlsruhe, Germany — [2]DFG-Center for Functional Nanostructures (CFN), Karlsruhe Institute of Technology (KIT) — [3]Institut für Nanotechnologie, Karlsruhe Institute of Technology (KIT)

We use atomic-layer deposition to grow ZnO films doped with Al (and Ti) at different concentrations and study their optical spectra. The measured spectra are well described by fits using a Drude free-electron model and the derived plasma frequencies are consistent with the expected amount of doping. The losses (damping) are also quantified.

We demonstrate that control of the doping concentration allows for continuously and controllably tunable plasma frequencies spanning almost an octave from 193 THz to 383 THz. In order to demonstrate the applicability of our approach for three-dimensional designs we have also deposited smooth, conformal coatings on three-dimensional polymer templates made by direct laser writing. Altogether, Al:ZnO appears as an attractive “tunable metal” for three-dimensional infrared metamaterials or transformation-optics architectures.

O 26.9 Tue 12:30 MA 005

Ordered nanostar arrays as reliable substrates for surface enhanced Raman scattering (SERS) — •Lidiya Osinkina, Theobald Lohmüller, Frank Jäckel, and Jochen Feldmann — Photonics and Optoelectronics Group, Department of Physics and CeNS, Ludwig-Maximilians-Universität München, 80799, Munich, Germany

Multispiked metallic nanoparticles, or ”nanostars” - are intriguing substrates for surface enhanced Raman scattering (SERS) spectroscopy due to the strong field enhancements that are emerging on their tips upon excitation with light at their resonance frequency. Exciting optical properties can appear in ordered arrays of SERS active nanoparticles, and arrays of metallic nanostars should therefore have high potential as substrates for sensing and imaging applications.

Here we present a two-step approach to efficiently produce large ordered arrays of gold nanostars by using a combination of block copolymer nanolithography and seeded growth. First, hexagonally ordered arrays of gold nanoparticle seeds are produced on top of a glass substrate. The interparticle distance between the seeds can be changed in a range of 65-100 nm. Second, nanostars, with the average size of 50 nm are grown from these seeds by one-pot synthesis in the aqueous solution. In this work, we will demonstrate that the size of the nanostar and the distances between the particles can be tuned independently, influencing the optical properties and the performance of the SERS active substrates.

O 26.10 Tue 12:45 MA 005

Gold Nanocones for Biosensing Applications — •Christian Schaefer, Andreas Horrer, Katharina Broch, Frank Schreiber, Dieter Kern, and Monika Fleischer — Eberhard Karls Universitaet Tuebingen, Institut fuer Angewandte Physik, Auf der Morgenstelle 10, 72076 Tuebingen

The localized surface plasmons in gold nanostructures give rise to strong and strongly localized near-fields which can for example be used to enhance the Raman signal of molecules by several orders of magnitude. We present the fabrication of a highly efficient Raman signal enhancing surface consisting of gold nanocones with tip radii of 10 nm or less. The properties of the cones will be shown by Raman measurements on samples with arrays of nanocones covered by thin layers of Pentacene. With regard to further application in biosensors, the cones can be integrated in microfluidic channels which opens the opportunity to handle small amounts of solutions. Further steps for the capture of molecules out of solution by dielectrophoresis will be presented.

O 27: Graphene II

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

O 27.1 Tue 10:30 MA 041

How clusters bind to the graphene moiré on Ir(111) - XPS compared to DFT — •Timm Gerber[1], Jan Knudsen[2], Peter J. Feibelman[3], Elin Grånäs[2], Karina Schulte[4], Patrick Stratmann[1], Jesper N. Andersen[2], and Thomas Michely[1] — [1]II. Physikalisches Institut, Universität zu Köln — [2]Division of Synchrotron Radiation Research, Lund University — [3]Sandia National Laboratories, Albuquerque, New Mexico — [4]MAX-lab, Lund University

Our understanding of metal-atom cluster adsorption on graphene on Ir(111) is based on elementary chemical ideas, rehybridization and buckling, supported by density functional theory (DFT) calculations. We have tested the DFT picture by comparing calculated core level spectra to X-ray photoemission spectroscopy (XPS) measurements. For pristine graphene, which forms a gently undulating moiré on Ir(111), DFT predicts a 140 meV modulation of C 1s core level shifts (CLS), consistent with the measured spectrum. With Pt clusters adsorbed, measured Pt 4f CLS of the adsorbed clusters also support the calculations. The modulation of the C 1s spectrum is strengthened with clusters adsorbed, and C-atom ionization potentials under and in the vicinity of the Pt clusters are shifted enough to be experimentally distinguished as a broad shoulder of positive C 1s CLS. Further, DFT calculations imply that sp^2 to sp^3 rehybridization of C-atoms below the Pt cluster induce a 1.1 eV CLS-splitting between Pt and Ir bonded C atoms; this prediction is also consistent with the XPS data.

O 27.2 Tue 10:45 MA 041

The stretching vibration of hydrogen adsorbed on epitaxial graphene — Hyunil Kim, •Thorsten Balgar, and Eckart Hasselbrink — Universität Duisburg-Essen, Fakultät für Chemie, Essen, Germany

The adsorption of hydrogen is one favorable approach for opening a bandgap in the bandstructure of graphene[1]. However, the binding geometry is still a matter of debate. Vibrational spectroscopy is a powerful tool which provides insight into the binding situation of adsorbates. We use IR/Vis sum-frequency generation (SFG) spectroscopy to study the stretching vibration of hydrogen chemically bound to a graphene sheet epitaxially grown on an Ir(111) crystal surface. The assignment of the observed resonances to C-H (C-D) stretching vibrations is discussed in view of the propensity for local cluster formation[2,3].

[1] Balog et al., Nat. Mater. (2010) 9 (4) pp. 315-319
[2] Kim et al., Chem. Phys. Lett. (2011) 508 (1-3) pp. 1-5
[3] Ng et al., J. Phys. Chem. C (2010) 114 (43) pp. 18559-18565

O 27.3 Tue 11:00 MA 041

Phase Coexistence of Clusters and Islands: Europium on Graphene — Daniel F. Förster[1], Tim O. Wehling[2], •Stefan Schumacher[1], Achim Rosch[3], and Thomas Michely[1] — [1]II. Physikalisches Institut, Universität zu Köln, D-50937 Köln — [2]1. Institut für Theoretische Physik, Universität Hamburg, D-20355 Hamburg — [3]Institut für Theoretische Physik, Universität zu Köln, D-50937 Köln

The adsorption and equilibrium surface phases of Eu on graphene on Ir(111) are investigated in the temperature range from 35 K to 400 K and for coverages ranging from a small fraction of a saturated monolayer to the second layer by scanning tunnelling microscopy (STM). Using density functional theory (DFT) including the 4f-shell Coulomb interactions and modelling of the electronic interactions, excellent agreement with the experimental results for the equilibrium adsorbate phase, adsorbate diffusion and work function is obtained. Most remarkable, at 300 K in an intermediate coverage range a phase of uniformly distributed Eu clusters (size 10 - 20 atoms) coexists in two dimensional equilibrium with large Eu-islands in a $(\sqrt{3} \times \sqrt{3})$R30° structure. We argue that the formation of the cluster phase is driven by the interplay of three effects: First, the metallic Eu-Eu binding leads to the local stability of $(\sqrt{3} \times \sqrt{3})$R30° structures. Second, electrons lower their kinetic energy by leaving the Eu clusters, thereby doping graphene. Third, the Coulomb energy penalty associated with the charge transfer from Eu to graphene is strongly reduced for smaller clusters.

O 27.4 Tue 11:15 MA 041

Adsorption of beryllium atoms, dimers and clusters on graphene and in graphite investigated by DFT — •Yves Ferro[1], Alain Allouche[1], and Christian Linsmeier[2] — [1]Laboratoire de Physique des Interactions Ioniques et Moléculaires, Aix-Marseille Université /CNRS - UMR 6633, Campus de Saint Jérôme, Service 252, 13397 Marseille Cedex 20, France — [2]Max-Planck-Institut für Plasmaphysik, EURATOM Association, Boltzmannstrasse 2, 85748 Garching b. München, Germany

We here investigate the interaction of beryllium with graphene and a bilayer of graphite by means of periodic DFT calculations. While non-magnetic, graphene and beryllium dimer can yield to an interacting structure in a magnetic electronic configuration; the magnetization is 1μB in the unit-cell. Another non-magnetic interacting structure has been found, but is not the electronic ground state. In all cases, we found the beryllium atoms and dimers to be more weakly bonded on graphene than in the bilayer, which is supported by the two following findings : (i) a Be atom is physisorbed on graphene while it is chemically bonded in the bilayer with an energy of about 1eV, (ii) the magnetic and non-magnetic beryllium dimers are adsorbed on graphene with energies of about one electron-Volt (1.3eV and 0.8 eV, respectively), while Be2 is bonded into the bilayer with an energy of 2.1eV. We eventually found the stability of Be clusters to increase with the size of the beryllium clusters in the bulk of graphite. We also found a charge transfer to occur from beryllium to graphite.

O 27.5 Tue 11:30 MA 041

Electronic properties of Ni adatoms on graphene — •Mike Gyamfi[1], Thomas Eelbo[1], Marta Waśniowska[1], Tim O. Wehling[2], Stiven Forti[3], Ulrich Starke[3], Alexander I. Lichtenstein[2], Mikhail I. Katsnelson[4], and Roland Wiesendanger[1] — [1]Institute of Applied Physics, University of Hamburg, Hamburg, Germany — [2]1st Institute of Theoretical Physics, University of Hamburg, Hamburg, Germany — [3]Max Planck Institute for Solid State Research, Stuttgart, Germany — [4]Institute for Molecules and Materials, Radboud University of Nijmegen, Nijmegen,The Netherlands

We investigated Ni adatoms adsorbed on epitaxial monolayer graphene grown on the silicon terminated SiC(0001) surface by means of scanning tunneling microscopy (STM) and spectroscopy (STS).

The experiments were performed at 5 K and Ni was evaporated on the sample at 12 K which results in the adsorption of well isolated monomers. STM images with atomic resolution of the graphene lattice reveal all Ni atoms being located on the same adsorption site, i.e. on the center of a carbon hexagon. The electronic structure of the monomers is characterized by pronounced peaks below the Fermi energy which are related to Ni d-states. Due to the interaction with the substrate the electronic configuration of the Ni atoms is predominantly d^{10} and consequently the monomers are nonmagnetic. Furthermore, we observed an orbital selective coupling between the Ni adatoms and the Dirac electrons of graphene. The experimental results are compared to theoretical calculations.

O 27.6 Tue 11:45 MA 041

Role of electron correlations in cobalt adsorption on graphene: A quantum chemical perspective — •Alexander Rudenko and Frerich Keil — Hamburg University of Technology, Chemical Reaction Engineering, Eißendorfer Str. 38, D-21073 Hamburg, Germany

Correct theoretical description of transition metal (TM) complexes represents a challenging task due to the presence of strong electron correlations. Commonly used theoretical concepts, such as DFT or single-determinant (HF-based) approaches are often unreliable even in terms of qualitative description of these systems. In the present work we investigate the adsorption of a single cobalt atom on graphene within the finite cluster approach by means of the complete active space SCF approach (CASSCF), additionally corrected by the second-order perturbation theory. We construct the active space by considering 3d, 4s, and 4p cobalt orbitals as well as two pairs of the most relevant π and π^* surface orbitals. In contrast to standard DFT studies, we find that the Co adatom *physisorbs* on graphene without formation of any chemical bonds. As a result, the spin state of adsorbed Co remains to be the same as for the free cobalt atom, i.e., S=3/2. The ground orbital configuration changes, however, from $3d^74s^2$ to $3d^84s^1$ as Co approaches the surface. These results are in qualitative agreement with the LDA+U and hybrid-functional calculations, which really indicate an important role of the Coulomb repulsion in the bonding and electronic properties of Co on graphene. In addition, we analyze the obtained CASSCF results in terms of a simple model Hamiltonian.

O 27.7 Tue 12:00 MA 041

Visualizing quantum interference nearby individual magnetic impurities on graphene — T. Eelbo[1], M. Gyamfi[1], S. Forti[2], U. Starke[2], •M. Waśniowska[1], and R. Wiesendanger[1] — [1]Institute of Applied Physics, University of Hamburg, Jungiusstr. 11, D-20355Hamburg — [2]Max Planck Institute for Solid State Research, Heisenbergstr. 1, D-70569 Stuttgart, Germany

The presence of impurities or defects on graphene and their influence on the electronic properties of graphene is an important aspect for next generation electronic devices. On the one hand intrinsic defects on graphene have already been widely studied, on the other hand extrinsic defects, such as adatoms are currently under theoretical and experimental study. We report on the local density of states of graphene in the presence of Co adatoms investigated by scanning tunneling microscopy/spectrocopy. The interaction of an individual Co adatom with graphene modifies the electronic structure over a distance of 1 nm around the adatom, leading to a $(\sqrt{3} \times \sqrt{3})$R30° superstructure in the local density of states. The observed features of this wave pattern are consistent with the electronic intervalley scattering predicted to occur at adatoms' sites.

O 27.8 Tue 12:15 MA 041

Adsorption of polar molecules on graphene Ni(111) by substrate sensitive NEXAFS spectroscopy. — •Stefan Böttcher, Martin Weser, Hendrik Vita, Yuriy Dedkov, and Karsten Horn — Fritz-Haber-Institut der Max-Planck-Gesellschaft, 14195 Berlin, Germany

On account of its unusual properties, graphene has attracted an enormous interest. However, the interaction of graphene with metals and other adsorbates is still not well understood, for example the strength of its interaction with different metals. Here we investigate the adsorption of water and ammonia molecules on single layer graphene films grown on Ni(111), a lattice matched system. We use NEXAFS at the substrate carbon 1s and the adsorbate N 1s and O 1s absorption edges, and complement these data by angle resolved valence band photoemission. The data are compared with DFT calculations to assign possible adsorption geometries. The unique possibility to study adsorption-induced NEXAFS features *in the substrate* permits an analysis of the adsorbate-substrate interaction mechanism beyond a simple physisorption model.

O 27.9 Tue 12:30 MA 041

Electronic Structure of a Copper Phthalocyanine Monolayer on Graphene/Ru(0001) — •T Nguyen[1], M Scholz[1], A Schoell[1,2], M Mulazzi[1], D Ehm[3], and F Reinert[1,2] — [1]Experimentelle Physik VII und Wilhelm Conrad Röntgen Research Center for Complex Material Systems (RCCM), Universität Würzburg, D-97074 Würzburg — [2]Gemeinschaftslabor für Nanoanalytik, Karlsruher Institut für Technologie KIT, D-76021 Karlsruhe — [3]Carl Zeiss SMT AG, Rudolf-Eber-Str. 2, 73447 Oberkochen,

We have studied the electronic structure of single layers of copper phthalocyanine (CuPc) on graphene/Ru(0001). The CuPc monolayers were prepared on graphene/Ru(0001) by using organic molecular beam deposition (OMBD). The surface structure of CuPc was characterized by low energy electron diffraction (LEED) and angle-resolved photoemission spectroscopy (ARPES) was used to investigate the electronic structure and the interaction of the molercules with the substrate. We show that there is a strong coupling between the CuPc molecule and the gaphene/Ru(0001) surface. This is reflected by the ARPES data that shows a HOMO peak at a binding energy of 2.1 eV and an additional signal near the Fermi edge at about 0.8 eV. This can be assigned to the former LUMO (F-LUMO) state [1] which is (partly) occupied due to a charge transfer from the graphen/Ru(0001) surface and the CuPc [2].

Reference.

1. Zou, Y., et al., Surface Science, 2006. 600(6): p. 1240-1251.
2. Stadtmuller, B., et al., Physical Review B, 2011. 83(8).

O 27.10 Tue 12:45 MA 041

***Ab initio* and semi-empirical van der Waals study of graphene-boron nitride interaction at a molecular scale** — •Vasile Caciuc, Nicolae Atodiresei, Martin Callsen, and Stefan Blügel — Peter Grünberg Institut & Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, 52425 Jülich, Germany

In the present contribution we report on a theoretical study aimed to investigate the role of the London dispersion effects on the adsorption of a single benzene (C_6H_6), triazine ($C_3N_3H_3$) and borazine ($B_3N_3H_6$) molecule on a freestanding graphene and a single BN sheet. To determine the proper ground-state adsorption geometry, the van der Waals interactions were included in our density functional theory (DFT) calculations by using a semi-empirical [1] and an *ab initio* [2] approach, the latter as implemented in our JuNoLo code [3] recently updated [4] using the scheme proposed by Román-Pérez and Soler [5]. The importance of the non-local *vs.* semi-local correlations on the adsorption energy is also discussed.

[1] S. Grimme, J. Comput. Chem. **27**, 1787 (2006).
[2] M. Dion *et al.*, Phys. Rev. Lett. **92**, 246401 (2004).
[3] P. Lazić *et al.*, Comp. Phys. Commun. **181**, 371 (2010).
[4] M. Callsen, N. Atodiresei, V. Caciuc, and S. Blügel, to be published.
[5] G. Román-Pérez and J. M. Soler, Phys. Rev. Lett. **103**, 096102 (2009).

O 28: Heterogeneous catalysis II

Time: Tuesday 10:30–13:15 Location: MA 042

O 28.1 Tue 10:30 MA 042

Ethylene Oxide Formation over Ag: Investigation of the "electrophilic" Oxygen on Ag(111) — •Sebastian Böcklein[1], Miguel À. Niño[2], Tevfik O. Menteş[2], Andrea Locatelli[2], Sebastian Günther[3], and Joost Wintterlin[1] — [1]Ludwig-Maximilians-Universität München, Germany — [2]Sincrotrone Trieste S.C.p.A., Trieste, Italy — [3]Technische Universität München, Germany

The understanding of the ethylene oxide formation crucially depends on the active oxygen species on the Ag catalyst. We have used x-ray photoelectron spectroscopy (XPS), temperature-programmed desorption and reaction (TPD and TPR), low-energy electron- as well as photo electron emission microscopy (LEEM / XPEEM) and scanning tunneling microscopy (STM) to identify and characterize O species on Ag(111). In addition to the (4×4)O phase (O 1s BE 528.3 eV) assigned to "nucleophilic" oxygen, the "electrophilic" oxygen (most likely the active species for the partial oxidation) was prepared under UHV conditions applying a special treatment using NO_2. The latter phase has previously only been prepared by extremely high O_2 exposures. XPS reveals two species (O 1s BE 530.2 and 530.7 eV). STM and LEED show a $(7\times\sqrt{3})$rect structure, which is connected with a massive change of the surface morphology. STM and TPR experiments show that this phase reacts with ethylene to give ethylene oxide. In situ STM experiments, performed under reaction conditions in the mbar regime, show structures and surface morphology changes that had before been observed in UHV experiments.

O 28.2 Tue 10:45 MA 042

CO adsorbtion and oxidation study on different types of Au clusters on C/W(110) — •Magdalena Bachmann, Norbert Memmel, and Erminald Bertel — Institute of Physical Chemistry, University of Innsbruck, Austria

In the last years gold nanoparticles on oxidic supports have gained great attention due to their catalytic activity for oxidation reactions. Despite 20 years of research, it is not clear if this unexpected behavior originates either from support effects (charge transfer etc.) or from intrinsic properties of the clusters (quantum size effect, number of low coordinated atoms etc.). We introduce two different carburized W(110) substrates for the growth of gold nanoclusters: On R(15x12)C/W(110) regularly spaced nanodot arrays with a cluster size of ≈ 7 atoms are formed, whereas on R(15x3)C/W(110) larger particles of bilayer height are fabricated. The catalytic properties of both systems are studied; CO combustion is chosen as a well-explored test reaction. As TPD measurements clearly indicate, CO is adsorbed on both types of clusters as well as on extended gold islands on the bare W(110) substrate. Although in-situ STM investigations on the influence of oxygen on the clusters suggest dissociation (which is regarded as the most crucial step), TPR experiments do not indicate the formation of CO_2. Probable reasons for these observations are discussed as well as the position of our findings within the field of research.

O 28.3 Tue 11:00 MA 042

Computational screening approach to redox-active metal-organic frameworks — •Jelena Jelic[1], Dmytro Denysenko[2], Dirk Volkmer[2], and Karsten Reuter[1] — [1]Technische Universität München (Germany) — [2]Universität Augsburg (Germany)

Metal-organic frameworks (MOFs) have been suggested for a wide range of applications including gas storage, gas separation and drug delivery. For catalytic applications, MOFs possessing higly accessible, redox active metal centers are particularly interesting. The highly robust and modular MFU-4 structural family offers such sites, with MFU-4l in particular featuring catalytically appealing large pore apertures [1]. We perform large-scale density-functional theory calculations to support the successful postsynthetic metal ion exchange to Co-based MFU-4l [2]. With the compound exhibiting promising reversible gasphase oxidation properties, we computationally screen for other coordinatively unsaturated metal centers or ligands that yield equally redox-active frameworks.

[1] S. Biswas *et al.*, Dalton Trans. 6487 (2009).
[2] D. Denysenko *et al.*, Chem. Commun. (accepted).

O 28.4 Tue 11:15 MA 042

Structure and reactivity of PdAg/Pd(111) surface alloys — •Luis Mancera and Axel Gross — Institute of Theoretical Chemistry, Ulm University, D-89069 Ulm, Germany

Bimetallic surface structures often exhibit catalytic activities and selectivities higher than their pure components. Therefore there is a strong interest in understanding the factors leading to the properties of bimetallic catalysts. Surface alloys often serve as model systems for bimetallic catalysts. Very recently, a study of the structural and catalytic properties of PdAg/Pd(111) upon CO exposure was carried out using a combination of various UHV techniques, i.e. STM, TPD and HREELS [1]. This study showed that the activity of this system is mainly driven by ensemble effects, i.e. by the configuration of Pd adsorption sites. It was also found that the CO bonding strength is significantly reduced upon increasing the Ag concentration. In this contribution, we address the reactivity of bimetallic PdAg/Pd(111) surface alloys based on density functional theory (DFT) calculations. Since changes in the relative metal composition often lead to a nonlinear variation of their catalytic properties, mainly due to the interplay of electronic ligand and geometrical effects, we investigate their dependence on the concentration and configuration of Ag atoms in the surface alloy. Furthermore, we also study trends in the CO adsorption energies as a function of CO coverage.

[1] Y. Ma, T. Diemant, J. Bansmann and R. J. Behm. Phys. Chem. Chem. Phys. **13**, 10741 (2011)

O 28.5 Tue 11:30 MA 042

HR-EELS studies on zinc oxide powder samples — •Sebastian Frey, Martin Kroll, and Ulrich Köhler — Ruhr-Universität, Bochum, Deutschland

High resolution electron energy loss spectroscopy is a useful tool in heterogeneous catalysis as it provides information about vibration states of adsorbates. With this, not only the adsorbed species can be identified, but also their orientation can be determined. In methanol synthesis HR-EELS is successfully applied to doped oxide single crystals [1] while studies on oxide powders, which are more similar to real catalysts, rely on infrared spectroscopy (FTIRS, [2]) due to their low conductivity.

However, with a thoroughly preparation it is possible to sediment a thin powder layer on a gold plate substrate. This avoids the conductivity problem and enables HR-EELS studies also on powders. Results show a distinct signal of Fuchs-Kliewer phonons and their multiples decreasing during adsorption which is comparable to ZnO single crystal samples. Further measurements contain CO, CO2, Methanol and other gases.

[1] Y. Wang et al., Angew. Chem. Int. Ed., 46, 5624-5627 (2007)
[2] H. Noei et al., Appl. Catalysis A, 391, 31-35 (2011)

O 28.6 Tue 11:45 MA 042

MgO on Mo(001) — Growth Study of a Model System for Heterogeneous Catalysis — •Stefanie Stuckenholz, Christin Büchner, Leonid Lichtenstein, Markus Heyde, and Hans-Joachim Freund — Fritz-Haber-Institut der Max-Planck-Gesellschaft, Faradayweg 4-6, 14195 Berlin, Germany

The morphology and electronic structure of oxide surfaces play an important role in surface reactions and thus in heterogeneous catalysis [1]. Insight into reactivity influencing parameters at the atomic level can be gained by incorporating scanning probe techniques.

The main tool we use is a microscope combining frequency modulation dynamic force microscopy (FM-DFM) with scanning tunneling microscopy (STM) [2]. This custom-built instrumentation provides atomically resolved complementary information about the morphology and the electronic properties of local surface sites.

Following previous studies on thin MgO films [3] we want to use our versatile microscope to characterize the change in morphology and the electronic structure of the oxide surface with respect to the transition from a thin film to a bulk-system. In this study we use MgO on Mo(001) as a model system for catalysis. We will present findings which were made during the growth study of the model system.

[1] L. Giordano, *et al.*, Acc. Chem. Res. **44**, 1244 (2011)
[2] M. Heyde, *et al.*, Appl. Phys. Lett. **89**, 263107 (2006)
[3] T. König, *et al.*, J. Am. Chem. Soc. **131**, 17544 (2009)

O 28.7 Tue 12:00 MA 042

ZnO micro- and nanostructures for photocatalytic applications — Ingo Paulowicz, Yogendra Kumar Mishra, Sebastian Wille, and •Rainer Adelung — Institute for Materials Science, Functional Nanomaterials, University of Kiel, Kaiserstr. 2, D-24143 Kiel, Germany

Photocatalysis has demonstrated great potential in degrading organic pollutants and thus is a promising mechanism in environmental and medical cleaning applications.

We present results on ZnO micro- and nanostructures which were produced employing two variants of a novel synthesis route.

ZnO microstructures were synthesized using a batch process, called the Flame Transport Synthesis (FTS, patent pending, DE 10 2010 012 385.4). The resulting powder can be formed into various shapes like tetrapods or core spike particles. Density as well as porosity can be tuned over a wide range by applying a post synthesis sintering step, underlining the possibility for upscaling.

ZnO nanostructures were synthesized using a modification of the FTS, which allows a continuous and ultra-rapid fabrication process, in which ZnO structures are produced from Zn in less than 20 ms.

Both systems were evaluated using a test-dye (methylene blue) and showed high conversion rates, where the nanostructured ZnO samples were about 20 times more efficient than their micro structured counterparts. First experiments with waste water were conducted.

O 28.8 Tue 12:15 MA 042

Oxidation of Platinum Nanoparticles on Gallium Nitride Surfaces: the effect of semiconductor doping on nanoparticle reactivity — •Susanne Schäfer[1], Sonja A. Wyrzgol[2], Michael Hävecker[3], Axel Knop-Gericke[3], Johannes A. Lercher[2], Ian D. Sharp[1,4], and Martin Stutzmann[1,2] — [1]WSI, Technische Universität München, Am Coulombwall 4, 85748 Garching — [2]Catalysis Research Center, Technische Universität München, Garching — [3]Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin — [4]Joint Center for Artificial Photosynthesis, LBNL, Berkeley, USA

Platinum nanoparticles supported on p- and n-type GaN are investigated as novel hybrid systems for the electronic control of catalytic activity. In-situ oxidation and reduction were studied with high pressure XPS. The experiments revealed that the underlying wide bandgap semiconductor has a large influence on the surface properties and reactivity of supported nanoparticles. For as-deposited Pt cuboctahedra supported on n-type GaN, a higher fraction of oxidized surface atoms was observed compared to cuboctahedral particles supported on p-type GaN. Under an oxygen atmosphere, immediate oxidation was recorded for nanoparticles on n-type GaN, whereas little oxidation was found for nanoparticles on p-type GaN. Together, these results indicate that changes of the Pt chemical activity under X-ray irradiation are dependent on the type of GaN doping. The strong nanoparticle-support interaction is consistent with charge transfer of

X-ray photogenerated free carriers at the GaN/Pt interface and suggests that GaN is a promising support material for photocatalysis and catalysis on demand.

O 28.9 Tue 12:30 MA 042

Composition-dependent size and shape changes of Pt-Rh alloy nanoparticles on α-Al_2O_3(0001) during CO oxidation reactions — •Uta Hejral[1], Patrick Müller[1], Olivier Balmes[2], Diego Pontoni[2], and Andreas Stierle[1] — [1]University of Siegen, 57068 Siegen, Germany — [2]European Synchrotron Radiation Facility, 38043 Grenoble, France

Pt-Rh nanoparticles are widely used in chemical industry and in automotive exhaust control where they catalyze the oxidation of CO among other reactions. Major attention has in recent years been paid to the study of alloy nanoparticles with the aim to identify systems that allow to control the catalyst selectivity and to enhance its activity and lifetime [1]. Sintering is regarded as one of the major causes of catalyst deactivation and it is of utmost scientific and economic interest to find ways to prevent it. Here we present concentration-dependent size and shape changes of epitaxial Pt-Rh alloy nanoparticles on α-Al_2O_3(0001) substrates observed in-situ during CO oxidation at near atmospheric pressures. The experiments were performed in a flow-reactor at the high energy beamline ID15A (ESRF, E=78.8 keV) by means of grazing incidence x-ray diffraction, x-ray reflectivity measurements and in-situ mass-spectrometry [2]. During the experiments the O_2 pressure ranged between 0 and 14 mbar while the temperature and CO pressure were kept at 550 K and 20 mbar, respectively. Our results demonstrate that a higher Rh concentration reduces sintering significantly.

[1] J.Y. Park et al., Nano Lett. 8 673 (2008)

[2] R. v. Rijn et al., Rev. Sci. Instr. 81 014101 (2010)

O 28.10 Tue 12:45 MA 042

Concentration dependent oxidation of Pd-Rh alloy nanoparticles on $MgAl_2O_4$(001) — •Patrick Müller[1], Uta Hejral[1], Uta Rütt[2], and Andreas Stierle[1] — [1]University of Siegen, Walter-Flex-Str. 3, 57068 Siegen, Germany — [2]Deutsches Elektronen-Synchroton (DESY), Notkestraße 85, 22607 Hamburg, Germany

Noble metal alloy nanoparticles play an eminent role in heterogeneous catalysis, especially as catalyst in automotive exhaust control (*CO* oxidation, NO_x reduction). Understanding oxidation and reduction behavior of Pd-Rh alloy nanoparticles on the nanoscale is of great importance for improving their functionality [1]. To this end we prepared a combinatorial sample containing five stripes of epitaxial alloy nanoparticles of varying Pd-Rh concentrations on an $MgAl_2O_4$ (001) support.

We present concentration-dependent size and shape changes of epitaxial Pd-Rh alloy nanoparticles as well as bulk oxide formation observed in-situ during oxidation. The experiments were carried out in a high pressure compatible UHV chamber at the high energy materials science beamline P07 at DESY in the temperature range between 570 K and 670 K and at oxygen pressures from UHV up to 0.1mbar. We employed grazing incidence x-ray reciprocal space mapping using a 2D detector and complementary x-ray reflectivity at an energy of 85 keV [2]. Our results demonstrate a strong influence of the nanoparticles composition on the oxidation behavior.

[1] F. Tao, et al., Science Vol. 322, 1164170 (2008)

[2] P. Nolte, et al., Phys. Rev. B 77, 115444 (2008)

O 28.11 Tue 13:00 MA 042

Cu clusters on ZnO: Atomistic Insights into Strong Metal–Support Interaction — •Luis Martinez Suarez[1], Johannes Frenzel[1], Bernd Meyer[2], and Dominik Marx[1] — [1]Ruhr–Universität Bochum, Theoretical Chemistry, Bochum, Germany — [2]Interdisziplinäres Centrum für Molekulare Materialen (ICMM) and ComputerChemieCentrum (CCC), Department Chemie und Pharmazie, Friedrich-Alexander-Universität Erlangen–Nürnberg, Erlangen, Germany

The morphology of nanodispersed Cu on ZnO surfaces, used as a catalyst for the industrial synthesis of methanol, directly depends on the interplay of chemical and physical processes of the environment.[1] In the present study, the underlying complex phase diagram of a ZnO–supported copper cluster exposed to wide ranges of H_2 and O_2 pressures is generated in the first place by *ab initio* thermodynamics. After having identified the relevant mechanisms of surface stabilization and Cu cluster morphology, i. e. hydrogen adsorption, oxygen vacancy formation and the experimentally observed[1] brass formation, insights into the strong metal–support interaction are obtained based on exploring the electronic structure of the catalyst under high temperature and reducing gas phase conditions of the industrial process. Furthermore, the response of the support and metal nanoparticle upon surface chemical reactions are probed by studying such processes with H_2 and CO_2, which are the key reactants.

[1] J.–D. Grunwaldt et al., *J. Catal.*, **194**, (2000) 452

O 29: Metal substrates: Adsorption of organic / bio molecules II

Time: Tuesday 10:30–13:00 Location: MA 043

O 29.1 Tue 10:30 MA 043

Adsorption of Dodecahydro-N-Ethylcarbazole and N-Ethylcarbacole on Pd(111) – An XPS study — •Hans-Jörg Drescher, Stefan Schernich, Karin Gotterbarm, Marek Sobota, Christian Papp, Jörg Libuda, and Hans-Peter Steinrück — Friedrich-Alexander-Universität Erlangen-Nürnberg

Hydrogen is a promising alternative energy carrier for CO_2-free vehicle propulsion. Applications are, however, hampered by serious deficiencies of conventional storage at high pressures and cryogenic temperatures. Recently, a promising concept was put forward making use of "Liquid Organic Hydrogen Carriers", which are regenerable chemical hydrogen storage compounds with high capacity. N-ethylcarbazole (NEC) has been identified as a highly attractive candidate, with hydrogen storage being performed through reversible hydrogenation to dodecahydro-N-ethylcarbazole (H_{12}-NEC), typically over oxide-supported Pt or Pd catalysts. This contribution covers *in-situ* high-resolution XPS studies identifying the main surface species and reaction intermediates on a Pd(111) surface upon adsorption and heating. The thermal stability of the reactants and intermediates gives valuable information on reaction, decomposition and catalyst deactivation mechanisms and provides better understanding of more complex model catalysts like palladium nanoparticles on an alumina substrate. Financial support by the DFG within the Excellence Cluster *Engineering of Advanced Materials*, the DAAD, BMW, Fonds der Chemischen Industrie and the European Union is greatfully acknowledged.

O 29.2 Tue 10:45 MA 043

A three-state single molecular junction — •Yongfeng Wang[1], Nicolas Néel[2], Jörg Kröger[2], Hector Vázquez[3], Mads Brandbyge[3], Bin Wang[4], and Richard Berndt[1] — [1]Institut für Experimentelle und Angewandte Physik, Christian-Albrechts-Universität, D-24098 Kiel, Germany — [2]Institut für Physik, Technische Universität Ilmenau, D-98693 Ilmenau, German — [3]DTU Nanotech - Department of Micro and Nanotechnology, NanoDTU, Technical University of Denmark, DK-2800 Kongens Lyngby, Denmark — [4]Department of Physics and Astronomy, Vanderbilt University Nashville, TN 37235, USA

Single molecule electronics aims at using individual molecules as electronic components for miniaturizing electric circuits. Molecular switches, diodes, and transistor-like devices have been reported. Passing current through molecules inevitably causes heating which may be detrimental for their functionality. Here, Ag-Sn-Phthalocyanine-Ag junctions are shown to exhibit three conductance states. While the junctions are conductive at low bias, their impedance drastically increases above a critical bias. Two-level fluctuations occur at intermediate bias. These characteristics may be used to protect a nanoscale circuit. Further experiments along with calculations reveal that the self-limiting conductance of junctions is due to reversible changes of the junction geometry. Financial support through SFB 677 is acknowledged.

O 29.3 Tue 11:00 MA 043

Nucleation in action: BDA on Cu(001) studied by LEEM — •Daniel Schwarz, Raoul van Gastel, Harold Zandvliet, and Bene Poelsema — Physics of Interfaces and Nanomaterials, MESA+

Institute for Nanotechnology, University of Twente

The growth and structure of 4,4'-biphenyldicarboxylic-acid (BDA) on Cu(001) at temperatures between 300 K and 400 K was studied by LEEM and μ-LEED. BDA is a linear molecule consisting of two phenyl rings with a carboxylic-acid group at opposite ends. During growth on Cu(001) the adsorbed BDA molecules form first a disordered 2D gas phase. Once this phase reaches a sufficiently large density, a crystalline phase nucleates, in which the molecules form a hydrogen-bonded 2D supramolecular network. By a careful analysis of the bright-field image intensity we can measure the density of the 2D gas phase, which is up to 40% of that in the crystalline phase. From the equilibrium densities at different temperatures we can construct the 2D phase diagram and extract the cohesive energy (0.47 eV). During the distinct nucleation period we can observe a fascinating phenomenon: sub-critical nuclei form, grow up to 4000 nm^2 in size and decay with lifetimes of several seconds. These sizes are considerably larger than what is usually seen in epitaxial growth and we explain this observation with the relatively weak intermolecular interactions.

O 29.4 Tue 11:15 MA 043

Growth mode of formic acid on Au(111) surfaces — Christa Elsaesser[1,2], Mirko Müller[1,2], Christian Wagner[1,2], and •Gerhard Pirug[1,2] — [1]Peter Grünberg Institut (PGI-3), Forschungszentrum Jülich GmbH, 52425 Jülich — [2]JARA-Fundamentals of Future Information Technology

The adsorption of formic acid (HCOOH) on a Au(111) surface has already been characterized by vibrational spectroscopy and electron diffraction using HREELS and LEED, respectively. The vibrational signature indicates weak chemical substrate interaction of flat lying chains of H-bonded HCOOH molecules[1] well ordered in a $\begin{pmatrix}1.9 & -0.3\\ 1.7 & 2.7\end{pmatrix}$ surface structure, as shown by LEED. The formation of ß-chains, as identified in crystalline formic acid and proposed from the pg glide mirror plane symmetry in the LEED pattern could be proven by topographical STM images. The rectangular 6.0 x 6.8 Å^2 unit cell, azimuthally rotated by 8.3° with respect to the $[1\bar{1}0]$ substrate direction could be attributed to a line-on-line epitaxial growth mode[2]. This result is generally not expected on a (111)-oriented metal surface. While the intermolecular interaction due to H-bonding within the adsorbed layer results in a bulk-like periodic surface structure, the comparably weak adsorbate substrate interaction leads to its azimuthal alignment.

[1] M. Kazempoor, and G. Pirug, Appl. Phys. A 87, 435-441 (2007)

[2] S. C. B. Mannsfeld, K. Leo, and T. Fritz, Phys. Rev. Lett. 94, 056104 (2005)

O 29.5 Tue 11:30 MA 043

Investigation of Pentacene Submonolayers Adsorbed on Cu(110)-(2×1)O and Cu(110)-c(6×2)O — •Johannes Gall, Mariella Denk, Günther Weidlinger, Daniel Queteschiner, Lidong Sun, Michael Hohage, and Peter Zeppenfeld — Institut für Experimentalphysik, Johannes Kepler Universität Linz, 4040 Linz, Österreich

We have investigated the sub-monolayer adsorption behavior of pentacene molecules on both the Cu(110)-(2×1)O and the Cu(110)-c(6×2)O surface with RDS (reflectance difference spectroscopy), STM/STS (scanning tunneling microscopy and spectroscopy) and LEED (low energy electron diffraction).

In case of the Cu(110)-(2×1)O surface it was found that pentacene sub-monolayers undergo a temperature-dependent phase transition from a (densely packed) condensed phase at low temperatures to a (dilute) 2D-gas phase at higher temperatures. The characteristics of this phase transition could also be well reproduced by Monte Carlo simulations. From the experiments we were able to derive important adsorption parameters, such as the effective lateral molecule-molecule interaction energy, which also agree with the simulation results.

For the Cu(110)-c(6×2)O surface the situation is quite different: pentacene molecules were not observed to condense into densely packed islands at low temperature. Instead, a low-density frozen 2D-gas phase was observed. We attribute this behavior to a repulsive interaction between adsorbed species. Furthermore, we found strong evidence that those species in the 2D-gas phase actually consist of pentacene dimers.

O 29.6 Tue 11:45 MA 043

Density-Functional Theory with Screened van der Waals Interactions for the Modeling of Hybrid Inorganic/Organic Systems — •Victor Gonzalo Ruiz[1], Wei Liu[1], Egbert Zojer[2], Matthias Scheffler[1], and Alexandre Tkatchenko[1] — [1]Fritz-Haber-Institut der MPG — [2]Institute of Solid State Physics, Graz University of Technology

The electronic properties and the function of hybrid inorganic/organic systems (HIOS) are intimately linked to their geometry, with van der Waals (vdW) interactions playing an essential role for the latter. Here we show that the inclusion of the many–body collective response of the substrate electrons inside the inorganic bulk enables us to reliably predict the HIOS geometries and energies. Specifically, dispersion-corrected density-functional theory (the DFT+vdW approach) [*PRL* **102**, 073005 (2009)], is combined with the Lifshitz-Zaremba-Kohn theory [*PRB* **13**, 2270 (1976)] for the non–local Coulomb screening within the bulk. Our method (DFT+vdW$^{\mathrm{surf}}$) includes both image-plane and interface polarization effects. We show that DFT+vdW$^{\mathrm{surf}}$ yields geometries in remarkable agreement (≈ 0.1 Å) with normal incidence x–ray standing wave measurements for the 3,4,9,10–perylene–tetracarboxylic acid dianhydride ($C_{24}H_8O_6$, PTCDA) molecule on Cu(111), Ag(111), and Au(111). Similarly accurate results are obtained for xenon and benzene adsorbed on metal surfaces.

O 29.7 Tue 12:00 MA 043

Assessing Density-Functional Theory with Screened van der Waals Interactions (DFT+vdW$^{\mathrm{surf}}$) for Model Hybrid Inorganic/Organic Systems — •Nicola Ferri, Matthias Scheffler, and Alexandre Tkatchenko — Theory Department, Fritz-Haber-Institut der MPG, Faradayweg 4-6, 14195 Berlin, Germany

Hybrid inorganic/organic systems (HIOS) are widely investigated for usage in a variety of devices, e.g., for opto-electronic applications. The interface geometry plays a crucial role in HIOS, and its correct description is a requisite for predicting electronic properties. Here we study two model HIOS: diindenoperylene (DIP, $C_{32}H_{16}$) and C_{60} on coinage metal surfaces (Cu(111), Ag(111), and Au(111)). These systems are used to test the recently developed PBE+vdW$^{\mathrm{surf}}$ approach, which accurately treats hybridization and long-range Coulomb screening, and includes interface polarization effects [1]. We show that for both systems (DIP and C_{60}), the PBE+vdW$^{\mathrm{surf}}$ approach yields average equilibrium adsorption positions in excellent agreement (about 0.1 Å) with experimental data. In the case of DIP, measurements have been performed using X-ray standing wave technique plus X-ray photoelectron spectroscopy (XSW+XPS) [2]. In the case of C_{60}, STM and LEED results are available [3]. Finally, we assess the role of self-consistency of the vdW energy in the DFT+vdW$^{\mathrm{surf}}$ method, by adding the potential due to vdW energy to the DFT potential.

[1] V. G. Ruiz *et al.*, submitted to Phys. Rev. Lett. (2011).
[2] C. Bürker *et al.*, `http://ftp.esrf.eu/pub/UserReports/43789_A.pdf`.
[3] H.L. Li *et al.*, Phys. Rev. Lett. **103**, 056101 (2009).

O 29.8 Tue 12:15 MA 043

Semi-empirical versus ab-initio non-local correlation effects: Thiophene adsorbed on Cu(111) — •Martin Callsen, 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

The adsorption mechanism of single thiophene (C_4H_4S), 4-thiophene ($C_{16}H_{10}S_4$) and their dimers on the Cu(111) surface has been studied within the framework of density functional theory (DFT). The importance of the long-range dispersion interaction on the molecule-surface adsorption geometry and the corresponding binding energy was investigated by using a first-principles approach [1] implemented in the JuNoLo code [2] which was recently updated with the scheme developed by Román-Pérez and Soler [3,4] as well as semi-empirical methods [5,6]. Interestingly, the physisorption character of the thiophene bonding on Cu(111) suggested by the DFT calculations is changed to weak chemisorption even for the DFT ground-state geometry when a non-local correlation energy functional [1] is used.

[1] M. Dion *et al.*, Phys. Rev. Lett. **92**, 246401 (2004)
[2] P. Lazić *et al.*, Comput. Phys. Commun. **181**, 371 (2010)
[3] G. Román-Pérez, J. M. Soler, Phys. Rev. Lett. **103**, 096102 (2009)
[4] M. Callsen, V. Caciuc, N. Atodiresei, S. Blügel to be published.
[5] S. Grimme, J. Comput. Chem. **27**, 1787 (2006)
[6] S. Grimme *et al.*, J. Chem. Phys. **132**, 154104 (2010)

O 29.9 Tue 12:30 MA 043

Structure and energetics of benzene adsorbed on transition-metal surfaces: Density-functional theory with screened van

der Waals interactions — •Wei Liu, Victor G. Ruiz-López, Guo-xu Zhang, Xinguo Ren, Matthias Scheffler, and Alexandre Tkatchenko — Fritz-Haber-Institut der MPG

The adsorption of benzene on metal surfaces is an important benchmark system for more complex hybrid inorganic/organic interfaces. Here, the recently developed DFT+vdW^{surf} method (density-functional theory including screened van der Waals (vdW) interactions) [1] is used to study the structure and energetics of benzene on transition-metal surfaces (Cu, Ag, Au, Pd, Pt, Rh, and Ir). Benzene adsorbs in a planar configuration at coinage metal surfaces, with almost zero distortion and a flat potential-energy surface. In contrast, benzene is strongly bound to the (111) surface of Pd, Pt, Rh, and Ir, and located at the bridge-30° site. The vdW interactions significantly enhance the binding energy by more than 0.75 eV for all metals. The screening of the vdW energy plays a critical role in coinage metals, shortening the equilibrium distance by 0.2 Å, and lowering the binding energy by 0.25 eV. The validity of our results is confirmed by comparison with calculations using the random-phase approximation including renormalized single excitations (EX+cRPA+rSE scheme [2]), and the experimental data from temperature-programmed desorption and calorimetry measurements.

[1] V. G. Ruiz-López et al., submitted.
[2] X. Ren et al., Phys. Rev. Lett. 106, 153003 (2011).

O 29.10 Tue 12:45 MA 043

DFT Studies on the Adsorption of Alkanethiolates at Coinage Metal Surfaces — •Porntip Seema, Jörg Behler, and Dominik Marx — Lehrstuhl für Theoretische Chemie, Ruhr-Universität Bochum, D-44780 Bochum

A large number of theoretical and experimental studies has been carried out to determine the structures and the properties of sulfur-containing molecules adsorbed on coinage metal surfaces, but still several questions remain open. We present density-functional theory calculations for the adsorption of alkanethiolates ($CH_3(CH_2)_nS$-) adsorbed on Cu(111), Ag(111) and Au(111). Calculations have been performed for a variety of adsorbate coverages, binding sites and surface models. We find that the sulfur-metal interaction is stronger for Cu(111) than for Ag(111) and Au(111), with an increased binding strength at surface defects. Moreover, the experimentally suggested models consisting of $c(4\times2)$ with Au adatoms, $(\sqrt{7}\times\sqrt{7})R19.1^\circ$ and pseudo-(100) for Au(111), Ag(111) and Cu(111), respectively, have been studied.

O 30: Focussed session: Functional molecules at surfaces I

Time: Tuesday 10:30–13:15 Location: A 053

O 30.1 Tue 10:30 A 053

Activation of surface hydroxyl groups by modification of H-terminated Si(111) — •Peter Thissen[1], Tatiana Peixoto[1], Roberto Carlos Longo[1], Wolf Gero Schmidt[2], Kyeongjae Cho[1], and Yves Jean Chabal[1] — [1]Department of Materials Science and Engineering, University of Texas at Dallas, Richardson, USA — [2]Lehrstuhl für Theoretische Physik, Universität Paderborn, Paderborn, Germany

Most approaches to self assembled monolayer grafting on silicon surfaces rely on chemical reactions with hydroxyl groups. To date, such groups have only been prepared on silicon oxide surfaces, leading to poor reactivity with only low number of important organic molecules. For instance, phosphonic acids are attractive because they can in principle attach to surfaces in different (mono-, bi- or tri-dentate) configurations that control their arrangement. However, all attempts to directly graft phosphonic acids on silicon has in the past decades not been possible, requiring a perturbating annealing step at 140° C. Here, we demonstrate, using a model surface prepared by functionalizing atomically flat, hydrogen terminated Si(111) with exactly 1/3 hydroxyl monolayer, that hydroxyl on oxide free silicon is more reactive than on oxides. With this model surface, we demonstrate that a perfectly ordered layer of phosphonic acid molecules can be directly grafted at room temperature, and explain why it can remain completely stable in aqueous environments in contrast to phosphonates grafted on oxides. This work opens new possibilities for surface functionalization needed for sensors, photovoltaic devices and fundamental studies.

Topical Talk O 30.2 Tue 10:45 A 053

Surface-supported molecular assemblies: insight from scanning tunneling microscopy and photoemission experiments — •Meike Stöhr — Zernike Institute for Advanced Materials, University of Groningen, Netherlands

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. The understanding of the interplay of the underlying intermolecular and molecule substrate interactions is highly important since the resulting molecular structures are based upon these two interactions. For the formation of molecular structures with improved stability and conductivity, the concept of on-surface polymerization has been introduced recently.

In my presentation, I will focus - on the basis of perylene derivatives adsorbed on Cu(111) - on surface-supported molecular assemblies based on non-covalent interactions [1]. The assembly structures can be altered through post-annealing of the sample. Thereby, also the intermolecular interactions are varied. Through the combination of experimental and theoretical methods, the electronic and structural properties have been elucidated.

[1] J. Lobo-Checa et al., Science 325 (2009) 300; M. Matena et al., Chem. Eur. J. 16 (2010) 2079.

Topical Talk O 30.3 Tue 11:15 A 053

How metal surfaces control adsorbate functionality: cooperativity, adatoms, and substrate interactions — •Felix Hanke — University of Liverpool, Liverpool, UK

Achieving complete atomic-level control and understanding of functional nanostructures in contact with a metal surface is one of the outstanding challenges in surface science. One of the most interesting issues is the role of the surface in driving the function and assembly of adsorbates and molecular switches. Here I will outline the impact and control of substrate reactivity and adatom incorporation on different molecular systems. These theoretical concepts will be illustrated in detail for two systems using van der Waals density functional theory calculations and STM simulations. First, the assembly of single porphyrins on Cu(110) leads to highly oriented one-dimensional nanostructures despite the complete lack of functionality to direct the self-assembly [1]. The porphyrin macrocycles are coupled by covalent C-Cu-C bonds, which result from the incorporation of adatoms into the structure. The one-dimensional nature of the chains is inherited from the substrate structure. Second, the recent synthesis of graphene nanoribbons (GNR) on the Au(111) surface will be discussed [2]. Again, the substrate plays a fundamental role in catalyzing the coupling reactions from a polyanthracene precursor to the full GNR. Successive couplings start at one end of the precursor and proceed cooperatively through the molecule in a domino-like fashion [3].

[1]J. Am. Chem. Soc. **133** 12031 (2011); ACS Nano **5** 9093 (2011); [2] Nature **466** 470 (2010); [3] J. Am. Chem. Soc. **133** 14884 (2011)

O 30.4 Tue 11:45 A 053

On-surface covalent linking of organic building blocks on a bulk insulator — Markus Kittelmann[1], Philipp Rahe[1], Markus Nimmrich[1], •Robert Lindner[1], André Gourdon[2], and Angelika Kühnle[1] — [1]Institut für Physikalische Chemie, Johannes Gutenberg-Universität Mainz, Germany — [2]CNRS, CEMES, Nanoscience Group, 29 Rue J. Marvig, 31055 Toulouse, France

On-surface synthesis in ultra-high vacuum provides a promising strategy for creating thermally and chemically stable molecular structures at surfaces. Very recently, few pivotal experiments have been presented, demonstrating the potential of this concept on metallic substrates.

However, many of the envisioned applications require non-conductive rather than metallic substrates to prevent electronic coupling and leakage or non-radiative quenching. Thus, it becomes exceedingly important to transfer this technique to bulk insulators.

Here, we demonstrate the covalent linking of organic molecules on a bulk insulator, namely calcite. We deliberately employ the strong electrostatic interaction between the carboxylate groups of halide substituted benzoic acids and the surface calcium cations to reach homolytic cleavage temperatures before molecular desorption. This allows for the formation of aryl radicals and intermolecular coupling. By varying number and position of the halide substitution, we rationally design the resulting structures, revealing straight lines, zigzag structures as well as dimers, providing clear evidence for the covalent linking [1].

[1] Kittelmann, M., et al., ACS Nano 2011, 5 (10), 8420-8425

O 30.5 Tue 12:00 A 053

Redox mediation by immobilised centres in the pores of a SURMOF metal-organic framework — •André Dragässer[1], Osama Shekhah[2], Olexandra Zybaylo[2], Cai Shen[3], Manfred Buck[3], Christof Wöll[2], and Derck Schlettwein[1] — [1]Justus-Liebig-Universität Gießen, Institut für Angewandte Physik, Heinrich-Buff-Ring 16, D-35392 Gießen — [2]Karlsruhe Institute of Technology, Institute of Functional Interfaces, Hermann-von-Helmholtz-Platz 1, D-76344 Eggenstein-Leopoldshafen — [3]University of St Andrews, EaStCHEM School of Chemistry, St Andrews, KY169ST, UK

Functionalizing surfaces by a highly ordered porous layer and loading of its pores with functional molecules appears very attractive. Very flexible frameworks are available in the form of metal-organic frameworks (*MOFs*). These frameworks are highly oriented thermally stable porous powders with a pore size of about 1 - 10 nm useful for gas separation, chromatography, and also for electrical and electronic applications. *MOFs* can be prepared on highly ordered surfaces to yield so-called *SURMOFs*. Their charge transport characteristics and redox properties are of pronounced interest. In this work, a layer of a metal-organic framework (*SURMOF*) was prepared by liquid-phase epitaxy on a self-assembled thiol monolayer on polycrystalline Au. Cyclic voltammetry in contact with a redox-active electrolyte was performed to probe charge transport through such *SURMOF* phases. Charge transport across these insulating membranes could be established by ferrocene as an immobilised redox mediator. Reversibility of the immobilisation and its role in the electrode kinetics is discussed.

O 30.6 Tue 12:15 A 053

STM investigations of functional platform adlayers on Au(111) surfaces — •Sonja Kuhn[1], Frauke Claussen[1], Jiyapa Sripirom[2], Ulrich Jung[1], Jens Kubitschke[3], Sandra Ulrich[3], Albert Schulte[2], Rainer Herges[3], and Olaf Magnussen[1] — [1]Institut für Experimentelle und Angewandte Physik, Christian-Albrechts-Universität zu Kiel, Leibnizstr. 19, 24118 Kiel, Germany — [2]Biochemistry-Electrochemistry Research Unit, Suranaree University of Technology 30000, Thailand — [3]Otto-Diels-Institut für Organische Chemie, Christian-Albrechts-Universität zu Kiel, Otto-Hahn-Platz 4, 24098 Kiel, Germany

For preparation of functionalized molecular adlayers, we have introduced the platform approach, where derivatives of the Triaza- [1,2,3] or Trioxatriangulenium [4] ions are used, which can be functionalized at the central carbon atom to control orientation and spacing of the functionality as well as at side positions to control the steric demand. Here, we present STM studies of these platform adlayers on Au(111) surfaces in air and in electrochemical environment [1,2,4]. These compounds form highly ordered hexagonal structures and thus are important example systems exhibiting a high degree of lateral and vertical order. We will also present in situ STM studies by a novel kind of carbon fiber tips, which exhibit superior electrochemical properties [5].

[1] Baisch et al., J. Am. Chem. Soc. (2009), 131, 442, [2] Kuhn et al., PCCP (2010), 12, 4481, [3] Kubitschke et al., Eur. J. Org. Chem. (2010), 5041, [4] Kuhn et al., Chem. Commun., 2011, 47, 8880-8882, [5] J. Sripirom et al., Carbon, 49, 2011, H. 7, 2402-2412

O 30.7 Tue 12:30 A 053

Disorder-order transition at coverages above one monolayer in 2H-tetraphenylporphyrins on Cu(111) — •Michael Stark, Stefanie Ditze, Martin Drost, Florian Buchner, Hans-Peter Steinrück, and Hubertus Marbach — Lehrstuhl für Physikalische Chemie II and Interdisciplinary Center for Molecular Materials (ICMM), Universität Erlangen-Nürnberg, Egerlandstr. 3, D-91058

The understanding of the adsorption behavior of functional molecules on surfaces is a prerequisite for using them as building blocks in molecular devices. In this study, we investigate the coverage dependent supramolecular arrangement of 2H-tetraphenylporhpyrin (2HTPP) on Cu(111) with scanning tunneling microscopy at room-temperature (RT) in ultra-high vacuum. At low coverage, "slow" diffusion of individual 2HTPP molecules along the close- packed atomic rows of the substrate is observed [1,2]. Up to saturation of the first layer, no supramolecular ordering occurs. However, at higher coverage, the formation of ordered domains is found. This behavior is attributed to a complex interplay of intermolecular and molecule-substrate interactions upon increasing 2HTPP coverage..

This work has been funded by the DFG through Sonderforschungsbereich 583.

[1] F. Buchner et al., Chem. Eur. J., (2011), 17, 10226.

[2] F. Buchner et al., J. Phys. Chem. C ,(2011), DOI: 10.1021-jp206675u..

O 30.8 Tue 12:45 A 053

Lichtinduzierte Knüpfung von kovalenten Bindungen auf Isolatoren — •Robert Lindner, Markus Kittelmann, Philipp Rahe, Christopher Hauke, Markus Nimmrich und Angelika Kühnle — Institut für Physikalische Chemie, Johannes Gutenberg-Universität Mainz, Germany

Die Ausbildung von kovalent gebundenen Netzwerken auf Isolatoren ist ein vielversprechender Schritt auf dem Weg zu molekularer Elektronik. Die Knüpfung von kovalenten Bindungen ermöglicht stabile Netzwerke, deren Eigenschaften und Struktur sich über funktionelle Gruppen gezielt beeinflussen lassen. Thermisch induzierte Bindungsknüpfungen auf Metallen [1] und Isolatoren [2] wurden schon auf eindrucksvolle Weise gezeigt. Um das Wachstum der Lagen und die Vernetzung selektiv voneinander zu trennen, stellen photochemische Reaktionen eine sehr elegante Methode dar.

In diesem Beitrag stellen wir erstmals die Photoreaktion des C_{60}-Fullerens auf einem Isolator vor. C_{60} Monolagen wurden auf einer Calcit (10.4)-Oberfläche durch Laserbelichtung photochemisch zweidimensional vernetzt und mit einem Nicht-Kontakt AFM untersucht. Hierbei wurden, neben Änderungen der Molekülabstände auch Änderungen der C_{60}-Überstruktur beobachtet. Dadurch können umfangreiche Aussagen über die Polymerisation der Fullerene auf der Calcitoberfläche dargelegt werden.

[1] Grill, L., et al., Nature Nanotechnology 2007, 2, 687-691

[2] Kittelmann, M., et al., ACS Nano. 2011, 5 (10), 8420-8425

O 30.9 Tue 13:00 A 053

Molecular orientation of tetracene in ordered and disordered layers on Ag(111) — •Tomoki Sueyoshi[1], Martin Willenbockel[1], Michael Naboka[2], Alexei Nefedov[2], Sergey Soubatch[1], Christof Wöll[2], and Stefan Tautz[1] — [1]Peter Grünberg Institut (PGI-3), JARA, Forschungszentrum Jülich, Germany — [2]Institute of Functional Interfaces, Karlsruhe Institute of Technology (KIT), Germany

Tetracene on Ag(111) forms different structural phases depending on preparation condition. Based on scanning tunneling microscopic/spectroscopic studies, we indicated that variation of the tilt angle of tetracene molecule (and local molecular environment) results in different electronic properties of tetracene layers. This demonstrates how it is important to know the molecular orientation in the layer to understand the electronic structure of molecular layers. Here, we investigates tetracene molecular orientation in ordered and disordered layers on Ag(111) using near edge X-ray absorption fine structure (NEXAFS) spectroscopy. Quantitative analysis of NEXAFS intensity reveals that monolayer alpha-phase consists of flat-lying molecule with a tilt angle of less than 10 degrees whereas complex bi-layer beta-phase includes tilted molecule with an average tilt angle of 36 degrees. At room temperature the monolayer alpha-phase gets disordered and the average tilt angle of tetracene molecules changes to 15 degrees, accordingly. The increase in the tetracene tilt angle suggests that an order-disorder transition of tetracene monolayer is achieved by getting additional degree of freedom for tetracene to move.

O 31: Clean surfaces II

Time: Tuesday 10:30–13:00 Location: A 060

O 31.1 Tue 10:30 A 060

Characterisation of a ceria film on Si(111) with non-contact atomic force microscopy — •Reinhard Olbrich[1], Hans Hermann Piper[1], Marvin Zoellner[2], Thomas Schroeder[2], and Michael Reichling[1] — [1]Universität Osnabrück, Germany — [2]IHP Frankfurt (Oder), Germany

A 180nm thick film of ceria deposited on Si(111) is studied with atomic force microscopy operated in the non-contact mode (NC-AFM) and Kelvin probe force microscopy (KPFM). The thin film is prepared by annealing to different temperatures in an ultra-high vacuum environment. Up to a temperature of 845 K, pyramidal triangular structures are observed. In a temperature range from 515 K to 780 K, 6 to12 nm high spikes appear between the triangle structures. After annealing the film to 930 K and higher temperatures flat terraces and step structures develop on the film surface that are similar to structures observed on CeO_2(111) surfaces of bulk crystals. Annealing temperatures over 1130 K causes a decomposing of the thin film. Sputtering the ceria film and anealing at 1110 K generates the best results whith clear terraces and step structures. The KPFM measurement reveals a positive local charge at step edges and a lower charge on the terraces.

O 31.2 Tue 10:45 A 060

Structural, electronic and optical properties of the two isomers of Si(111)2x1 — •Claudia Violante[1], Adriano Mosca Conte[1], Friedhelm Bechstedt[2], and Olivia Pulci[1] — [1]ETSF, Dept. of Physics University of Rome Tor Vergata — [2]IFTO, Friedrich Schiller Universitaet, Jena, Germany

The Si(111)2x1 surface, which appears on cleaved surfaces at low and room temperature, has been among the most studied semiconductor surfaces ever. Although apparently simple, it shows several intriguing and not completely understood features. The atomic structure of the Si(111)2x1 surface has been known for decades to consist of Pandey chains, that can tilt with two possible directions, generating two almost energetically degenerate structures called isomers: the Si(111)2x1 negative buckling and the Si(111)2x1 positive buckling. Although it is currently believed that for a sample of Si(111)2x1 at room temperature the most stable configuration is the positive buckling structure, it has been recently shown by STS measurements that for highly n-doped Si(111)2x1, at low temperature, both positive and negative isomers may coexist on the surface. A confirmation of this experimental observations could come from the study of optical properties of these two isomers. In this talk we will show and discuss the results of our theoretical simulations for the calculation of structural, electronic and optical properties (RAS spectra) of the two structures, obtained by ab-initio calculations within the most reliable state-of-the-art methods based on density functional theory and many-body perturbative techniques.

O 31.3 Tue 11:00 A 060

Vibrational spectra of reconstructed Si(100) surfaces — •Charles H. Patterson — School of Physics, Trinity College Dublin, Dublin 2, Ireland

We present calculations of vibrational spectra of IR-active modes at the Si(100) (2x1), p(2x2) and c(4x2) surfaces and the (2x1)-H surface. Previous calculations of phonons at these surfaces have not included scattering cross-sections. In contrast to existing hypotheses regarding relative scattering cross-sections for vibrational motions parallel or perpendicular to the surface, we find that the largest scattering cross-sections for the clean surfaces are for motions parallel to the surface. This is because parallel motions of chemically unsaturated dimers are accompanied by large charge transfer between dimer atoms which is relatively weakly screened by the less polarisable bulk semiconductor. Results of calculations are compared to HREELS data for the clean and H-covereved Si(100) surfaces and some suggestions for new experiments are made.

O 31.4 Tue 11:15 A 060

STM measurements on MOVPE-prepared germanium and silicon surfaces — •Johannes Luczak[1], Peter Kleinschmidt[1,4], Sebastian Brückner[1,2], Henning Döscher[1,2], Oliver Supplie[1], Enrique Barrigón[3], and Thomas Hannappel[1,2,4] — [1]Helmholtz-Zentrum Berlin, Institut Solare Brennstoffe und Energiespeichermaterialien, D-14109 Berlin — [2]TU Ilmenau, Institut für Physik, Fachgebiet Photovoltaik, D-98693 — [3]Instituto de Energía Solar, Universidad Politécnica de Madrid, E-28040 Madrid — [4]CiS Forschungsinstitut für Mikrosensorik und Photovoltaik, D-99099 Erfurt

An important requirement to achieve low defect densities in the III-V epilayers deposited on group IV substrates is a suitable substrate surface preparation prior to heteroepitaxy. Generation of double layer steps on Si(100) or Ge(100) is desirable for subsequent anti-phase domain-free heteroepitaxy of III-V semiconductors. A contamination-free MOVPE-to-UHV transfer system allowed us to analyze different surfaces with various UHV based surface-sensitive techniques such as x-ray photo electron spectroscopy (XPS), low energy electron diffraction (LEED), and scanning tunneling microscopy (STM). STM measurements on Si(100) showed the formation of D_A or D_B - double-layer steps on a surface with an intermediate offcut of 2° in [011], depending on the process parameters. STM measurements on Ge(100) showed single-layer steps after homoepitaxial growth on substrates with 0.2° offcut in [011] direction, and double-layer steps after deoxidation on substrates with 6° offcut in [011].

O 31.5 Tue 11:30 A 060

Spectroscopy of single donors at ZnO(0001) surfaces — •Hao Zheng[1], Jörg Kröger[2], and Richard Berndt[1] — [1]Institut für Experimentelle und Angewandte Physik, Christian-Albrechts-Universität zu Kiel, D-24098 Kiel, Germany — [2]Institut für Physik, Technische Universität Ilmenau, D-98693 Ilmenau, Germany

ZnO has been widely investigated as a material for piezo-, micro-, and opto-electronic devices. Although the band-gap of ZnO in the wurtzite structure is as large as 3.4eV, undoped material exhibits n-type conductivity at room temperature. The conductivity has been attributed to native defects such as interstitial Zn, Zn with O vacancies, Zn with substitutional N, and H impurites. Despite its importance for applications the origin of the residual conductance is still controversial. Here, donors near the polar (0001) surface of nominally undoped ZnO were investigated with scanning tunneling microscopy at 5K. Spatially resolved spectroscopy reveals single and double charging. Equidistant peaks in spectra of ionized donors are attributed to polaron excitation. The data are consistent with doping due to Zn interstitials or complexes. Support by the DFG via SFB 855 is acknowledged.

O 31.6 Tue 11:45 A 060

Construction of High-Dimensional Neural Network Potentials for Surfaces: Applications to Copper and Zinc Oxide — •Nongnuch Artrith, Björn Hiller, and Jörg Behler — Lehrstuhl für Theoretische Chemie, Ruhr-Universität Bochum, D-44780 Bochum, Germany

Molecular dynamics simulations of large systems critically depend on the accurate description of the underlying potential energy surface (PES). First-principles methods like DFT can provide very accurate energies and forces, but at high computational costs. Therefore, the development of more efficient potentials is a very active field of research. High-dimensional Neural Networks (NN) trained to first-principles data have been shown to provide accurate PESs for systems containing a single atomic species, while they are several orders of magnitude faster than electronic structure calculations. Now, we have generalized this method to multicomponent systems with arbitrary chemical composition. This is achieved by introducing physically motivated terms to deal with long-range interactions and charge transfer. Here we report the capabilities of the NN method for systems containing a single atomic species as well as for multicomponent systems. We present structural energy differences, vacancy formation energies, and surface energies for different copper and zinc oxide surfaces. The predicted geometries, energies, forces, and atomic charges are in excellent agreement with reference DFT calculations.

O 31.7 Tue 12:00 A 060

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 hybrid inorganic/organic interfaces, ZnO is becoming more and more wide spread as inorganic component. To prevent charging or conductivity problems in surface sensitive characterization techniques such as scanning tunneling microscopy or photoemission spectroscopy, metal supported ultra-thin ZnO films can be used as model systems. By means of PBE density-functional theory (DFT) calculations we investigate to what extend ultra-thin ZnO on the (111) surfaces of Ag, Cu and Pd resembles the properties of bulk ZnO surfaces or if it should be regarded as a distinct nanosystem in its own right [1]. Free standing ZnO mono-layer thin films deviate from the wurtzite structure of the bulk material and adopt a planar, graphite-like geometry, in agreement with previous calculations [2]. By inspecting the stress/strain curve of the freestanding mono-layer the expected commensurability condition for different substrates can be estimated. The PBE calculations reveal that the ZnO/metal interaction is weak and a 8 x 9 reconstruction on Ag (111) is most stable [3]. The results will be analyzed in terms of the underlying electronic structure and the effect of the exchange-correlation functional and the thickness of the ZnO layers will be addressed. [1] C. Freysoldt *et al.*, Phys. Rev. Lett. **99**, 086101 (2007), [2] Z. C. Tu and X. Hu, Phys. Rev. B **74**, 035434 (2006), [3] C. Tusche *et al.*, Phys. Rev. Lett. **99**, 026102 (2007)

O 31.8 Tue 12:15 A 060

Preparation of vicinal Ge(100) surfaces in hydrogen ambient — •Oliver Supplie[1], Sebastian Brückner[1,2], Enrique Barrigón[3], Henning Döscher[1,2], Anja Dobrich[1], Claas Löbbel[1], Johannes Luczak[1], Peter Kleinschmidt[1,4], and Thomas Hannappel[1,2,4] — [1]Helmholtz-Zentrum Berlin, Institut Solare Brennstoffe und Energiespeichermaterialien, D-14109 Berlin — [2]TU Ilmenau, Institut für Physik, Fachgebiet Photovoltaik, D-98693 Ilmenau — [3]Instituto de Energía Solar, Universidad Politécnica de Madrid, E-28040 Madrid — [4]CiS Forschungsinstitut für Mikrosensorik und Photovoltaik, D-99099 Erfurt

Vicinal Ge(100) is the established substrate for III-V nucleation regarding high efficiency opto-electronic devices such as multi-junction solar cells. We studied vicinal Ge(100) surfaces prepared by H_2 annealing in metalorganic vapor phase epitaxy (MOVPE) environment prior to heteroepitaxy. A contamination-free MOVPE-to-UHV transfer system allowed to correlate in situ reflection anisotropy spectroscopy (RAS) and surface science techniques. Annealing in H_2 removed oxides and carbon from the substrates as confirmed by X-ray photoemission spectroscopy. Low energy electron diffraction patterns indicated a (2×1) majority surface reconstruction domain. The presence of coupled Ge-H monohydride was confirmed via Fourier-transform infrared spectroscopy. The RA spectrum of the hydrogen terminated Ge(100) surface featured characteristic differences compared to the RA spectrum of UHV-prepared clean Ge(100) in literature [1].
[1] Rossow et al., JVSTB**18**(2000)2229

O 31.9 Tue 12:30 A 060

Non-polar and semipolar InN surfaces — •abderrezak belabbes, Jürgen Furthmüller, and Friedhelm Bechstedt — Friedrich-Schiller-Universität Jena

Using density-functional-based total-energy calculations and the LDA-1/2 method to compute approximately quasiparticle band structures, we have studied clean relaxed InN surfaces with vanishing or small polarity. More in detail, the c-plane, a-plane, m-plane, and r-plane surfaces have been investigated. In contrast to the polar faces, which allow Fermi level pinning, the projected fundamental bulk gap of about 0.71 eV is free of surface states in the nonpolar cases. Consequently, freshly cleaved InN surfaces cannot lead to a surface accumulation layer. The different electronic structures modify the surface dipole and hence the ionization energy and electron affinity significantly when varying the surface normal from [0001] via [11-22] and [10-10] or [11-20] to [000-1].

O 31.10 Tue 12:45 A 060

Imaging and manipulation of ferroelectric domains by STM and STS — •Maik Christl[1], Stefan Förster[1], Hannes Bayer[1], and Wolf Widdra[1,2] — [1]Institute of Physics, Martin-Luther-Universität Halle-Wittenberg, Halle, Germany — [2]Max Planck Institute of Microstructure Physics, Halle, Germany

Piezoresponse force microscopy (PFM) has emerged as a basic tool for imaging and domain engineering on ferroelectric materials, however the lateral resolution is limited down to several nanometers [1].
Here we present an alternative approach of characterizing ferroelectric domain structures by using the scanning tunneling microscope (STM). Epitaxial $BaTiO_3$ films of various thickness which have been grown under ultra high vacuum conditions on a Pt(100) substrate [2] have been studied by STM and STS at room temperature. DI/dV maps allow to identify the out-of-plane domain structure in the $BaTiO_3$ films as prepared. Upon applying higher STM bias voltages, the ferroelectric polarization can be reversed and domain structures will be written. With STS a clear contrast between positively and negatively poled areas becomes visible. Additionally, downward polarized areas appear higher in the STM topography. The manipulated areas are stable for days. All STM data will be compared with PFM measurements of the same sample.
[1] M. Alexe and A. Gruverman, *Nanoscale Characterisation of Ferroelectric Materials*, Springer, Berlin Heidelberg **2004.**
[2] S. Förster, M. Huth, K.-M. Schindler, and W. Widdra, *J. Chem. Phys. 135*, 104701 **2011.**

O 32: [DS] Organic electronics and photovoltaics: simulations and optics II (jointly with CPP, HL, O)

Time: Tuesday 11:30–13:00 Location: H 2032

O 32.1 Tue 11:30 H 2032

Fast, stable and high-brightness light-emitting electrochemical cells — •Sebastian B. Meier[1,2], Daniel Tordera[3], Henk J. Bolink[3], Wiebke Sarfert[2], and Albrecht Winnacker[1] — [1]University of Erlangen-Nuremberg, Department of Materials Science, Chair VI: Materials for Electronics and Energy Technology, Erlangen, Germany — [2]Siemens AG, Corporate Technology, GTF Organic Electronics, Erlangen, Germany — [3]Instituto de Ciencia Molecular, Universitat de València, Paterna, Spain

Light-emitting electrochemical cells (LECs) are among one of the simplest class of light-emitting devices based on organic semiconducting materials. In its most facile form they just comprise a single solution-processed layer of an ionic transition metal complex (iTMC) sandwiched between two air-stable electrodes, which supports all the three events of charge injection, charge transport and radiative recombination. The ordinary architecture and the possibility to use stable electrode materials is a direct consequence of the ionic nature of the active layer enabling efficient charge injection with concomitant in-situ electrochemical doping resulting in the formation of a light-emitting p-i-n junction. There has been a longstanding issue in iTMC device operation between fast response and high stability when standard constant DC voltage is used, which is due to the dynamic nature of the junction. We will show how to stabilize the dynamic junction to achieve long-living ($>$ 1000 h) high-brightness ($>$ 1200 cd/m^2) iridium(III) iTMC-based LECs possessing simultaneous fast turn-on times ($<$ 20s) at considerable light intensity ($>$ 200 cd/m^2).

O 32.2 Tue 11:45 H 2032

Charge Carrier Storage on Emitter Molecules in Organic Light-Emitting Diodes — •Caroline Weichsel[1], Sebastian Reineke[1,2], Björn Lüssem[1], and Karl Leo[1] — [1]Institut für Angewandte Photophysik, Technische Universität Dresden, George-Bähr-Str. 1, D-01069 Dresden, Germany — [2]Massachusetts Institute of Technology, 77 Massachusetts Avenue, Cambridge, MA 02139, USA

In this contribution, we study trapping of charge carriers in phosphorescent organic light-emitting diodes (OLED) using the red emitter iridium(III)bis(2-methyldibenzo[f,h]quinoxaline) (acetylacetonate) [Ir(MDQ)2(acac)] by transient electroluminescence. We observe a transient overshoot exceeding regular light emission after voltage turn-off, which can be explained by delayed charge carrier recombination of charges stored in the emission layer. We study this mechanism by variation of the off-voltage and by adding thin quenching layers, which allow to determine the position of the emission zone during regular light emission and after voltage turn-off. Additionally, we show that the signal intensity is linearly proportional to the doping concentration. Investigations on the applied current and the pulse length show a saturation of the overshoot intensity, which we ascribe to the limited ability of emitter molecules to store electrons. We propose that this storage process negatively affects the external quantum efficiency of the OLED. We assume that the effect can also take place in other OLED structures and suggest that the methods presented here can help identifying charge carrier storage on emitter molecules.

O 32.3 Tue 12:00 H 2032

Surface Modification Effect on Optical Anisotropy and Molecular Orientation of CuPc Thin Films — •L. Ding, M. Friedrich, O. Gordan, and D. R. T. Zahn — Semiconductor Physics, Chemnitz University of Technology, D-09107 Chemnitz, Germany

Copper phthalocyanine (CuPc), as an organic semiconductor, attracts much attention currently due to its potential application in organic electronic and photovoltaic devices. Molecular orientation plays a significant role to improve the device performance. In situ spectroscopic ellipsometry (SE) and reflection anisotropy spectroscopy (RAS) are employed simultaneously to investigate the out-of-plane and in-plane anisotropy as well as molecular orientation of CuPc thin films, respectively.

Chemically prepared octadecyltrichlorosilane (OTS) monolayer with upright standing molecules shows a significant influence on the out-of-plane anisotropy with an average out-of-plane tilt angle of 69.3° +/- 4.1° but little impact on the in-plane anisotropy. Nearly flat lying CuPc molecules are observed on thermally evaporated Perylene-3,4,9,10-tetracarboxylic-3,4,9,10-dianhydride (PTCDA) layers thicker than 3.4 nm, giving an average tilt angle of 19.7° +/- 8.0° due to the flat lying PTCDA molecules on Si. Meanwhile, the in-plane anisotropy of CuPc is much lower than that without PTCDA. The influence of the PTCDA layer thickness on molecular orientation can be explained by the island growth mode of PTCDA.

O 32.4 Tue 12:15 H 2032

Stability of perfluroro-pentacene thin films on coinage metals — •Christian Schmidt[1], Tobias Breuer[1], Stefan Wippermann[2], Wolf Gero Schmidt[2], and Gregor Witte[1] — [1]Molekulare Festkörperphysik, Philipps-Universität Marburg, Germany — [2]Theoretische Physik, Universität Paderborn, Germany

The development of organic electronics greatly benefits from the systematic improvement of molecular properties by chemical functionalization. One example constitutes pentacene that can be prevented from oxidization by perfluorination. Topical investigations of the interface properties of perfluoropentacene (PFP) are frequently conducted only from an electronic point of view, measuring either macroscopic device properties or valence band spectra. In these studies possible chemical interactions have not been addressed since PFP is especially designed to be more stable than PEN. It was therefore unexpected that PFP monolayers on Cu(111) undergo degradation upon heating and that decomposition also occurs on Ag(111). This means that PFP is less stable than PEN, which desorbs intact from Ag(111). This behaviour is especially remarkable when considering that PFP is farther above metal surfaces than PEN. This unclear situation is very problematic, as the PFP-metal interface itself serves as a model system for electronic effects and is of vital interest in this field. Therefore, we systematically studied the thermal behaviour of PFP on the coinage metals by means of temperature NEXAFS and XPS. In order to understand underlying mechanisms we accompany our experimental data with density functional theory (DFT) calculations including chemical reactions.

O 32.5 Tue 12:30 H 2032

Two dimensional band structure mapping of organic single crystals using the new generation electron energy analyzer ARTOF — •A. Vollmer[1], R. Ovsyannikov[1], M. Gorgoi[1], S. Krause[1], M. Oehzelt[1], N. Martensson[2], S. Svensson[2], P. Karlsson[3], M. Lundquist[3], J. Pflaum[4], T. Schmeiler[4], and N. Koch[1,5] — [1]Helmholtz Zentrum Berlin für Materialien und Energie GmbH, Berlin, Germany — [2]Uppsala University, Uppsala, Sweden — [3]VG Scienta, Uppsala, Sweden — [4]Universität Würzburg, Würzburg, Germany — [5]Humboldt-Universität zu Berlin, Berlin, Germany

We report on a novel type of photoemission instrument, the Angle Resolved Time Of Flight analyzer (ARTOF 10k)electron energy analyser. The instrument facilitates the simultaneous recording of kinetic energy and angular pattern of photoelectrons in a cone of up to 30° opening angle with very high energy resolution (100 μeV). Its transmission (250 times higher than in hemispherical analysers)allows for very mild conditions during the experiment turning the ARTOF into the predestined instrument to investigate sensitive specimens such as organic single crystals, as extremely low photon fluxes can be used. Even though organic single crystals are of increasing fundamental and applied scientific interest, knowledge of their electronic properties is still mainly based on theoretical calculations due to major experimental challenges in measuring photoemission. Here we present the band structures of rubrene and tetracene single crystals obtained with unprecedented quality using the ARTOF instrument within only a few hours of measurement time.

O 32.6 Tue 12:45 H 2032

Electronic structure of prototypical organic-organic heterojunctions for photovoltaic applications — •Andreas Wilke[1], Raphael Schlesinger[1], Ullrich Hörmann[2], Jens Niederhausen[1], Johannes Frisch[1], Antje Vollmer[3], Julia Wagner[2], Mark Gruber[2], Andreas Opitz[1], Wolfgang Brütting[2], and Norbert Koch[1,3] — [1]Humboldt-Universität zu Berlin — [2]Universität Augsburg — [3]Helmholtz-Zentrum Berlin für Materialien und Energie GmbH

In organic photovoltaic cells (OPVCs) typically two organic materials with electron acceptor and donor character are sandwiched between anode and cathode, forming either layered planar (PHJ) or bulk heterojunctions, where charge separation occurs. We report ultraviolet photoelectron spectroscopy (UPS) measurements done for three different organic-organic PHJs, comprising the donors sexithiophene (6T) and poly(3-hexylthiophene) (P3HT), and the acceptors diindenoperylene (DIP) and C60. The respective heterojunctions were formed on poly(ethylenedioxythiophene) : poly(styrenessulfonate) (PEDT:PSS) electrodes. The energy level alignment found experimentally for these heterojunctions are discussed in relationship to the open circuit voltages achieved in corresponding PHJ OPVCs. The offset between the highest occupied molecular orbital of the donor and the lowest unoccupied molecular orbital of the acceptor, an estimate for the maximum achievable open circuit voltage, peaked at 1.75 eV for the 6T/DIP PHJ. In actual OPVCs based on 6T/DIP, an open circuit voltage of up to 1.38 V was observed.

O 33: Gaede Prize talk (Mato Knez)

Time: Tuesday 13:30–14:00 Location: HE 101

Prize Talk O 33.1 Tue 13:30 HE 101

Material Design by Atomic Layer Deposition — •Mato Knez — Max Planck Institute MSP, Halle, Germany — CIC nanoGUNE Consolider, San Sebastian, Spain

Atomic layer deposition (ALD) is a thin film deposition technique which was developed in the 1970s. In contrast to chemical vapor deposition (CVD), ALD incorporates the separation of the chemical reaction into two half-reactions with a growth control in a cycle by cycle manner, allowing good coating conformality even on structures with high aspect ratios. A combination of diffusion effects and ALD coating can largely extend the variation parameters of the materials design. For example, using the deposited films as platform for further chemical or physical manipulation by means of interfacial diffusion or as sacrificial spacers enables the synthesis of nanovoids or nanoparticle assemblies in a very elegant way. A further side-effect of the ALD process was investigated in more detail: If polymers are used as substrates, the highly reactive precursors can diffuse into the bulk of the polymer and chemically interact with it. As a result, physical properties of the substrates in many cases significantly alter during the process. Our focus is primarily on the mechanical properties of (bio)polymers which in many cases are most seriously changed. In summary, ALD is a method-of-choice for many applications in materials design and functionalization. Instead of being just an instrument for coating, it opens possibilities for research and development in various fields. Especially the infiltration of metals into soft materials shows a distinct, but important difference between ALD and CVD and thus its uniqueness.

O 34: Poster Session I (Graphene; Plasmonics and nanooptics; Coherence and coherent control in nanophotonics and plasmonics)

Time: Tuesday 18:15–21:45 Location: Poster E

O 34.1 Tue 18:15 Poster E

Oxidation of monovacancies in graphene by oxygen molecules — •Udo Schwingenschlögl, Thaneshwor Kaloni, and Yingchun Cheng — KAUST, PSE Division, 23955-6900 Thuwal, Kingdom of Saudi Arabia

We study the local magnetic moments develop at monovacancies in graphene due to the presence of dangling carbon bonds. These moments remain intact when an oxygen molecule is adsorbed such that the dangling bonds are not fully saturated. We obtain values of 1.35 and 1.86 μ_B for the magnetic moments of monovacancies and oxidized monovacancies, respectively. A transition from semimetallic to semiconducting behavior appears if at least one C–O–C bridge is present, whereas the formation of C=O groups makes the system metallic. Our results explain the experimentally observed behavior of graphene under exposure to an oxygen plasma.

Reference: J. Mater. Chem. **21**, 18284 (2011).

O 34.2 Tue 18:15 Poster E

Growth of epitaxial graphene on Rh(111) — •Karin Gotterbarm, Christian Papp, Oliver Höfert, Wei Zhao, and Hans-Peter Steinrück — Lehrstuhl für Physikalische Chemie II, Universität Erlangen-Nürnberg, Egerlandstr. 3, 91058 Erlangen

Epitaxial graphene was grown on a Rh(111) single crystal surface by chemical vapor deposition of propylene at elevated temperatures. The growth process was observed by fast XPS performed at the synchrotron facility BESSY II. The quality of the produced graphene sheets was checked by LEED. Different preparation parameters such as propylene pressure and preparation temperature were varied in order to investigate the influence of these parameters on corrugation and regularity of the produced graphene sheet. Additionally we explored the thermal stability of the produced graphene layers as well as the possibility to oxidise these layers. 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.* The binding energy separation of the two species becomes more distinct at lower temperatures and varies depending on the preparation parameters mentioned above.

Support is acknowledged from the BMBF (05 ES3XBA/5) and the Cluster of Excellence "Engineering of Advanced Materials".

* A. B. Preobrajenski, May Ling Ng, A. S. Vinogradov, N. Mårtensson, Phys. Rev. B 78, 2008, 073401.

O 34.3 Tue 18:15 Poster E

Investigation of excitonic Fano resonances in graphene using optical spectroscopy — •Patrick Herlinger[1,2], Daniela Ullrich[1,2], Dong-Hun Chae[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 optical absorbance spectrum shows an asymmetric peak of about 10% at around 4.7 eV. We introduced a Fano model which is in excellent agreement with our experimental data. Our model includes an excitonic state beneath the saddle point M of the band structure [1]. We study the influence of the environment on the excitonic Fano resonance. We compare the optical response of free-standing and supported graphene and investigate the dependence on the ambient conditions.

[1] Chae et al., Nano Lett. 11, 1379 (2011)

O 34.4 Tue 18:15 Poster E

Graphene on mica: corrugation of monolayer and stacking faults within few-layer graphene studied by scanning tunneling microscopy (STM) — •Silke Hattendorf, Alexander Georgi, Viktor Geringer, Marcus Liebmann, and Markus Morgenstern — II. Institute of Physics B and JARA-FIT, RWTH-Aachen

Graphene flakes were prepared on freshly cleaved mica by exfoliation. The topography of mono- and few-layer flakes was studied down to atomic resolution revealing an overall roughness of (61 ± 13) pm on the monolayer, which is a bit more than measured recently with atomic force microscopy (24,1 pm) [2] but flat compared to graphene on silicon dioxide (320 pm) [1]. The corrugations are analyzed in respect to height and correlation length. The latter is determined by analyzing the auto correlation functions. The results are compared to those on silicon dioxide [1] and earlier measurements on a few-layer flake on mica.

On few-layer graphene on mica a large triangular network of partial dislocations separating differently stacked graphene areas was studied. Such networks have been observed before on HOPG [3,4]. Due to differences in the electronic structure of hexagonal and rhombohedral graphite, the differently stacked areas appear to be separated by edges of 1-4 Å height. This apparent height depends on the bias voltage. This dependency is studied by scanning tunneling spectroscopy (STS).

[1] V. Geringer et. al., Phys. Rev. Lett.102, 76102 (2009).

[2] C. Lui et. al., Nature 462, 339 (2009).

[3] S. Amelinckx and P. Delavignette, J. Appl. Phys. 31, 2126 (1960).

[4] S. Snyder et. al., Phys. Rev. B 47, 10823 (1993).

O 34.5 Tue 18:15 Poster E

An electron lens out of strained graphene — Lukas Gerhard[1], Eric Moyen[2], •Timofey Balashov[1], Igor Ozerov[2], Marc Portail[3], Houda Sahaf[2], Laurence Masson[2], Wulf Wulfhekel[1], and Margrit Hanbücken[2] — [1]Physikalisches Institut, Karlsruhe Institute of Technology, Germany — [2]CINaM-CNRS, Aix-Marseille University, Marseille, France — [3]CRHEA-CNRS, Valbonne, France

An epitaxial layer of graphene was grown on a 6H-SiC(0001) crystal, prepatterned with hexagonal nano-holes. The graphene layer covers the surface smoothly, without dislocations or grain boundaries. The necessary elastic deformation of graphene leads to a strain-induced modification of electron group velocity in the graphene layer, and to an increased time-of-flight across the nano-hole. We propose to use this effect to focus two-dimensional electrons in analogy with simple optical lenses.

O 34.6 Tue 18:15 Poster E

Local transport measurements in graphene and graphene nanostructures — •Frederik Edler, Jens Baringhaus, Thomas Langer, Herbert Pfnür, and Christoph Tegenkamp — Institut für Festkörperphysik, Leibniz Universität Hannover, Abteilung Atomare und Molekulare Strukturen, Appelstrasse 2, 30167 Hannover, Germany

Graphene exhibits interesting transport signatures. The non-vanishing conductivity in neutral graphene was believed to be a signature of a ballistic system. However, diffusive transport theory including long range ordered defects reveal similar conductance values. Therefore, the control of the structure is important in order to interpret transport data, affected by in impurities, defects, or finite size effects, correctly. We have studied the morphology and the resistivity of graphene and graphene nanostructures by means of a 4-tip STM SEM system.

Due to inhomogeneous growth and the residual influence of substrate, the sheet resistance for monolayer graphene, grown on SiC(0001) and SiC(000$\bar{1}$) substrates, was around 40-50 kΩ/□. After further graphitization it decreased to 8 kΩ/□. Graphene bilayers on SiC(000$\bar{1}$) reveal values close to those reported for exfoliated graphene. Besides 2d graphene, uniaxial graphene nanoribbon structures (width ≈ 100 nm), grown by using appropriate SiC-MESA structures, have been studied. The resistances measured on them were found to be significantly lower and are almost independent on the contact separation, as expected for graphene ribbons with robust edge channels.

O 34.7 Tue 18:15 Poster E

Production of Nitrogen-Doped Graphene via Low Energy Nitrogen Bombardment — •Wei Zhao[1], Olive Höfert[1], Karin Gotterbarm[1], Junfa Zhu[2], Christian Papp[1], and Hans-Peter Steinrück[1] — [1]Lehrstuhl für Physikalische Chemie II, Universität Erlangen-Nürnberg, Egerlandstr. 3, 91058 Erlangen — [2]National Synchrotron Radiation Laboratory, UniVersity of Science and Technology of China, Hefei 230029, Peoples Republic of China

Tailoring the electronic structure of graphene by chemical modification of graphene represents a crucial route to the synthesis of a new class of semiconductor materials. The covalent introduction of nitrogen might pave a way to use tailored graphene in electronic devices. Herein, we report a simple procedure to insert nitrogen atoms into graphene by low energy nitrogen bombardment, forming nitrogen-doped graphene. Applying high resolution X-ray photoelectron spectroscopy, different carbon-nitrogen species in the nitrogen-doped graphene sheet are identified. Additionally, the distribution of nitrogen in its doping sites and the doping level becomes available. The doping level and doping sites of nitrogen-doped graphene can be varied by changing the nitrogen bombardment energies and times.

Support is acknowledged from the BMBF (05 ES3XBA/5) and the Cluster of Excellence "Engineering of Advanced Materials".

O 34.8 Tue 18:15 Poster E

Graphene as a supporting layer for nanoparticles — •Torsten Veltum, Wolfgang Rosellen, Hendrik Bettermann, and Mathias Getzlaff — Institute of Applied Physics, University Duesseldorf

In the past few years graphene has gained the attention of scientists due to its unique mechanical and electrical properties. On the other hand, fabrication and deposition of nanoparticles on a substrate is of great interest for studies of, e.g. model catalysts. In this study we want to get a better understanding of the interaction between the nanoparticles and graphene substrate.

A thin Ni(111) film is 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 in-situ by means of scanning tunneling microscopy (STM), low energy electron diffraction (LEED) and auger electron spectroscopy (AES).

The well-characterized FeCo 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 34.9 Tue 18:15 Poster E

Strain Modulation of Graphene Nanoribbons — •Yingchun Cheng[1], Hongtao Wang[2], Zhiyong Zhu[1], Xixiang Zhang[3], and Udo Schwingenschlogl[1] — [1]PSE Division, KAUST, Thuwal 23955-6900, Kingdom of Saudi Arabia — [2]Institute of Applied Mechanics, Zhejiang University, Hangzhou 310027, China — [3]Advanced Nanofabrication, Imaging and Characterization Core Lab, KAUST, Thuwal 23955-6900, Kingdom of Saudi Arabia

The edge structure and width of graphene nanoribbons (GNRs) are crucial factors determining the electronic structure. A combination of experiment and first-principles calculations allows us to study the mechanism of transformation from hexagon-hexagon (66) to pentagon-heptagon (57) configuration. Thin GNRs (< 2 nm) are fabricated by bombardment of a graphene sheet with high-energetic Au clusters. The edges of the GNRs are modified *in-situ* by electron irradiation. Tensile strain along the edge decreases the transformation energy barrier from the 66 to the 57-GNR. A thin 66-GNR is antiferromagnetic with direct band gap, a 57-GNR turns out to be an indirect semiconductor, and a GNR transformed on only one edge is ferromagnetic. We propose that strain can be an effective method to tune the edge (and electronic) structure of thin GNRs for graphene based electronics.

O 34.10 Tue 18:15 Poster E

Strain Modulation of Graphene Nanoribbons — •Yingchun Cheng[1], Hongtao Wang[2], Zhiyong Zhu[1], Xixiang Zhang[3], and Udo Schwingenschlogl[1] — [1]PSE Division, KAUST, Thuwal 23955-6900, Kingdom of Saudi Arabia — [2]Institute of Applied Mechanics, Zhejiang University, Hangzhou 310027, China — [3]Advanced Nanofabrication, Imaging and Characterization Core Lab, KAUST, Thuwal 23955-6900, Kingdom of Saudi Arabia

The edge structure and width of graphene nanoribbons (GNRs) are crucial factors determining the electronic structure. A combination of experiment and first-principles calculations allows us to study the mechanism of transformation from hexagon-hexagon (66) to pentagon-heptagon (57) configuration. Thin GNRs (< 2 nm) are fabricated by bombardment of a graphene sheet with high-energetic Au clusters. The edges of the GNRs are modified *in-situ* by electron irradiation. Tensile strain along the edge decreases the transformation energy barrier from the 66 to the 57-GNR. A thin 66-GNR is antiferromagnetic with direct band gap, a 57-GNR turns out to be an indirect semiconductor, and a GNR transformed on only one edge is ferromagnetic. We propose that strain can be an effective method to tune the edge (and electronic) structure of thin GNRs for graphene based electronics.

O 34.11 Tue 18:15 Poster E

Non-linear optics in graphene — •Evgeny Bobkin, Torben Winzer, Ermin Malic, and Andreas Knorr — Institut für Theoretische Physik, Nichtlineare Optik und Quantenelektronik, Technische Universität Berlin, 10623 Berlin, Germany

We present a microscopic study on non-linear optics in graphene including the investigation of Rabi oscillations, adiabatic following, and detuning effects. Our approach is based on the density matrix formalism, which allows a straight-forward inclusion of many-body interactions, such as excitonic effects. By solving the microscopic graphene Bloch equations we gain a time- and momentum-resolved access to the non-linear dynamics of the charge carriers and the coherence [1]. We investigate the appearance of Rabi oscillations as a function of time and pump fluence for different excitation regimes. Furthermore, we compare the free-particle and the excitonic picture to extract the influence of the Coulomb interaction.

[1] Ermin Malic, Torben Winzer, Evgeny Bobkin and Andreas Knorr, "Microscopic theory of excitonic absorption and ultrafast many-particle kinetics in graphene", Phys. Rev. B 84, 205406 (2011)

O 34.12 Tue 18:15 Poster E

Local anodic oxidation of graphene by scanning force microscopy — •Marcus Liebmann, Theresa Hecking, Alexander Nent, Lena Jung, Jonas van Bebber, Jens Kellner, Lisa Felker, Silke Hattendorf, Nils Freitag, and Markus Morgenstern — II. Phys. Inst. B, RWTH Aachen University and JARA-FIT, Germany

For structuring graphene flakes exfoliated on a substrate, local anodic oxidation (LAO) is an interesting tool which avoids the contamination of large parts of the flake during processing using conventional lithography. Being well-established for semiconductor nanostructures [1], this technique has also been applied to graphene more recently [2]. It makes use of the oxidation of the surface at the contact area between a sample and a scanning tip of an atomic force microscope (AFM) when a bias voltage is applied under ambient conditions.

Graphene flakes exfoliated on SiO_2 and contacted by Indium soldering are modified by LAO. We observe two main processes: oxidation and cutting, depending on parameters like voltage, load force, tip velocity, and humidity. Appropriate sets of parameters are investigated and first nanostructures are tested. Line widths of 40 nm could be achieved. Conductivity measurements indicate that cut lines are insulating and oxidized structures show sheet resistances of at least 300 GΩ. Graphene samples have also been prepared on BN and the morphology has been analyzed by AFM.

[1] R. Held et al., Appl. Phys. Lett. 71, 2689 (1997).

[2] A. J. M. Giesbers et al., Solid State Commun. 147, 366 (2008).

O 34.13 Tue 18:15 Poster E

Mechanical exfoliation of epitaxial graphene on Ir(111) enabled by Br_2 intercalation — •Charlotte Herbig[1], Markus Kaiser[2], Nedjma Bendiab[3], Johann Coraux[3], Klaus Meerholz[2], Thomas Michely[1], and Carsten Busse[1] — [1]II. Physikalisches Institut, Universität zu Köln, Germany — [2]Institut für Physikalische Chemie, Universität zu Köln, Germany — [3]Institut Néel, CNRS-UJF, France

For a technological use of graphene, it is desirable to grow it on a large scale with a reproducible high quality. The best quality up to date is achieved by growth on metal substrates. Especially on Ir(111), strictly monoatomic graphene sheets of well defined orientation and macroscopic extension are achieved [1]. For application graphene on metals is non-suitable. Therefore, a transfer is necessary. Here, we present a method for a dry transfer of graphene grown on Ir(111).
First, the epitaxially grown graphene layer was investigated by LEED and STM. Afterwards, graphene was intercalated by Br_2 and examined by SEM. The transfer process was conducted by attaching adhesive tapes as supporting material and subsequent removal. Finally, the surface was analyzed by SEM. Raman spectroscopy was carried out to prove the transfer of graphene onto the adhesive tapes.
[1] R. van Gastel et al., Appl. Phys. Lett. 95 (2009) 121901

O 34.14 Tue 18:15 Poster E

Microscopic derivation of screened Graphene-Bloch equations — •Eike Verdenhalven[1], Ermin Malic[1], Rolf Binder[2], and Andreas Knorr[1] — [1]Institut für Theoretische Physik, Technische Universität Berlin, Germany — [2]College of Optical Sciences and Department of Physics, University of Arizona, Tucson, USA

The Coulomb interaction is known to be very strong in low-dimensional carbon-nanostructures, such as carbon nanotubes and graphene. Earlier calculations and experiments have revealed that excitonic effects significantly change the optical properties even of metallic nanotubes and graphene [1, 2]. However many-particle interaction also leads to the reduction of the Coulomb interaction strength by introducing an internal screening. In this work, we present a fully microscopic derivation of the dielectric function in the static limit. Within a density-matrix formalism we derive screened graphene-Bloch equations and a screened microscopic Boltzmann equation in second order Born-Markov approximation. We calculate the dielectric function in dependence of the momentum transfer along different directions in the Brillouin zone of graphene, showing its highest value of about 4.7 for small momentum transfer.

[1] E. Malić, T. Winzer, E. Bobkin, and A. Knorr, Phys. Rev. B 84, 205406, (2011)

[2] E. Malić, J. Maultzsch, S. Reich, and A. Knorr, Phys. Rev. B 82, 035433 (2010)

O 34.15 Tue 18:15 Poster E

Mechanical exfoliation of graphene in UHV — •Gerrit Begall, Oliver Ochedowski, and Marika Schleberger — Universität Duisburg-Essen, Duisburg, Germany

Our new approach to graphene preparation is mechanical exfoliation under UHV-conditions.

There are typically two ways of preparing graphene on an arbitrary substrate: The mechanical exfoliation (known as the scotch tape method) and the transfer of CVD-graphene (graphene grown on Ni by chemical vapor deposition), using a polymer which is dissolved later.

Both techniques are far from being perfect, regarding cleanliness of the samples and graphene properties. Scotch tapes, used in the mechanical exfoliation method, leave adhesives and there is usually water intercalated inbetween substrate and graphene. The quality of CVD-graphene is inferior to the quality of exfoliated graphene regarding its physical properties, since it consists of small domains. The chemicals involved in the transfer (acetone, PMMA) can be problematic as well.

With the possibilities of an UHV-system, we can prepare atomically clean substrates by sputtering and heating. After this cleaning, a graphenium-flake or a HOPG-crystal is pressed onto the sample. We plan to prepare graphene on Ni, Si (7x7) and SiO_2 surfaces. The results will be compared to classically prepared graphene.

O 34.16 Tue 18:15 Poster E

Theoretical modelling and interpretation of the C $1s \rightarrow \pi^*, \sigma^*$ X-ray absorption spectra of $H_2O(NH_3)$/graphene — •Elena Voloshina[1], Roman Ovcharenko[1,2], Aleksander Shulakov[2], Beate Paulus[1], and Yuriy Dedkov[3] — [1]Physikalische und Theoretische Chemie, Freie Universität Berlin, Germany — [2]V. A. Fock Institute of Physics, Saint-Petersburg State University, Russia — [3]SPECS Surface Nano Analysis GmbH, Germany

Recently, adsorption of polar molecules on graphene/Ni(111) was investigated by means of angle-resolved photoelectron spectroscopy (ARPES) and X-ray absorption spectroscopy (XAS) [1]. It was found, that adsorption of H_2O and NH_3 leads to the noticeable modification of the XAS C K-edge spectra indicating the orbital mixing of the valence band states of graphene and adsorbates. Further analysis of the obtained results allows assuming the site-selective adsorption for the two studied adsorbates. However, neither position nor orientation of the adsorbate were determined. In order to clarify these aspects, we performed the first-principles electronic structure calculations on the H_2O/graphene and NH_3/graphene systems as well as modelling the C K-edge XAS spectra of these systems. The dynamical core-hole screening effects in the XAS spectra were taken into account via the multiband Mahan-Nozieres-De Dominicis (MND) theory [2]. The presented theoretical results are compared to available previously published theoretical data as well as experimental observations.

[1] S. Böttcher *et al.* Nanoscale Res. Lett. **6**, 214 (2011).

[2] O. Wessely *et al.* Phys. Rev. B **73**, 075402 (2006).

O 34.17 Tue 18:15 Poster E

Quasi-free standing trilayer epitaxial graphene on SiC(0001) — •Stiven Forti[1], Camilla Coletti[2], Konstantin V. Emtsev[1], Alexei Zakharov[3], Kevin Daniels[4], Biplob Daas[4], M.V.S. Chandrashekhar[4], and Ulrich Starke[1] — [1]Max Planck Institute for Solid State Research, Heisebergstr. 1, 70569 Stuttgart, Germany — [2]Center for Nanotechnology Innovation @ NEST, Istituto Italiano di Tecnologia, Piazza San Silvestro 12, 56127 Pisa, Italy — [3]Max Lab, Lund University, Box 118, Lund, S-22100, Sweden — [4]University of South Carolina, 301 S. Main St, Columbia, SC 29208, USA

The control of the thermal decomposition of the 6H-SiC(0001) surface to grow a homogeneous coverage of epitaxial few-layers graphene remains not easily achievable in the experiments. In the present work, we report on high resolution ARPES data, showing the electronic band structure of quasi-free standing trilayer epitaxial graphene. The system is characterized in different doping conditions, from p-type to charge neutrality. LEEM data provide evidence that the number of graphene layers is homogeneous over the surface up to a several micron scale. The question of different stacking sequences will be addressed with the aid of theoretical calculations to fit the experimental band structures.

O 34.18 Tue 18:15 Poster E

Excited electron dynamics in Au-intercalated Graphene on Ni(111) — •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 advancd materials, University of Groningen

Theoretical calculations predict an initial ultrafast relaxation of hot electrons accompanied by a population of optical phonons, which decays on a picosecond time scale[1]. We present an experimental set-up suited to measure the lifetime of excited electrons and their relaxation dynamics in Graphene via time-resolved two-photon photoemission. The set-up utilizes an amplified Ti:sapphire laser to generate intense femtosecond pulses with high repetition rates. 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. The fundamental radiation of the Ti:Sa laser is used to excite the carriers.

Graphene was produced by decomposition of ethylene on a Ni(111) substrate. The Laser-Assisted Photoelectric Effect (LAPE) was utilized to determine the XUV pulse duration to 28 fs. First experiments reveal a Ni(111) nonthermal electron lifetime of less than 20 fs. Additional measurements on Au-intercalated Graphene and Graphene on SiC will be presented.

[1]T. Elsaesser et al., Phys. Rev. Lett. 66 (1991) 1757

O 34.19 Tue 18:15 Poster E

Water adsorption on heteroepitaxial graphene — •Janine Scherer, Samir Mammadov, Thomas Seyller, and Sabine Maier — Department für Physik, Universität Erlangen-Nürnberg

Graphene devices operated in ambient conditions are exposed to a variety of molecules. Here, we focus in particular on water, which can act as dopant and might alter the electronic properties of such devices. We study epitaxial graphene grown on 6H-SiC(0001) upon water adsorption using high resolution scanning tunneling microscopy operated in ultrahigh vacuum conditions at low temperature. We will discuss the adsorption structures of water on clean graphene surfaces with respect to the number of graphene layers. While water forms clusters on the interface layer, it leads to significant topographical changes for single and multiple graphene layers. We observe that graphene is split into small flakes in the vicinity of step edges, which is unfavorable for technological applications.

O 34.20 Tue 18:15 Poster E

Interaction of manganese and nickel with epitaxial graphene on Ir(111) — •Hendrik Vita, Stefan Böttcher, Martin Weser, Yuriy Dedkov, and Karsten Horn — Fritz-Haber-Institut der Max-Planck-Gesellschaft, 14195 Berlin, Germany

In view of an application as spin filter, the interaction of graphene with magnetic materials is interesting. Here we report on a LEED as well as core and valence level photoemission study of the interaction of manganese and nickel adlayers and intercalated layers with graphene grown epitaxially on Ir(111). We examine the doping effect of the adlayers and intercalates through a shift of the Dirac cone to higher binding energies. In a second step, the growth of alloys films of Mn and Ni by stepwise deposition and annealing is examined. We compare our data to Al and Fe intercalated layers in graphene grown on Ni(111).

O 34.21 Tue 18:15 Poster E

Interaction of Water Molecules with Graphene — •Sebastian Standop, Thomas Michely, and Carsten Busse — II. Physikalisches Institut, Universität zu Köln

Graphene is a promising candidate as an electrode material in future electronics including ultracapacitors [1] and dye sensitized solar cells [2]. With the potential of graphene to be used in electrochemical applications it is of great interest to understand in detail structure as well as adsorption kinetics and energetics of water on graphene. Therefore we dosed water onto a graphene covered Ir(111) surface and performed both scanning tunneling microscopy (STM) and thermal desorption spectroscopy (TDS). For low coverages adsorbed at 20 K the water layer shows zero order desorption with an high temperature shoulder increasing with coverage, eventually leading to a complete suppression of the initial peak in favor of the high temperature structure. When elevating the adsorption temperature above 100 K the formation of the second structure is preferred over the low coverage phase indicating its metastable character. We presume that this transition corresponds to a reduced number of dangling bonds within the water layer which is due to the hydrophobicity of the graphene substrate [3]. Our real space analysis corroborates these findings by showing heavy manipulation of the low coverage phase even at 20 K. When increasing the coverage the water molecules organize in extended islands aligned to the inherent moiré supercell of epitaxially grown graphene. [1] C. Liu *et al.*, Nano Lett. 10, 4863 (2010); [2] X. Wang *et al.*, Nano Lett. 8, 323 (2008); [3] G. A. Kimmel *et al.*, J. Am. Chem. Soc. 131, 12838 (2009)

O 34.22 Tue 18:15 Poster E

Intercalation of Cs through wrinkles of epitaxial graphene — Marin Petrović[1], Iva Šrut[1], Ivo Pletikosić[1], Petar Pervan[1], Milorad Milun[1], Sven Runte[2], Carsten Busse[2], Thomas Michely[2], Jurek Sadowski[3], Tonica Valla[3], and •Marko Kralj[1] — [1]Institut za fiziku, Zagreb — [2]II. Physikalisches Institut, Köln — [3]Brookhaven National Lab, New York

Interclation of alkali atoms is a straightforward route for the chemical doping of epitaxial graphene (G). This has been demonstrated for graphene on SiC [1] as well as for graphene on metals [2], where dopings/shifts of the Dirac cone at the K-point near the Fermi level have been followed by angle-resolved photoemission spectroscopy (ARPES). However, ARPES is area-averaging technique which does not provide a clear picture on the process of the penetration of alkali atoms to a position between graphene layer and its support. Our ARPES studies for intercalation of Li, Na, K, and Cs to G/Ir(111) have indicated that dynamics of alkali intercalation depend on the size of the alkali atom and we have focused to the intercalation of large alkali atom, Cs. By the combination of ARPES, scanning tunneling microscopy and low-energy electron microscopy we reveal two different doping effects from Cs on top and intercalated compact layer which is formed by a diffusion of Cs atoms through wrinkles network of graphene.

[1] J. L. McChesney, et al., Phys. Rev. Lett. 104, 136803 (2010).

[2] M. Bianchi, et al., Phys. Rev. B 81, 041403(R) (2010).

O 34.23 Tue 18:15 Poster E

Raman spectrum of the $(6\sqrt{3}\times6\sqrt{3})$R30° reconstructed surface of 6H-SiC(0001) — •Felix Fromm[1], Martin Hundhausen[1], Myriano Henriques de Oliveira Jr.[2], Marcelo Lopes[2], Henning Riechert[2], and Thomas Seyller[1] — [1]Universität Erlangen-Nürnberg, Lehrstuhl für Technische Physik, 91058 Erlangen — [2]Paul-Drude-Institut für Festkörperelektronik, 10117 Berlin

The epitaxial growth of graphene on silicon carbide (SiC) by thermal sublimation of silicon in an argon atmosphere is a prominent method to produce high quality graphene layers. There are two approaches to obtain graphene on SiC: As an initial step of graphene formation a $(6\sqrt{3}\times6\sqrt{3})R30^\circ$ reconstructed overlayer of carbon, the so-called buffer layer (BL) is formed. Further graphitisation converts the BL to graphene and forms a new BL underneath (MLG). Another path is the conversion of the BL to graphene via intercalation of hydrogen. This results in quasi-free-standing graphene on hydrogen saturated SiC (QFMLG). In this work we analysed Raman spectra of QFMLG and MLG. Since graphene is highly transparent the substrate underneath the garphene contributes to the Raman spectrum. Therfore a SiC Raman spectrum has to be subtracted to obtain the Raman signal of the graphene layers. Whereas the Raman spectrum of QFMLG shows symmetric D and G lines, the spectrum of MLG shows additional broad features in the D and G range. We assign these broad contributions to the Raman spectrum of the BL.

O 34.24 Tue 18:15 Poster E

Giant Rashba splitting in graphene/SiC(0001) after Au intercalation — •Dmitry Marchenko[1], A. Varykhalov[1], J. Sánchez-Barriga[1], M. R. Scholz[1], Th. Seyller[2], and O. Rader[1] — [1]Helmholtz-Zentrum Berlin — [2]Universität Erlangen

We have recently demonstrated a giant spin-orbit splitting in graphene/Ni(111) after intercalation of a Au monolayer. The spin-orbit splitting is by 4 orders of magnitude larger than the intrinsic splitting of graphene. The intercalation approach works also for graphene on SiC(0001) which is one of the most popular substrates for high quality graphene growth. We show that in graphene/SiC the spin splitting of the Dirac-cone is zero, but intercalation of a gold layer under the graphene dramatically increases the splitting up to 120 meV.

O 34.25 Tue 18:15 Poster E

Characterization of functional plasmonic elements: a far-field approach — •Christian Rewitz[1], Thomas Keitzl[1], Philip Tuchscherer[1], Jer-Shing Huang[2], Peter Geisler[3], Gary Razinskas[3], Bert Hecht[3,4], and Tobias Brixner[1,4] — [1]Institut für Physikalische und Theoretische Chemie, Universität Würzburg, Am Hubland, 97074 Würzburg, Germany — [2]Department of Chemistry, National Tsing Hua University, Hsinchu 30013, Taiwan — [3]Nano-Optics and Biophotonics Group, Experimentelle Physik 5, Universität Würzburg, Am Hubland, 97074 Würzburg, Germany — [4]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. In view of applications in the field of optical communication the dispersion and group velocity of plasmon propagation are of high interest. Here, we present a microscope setup that employs a far-field technique to measure the spectral and spatial transfer functions of plasmonic elements thus enabling us to determine the dispersion and group velocity of plasmon propagation. For the exact determination of the plasmon group velocity, i.e., the speed of ultrashort propagating pulses representing bits of information, a detailed knowledge of the setup transfer function is needed, which we provide here. The setup inherent time delay of signals due to different path lengths is measured with 1 fs accuracy and is used to obtain corrected results for plasmon group velocities.

O 34.26 Tue 18:15 Poster E

Photochemical metal deposition in nanoporous aluminum oxide matrices — •Julia Katzmann and Thomas Haertling — Fraunhofer Institute for Nondestructive Testing, Maria-Reiche-Str. 2, 01109 Dresden, Germany

Well-ordered arrays of metal nanorods show highly interesting optical properties which make them promising structures for sensor applications [1]. Such arrays can be fabricated via template-based methods at low cost and on large areas.

We report on a proof-of-concept investigation which demonstrates the targeted photochemical deposition [2] of gold into the pores of anodized aluminum oxide (AAO). We exploit a thin layer of gold sputtered onto one side of the AAO membrane as a seed layer for the photochemical process. A solution of $HAuCl_4$ is applied onto the other side of the membrane. Upon UV light irradiation, nanorods grow within the oxide matrix without the need of an electrical contact. The optical properties of the gold-filled matrices, i.e., the excitation of plasmons in the nanorods were measured by means of optical transmission spectroscopy, while the rod length was determined by scanning electron microscopy. We observe a spectral blue shift of the transversal plasmon resonance with increasing rod length. This finding is correlated with different fabrication parameters to obtain a detailed understanding of the photochemical growth process.

[1] A.V. Kabashin et.al, Nature Materials 8, 857 (2009)

[2] T. Haertling et.al, Optics Express 16, 12362 (2008)

O 34.27 Tue 18:15 Poster E

Mapping of gold nanostructure-induced near-field enhancement — •Oksana Kostiuchenko[1,2], Jacek Fiutowski[2], Christian Maibohm[2], Jakob Kjelstrup-Hansen[2], Horst-Günter Rubahn[2], and Heinz Sturm[1] — [1]BAM - Div. Nanotribol. & Nanostruct., Berlin — [2]Univ. of Southern Denmark, Mads Clausen Inst., NanoSYD, 6400 Sønderborg, DK

Sub-diffraction spatially resolved, quantitative mapping of strongly localized field intensity enhancements on gold nanosquares and nanotriangles via laser scanning femtosecond (fs) ablation of polymer thin films and via second harmonic generation (SHG) is reported. Using electron beam lithography, periodical patterns of gold squares and triangles on gold thin films are fabricated. Subsequently, poly(methyl methacrylate) (PMMA) is spin coated on top of such nanostructures. Illumination by a scanning fs laser beam induces an electromagnetic surface field, which is locally enhanced at the edges of the nanostructures and - under appropriate excitation wavelength conditions - also between the structures due to surface plasmon excitation. This enhancement lowers the threshold for nonlinear optical effects such as surface second harmonic generation or deformation and ablation of the polymer coating. The scanning laser beam thus results in a two-dimensional map of near field enhancement, imprinted into the polymer and directly seen via SHG. A variation of the polymer film thickness enables one to discriminate between edge and surface plasmon enhancement effects.

O 34.28 Tue 18:15 Poster E

Plasmons in Ag-Nanowires Grown on Si (557) — •Yu Zhang, Ulrich Krieg, Christian Brand, Herbert Pfnür, and Christoph Tegenkamp — Institut für Festkörperphysik, Leibniz Universität Hannover, Appelstrasse 2, D-30167 Hannover, Germany

We present electron energy loss spectroscopy data of wire like Ag-structures grown via self assembly of on vicinal Si(557) at a coverage of 0.3 monolayers.

Using an instrument with both high energy and high momentum resolution (ELS-LEED) we observed a linearly dispersing plasmon loss parallel to the step-edges and a plasmon loss without dispersion in perpendicular direction.

Spot profile analysis LEED (SPA-LEED) and STM measurements show that the step-structure remains unchanged and the step-edges are still undecorated after the evaporation and annealing process. Both results are strong indications for well separated nanowires with a defined width resulting in a confinement of the plasmon to the individual nanowire.

Further effects of finite wire width and of residual coupling between the wires are discussed.

O 34.29 Tue 18:15 Poster E

Investigation of Si/chalcogenide hybrid slot waveguides — •Peter Nolte, Christian Bohley, and Jörg Schilling — Martin-Luther-Universität Halle-Wittenberg, ZIK SiLi-nano, Halle, Germany

In the last years great efforts lead to a strong miniaturization of optical components, as several devices were realized on the silicon-on-insulator (SOI) platform which is to CMOS technology. The very high refractive index contrast between the Si core, oxide cladding and air, leads to a high confinement of light inside a waveguide. However, for many applications active devices exhibiting a nonlinear optical behavior are needed. One possible way to boost the nonlinear optical properties in integrated optics is the functionalization of SOI-structures with chalcogenide glasses. These glasses (e.g. As_2S_3) exhibit a nonlinear figure of merit of about $\mathrm{Re}(\chi^{(3)})/\mathrm{Im}(\chi^{(3)}) = 10$ in the near infrared. We present slotted SOI-waveguides which have been clad and infiltrated by chalcogenide glasses. The linear optical properties of the clad waveguides were investigated using a fiber coupled laser setup, tuned from 1490 nm to 1640 nm with 1 pm steps. The nonlinear properties have been studied by means of degenerate four wave mixing. Here, two laser beams with frequencies ω_1 and ω_2 interact with each other through the 3rd order nonlinear susceptibility of the waveguides. Thus two new beams formed. From the conversion efficiency and its intensity dependence the averaged 3rd order nonlinear susceptibility $\chi^{(3)}$ for the hybrid waveguide device is determined. We demonstrate how hybrid silicon/As_2S_3 waveguides can perform nonlinear frequency conversion via four wave mixing extending the functionality on integrated SOI photonics.

O 34.30 Tue 18:15 Poster E

Optical fiber sensor with concentric circular gold grating sensitive to change of ambient refractive index — •Sabrina Darmawi[1], Shengfei Feng[2], Torsten Henning[1], Xingping Zhang[2], and Peter J. Klar[1] — [1]I. Physikalisches Institut, Justus-Liebig-Universität, Heinrich-Buff-Ring 16, 35392 Gießen — [2]College of Apllied Sciences, Beijing University of Technology, Beijing 100124

Metallic nanostructures on top of the end facet of an optical fiber can be employed as probes or sensors. Due to their flexibility, durability and large aspect ratio, optical fibers are well-suited for remote sensing. We present a polarization-independent optical sensor consisting of a concentric gold ring grating with a period of 900 nm transferred onto the end facet of an optical fiber. The sensing function of the device is realized by sending white light through the unstructured end and collecting the reflected response signal. A distinct peak due to the Rayleigh anomaly of the gold ring grating is observed in the reflection sprectrum. We show that this peak is sensitive to the change in the environmental refractive index of the end facet of the fiber.

O 34.31 Tue 18:15 Poster E

Multi-wavelength superlensing with layered phonon-resonant dielectric — •Peining Li and Thomas Taubner — I. Institute of Physics (IA), RWTH Aachen University, Sommerfeldstraße 14, 52074 Aachen, Germany

A superlens is a very promising device to overcome the diffraction limit and resolve subwavelength features [1]. However, the practical application of the superlens is limited by its narrow bandwidth since a superlensing condition should be met. For dispersive materials, this condition limits operation to a very small wavelength range for each material system. For example, the superlensing condition for the silicon carbide (SiC) case is met at a wavelength of around 11 μm [2]. Therefore, in order to cover a relatively wide wavelength range, different superlenses should be used [3].

Here, we theoretically propose a possibility of employing a multilayered polar-dielectric system to achieve sub-diffraction limited imaging at different wavelengths. Our theory and simulation results show that this multilayered lens can fulfill the superlensing condition at multiple different wavelengths simultaneously due to the phonon resonances of polar dielectrics, and the number of superlensing wavelengths of the lens can be easily tuned by controlling the number of polar dielectrics. Ideally, by suitably choosing the polar dielectrics, the wavelength range of our lens can cover from infrared to THz frequencies.

O 34.32 Tue 18:15 Poster E

Comparative study of localized surface plasmons in gold ring structures performed by SNOM and PEEM. — •Cristian Gonzalez, Daniela Bayer, Pascal Melchior, Alexander Fischer, Christian Schneider, Bernhard Schaaf, Egbert Oesterschulze, and Martin Aeschlimann — University of Kaiserslautern, Department of Physics, 67663 Kaiserslautern, Germany

We will present a first comparative study on plasmonic nanostructures performed by SNOM (Scanning Near-field Optical Microscopy) and PEEM (Photo-Electron Emission Microscopy). Our new PEEM setup allows measurements under normal and 65° incidence of the laser beam. Hence, we are able to compare directly local near field enhancement in the vicinity of nanostructures obtained by both techniques, PEEM and SNOM under the same geometrical conditions.

With these two complementary microscopy techniques, we have the possibility to address both plasmonic damping channels, the radiative channel by SNOM and the non-radiative channel (electron-hole pair creation) by PEEM. In our first studies we focus on Au ring structures and ring segmented arrays made by electron beam lithography deposited on Indium Tin Oxide (ITO). Ring structures are of special interest because of the high tunability of their optical properties. Besides the interest in fundamental physics of the excitation of multipolar modes, they can be implemented in technological applications as, for example, bio-sensors and resonators.

O 34.33 Tue 18:15 Poster E

ToF-PEEM on Metallic Structures using Attosecond XUV Pulses — •Soo Hoon Chew[1,2], Frederik Süssmann[2], Christian Späth[1], Adrian Wirth[2], Alexander Guggenmos[1,2], Jürgen Schmidt[1], Sergey Zherebtsov[2], Kellie Pearce[1], Andreas Oelsner[3], Nils Weber[4], James Kapaldo[2], Alexander Gliserin[1,2], Ferenc Krausz[1,2], Mark Stockman[5], Matthias Kling[4], and Ulf Kleineberg[1] — [1]Department of Physics, Ludwig Maximilian University of Munich, Garching, Germany — [2]Max Planck Institute of Quantum Optics, Garching, Germany — [3]Surface Concept GmbH, Staudingerweg 7, 55128 Mainz, Germany — [4]Focus GmbH, Hünstetten Kasselbach, 65510, Germany — [5]Department of Physics and Astronomy, Georgia State University, Atlanta, Georgia, 30303 USA

We report on the imaging of gold structures by time-of-flight-photoemission electron microscopy (ToF-PEEM) in combination with extreme ultraviolet (XUV) attosecond pulses from a high harmonic generation (HHG) source. Characterization of lithographically fabricated gold structures using these ultrashort XUV pulses by ToF-PEEM shows a spatial resolution of 200 nm. Energy-filtered imaging of the secondary electrons resulting in reduced chromatic aberrations as well as microspectroscopic identification of core and valence band electronic states have been successfully proven. We also find that the fast valence band electrons are not infuenced by the space charge effects, which is essentially important for attosecond nanoplasmonic field microscopy realization.

O 34.34 Tue 18:15 Poster E

Coherent two-dimensional nanoscopy – insights into an advanced spectroscopic technique — Martin Aeschlimann[1], Tobias Brixner[2], Alexander Fischer[1], •Christian Kramer[2], Pascal Melchior[1], Walter Pfeiffer[3], Christian Schneider[1], Christian Strüber[3], Philip Tuchscherer[2], and Dmitri V. Voronine[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]Institute for Quantum Science and Engineering, Texas A&M University, College Station, TX 77840, USA

Coherent two-dimensional nanoscopy combines the principle of coherent two-dimensional spectroscopy with photoemission electron microscopy (PEEM). Using a sequence of four ultrashort laser pulses for excitation ensures high temporal resolution and detection of the emitted photoelectrons with a PEEM guarantees high spatial resolution below the optical diffraction limit. We present the concept of 2D nanoscopy for a quantum three-level system and compare the technique with conventional 2D spectroscopy. Furthermore we go into details about the experimental realization of this method and explain the evaluation of the measured data, i.e. the calculation of the local 2D nanospectra.

O 34.35 Tue 18:15 Poster E

A Point-Dipole Model for fast Computation of Plasmonic Structures and Nanoantennas — •Thorsten Schumacher[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

Optical nanoantennas based on plasmonic nanostructures are a novel tool to investigate previously inaccessible single nanoobjects [ref. Natcom]. Here the optical and geometric properties of the nanoantenna play an important role and have to be designed very accurately to achieve the desired effects. Several numerical methods such as FEM, FDTD, or multiple multipoles (MMP) are available to compute the linear optical behavior of such plasmonic nanostructures. They all have in common, that the required computation time is relatively long and that a deeper understanding of the coupling behavior is not obtained. Here we present a simple and very fast alternative to these methods to predict the coupling behavior of plasmonic nanoparticles in dependence of their spatial arrangement and individual plasmonic eigenmodes. Our approach is based on the discrete dipole approximation with a maximum reduction of used dipoles. We show the range of validity and demonstrate how our method can be used to obtain a deeper understanding of plasmonic interactions in complex nanostructures.

O 34.36 Tue 18:15 Poster E

Investigations of silver and copper nanoparticles for photocatalysis — •Hannes Hartmann[1], Vladimir Popok[2], Alexandra Pazidis[1], Antje Neubauer[1], I. Barke[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 for hydrogen production. Here the interaction of clusters with Ir based photosensitizers (PS) is investigated. These molecules are known to be promising systems for reduction of water to hydrogen in combination with metal-complex catalysts [1].

Using arc-discharge and magnetron sputtering cluster ion sources, silver and copper nanoparticles are produced and deposited on fused silica substrates. The PS is then deposited on cluster-covered samples. Their optical properties are characterized by absorption and fluorescence measurements. For understanding the detailed processes investigations with PEEM (photoemission electron microscopy) are planned. The current status of the experimental setup is presented.

[1] Beller et al., Angew. Chem. 2009, 48, 9962-9965

O 34.37 Tue 18:15 Poster E

Simulation of the nonlocal optical response of metallic nanostructures — •Mathias Wand, Peter Kölling, Torsten Meier, and Jens Förstner — Department Physik and CeOPP, University of Paderborn, 33098 Paderborn, Germany

Recent developments for the theoretical description of plasmonic nanostructures have shown that nonlocal effects in the motion of electrons can have a significant influence on the optical properties [1]. We present two quantum theories for the nonlinear optical response of metals and their application to the simulation of plasmonic nanostructures: The first theory is based on the time-dependent density functional theory (TDDFT) [2]. The second theory is based on the quantum generalized Vlasov equations [3], which describe the time-evolution of the single-particle Wigner functions for a two-component plasma. Both quantum theories take nonlocal effects into account. We compare our results with those from classical hydrodynamic model calculations regarding ground-state charge distribution, linear response, nonlocality, and higher harmonic generation.

[1] J. M. McMahon, S. K. Gray, and G. C. Schatz, Phys. Rev. Lett. 103, 097403 (2009).

[2] M. Wand, T. Meier, and J. Förstner, phys. stat. sol. (b) 248, 887 (2011).

[3] Y. Zeng, W. Hoyer, J. Liu, S. W. Koch, and J. V. Moloney, Phys. Rev. B 79, 235109 (2009).

O 34.38 Tue 18:15 Poster E

A SPA-LEED Study of Ag Nanowires grown on vicinal Si(557) via self-assembly — •Viktoria Meier, Ulrich Krieg, and Herbert Pfnür — Institut für Festkörperphysik, Leibniz Universität Hannover, Appelstrasse 2, D-30167 Hannover, Germany

To be able to study plasmonic excitations on Ag-nanowires we first must find a reproducible process to prepare uniaxial nanowires of well defined width. In this work we try to measure the averaged width of the nanowires via spot profile analysis LEED (SPA-LEED).

We prepared our samples by evaporation of different amounts of silver (0.2, 0.3 and 0.5 ML) on Si(557). After a precise heating and annealing cycle a single domain system of Ag-nanowires is formed on the surface via self assembly.

Studying the so-prepared sample with SPA-LEED we show that the step-structure of the substrate remains unchanged and the step-edges remain undecorated after the evaporation process. Already at 0.3 as well as 0.5 ML the silver forms a $\sqrt{3} \times \sqrt{3}$ reconstruction on the (111) terraces.

To access the width of the nanowires we made a $\left(K_{\|}, K_{\perp}\right)$ plot of the Γ-Point. We compute the terrace width from the angle between the diffraction-rods of the step-train and the (111)-structure.

O 34.39 Tue 18:15 Poster E

Ferroelectric-metal core-shell nanoparticles — •Thomas Kämpfe, Philipp Reichenbach, Stefan Grafström, and Lukas M. Eng — Institute of Applied Photophysics, University of Technology Dresden, 01062 Dresden

The optical properties of plasmonic nanoparticles (NPs) are widely used in linear-optical microscopy techniques as well as in many nanotechnological applications. However, in coherent nonlinear optical microscopy the narrow adjustment range of the localized surface plasmon (LSP) resonance wavelength practically restricts the application to far-off-resonant excitation, hence dramatically limiting the efficiency of the invoked nonlinear processes. Here, we show how to increase the nonlinear particle scattering by using dielectric-metallic core-shell NPs. Such a core-shell nanosystem provides plasmon-resonance tuning from the visible into the near-infrared wavelength range, allowing to resonantly excite LSPs with standard femtosecond laser sources. Moreover, a ferroelectric core will give rise to strongly enhanced second-harmonic generation due to the field enhancement produced by the plasmonic shell. We demonstrate (a) the fabrication steps for $BaTiO_3$@Au core-shell NPs, (b) the optically controlled in-situ adjustment of their plasmonic resonance by laser-induced metal precipitation [1], and (c) the ability of such $BaTiO_3$@Au core-shell NPs to emit enhanced SHG. The approach sketched here is very versatile, and paves the way to nonlinear-optical read-out of nearfields by means of a single core-shell NP probe via the emitted second-harmonic radiation.

[1] T.Härtling *et.al.*, Nanotechnology **21**, 145309 (2010)

O 34.40 Tue 18:15 Poster E

Fabrication of bow-tie like infrared antennas with small gaps by nanosphere lithography — Hendrik Janssen, •Jón Mattis Hoffmann, and Thomas Taubner — I. Institute of Physics (IA), RWTH Aachen University, Sommerfeldstraße 14, 52074 Aachen, Germany

Infrared absorption spectroscopy allows for the investigation of characteristic molecule absorption bands of sample materials by directly probing molecular vibrations. The sensitivity of infrared spectroscopy has been increased by several orders of magnitude with optical antennas.[1-3] Decreasing the distance between two antennas leads to antenna coupling and increased field-enhancement [4], resulting in even higher enhancement factors over non-coupling antennas.

In this work we present metallic bow-tie like structures with gap sizes down to sub 20 nm. To prepare these structures we use the easy method of nanosphere lithography (NSL) and two steps of evaporation on a tilted sample. For spectral characterization of the infrared resonances we use polarization resolved far-field measurements.

[1] R. Adato et al.; PNAS, 106, 19227 (2009)
[2] F. Neubrech et al.; PRL 101, 157403 (2008)
[3] R. Bukasov et al.; Analyt. Chem. 81, 4531 (2009)
[4] P. J. Schuck, et al, Phys. Rev. Lett. 94, 017402 (2005)

O 34.41 Tue 18:15 Poster E

Leakage radiation microscopy of laterally manipulated surface plasmons — •Manuel Roth, Stephen Riedel, Paul Leiderer, Elke Scheer, and Johannes Boneberg — Universität Konstanz

In a Kretschmann-configuration for an ATR (attenuated total reflection) setup, we excite SPPs (surface plasmon polaritons) on thin gold layers with a laser diode at 965 nm. Due to natural surface roughness, a fraction of the SPPs is scattered into the half space above the metal layer and recorded by a camera on top of a microscope (leakage radiation microscopy). Standing wave patterns and scattering centers can be observed on the images.

We report on SPP interference patterns which are created by different surface structures. The results are compared to simulations done by a FDTD (finite-difference time-domain) algorithm provided by Lumerical Solutions.

O 34.42 Tue 18:15 Poster E

Plasmonically enhanced electro-optical effects in metal-semiconductor nanodevices — •Markus Parzefall[1], Johannes Kern[1], Monika Emmerling[2], Martin Kamp[2], Jord C. Prangsma[1], and Bert Hecht[1] — [1]Experimental Physics 5, University of Würzburg, Germany — [2]Technical Physics, University of Würzburg, Germany

Surface plasmon enhanced internal photoemission in nanostructured Schottky devices has recently gained attention due to its promising application in photodetection and solar energy conversion. Due to their resonant nature, metallic nanostructures have shown to increase the photocurrent generated in such devices by orders of magnitude. We experimentally investigate electro-optical effects in nanostructured Schottky diodes based on gold and titanium dioxide. Our main focus lies on the evaluation of new design principles for optimized incident photon to current conversion efficiency, spectral tunability and the achievement of a deeper understanding of the underlying physics.

O 34.43 Tue 18:15 Poster E

Numerical study of circular dichroism in bi-chiral plasmonic crystals — •Yevgen Grynko[1], Jens Förstner[1], Torsten Meier[1], André Radke[2], Timo Gissibl[2], Paul V. Braun[3], and Harald Giessen[2] — [1]Department of Physics & CeOPP, University of Paderborn, Warburger Str. 100, D-33098 Paderborn, Germany — [2]4. Physikalisches Institut, University of Stuttgart, 70569 Stuttgart, Germany — [3]Department of Materials Science and Engineering, Frederick Seitz Materials Research Laboratory, Beckman Institute, University of Illinois at Urbana-Champaign, Urbana, IL 61801, USA

We study the optical properties of bi-chiral plasmonic nanostructures using the Discontinuous Galerkin Time Domain method [1], utilizing its advantages in the description of nanostructures with complex shapes. We simulate experimental measurements of transmission spectra of silver helix structures presented in [2]. Our numerical results reproduce the phenomenon of selective transmission of different circular polarizations well and qualitatively agree with the experiment for all types handednesses of bi-chiral crystals. The numerical analysis of the near fields provides information towards an understanding of the effects.

[1] J. S. Hesthaven, T. Warburton, 2002, J. Comp. Phys., 181, 186-221. [2] A. Radke, T. Gissibl, T. Klotzbücher, Paul V. Braun, and H. Giessen, 2011, Adv. Mater., 23, 3018.

O 34.44 Tue 18:15 Poster E

Enzymatically generated silver nanoparticles for surface enhanced Raman spectroscopy (SERS) — •Henrik Schneidewind[1], Karina Weber[1,2], Dana Cialla[1,2], Marco Diegel[1], Roland Mattheis[1], Andreas Berger[3], and Jürgen Popp[1] — [1]Institute of Photonic Technology (IPHT) Jena, Germany — [2]Institute of Physical Chemistry and Abbe-Center of Photonics, Friedrich-Schiller University Jena, Germany — [3]Max Planck Institute of Microstructure Physics Halle, Germany

Silver nanoparticles (Ag-NP) synthesized by an enzymatic induced growth process onto solid substrates form structures called as desert roses or nanoflowers. In order to customize the enzymatically grown nanoparticles to analytical applications in bio-molecular research, studies were carried out on the time evolution of the formation of the Ag-NP, their morphology, and their chemical composition. Therefore, Ag-NP films of different densities were investigated using SEM, TEM as well as energy dispersive X-ray spectroscopy. The surface coverage of substrates with Ag-NP and the maximum particle height were determined using Rutherford backscattering spectroscopy. It is shown, that the desert rose like Ag-NP consist of single crystalline silver plates containing only pure silver. Surface enhanced Raman spectroscopic (SERS) measurements of the vitamin riboflavin incubated on the Ag-NP are shown as an exemplary application for quantitative analysis.

O 34.45 Tue 18:15 Poster E

Electroluminescence in STM junction: nanostructures on Cu(3)N insulating layer — •Anna Strozecka, Jingcheng Li, Gunnar Schulze, Martina Corso, Katharina J. Franke, and Jose I. Pascual — Institut für Experimentalphysik, Freie Universität Berlin, Arnimallee 14, 14195 Berlin

Photons emitted in a scanning tunneling microscope (STM) junction can provide rich information about the electronic structure of investigated systems. However, on metal surfaces the light emission spectra are usually dominated by plasmonic excitations of the tip-sample cavity and the direct optical transitions are strongly quenched due to the short lifetime of the involved resonances. The decoupling from the metal support is neccessary in order to observe light emission directly from the nanostructure. Our experiments aim at getting closer insight into the coupling between plasmonic and electronic degrees of freedom in such systems. We investigated different types of nanostructures grown on Cu(3)N insulating layer on Cu(110). In three-dimensional Cu(3)N nanocrystals the narrow resonances corresponding to localized images potential states give rise to a direct optical transition. We studied also light emitted from molecules supported on a single Cu(3)N layer. The resulting spectra show that the molecular fluorescence is mediated by the plasmonic excitations in the cavity. Depending on the molecular structure we observe enhancement or quenching of the light emission.

O 34.46 Tue 18:15 Poster E

Fano resonances in plasmonic nanostructures — •Manuel Gonçalves and Othmar marti — Ulm University - Inst. of Experimental Physics, Albert-Einstein-Allee 11, 89069 Ulm, Germany

Fano resonances arise from the interference between a resonant process and the continuum (background) [1]. Recently, it was found that resonances in plasmonic nanostructures may also give rise to asymmetric resonance line shapes (Fano modes) [2]. These modes arise from interferences between electric dipole resonances, between electric dipole and quadrupole and, in some cases, between electric dipole and magnetic dipole. On the other hand, resonant modes in arrays of gold nanospheres have pronounced dips in the transmission spectrum and large figure of merit (FOM)[3]. These resonances are very sensitive to changes in the refractive index of the medium and are therefore good candidates for sensing applications.

We present a study of the Fano resonances in several plasmonic nanostructures, using the finite-element method (COMSOL Multiphysics). The dependence of the resonances on the excitation conditions, shape, size of the nanostructures and embedding medium was investigated.

[1] U. Fano, Phys. Rev., 124 1866 (1961).
[2] B. Lukyanchuk *et al.*, Nature Materials, 9 707 (2010).
[3] Arseniy I. Kuznetsov *et al.*, ACS Nano, 5 4843 (2011).

O 34.47 Tue 18:15 Poster E

Plasmons in Pb nanowire arrays : Between one and two dimensions — •Tammo Block, Christoph Tegenkamp, Jens Baringhaus, Karthiga Kanthasamy, and Herbert Pfnür — Institut für Festkörperphysik, Leibniz Universität Hannover, Appelstrasse 2, 30167 Hannover, Germany

Electron energy loss spectroscopy with both high energy and momentum resolution (ELS-LEED) was used to investigate the plasmon dispersion of arrays of Pb nanowires in the monolayer regime on a vicinal Si(557) substrate. While for coverages close to the physical monolayer (at 1.3ML) a true one-dimensional (1D) plasmon loss can be found, a wavelength-dependent transition from 1D to 2D properties takes place in the range from 1.2 to 1.4 monolayers. Due due to the high anisotropy in the system at all coveragess, the dispersion curves exhibit 1D characteristics in both directions, perpendicular and along the Pb wire direction. The Pb-induced refacetting of the Si(557) surface, which depends on Pb coverage seems to be the reason for this behavior, because both effective system sizes and coupling strength between miniterraces changes while increasing the Pb coverage.

O 34.48 Tue 18:15 Poster E

Interaction of Carbon Nanotubes with periodic Plasmonic Surfaces — •Christian Lehmann, Eser Akinoglu, Michael Giersig, and Stephanie Reich — FU Berlin, Fachbereich Physik, Arnimallee 14, 14195 Berlin

We investigate the interaction of carbon nanotubes with plasmonic particles using Raman spectroscopy. Our goal is to understand the influence of the shape and dielectric environment of the plasmonic particles on the Raman signal. Therefore we use shadow nanosphere lithography to create plasmonic surfaces with homogeneously shaped triangular gold particles aligned in a hexagonal lattice structure. Depending on the deposition parameters, the plasmonic resonance was shifted to available excitation wavelengths for Raman measurements. The parameters were obtained by finite difference time domain simulations, which agree well with the measured resonances. The resonances were obtained using dark field and UV/VIS absorption spectroscopy. As marker molecules we used carbon nanoubes because of their well known Raman spectrum. We observed an additional plasmonic amplification of the Raman signal. The effect was observed only when the particle was in resonance with the exciting laser wavelength. Under certain conditions additional Raman modes were observed. These modes are strongly dependend on the distance between the carbon nanotube and the plasmonic particles. We will discuss the origin of these additional modes. Furthermore, a strong luminescence amplification of the gold particles was observed for certain shapes. It is likely that this effect originates from clustering of the gold particles.

O 34.49 Tue 18:15 Poster E

Fabrication and characterization of complex nano antennas generated by evolutionary algorithms — •Oleg Selig, Thorsten Feichtner, Markus Kiunke, and Bert Hecht — 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

Plasmonic nano antennas are used to enhance visible light-matter interaction on the nanometer scale and thus can improve e.g. single molecule detection and the coupling of light into plasmonic waveguides. Most of the established nano antenna designs are inspired by well-known concepts from the radio-frequency regime. In order to find new designs, which account for the plasmonic behavior of metals in the optical regime we used an evolutionary algorithm which finds optimized structures for defined properties. The working principal is basically to etch holes in an array of gold in the right position and size to get an good value for the desired property and then recombine and mutate good structure to further improve them. By using rounded corners, gaussian excitation and realistic material thickness a very good approximation to feasible experimental conditions was achieved. For the realization we dropcasted mono crystalline gold flakes on ITO-covered glass. The structures calculated by the evolutionary algorithms were then written by means of focused ion beam milling. The optical properties were measured by confocal two-photon-photo-luminescence and compared to the simulation results, showing a substantial agreement.

O 34.50 Tue 18:15 Poster E

Fabrication of nanometer-sized gaps between nanoantenna dimers by photo-chemical metal deposition for SEIRS measurements — •Christian Huck[1], Daniel Weber[1], Frank Neubrech[1], Julia Katzmann[2], Thomas Härtling[2], Andrea Toma[3], Enzo Di Fabrizio[3], and Annemarie Pucci[1] — [1]Kirchhoff-Institute for Physics, Im Neuenheimer Feld 227, Heidelberg, Germany — [2]Fraunhofer Institute for Non-Destructive Testing, Dresden, Germany — [3]Istituto Italiano di Tecnologia (IIT), Genova, Italy

Metal nanoparticles exhibit surface plasmons, which are able to strongly enhance electromagnetic fields when excited by electromagnetic radiation. If the resonance frequency matches specific IR active vibrations of molecules, the detection of such vibrations of molecules adsorbed on the antennas can be improved up to 5 orders of magnitude. Additional enhancement can be achieved by exploiting the extraordinary field enhancement of two antennas interacting across a very small gap. Constraints in the lithographic fabrication limit the gap size to $\geq 20nm$.

To overcome these limitations, we applied the method of optically induced metal deposition to lithographically prepared gold nanoantennas. The technique was demonstrated for nm-sized structures and is applied here in the μm range.Covering the nanorods on the substrate with a solution of HAuCl4 and illuminating them by a focused 532nm laser beam leads to the reduction of the gold salt and to a gradual growth of the nanorods. The changes of the optical particle properties can be monitored by IR-spectroscopy.

O 34.51 Tue 18:15 Poster E

Transfer of Angular Momentum by Circularly Polarized Near Fields — •Peter Klaer, Florian Schertz, Keno Krewer, Gerhard Schönhense, and Hans-Joachim Elmers — Institut für Physik, Johannes Gutenberg-Universität Mainz, 55122 Mainz

A locally rotating electrical near field generated by special nanoantennas might have properties similar to a circularly polarized plane light wave.[1] In particular, the photons of the near field possess spin momenta of $\pm\hbar$ and all effects related to the photon spin should exist for near fields as well. The plasmonic near field concentrates large amounts of electromagnetic energy and, for rotating fields, also large amounts of photon spin momentum in a very small spatial volume far below the diffraction limit.

We show first results confirming the transfer of angular momentum by circularly polarized near fields using spin-polarized photoemission electron microscopy (SP-PEEM) to detect the spin polarization of electrons excited by 100fs light pulses with 800nm wavelength from localized plasmons on a Ag/GaAs(100) surface. We thank the DFG EL172/16-1 for financial support.

[1] R. Mohammadi et al., Appl. Phys. B, publ. online (2011).

O 34.52 Tue 18:15 Poster E

Fabricating Confined Nanorod Arrays for Nano-optical Applications — •Vera Hoffmann[1], René Kullock[1], Mathias Böhm[1], Gunther Scheunert[2], and Lukas M. Eng[1] — [1]Department of Applied Photophysics, TU Dresden, Dresden, Germany — [2]Department of Physics and Astronomy, Queen's University Belfast, Belfast, UK

Two-dimensional nanorod arrays made of materials such as gold, silver, cobalt etc. show optical properties [1,2] that provide the basis for novel plasmonic devices [3]. To go a step further towards low-cost integration into existing technologies, the electrochemical growth of such nanorods in self-organized porous alumina masks deposited onto a thin gold film is of great interest. In this study, we present a novel technique in which we restrict the nanorod growth to a confined nanoscale surface area only. By pre-structuring the underlying gold metal film, the growth of nanorods is confined to the edges of this structured area. Hence, the geometry and the plasmonic properties of the arrays can be modified, which makes them very promising and tunable for applications such as waveguides, nanoantennas, or in data storage devices.

[1] R. Kullock et al., Optics Express 16, 21671 (2008) [2] R. Kullock et al., J. Opt. Soc. Am. B 27, 1819 (2010) [3] A.V. Kabashin et al., Nat. Mater. 8, 867 (2009)

O 34.53 Tue 18:15 Poster E

Towards Quantum Plasmonics on a Chip: An Efficient Photon-Plasmon-Coupler for Single-Mode Operation — •Günter Kewes[1], Andreas W. Schell[1], Rico Henze[1], Sven Burger[2], and Oliver Benson[1] — [1]Institut für Physik, Humboldt-Universität zu Berlin — [2]Konrad-Zuse-Zentrum für Informationstechnik Berlin

Not only the ability of surface plasmon polaritons to guide energy and information below the diffraction limit of light [1] but also their quantum nature [2], hold great potential for highly integrated photonic/plasmonic circuits or on-chip experiments. We numerically investigate and design a photon to plasmon coupler which consists of a tapered dielectric waveguide and a V-shaped metal part, using adaptive finite-element methods. We pay special attention on an easy-to-fabricate approach and focus on single-mode operation since this will simplify quantum plasmonic experiments.

[1] W. L. Barnes et al., "Surface plasmon subwavelength optics", Nature 424, 824-830 (2003) [2] A. V. Akimov et al., "Generation of single optical plasmons in metallic nanowires coupled to quantum dots", Nature 450, 402-406 (2007)

O 34.54 Tue 18:15 Poster E

Near-Field of Strongly Coupled Plasmons - Uncovering Dark Modes Using PEEM — •Florian Schertz[1], Marcus Schmelzeisen[2,3], Reza Mohammadi[2,4], Maximilian Kreiter[2], Hans-Joachim Elmers[1], and Gerd Schönhense[1] — [1]Insitut für Physik, Johannes Gutenberg-Universität, D-55099 Mainz, Germany — [2]Max-Planck-Institut für Polymerforschung, D-55128 Mainz, Germany — [3]Center of Smart Interfaces, TU Darmstadt, D-64287 Darmstadt, Germany — [4]Department of Physics, Payame Noor University, Tehran, Iran

Strongly coupled plasmons in a system of individual Au nanoparticles placed at sub-nm distance to a Au film (nanoparticle-on-plane, NPOP) are investigated using two complementary single particle spectroscopy techniques. Optical scattering spectroscopy exclusively detects plasmon modes that couple to the far-field via their dipole moment (bright modes). By using photoemission electron microscopy (PEEM) we detect in the identical NPOPs near-field modes that do not couple to the scattered far-field (dark modes) and are characterized by a strongly enhanced non-linear electron emission process. To our knowledge, this is the first time that both far-field and near-field spectroscopy are carried out for identical individual nanostructures interacting via a sub-nm gap. Strongly resonant electron emission occurs at excitation wavelengths far off-resonant in the scattering spectra. Simulations based on classical electrodynamics confirm the observed differences of near- and far-field characteristics for a strongly coupled plasmonic model system. We thank DFG EL172/16-1 for financial support.

O 34.55 Tue 18:15 Poster E

Surface passivation and dark field spectroscopy of metallic nanocones — •Dominik Gollmer, Christian Schäfer, Yuliya Fulmes, Andreas Horrer, Dieter P. Kern, and Monika Fleischer — Institut für Angewandte Physik, Eberhard Karls Universität Tübingen, Auf der Morgenstelle 10, 72076 Tübingen

The external electromagnetic excitation of plasmonic nanostructures is accompanied by a localized enhanced near field, which makes these structures promising candidates for several applications like near-field imaging or sensing. We fabricated conical nanostructures with sharp tips (tip radii less than 10 nm) [1] using different unique fabrication methods. Because of their shape, these nanocones are suitable candidates for the applications mentioned above. The tunability of the optical properties of nanocones is an important precondition for efficient excitation. We showed via dark field spectroscopy of single structures that this can be achieved by variation of size, aspect ratio and material. For non-stable materials a passivation is essential to keep the optical properties constant over time. Aluminum oxide has been suggested as an appropriate material for this purpose [2]. We showed that it is possible to passivate silver nanocones by oxidized thin sputtered aluminum layers. The fabrication processes will be presented together with dark field images and spectra of gold and silver nanocones in different sizes. The changes in unprotected and passivated silver cones with time will be illustrated by SEM and dark field images. [1] M. Fleischer et al.; Nanotechnology 21 (2010); 065301 [2] C. A. Barrios et al.; The Journal of Physical Chemistry C 113 (2009); 8158-8161

O 34.56 Tue 18:15 Poster E

Interaction of Light and Surface Plasmon Polaritons in Ag Islands Studied by Nonlinear Photoemission Microscopy — Philip Kahl, •Simone Wall, Niemma Buckanie, Pierre Kirschbaum, Simon Sindermann, Michael Horn-von Hoegen, and Frank-J. Meyer zu Heringdorf — Faculty of Physics and Center of Nanointegration Duisburg-Essen (CeNIDE), Universität Duisburg-Essen, Lotharstrasse. 1, 47057 Duisburg

Two Photon Photoemission Microscopy was used to study the interaction of femtosecond laser pulses with Ag islands on Si(111) and SiO_2. The fs laser pulses initiate surface plasmon polariton (SPP) waves at the edges of the island. The superposition of the electrical fields of the fs laser pulses with the electrical fields of the SPP results in a moiré pattern, the analysis of which gives access to the wavelength and direction of the SPP wave. If the SPPs reach edges of the Ag islands, they may be converted back into light waves. The incident and refracted light waves result in an interference pattern that can again be described with a moiré pattern, showing that Ag islands can be used as plasmonic beam deflectors for light.

O 34.57 Tue 18:15 Poster E

Calculation of enhanced up-conversion intensity from Er^{3+} ions near gold nanospheres — •Florian Hallermann[1], Stefan Fischer[2], Deepu Kumar[1], Alexander Sprafke[1], Jan Christoph Goldschmidt[2], and Gero von Plessen[1] — [1]Institute of Physics (1A), RWTH Aachen University, 52056 Aachen, Germany — [2]Fraunhofer ISE, Heidenhofstr. 2, 79110 Freiburg, Germany

In conventional silicon solar cells, photons with energies below the silicon band gap (1.12 eV) do not contribute to current generation. The near-infrared part of the solar spectrum could be exploited by using up-conversion processes, such as the excitation of electrons via sequential absorption of infrared photons in suitable rare-earth ions. The electrons subsequently relax from the final state by emitting photons whose energy is high enough to be absorbed in the silicon. Here, we show on the basis of model calculations by how much the up-conversion intensity from Er^{3+} ions can be enhanced using spherical gold nanoparticles. In the vicinity of the nanoparticles, the excitation rate of the ions is changed due to the near-field of the particles. In addition, the relaxation times of all involved excited states of the ions are changed by the presence of metal nanoparticles due to energy transfer from the ions to the nanoparticles, which offer additional radiative and nonradiative decay channels. We calculate the effects that these changes have on the up-conversion intensity by using Mie theory combined with a rate equation system. We find a 17% enhancement for the most prominent up-conversion line emitted by Er^{3+} ions that are distributed over a volume around a 200 nm particle.

O 34.58 Tue 18:15 Poster E

Theoretical and Experimental Studies of Surface Plasmon Polaritons on Gold Microstructures Using Photoemission Electron Microscopy — •Martin Piecuch[1], Christian Schneider[1], Daniela Bayer[1], Alexander Fischer[1], Pascal Melchior[1], Christoph Lemke[2], Michael Bauer[2], and Martin Aeschlimann[1] — [1]TU Kaiserslautern — [2]Christian-Albrechts-Universität zu Kiel

Collective electron excitations at metal surfaces are currently a rapidly developing research field. Surface plasmon polaritons (SPPs) for instance are promising candidates for future ultrafast subwavelength electronic devices. By using photoemission electron microscopy (PEEM), we investigate coherent excitations with spatial resolution which is well below the diffraction limit defined by the laser wavelength. Applying a laser pulse to a gold microstructure results in a beating pattern due to interference between the incident light source and excited SPPs which can be observed by PEEM. Using a phase stabilized Mach-Zehnder-interferometer that manipulates the excitation spectrum of the laser enables us to control the phase sensitive interference pattern. Theoretical simulations of the full electrical field with a fast algorithm based on the Huygens principle give insight into the underlying SPP dynamics. We show the high potential of the developed algorithm by a comprehensive comparison between experimental data and the simulation.

O 34.59 Tue 18:15 Poster E

Coherent Control of the Electron Emission from Metal Nanotips due to Ultrashort Laser Pulses — •Steve Lenk and Erich Runge — Institut für Physik und Institut für Mikro- und Nanotechnologien, Technische Universität Ilmenau, 98693 Ilmenau, Germany

Recent experiments show the possibility for a novel scanning microscope using ultrafast laser-induced photoelectron emission. The analysis of the experimental data requires a detailed theoretical knowledge of the emission process and the underlying physics. We investigate the electron emission from sharp gold nanotips illuminated by ultrashort femtosecond laser pulses theoretically. The emission processes under discussion for few-femtosecond laser pulses are multiphoton emission and optical field emission. We calculate the probability current and the Wigner distribution of the emitted electrons from a numerical solution of the time-dependent Schrödinger equation via a real-space product-formula algorithm. By the use of an optimization routine, we study the dependence of several target functions, like the emission current, on laser pulse properties and on confined potential energy profiles. By comparing experimental and theoretical findings, we can distinguish the dominant physical processes for different energy profiles and pulse shapes. Generally speaking, such investigation allow us to find optimized laser pulse properties to achieve the best electron emission characteristics for different experimental requirements.

O 34.60 Tue 18:15 Poster E

Far-field control of optical near-field enhancement — •Riko Kiessling, David Leipold, and Erich Runge — Technische Universität Ilmenau, 98693 Ilmenau, Germany

Controlling optical near-fields by shaping the temporal envolope of an incoming far-field laser pulse is a new and interesting topic with most promising applications in optical nano-circuitry. Recent experiments proof the possibility to tailor the near-fields in an arrangement of nano-antennas spatially and temporally [1].

In this theoretical work, we study how strong the fields near one out of some randomly arranged nano-anntennas can be enhanced. We quantify the relative near-field enhancement dependent on the number of far-field degrees of freedom allowed in the optimization. In particular, we consider superpositions of incident plane-waves with different frequencies, directions and polarizations. For this purpose, we explore a huge configuration space with a discrete-dipole approximation (DDA). DDA calculations are numerically cheap and inherently well suited for sytems of small antennas. The optimization itself is then performed semi-analytically.

[1] M. Aeschlimann, et. al, PNAS **107**, 5333 (2010)

O 35: Poster Session II (Polymeric biomolecular films; Nanostructures; Electronic structure; Spin-orbit interaction; Phase transitions; Surface chemical reactions; Heterogeneous catalysis; Particles and clusters; Surface magnetism; Electron and spin dynamics; Surface dynamics; Methods; Electronic structure theory; Functional molecules)

Time: Tuesday 18:15–21:45 Location: Poster B

O 35.1 Tue 18:15 Poster B

Interfacial behaviour of thin films of ionic liquids on mica — •Alexey Deyko, Florian Rietzler, Hans-Peter Steinrück, and Florian Maier — Lehrstuhl für Physikalische Chemie II, Egerlandstr. 3, Erlangen, 91058, Germany

We present a comprehensive study of ultrathin films of ionic liquids (ILs) deposited on mica surface. The ILs used are [C1C1Im][Tf2N] (1,3-dimethylimidazolium bis(trifuoromethyl)imide), and [C4C1Im][Tf2N] (1-butyl-3-octylimidazolium bis(trifuoromethyl)imide). These ILs can be successfully employed in a variety of electrochemical applications, for instance in solar cells. However, little information is available on the interfacial structure of ILs at charged surfaces. Due to its atomically flat surface and relatively simple preparation, mica is an ideal candidate for our studies. Ultra thin films of ILs in the sub-monolayer regime up to several nm thicknesses were prepared using a physical vapour deposition method under ultra high vacuum conditions. Employing angle resolved x-ray photoelectron spectroscopy (ARXPS), top and interface layers were probed with respect to adsorption behaviour, molecular orientation, and growth mode. It was found that the investigated ILs grow in a three-dimensional fashion and form islands on mica surface, even at coverages below one monolayer. That result is noticeably different to a case, when ILs are deposited on a metal surface, such as Au(111), where films grow in a layer-by-layer fashion wetting the Au surface. Supported by the DFG through SPP 1191 and by the Cluster of Excellence Engineering of Advanced Materials.

O 35.2 Tue 18:15 Poster B

Photonic Crystal Fibres Coated with Ionic Liquids in a Surface Science Approach — •Florian Rietzler[1], Till Cremer[1], Alexey Deyko[1], Florian Maier[1], Mathias Schmidt[2], Bastian Etzold[2], Peter Wasserscheid[2], and Hans-Peter Steinrück[1] — [1]Lehrstuhl für Physikalische Chemie II, Egerlandstr. 3, 91058 Erlangen — [2]Lehrstuhl für Chemische Reaktionstechnik, Egerlandstr. 3, 91058 Erlangen

Ionic liquids (ILs), organic salts with melting points below 100 °C, are often denoted as "green" solvents because of their extremely low vapour pressure. In catalysis one major problem of ILs is related to their high viscosity-induced mass transfer limitations. In the so-called Supported Ionic Liquid Phase concept this problem can be overcome by immobilizing a thin layer of IL on a solid support. Transferring this concept to Photonic Crystal Fibres (PCFs), i.e. coating the inner surface of light transmitting PCFs with a thin IL film, potentially allows in-situ monitoring of chemical reactions. Until now, the morphology of the IL film and the IL-glass interface is not well understood. In a surface science approach ultrathin films of the IL 1,3-dimethylimidazolium bis(trifluoromethylsulfonyl)imide were evaporated onto flat silica glass (as a model for the PCF surface) and investigated by ARXPS. In order to overcome the observed island formation of the IL on pristine Suprasil, two types of surface modifications were performed, both leading to a better wetting. This work was supported by DFG-SPP1191 and the Cluster of Excellence "Engineering of Advanced Materials".

O 35.3 Tue 18:15 Poster B

Silver nanosctructure formation in cinnamyl alcohol — •Sebastian Dahle[1,2], Lienhard Wegewitz[1,3], and Wolfgang Maus-Friedrichs[1,3] — [1]Institut für Physik und Physikalische Technologien, Technische Universität Clausthal, Leibnizstrasse 4, 38678 Clausthal-Zellerfeld, Germany — [2]Hochschule für Angewandte Wissenschaft und Kunst, Fakultät für Naturwissenschaften und Technik, Von-Ossietzky-Straße 99, 37085 Göttingen, Germany — [3]Clausthaler Zentrum für Materialtechnik, Technische Universität Clausthal, Leibnizstrasse 4, 38678 Clausthal-Zellerfeld, Germany

Metastable Induced Electron Spectroscopy, Ultraviolet Photoelectron Spectroscopy, X-ray Photoelectron Spectroscopy, and Atomic Force Microscopy have been employed to study the adsorption of silver and cinnamyl alcohol on Au(111) and Si(100) substrates. Initially, these investigations were carried out preceding the investigation of the adsorbtion behavior of silver on wood surfaces, where cinnamyl alcohol is used as precursor for lignin. Even though cinnamyl alcohol has only one technical application by now, some interesting properties of nanostructure formation and catalytic decomposition have been found.

O 35.4 Tue 18:15 Poster B

Inelastic tunnelling spectroscopy of protein monolayers — •Robert Lovrincic[1], Lior Sepunaru[1], Israel Pecht[2], and David Cahen[1] — [1]Department of Materials and Interfaces, Weizmann Institute of Science, Rehovot, Israel — [2]Department of Immunology, Weizmann Institute of Science, Rehovot, Israel

Electron transfer (ET) through proteins has been studied intensively in aqueous solutions. Based on our previous work on temperature-dependent current-voltage measurements across proteins in a solid-state configuration[1], we tried to gain deeper insight to the ET mechanism through macroscopic solid-state protein junctions, using inelastic tunnelling spectroscopy (IETS). IETS is a is an all-electronic spectroscopy that measures the vibronic structure of non-equilibrium molecular transport, where even Raman- and IR-forbidden transitions may be observed as strong bands. By assigning the observed peaks to known vibrations of the protein, we prove that at least some of the electrons actually pass through the proteins, a finding that presents a first step towards tracing the electron transport pathways through complex biomolecules.

1 L. Sepunaru, I. Pecht, M. Sheves, and D. Cahen, Journal of the American Chemical Society 133, 2421-2423 (2011).

O 35.5 Tue 18:15 Poster B

Covalently bonded mixed chains of Br-NDI and Br-TTP molecules — •Finn Lorbeer[1], Isabel Fernandez Torrente[1], Martina Corso[1], Lena Kaufmann[2], Max Kerbs[2], Arno Wiehe[2], Christoph A. Schalley[2], Andrew DiLullo[3], Saw-Wai Hla[3], José Ignacio Pascual[1], and Katharina J. Franke[1] — [1]Institut für Experimentalphysik, Freie Universität Berlin, Arnimallee 14, 14195

Berlin, Germany — [2]Insitut für Chemie und Biochemie, Freie Universität Berlin, Takustraß e 3, 14195 Berlin, Germany — [3]Dept. of Physics and Astronomy, Clippinger Lab 251B, Athens, OH 45701, USA

A promising route for the synthesis of a junction composed of a molecular charge donor and an acceptor on a surface resembling a diode, is the controlled formation of a covalent bond between individual organic donor and acceptor species. Here we use low temperature scanning tunneling microscopy (STM) and scanning tunneling spectroscopy (STS) to investigate the brominated naphthalenediimide (Br-NDI) and tetra(4-bromophenyl)porphyrin (Br-TPP) bond formation on Au(111).

For preparation temperatures of 300 K the Br-NDI and Br-TPP form H-bonded networks. Above 650 K annealing temperature we debrominate the two species and covalently bonded chains are formed. The electronic properties of the TPP remain unaffected after the bond formation. In contrast the flexible NDI molecule is geometrically distorted in the chains and the energy level alignment depends on this deformation as well as on the neighbors in the chain. We can change the geometric configuration of the NDI by vertical manipulation and hence shift the energy levels without affecting the covalent chains.

O 35.6 Tue 18:15 Poster B

Formation of Dysprosium clusters on Si(111)7x7 and Si(001)2x1 surfaces — •Martin Franz, Stephan Appelfeller, Michael Theurer, Monir Rychetsky, and Mario Dähne — Institut für Festkörperphysik, Technische Universität Berlin, Hardenbergstr. 36, D-10623 Berlin, Deutschland

Clusters on surfaces are of high interest because of their fascinating quantum properties and their possible application in future nanodevices or catalysis. Here, dysprosium induced clusters on the Si(111)7x7 and on the Si(001)2x1 surface were studied using scanning tunneling microscopy. The clusters were grown by molecular beam epitaxy using submonolayer metal coverages and moderate annealing temperatures. It was found that the 7x7 reconstructed Si(111) surface acts as a template for cluster formation, where the clusters grow self-organized preferentially on the faulted halves of the 7x7 unit cells. Here different cluster types could be observed, depending on the growth conditions. For post-growth annealing off-center clusters which are located at an edge of the 7x7 half unit cells form, while at deposition directly on the heated substrate the preferential growth of centered clusters is observed. On the Si(001) surface no such template effect exists. Here, clusters are observed that show a one-dimensional ordering resulting in the presence of cluster-chains on the surface. This project was supported by the DFG through FOR 1282 project D.

O 35.7 Tue 18:15 Poster B

Fabrication of nanostructures for detecting single nanoparticles using the meniscus-force-method — •Daniela Schön, Kathrin Kroth, Sabrina Darmawi, and Peter J. Klar — I. Physikalisches Institut, Justus-Liebig-Universität, Heinrich-Buff-Ring 16, DE-35392 Gießen, Germany

We present an array of holes that can be used for separating and arranging nanoparticles. The structure is created on a glass substrate via electron beam lithography (EBL), using PMMA as resist. In order to remove electrostatic charges during the EBL, a conductive polymer is applied on top of the PMMA. By creating a cavity array with lateral and vertical dimensions in the sub-micrometer range, particles with diameters smaller than 100 nm can be separated. A drop of a solution containing nanoparticles, such as TiO_2, CaO or ZnO, can be applied on top of the structure. During the evaporation of the drop the particles are drawn into the cavities by the meniscus-force. The structure containing the separated nanoparticles can be investigated by SEM and Raman imaging.

O 35.8 Tue 18:15 Poster B

Combined experimental STM and atomistic KMC modelling study of Ru cluster growth on graphene/Ru(0001) — •Albert K. Engstfeld[1], Christoph U. Lorenz[1], Harry E. Hoster[2], Yong Han[3], Jim W. Evans[3], and R. Jürgen Behm[1] — [1]Ulm University, Institute of Surface Chemistry and Catalysis, D-89069 Ulm, Germany — [2]Technische Universität München, Centre for Electromobility, 50 Nanyang Drive, Singapore 637553 — [3]Iowa State University, IPRT and Department of Physics & Astronomy, Ames, IA 50011 USA

The inhomogeneous potential energy surface (PES) for Ru on graphene/Ru(0001) leads to the formation of Ru clusters on specific trap sites within the moiré unit cells. We determine the fraction of populated moiré cells (versus coverage, deposition flux, and temperature), as well as the spatial distribution of clusters quantified by a SRO analysis. Behaviour is elucidated by KMC simulations of an atomistic model for cluster formation on a suitable non-uniform PES. The simulated evolution of the cluster density versus coverage, and the spatial cluster distribution, agree with experiments. An unusually weak dependence on deposition flux seen in experiment is not yet recovered by the current simulation parameters. Simulation also provides the cluster size distribution, not readily accessible with STM. Varying diffusion barriers for Ru used in the simulation are compatible with DFT results for Ru on flat graphene.

O 35.9 Tue 18:15 Poster B

Self-organized controlled positioning of nanoparticles based on the meniscus-force method — •Kathrin Kroth, Sabrina Darmawi, Torsten Henning, and Peter J. Klar — I. Physikalisches Institut, Justus-Liebig-Universität, Heinrich-Buff-Ring 16, DE-35392 Gießen, Germany

With the help of a periodic array of cavities, nanoparticles in solution can be separated and arranged. Arrays of cavities in the micrometer range were created in a thin layer of PMMA on a silicon substrate via EBL. A drop of solution containing nanoparticles, such as polystyrene-latex, Au and SiO_2 in the range of (300 ... 500) nm were deposited onto the array. During the evaporation of the drop the nanoparticles are shoved into the cavities by the meniscus-force. Since the meniscus-force is dependent on the contact angle, different surfactants were added to the solution. The approach of evaporating a thin film of metal on top of the structure was also used to manipulate the contact angle. A characterization of the particles inside the cavities was carried out via SEM and Raman mapping.

O 35.10 Tue 18:15 Poster B

Spin polarized surface states on stepped magnetic surfaces : ab-initio approach. — •Oleg Stepanyuk[1], Oleg Polyakov[1], and Valeri Stepanyuk[2] — [1]Faculty of Physics, Moscow State University, 119899 Moscow, Russia — [2]Max-Planck-Institut für Mikrostrukturphysik, Weinberg 2, D-06120 Halle, Germany

It was shown that surface states electrons become spin polarized above magnetic layers and nanoislands[1]. In the present work we perform the state of the art ab-initio studies of surface state electrons at steps of magnetic metals. We focus on steps of 3d metals on Cu(111) surface. We have revealed a spin-dependent charge transfer at step ages which is explained by Smoluchowski effect. Strongly inhomogeneous spin polarization of surface statates[1] at steps is revealed. Our results indicate that tunneling magnetoresistance at steps can exhibit very strong changes at the atomic scale. [1]* L. Diekhoner et. al. Phys. Rev. Lett. 90, 236801

O 35.11 Tue 18:15 Poster B

Characterization of Pt and Au nanoparticles on Fe3O4/Pt(111) thin film — •Alessandro Sala, Francesca Genuzio, Hagen Klemm, Thomas Schmidt, and Hans-Joachim Freund — Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, Germany

Pt and Au nanoparticles are catalytically active systems which show a peculiar strong metal-support interaction [1]. The formation of such nanoparticles over a iron oxide thin film has been observed in-situ and in real-time with SMART; this Low Energy and PhotoEmitted Electron Microscope can combine microscopy, spectroscopy and diffraction with high resolution and transmission to collect information about the morphology, the chemical distribution and the structural and electronic properties of complex systems. Particularly, XPEEM images reveal under particular conditions the formation by dewetting of FeO domains and the different nucleation of Au nanoparticles on this domains respect to the Fe3O4 area. LEEM, LEED, XPEEM and XPS permits to characterize the growth, the morphology and the electronic properties of Pt nanoparticles and their encapsulation by FeO, under different deposition conditions. [1] Z.-H. Qin, M. Lewandowski, Y.-N. Sun, S. Shaikhutdinov, and H.-J. Freund, J. Phys. Chem. C 2008, 112, 10209-10213

O 35.12 Tue 18:15 Poster B

Three-dimensional TiO2 nanotube arrays for photo-device application — •Ahmed al-Haddad[1,2], Yaoguo Fang[1], Huaping Zhao[1], and Yong Lei[1] — [1]Fachgebiet 3D-Nanostrukturierung, Institut für Physik & Zentrum für Mikro- und Nanotechnologien (ZIK MacroNano), Technische Universität Ilmenau, 98693 Ilmenau, Germany. — [2]Department of Physics, College of Science, University of

Al-Mustansiryah, Baghdad, Iraq

Thin films of high purity titanium were deposited on p-Si surface by physical vapour deposition (electron beam deposition) and followed by anodization of the deposited titanium thin film in an ethylene glycol solution at room temperature. TiO2 nanotubes are well aligned and organized into high-order uniform arrays. The morphology and crystallization of the resulting three-dimensional TiO2 nanotubes were investigated by scanning electron microscopy and X-ray diffraction. Current-voltage and capacitance-voltage characteristics and photo responsivity was measured for these arrays.

O 35.13 Tue 18:15 Poster B

Surface morphology of Silicon nanowires in dependence of different doping concentrations — •Stefan Weidemann, Ulrike Heiden, Jürgen Sölle, and Saskia Fischer — Neue Materialien, Institut für Physik, Humboldt-Universität zu Berlin, 12489 Berlin

Silicon nanowires (SiNWs) with rough surfaces have strongly decreased thermal conductivities and, hence, are promising candidates for thermoelectric devices [1]. However, the mechanism of formation of rough surfaces is still unclear and remains to be investigated. Here, we concentrate on producing NWs of defined length and study their structural and surface properties.

We fabricate SiNW arrays on wafer scale with tuneable lengths between 10-50 μm, and diameter in the range between 50-300 nm by the method of metal-assisted chemical etching [2]. We investigate the preparation of solid, rough and porous NW surfaces of different Boron-doped Si-substrates with resistivities of 5 mΩcm, 20Ωcm and >10kΩcm.

[1] A. I. Hochbaum et al., Nature 451, 163 (2008)

[2] M.-L. Zhang et al., J. Phys. Chem. C, 112 2008

O 35.14 Tue 18:15 Poster B

Manipulating and contacting single InAs Nanowires at GaAs edges — •Kilian Flöhr[1], Yusuf Günel[2], Kamil Sladek[2], Robert Frielinghaus[2], Hilde Hardtdegen[2], Carola Meyer[2], Marcus Liebmann[1], Thomas Schäpers[1,2], and Markus Morgenstern[1] — [1]II. Physikalisches Institut, RWTH Aachen and JARA Jülich Aachen Research Alliance, 52074 Aachen, Germany — [2]Peter Grünberg Institut, Forschungszentrum Jülich and JARA Jülich Aachen Research Alliance, 52425 Jülich, Germany

We investigated methods to spatially control InAs nanowires on a substrate using micromanipulators attached to an optical microscope with the goal of producing InAs tips for scanning tunneling microscopy. The wires, which were grown by metalorganic vapor phase epitaxy (MOVPE) on a GaAs wafer without catalysts, could be picked up individually using a sharp indium tip exploiting adhesion forces. Later, the wires were placed with submicrometer precision onto the desired position somewhere at the edge of a cleaved GaAs wafer or on other substrates, e.g. a perforated Si_3N_4 membrane [1]. We established a new method to realize ohmic contacts for partly suspended nanowires at the wafer edge with standard electron beam lithography.

[1] K. Flöhr, M. Liebmann, K. Sladek, H.Y. Günel, R. Frielinghaus, F. Haas, C. Meyer, H. Hardtdegen, Th. Schäpers, D. Grützmacher, M. Morgenstern, Rev. Sci. Instrum. 82, 113705 (2011)

O 35.15 Tue 18:15 Poster B

***p*- and *n*-type Silicon Nanowires from Metal-Assisted Chemical Etching** — •U. Heiden[1], J. Sölle[1], S. Weidemann[1], R. Heimburger[2], T Teubner[2], T. Boeck[2], R. Fornari[2], and S.F. Fischer[1] — [1]Neue Materialien, Institut für Physik, Humboldt-University zu Berlin, D-10099 Berlin — [2]Leibniz-Institut für Kristallzüchtung, Max-Born-Str. 2, D-12489 Berlin

Metal-assisted chemical etching (MACE) is a top-down procedure to form silicon nanowires (SiNWs) [1]. A precise control of etching parameters and the understanding of their influence on the nanowire morphology are topical research issues. They are extremely important to achieve process reproducibility.

Vertical and single crystalline SiNWs were produced with a two-step MACE procedure. Silver nanoparticles are used as catalyst. The etchant includes hydrofluoric acid (HF) and hydrogen peroxide (H_2O_2). We investigate the difference between highly doped p and n SiNWs regarding to the length, porosity and their density on the wafer.

p-type SiNWs are longer and show a higher density on the wafer compared to n-type NWs. Longer etching times lead to longer NW lengths. Increasing the concentration of H_2O_2 in the etchant, accelerates the etching reaction and decreases the NW density. A higher growth rate causes the NWs to stick together at the top and form sheaves which is in accordance with the previous report in [1].

[1] M. Zhang et al., J. Phys. Chem. C 112, 4444-4450 (2008).

O 35.16 Tue 18:15 Poster B

Stability of In/Si(111)-(4x1) nanowires — •Martin Babilon, Stefan Wippermann, Uwe Gerstmann, and Wolf Gero Schmidt — Universität Paderborn, Germany

Quasi one-dimensional structures, such as artificial atomic-scale wires, have attracted considerable attention recently [1]. They do not only show fascinating physical properties, but also have a large technological potential, e.g., as atomic-scale interconnects. Highly anisotropic surface superstructures are suitable model systems to explore atomic-scale wires both experimentally and computationally. The In/Si(111)-(4x1) surface [2, 3] is probably the most intensively investigated system in this context.

In this work, we present first-principles calculations on the influence of relativistic effects affecting the stability of (4x1) and (8x2) surface. A reversible phase transition from the metallic Si(111)-(4x1)-In zigzag chain structure to an insulating (8x2) reconstruction below 125 K is observed [4]. Here, our goal is to investigate the influence of relativistic effects and the treatment of the In core electrons on the phase transition temperature.

[1] N. Nilius, T. M. Wallis and W. Ho, Science 297, 1853 (2002).

[2] O. Bunk et al., Phys. Rev. B 59, 12228 (1999).

[3] S. Wippermann, N. Koch, W. G. Schmidt, Phys. Rev. Lett. 100, 106802 (2008).

[4] A. A. Stekolnikov, K. Seino, F. Bechstedt, S. Wippermann, W. G. Schmidt, Phys. Rev. Lett. 98, 026105 (2007).

O 35.17 Tue 18:15 Poster B

Tomonaga-Luttinger Liquid Behavior in Au/Ge(001) Nanowires — •Sebastian Mietke[1], Christian Blumenstein[2], Jörg Schäfer[2], Sebastian Meyer[2], Michael Lochner[1], René Matzdorf[1], and Ralph Claessen[2] — [1]Fachbereich Naturwissenschaften, Experimentalphysik II, Universität Kassel, 34132 Kassel, Germany — [2]Physikalisches Institut, Universität Würzburg, 97074 Würzburg, Germany

Atomic nanowires formed by self-organization of metal adatoms on semiconductor surfaces offer a vast playground for physics in low dimensions. Recently, Au-induced chains on Ge(001) have been found to exhibit Tomonaga-Luttinger liquid behavior (TLL) [1], which has not been found in a surface system before. Here we scrutinize the electronic properties of these Au chains by scanning tunneling spectroscopy (STS) and angle-resolved photoemission (ARPES) over a wide temperature range. Density of states maps reveal a 1D conduction path in real space, thereby clearly identifying conducting filaments in chain direction over a wide energy range. A power-law behavior upon energy is found in the density of states, characteristic of a TLL. The corresponding exponent α is found independently by both STS and ARPES. Furthermore, *universal scaling behavior* is observed as a hallmark of TLL physics. This renders the Au/Ge(001) chains the first TLL system at a surface, opening new possibilities to probe modified interactions from specific atomic configurations. [1] Nature Physics, Vol. 7, 776-780 (Oct. 2011).

O 35.18 Tue 18:15 Poster B

Sensitive gas sensor device obtained from the combination of 3D surface nano-patterns technique with atomic layer deposition — Zhibing Zhan[1,2], Yan Mi[1,2], Hui Sun[1,2], Fabian Grote[1,2], Huaping Zhao[1,2], and •Yong Lei[1,2] — [1]Fachgebiet 3D-Nanostrukturierung, Institut für Physik & Zentrum für Mikro- und Nanotechnologien (ZIK MacroNano), Technische Universität Ilmenau, 98693 Ilmenau, Germany — [2]Institut für MaterialPhysik, Westfälische Wilhelms-Universität Münster, 48149 Münster, Germany

Combined atomic layer deposition (ALD) with an innovative three-dimensional (3D) surface nano-structuring technique, ultrathin alumina membranes (UTAMs), we obtained a gas sensor device with sensitivity reaching PPB level to NO2. To our knowledge, this value has not been reported before for commercial gas sensors. Due to the characteristic of high regularity and controllability from ALD and our 3D nano-patterns technique, it is feasible to investigate the surface chemistry and physics, and hence to optimize the parameters of the gas sensor device. Our method used to prepare this gas sensor device is compatible to semiconductor device industry, which exhibit tremendous application potentials in the fields of environmental protection and atmospheric quality monitoring.

O 35.19 Tue 18:15 Poster B

Confined metallic thin films obtained by epitaxy on Si nanorods — •Lisa Kühnemund, Christoph Tegenkamp, and Herbert Pfnür — Institut für Festkörperphysik, Leibniz Universität Hannover

Understanding the properties of structures on the nanoscale is the key to realize miniaturization in electronic systems. Transport and local spectroscopy of thin but spatially extended Ag layers performed so far have revealed that indeed the morphology in metallic films is essential for (mesoscopic) transport [1,2]. We are interested in the effect of confining these films to structures on the nanoscale. This enables us to control also the current paths and monitor the effective defect structures.

To obtain these structures we used Si nanorods as masks for growing constricted nano-sized Ag films. The Si nanorods of 1μm in length and 100 nm in diameter [3] were transferred, after an HF-dip, onto Si substrates. The deposition of Ag at low temperatures reveals metallic and contiguous films of a few atomic layer thickness. First results of this technique as well as local transport measurements obtained by means of a 4 point probe STM-SEM system will be presented.

[1] M. Henzler et al., Phys. Rev. B **58**, 10046 (1998).

[2] J. Schmeidel et al., Phys. Rev. B **80**, 115304 (2009).

[3] The Si rods were grown by phase shift lithography and plasma etching at the IMTEK, Freiburg.

O 35.20 Tue 18:15 Poster B

Large area Zirconium carbide surface nanopatterns towards smart sunlight-heat conversion — Zhenyang Wang[1,2], Hui Sun[1,2], Yan Mi[1,2], Fabian Grote[1,2], Huaping Zhao[1,2], and •Yong Lei[1,2] — [1]Fachgebiet 3D-Nanostrukturierung, Institut für Physik & Zentrum für Mikro- und Nanotechnologien (ZIK MacroNano), Technische Universität Ilmenau, 98693 Ilmenau, Germany. — [2]Institut für MaterialPhysik, Westfälische Wilhelms-Universität Münster, 48149 Münster, Germany

Manipulation and/or conversion of sunlight energy are eternal research topics, since the inexhaustible solar energy is one of the most ideal candidates to conquer the increasingly terrible energy sources crisis. In this work, highly regular ZrC nanopatterns were assembled, by combination of an atomic layer deposition (ALD) and ultra-thin alumina membranes (UTAMs). The as-grown ZrC nanopatterns are in large area up to several square centimeters, and can be self-supported. Assisted with the sacrificed zinc oxide, size and spacing of the nanopatterns can be manipulated in even larger scale. Solar thermal property investigation shows that this kind of carbide of the transition metal can efficiently convert the sunlight into heat. This kind of nanopatterns has great potential in both solar-thermo usage and solar-thermo enhanced thermo-chromic smart windows.

O 35.21 Tue 18:15 Poster B

Single one-dimensional nanolines and atom chains on the semiconductiong Si(001) surface — •Sigrun A. Köster[1], François Bianco[1], James G. H. Owen[1], David R. Bowler[2], and Christoph Renner[1] — [1]University of Geneva, Switzerland — [2]University College London/London Centre of Nanotechnology, UK

Single-atom chains on a wide gap substrate are a very attractive embodiment of a truly one-dimensional system to explore the remarkable physical properties emerging in such low dimensions. We present examples of self-assembled one-dimensional systems on the Si(001) surface, that is, Bi nanolines [1], Haiku stripes [2,3] and single atom Mn chains. All lines grow perpendicular to the Si(001) dimer rows, at densities which can be adjusted by means of the growth parameter. Therefore we can establish chains isolated on a semiconducting background or produce a dense array of possibly interacting chains. High resolution scanning tunneling microscopy (STM) micrographs are in perfect agreement with density functional theory (DFT), providing detailed insight into the chain structures. We further discuss low temperature STM spectroscopy suggesting that our chains are indeed suitable candidates to investigate the electronic properties in one dimension.

[1] J. H. G. Owen, K. Miki, D. R. Bowler, J. Mater. Sci. **41** (2006) 4568

[2] F. Bianco, J. H. G. Owen, S. A. Köster, D. Mazur, Ch. Renner and D.R. Bowler, Phys. Rev. B **84**, 035328 (2011)

[3] J. H. G. Owen, F. Bianco, S. A. Köster, D. Mazur, D. R. Bowler and Ch. Renner, Appl. Phys. Lett. **97** (2010) 093102

O 35.22 Tue 18:15 Poster B

Fabrication and the characterization of the electrical, optical and field emission properties of regular ZnO and PbSe nanowires arrays — •Yaoguo Fang[1,2], Kin Mun Wong[1,2], André Devaux[3], Liaoyong Wen[1,2], Luisa De Cola[3], and Yong Lei[1,2] — [1]Fachgebiet 3D-Nanostrukturierung, Institut für Physik & Zentrum für Mikro- und Nanotechnologien (ZIK MacroNano), Technische Universität Ilmenau, 98693 Ilmenau, Germany. — [2]Institut für Materialphysik, Westfälische Wilhelms-Universität Münster, 48149 Münster, Germany. — [3]Physikalisches Institut, Westfälische Wilhelms-Universität, 48149 Münster, Germany.

ZnO nanowires (NWs) and nanostructures of different length and shape were fabricated on silicon substrates by different methods such as chemical vapour deposition (CVD), hydrothermal or by chemical etching of the NWs grown by the CVD process. Well aligned ZnO NWs arrays of different length and size could be obtained by the CVD method and the shape of the NWs could be modified by chemical etching which produces needlelike ZnO NWs arrays. Conversely, doping the ZnO NWs with indium produces leaf-like ZnO nanostructures. With the use of the dry contact printing method, the regular and long ZnO NWs arrays could be used for the realizations of the NWs in Schottky device applications. In addition, the electrical, optical, stoichiometric, doping concentrations, field emission as well as the defect properties of the different morphologies of the ZnO nanostructures were obtained by a number of different spectroscopic techniques. On the other hand, p-PbSe nanowire arrays have also been fabricated and characterized.

O 35.23 Tue 18:15 Poster B

Fabrication and Characterization of Self-Assembled and Self-Aligned Single-Walled Carbon Nanotubes — •Harald Budde, Nicolai Hartmann, Nina Rauhut, and Achim Hartschuh — Department Chemie und CeNS, LMU, München, Germany

We report on the fabrication of horizontally aligned single-walled carbon nanotube arrays and their electro-optical properties. The arrays were obtained via a simple solution-based evaporation method on different substrates and were characterized by atomic force and optical microscopy [1, 2]. The nanotube alignment was determined by polarization-sensitive photoluminescence (PL) measurements. Electrically contacted arrays exhibit ohmic transport characteristics. Upon applying a bias voltage, electroluminescence (EL) from semiconducting nanotubes could be detected [3]. We investigate the bias dependence of the electroluminescence and compare PL and EL spectra for the same sample position. Arrays of aligned nanotubes are rather robust and bright sources of broad range emission as compared to single nanotubes and could be useful for optoelectronic applications.

[1] P. Yunker, T. Still, M. Lohr, A. Yodh, Nature 476, 308-311, 2011.

[2] M. Engel, J. Small, M. Steiner, M. Freitag, A. Green, M. Hersam, P. Avouris, ACS Nano 2 (12), 2445-2452, 2008.

[3] M. Freitag, J. Chen, J. Tersoff, J. Tsang, Q. Fu, J. Liu, P. Avouris, Phys. Rev. Lett. 93 (7), 076803, 2004.

O 35.24 Tue 18:15 Poster B

Embedding Nanowires by means of Spin Coating — •Jan Schmidtbauer, Franziska Schuette, Roman Bansen, Thomas Teubner, and Torsten Boeck — Leibniz-Institute for Crystal Growth

Nanowires are promising structures for future optoelectronic devices as well as for thermoelectric applications, gas sensors and Li-ion batteries. Typically, nanowires are removed from the substrate for electric characterization. However, contacting nanowires turns out to be challenging without removing them from the substrate. For this purpose, embedding nanowires in an insulating matrix which is protruded by the nanowire tips can provide a promising way to contact the wire using an AFM. We propose an embedding process by means of spin coating hydrogen silsesquioxane (HSQ) and curing the layer subsequently. The curing process is conducted at temperatures up to 700°C. Thus, the HSQ layer transforms from a Si-O-Si cage-like structure into a Si-O-Si network (SiO_2). Different approaches are compared to uncover the nanowire tips.

O 35.25 Tue 18:15 Poster B

Directional photochemical growth in gold nanoparticle arrays — •Susan Derenko[1], Andrew Sarangan[2], and Thomas Härtling[1] — [1]Fraunhofer Institute for Nondestructive Testing, Dresden Branch, Maria-Reiche-Str. 2, 01109 Dresden, Germany — [2]Electro-Optics Program, University of Dayton, 300 College Park, Dayton, Ohio, USA

Plasmonic nanoparticle arrays are interesting building blocks for optical sensors. For their integration into devices one may wish to modify their geometry locally within an array to tune the surface plasmon resonance in certain array sections. We present a method to induce local particle growth by exposure of lithographically fabricated Au-nanoparticle arrays to a HAuCl4 solution. Illumination of the system activates the gold ions in solution, whereas the nanoparticles act as seeds and induce particle growth. We monitor the modification via the shift of the plasmon resonance wavelength. For discoidal particles a growth preferentially perpendicular to the array plane is obtained resulting in a blue-shifted resonance. These findings are supported by AFM and SEM measurements and simulations.

O 35.26 Tue 18:15 Poster B

Coupling of plasmons to molecular excitons — •Hongdan Yan[1], Peter Lemmens[1], Johannes Ahrens[2], Martin Bröring[2], Sven Burger[3], Gerhard Lilienkamp[4], Winfried Daum[4], Ulrich Krieg[5], Herbert Pfnür[5], Fatih Kalkan[5], Karina Morgenstern[5], Aidin Lak[6], and Meinhard Schilling[6] — [1]IPKM, TU-BS, Braunschweig, Germany — [2]IAAC, TU-BS, Braunschweig, Germany — [3]ZIB, Berlin, Germany — [4]IEPT, TU Clausthal, Germany — [5]FKP, LU Hannover, Germany — [6]EMG, TU-BS, Braunschweig

We investigate plasmon/molecule interaction using Au nanowire arrays that have strongly polarized plasmonic modes. The energy of the longitudinal mode is tuned by varying the aspect ratio of the nanowires. A coupling to molecular excitons is evident from an analysis of the lineshape of the optical absorption. Theoretical modelling of the plasmonic spectrum confirms our experimental findings. Work supported by B-IGSM and NTH School for Contacts in Nanosystems.

O 35.27 Tue 18:15 Poster B

Instability types at ion-assisted alloy deposition: from surface to bulk nanopatterning — Gintas Abrasonis[1] and •Klaus Morawetz[2,3] — [1]Institute of Ion Beam Physics and Materials Research, Helmholtz-Zentrum Dresden Rossendorf, PF 51 01 19, 01314 Dresden, Germany — [2]Münster University of Applied Sciences, Stegerwaldstrasse 39, 48565 Steinfurt, Germany — [3]International Institute of Physics (IIP) Av. Odilon Gomes de Lima 1722, 59078-400 Natal, Brazil

Ion irradiation assistance of the film growth has a strong impact on structural properties. Here, we demonstrate that ion irradiation of growing binary alloys leads to the formation of composition-modulated surface patterns. Be means of linear stability analysis we show that the ion-to-atom arrival ratio is the pattern control parameter. Close to the instability threshold we identify different regimes of instabilities driven by ion-induced surface roughness processes or roughness-composition feedback interactions. In particular, the synergistic effects of the curvature-dependent displacement coupling to the preferential sputtering or to the diffusivity are found to induce instabilities and pattern formation. Depending on the film growth and ion-irradiation conditions the instabilities show stationary or oscillating behavior. This presents opportunities to grow 3D laterally or vertically ordered nanostructures.

O 35.28 Tue 18:15 Poster B

Diamond-Like Carbon Coatings on Industrial Polyethylene Surfaces — •Magdalena Rohrbeck[1], Christian B. Fischer[1], Stefan Wehner[1], Matthias Richter[2], and Dieter Schmeisser[2] — [1]Universität Koblenz-Landau, IfIN - Physik, 56070 Koblenz, Germany — [2]BTU Cottbus, Angewandte Physik II / Sensorik, 03046 Cottbus, Germany

Synthetic materials are used in a wide variety of fields. Depending on the intended application the plastic material must meet specific requirements. Since the material always interacts with its environment, particular attention is required regarding the surface. Possible damage of the plastic material and further risks could be caused by the adhesion of bacteria, biofilm formation and encrustations. Therefore, bacteria-repellent coatings and surface-modified materials that allow for an effective removal of adhered bacteria are of extremely high interest for many applications. In this study Polyethylene (PE) is chosen as simplest model for relevant plastic materials. Surface modification of PE samples is accomplished by plasma-deposited diamond-like carbon (DLC) coatings to achieve increased abrasion strength and bacterial resistance. Two types of nanometer-scaled DLC films with different layer thicknesses are compared by multiscale microscopic analysis. Further spectroscopic measurements with synchrotron radiation are performed. These results will provide an enhanced understanding of layer formation at the interface between the basic plastic material and the DLC coating and will possibly lead to optimal parameters for the surface coating to achieve improved product characteristics.

O 35.29 Tue 18:15 Poster B

Replication of nanometer size structures by laser embossing in thin metal foils — •Martin Ehrhardt, Pierre Lorenz, and Klaus Zimmer — Leibniz Institut für Oberflächenmodifizierung, Permoserstr. 15, 04318 Leipzig

Laser embossing is a micromanufacturing technology which enables the direct fabrication of three dimensional structures in metal foils. In the present study a novel arrangement of pulsed laser microembossing is introduced which allows a more flexible fabrication process with laser microembossing. To demonstrate the capability of the manufacturing process micro and nanostructures were successfully transferred from moulds into silver and copper foils by using UV Excimer laser pulses. The replicated patterns had high accuracy regarding the shape and the spatial resolution. An almost linear correlation between the used laser fluence and the height of the embossed microstructures was observed for both investigated materials. The achieved surface qualities were analysed with scanning electron microscopy (SEM), Atomic Force Microscopy (AFM) and reflection measurements.

O 35.30 Tue 18:15 Poster B

Complex quantum well states/resonances in magnetic thin films — •Christoph Seibel[1], Andreas Nuber[1], and Friedrich Reinert[1,2] — [1]Physikalisches Institut, Experimentelle Physik VII und Wilhelm Conrad Röntgen Research Center for Complex Material Systems (RCCM), Universität Würzburg, D-97074 Würzburg — [2]Gemeinschaftslabor für Nanoanalytik, Karlsruher Institut für Technologie KIT, D-76021 Karlsruhe

Low dimension effects are attracting more interest as they are becoming more relevant for future applications. In particular ultra thin Ni or Fe films are suitable model systems for nanostructured magnetic devices.

Using angle-resolved photoelectron spectroscopy (ARPES) we measured quantum well states/resonances in the close vicinity to the Fermi energy along high symmetry directions and the Fermi surface of the Fe/W(110) and Ni/W(110) films. In Fe/W(110) we find minority quantum well states, which are highly anisotropic in their dispersion due to the rather weak structural anisotropy of the bcc (110) crystal surface. Due to hybridisation effects of the measured quantum well states in Ni/W(110), the origin of the apparent splitting remains to be discussed.

O 35.31 Tue 18:15 Poster B

Two-site Kondo effect in atomic chains — Nicolas Néel[1], Richard Berndt[1], •Jörg Kröger[2], Tim Wehling[3], Alexander Lichtenstein[3], and Mikhail Katsnelson[4] — [1]University of Kiel, Germany — [2]Technical University of Ilmenau, Germany — [3]University of Hamburg, Germany — [4]University of Nijmegen, The Netherlands

Linear $\mathrm{CoCu}_n\mathrm{Co}$ clusters on Cu(111) are fabricated by means of atomic manipulation. They represent a two-site Kondo system with tunable interaction. Scanning tunnelling spectroscopy reveals oscillations of the Kondo temperature T_K with the number n of Cu atoms for $n \geq 3$. Density functional calculations show that the Ruderman-Kittel-Kasuya-Yosida interaction mediated by the Cu chains causes the oscillations. Calculations find ferromagnetic and antiferromagnetic interaction for $n = 1$ and 2, respectively. Both interactions lead to a decrease of T_K as experimentally observed. Financial support through SFB 668 is acknowledged.

O 35.32 Tue 18:15 Poster B

X-ray spectroscopic investigation of $\mathbf{YVO_3}$ — •Olga Schuckmann[1], Stefan Bartkowski[1], Anna Buling[1], Christine Derks[1], Karsten Küpper[2], Stephen Blundell[3], Ewa Talik[4], and Manfred Neumann[1] — [1]Fachbereich Physik, Universität Osnabrück, Germany — [2]Abteilung Festkörperphysik, Universität Ulm, Germany — [3]Clarendon Laboratory, University of Oxford, United Kingdom — [4]University of Silesia, Institute of Physics, Katowice, Poland

Orthovanadate $\mathrm{YVO_3}$ is a particularly interesting material, due to multiple orbital-, spin ordering and structural phase transitions as a function of temperature. The dynamic of such phase transition plays a key role in optical rewritable data storages, due to the limitation of the switching rate by the phasechange rate.

Moreover YVO_3 is a strongly correlated electron system, thus the interplay between the kinetic energy and Coulomb interaction manipulates the electronic and magnetic properties of matter. Due to the strong correlation between d electrons a variety of physical properties, such as Mott transition and so insulating phases, can occur.

By means of X-ray spectroscopic techniques XPS, XES and XAS, the electronic structure and microscopic formation of physical properties of YVO_3, as the origin of the band gap, satellites and the valence states are investigated. As a first result we identified YVO_3 as a real Mott-insulator with a nominal band gap of minimum 1.1 eV.

O 35.33 Tue 18:15 Poster B

Formation of an ideal Schottky barrier by Au/n-type β-Ga_2O_3

— •Mansour Mohamed[1], Christoph Janowitz[1], Klaus Irmscher[2], and Recardo Manzke[1] — [1]Institute of Physics, Humboldt University of Berlin, Newtonstr. 15, D-12489 Berlin, Germany — [2]Leibniz Institute for Crystal Growth, Max-Born-Str. 2, D - 12489 Berlin, Germany

High resolution angular-resolved photoelectron spectroscopy (ARPES) was applied to study the formation of a Schottky barrier on cleaved β-Ga_2O_3 single crystals with a carrier concentration of $6x10^{16}$ cm^{-3}, which were grown by the Czochralski method. A coverage-dependent surface photovoltage effect induced by the synchrotron radiation was observed. The shift of the valence band- and semicore- states at low Au- coverage and the work functions of Au and β-Ga_2O_3 were determined in situ by ARPES. From these experimental data the Schottky barrier height was found to be 1.01 eV in nearly perfect agreement to the value of 1.07 eV obtained from the current-voltage characteristics. The system Au/n-type β-Ga_2O_3 matches nearly ideally the characteristics of a pure Schottky barrier.

O 35.34 Tue 18:15 Poster B

Spin-orbit splitting in the valence bands of ZrS_xSe_{2-x}

— •Mohamed Moustafa, Ali Ghafari, Christoph Janowitz, and Recardo Manzke — Institut für Physik, Humboldt Universität zu Berlin, Newtonstr. 15, D-12489 Berlin, Germany

Angle-resolved photoemission spectroscopy using synchrotron radiation was performed for ternary layered transition metal dichalcogenides ZrS_xSe_{2-x}, where x varies from 0 to 2. A characteristic splitting of the chalcogen p-derived valence bands along high symmetry directions was observed. The splitting size at the A point of the Brillouin zone is found to increase from 0.06 eV to 0.31 eV with increasing atomic number of the chalcogenide as progressing from ZrS_2 towards $ZrSe_2$, respectively. An almost linear behaviour of the splitting size upon the composition parameter x is observed. Our electronic structure calculations based on the density functional theory prove that this splitting is due to spin-orbit (SO) coupling. When considering spin-orbit coupling, the degeneracy of the valance bands is lifted.

O 35.35 Tue 18:15 Poster B

Two dimensional Rare-Earth ordered alloys

— •Lucia Vitali[1,2] and Enrique Ortega[1,3] — [1]Material Physics Center- University of Basque Country, San Sebastian (Spain) — [2]Ikerbasque Foundation, Bilbao (Spain) — [3]Fisica Aplicada, University of Basque Country (spain)

The reported fast magnetization/demagnetization, key features for spintronics and data storage, has raised the scientific and technological interest for thin ferromagnetic layers supported on non-magnetic metal-substrates. The physical principle behind these observations is the interaction between quasi-particles and the role of the interface. Recent work has reported on the formation of a new ordered stoichiometric alloy of GdAu2 formed by deposition of Gd atoms on Au(111) surface at high temperatures [1]. The observed layer by layer growth shows different structural, electronic and magnetic properties with respect to bulk GdAu2 structure although the stoichiometric structure is preserved. Indeed, contrary to the antiferromagnetic behaviour of this alloy as bulk material, the first two layers of GdAu2 grown on Au(111) show a ferromagnetic character [1]. Here, we report that, similarly to GdAu2, also GdAg2 and GdCu2 surface alloys can be obtained. Topographic and spectroscopic characterization of the local density of state of the three epitaxially grown surface alloys of Gd have been performed with a commercial 1K-STM. Here, the similarity and peculiarity of these surface alloys will be explained in terms of the influence of the s, p and d orbitals of the supporting substrates. [1] M.Corso, et al. PRL 105, 016101 (2010)

O 35.36 Tue 18:15 Poster B

Two-dimensional fitting data analysis in Angle-resolved photoemission spectroscopy

— •Lucas Barreto, Richard Hatch, Marco Bianchi, and Philip Hofmann — Department of Physics and Astronomy, Interdisciplinary Nanoscience Center, Aarhus University, 8000 Aarhus C, Denmark

Angle-resolved photoemission spectroscopy (ARPES) is a well-established technique used to investigate the electronic properties of materials. ARPES data is frequently analyzed by considering scans taken at fixed emission-angle (EDC) or binding energy (MDC). In a number of cases, however, this approach does not permit one to extract all the useful information and may even lead to a misinterpretation of results [1]. Furthermore, recent ARPES developments have heightened the importance of analyzing the entire two-dimensional data set. Assuming an initial dispersion and a self-energy, the spectral function is calculated and then, using a search procedure, the parameters are optimized in order to obtain a good agreement between the measured and calculated spectra. The customary way to perform this search is to minimize χ^2. In this work, we propose an alternative way of comparing the calculated and the measured spectra that gives more weight to the regions with higher intensities by using derivatives. We will present results of both methodologies for ARPES measurements on Bi_2Se_3 exposed to CO [2] and compare the two methods in order to verify the applicability of the suggested approach.

[1] I. A. Nechaev et al. PRB, **80**,113402 (2009).

[2] M. Bianchi et al. PRL,**107**,086802 (2011).

O 35.37 Tue 18:15 Poster B

Nitridation of diamond - a possible way to n-type surface-conductivity?

— •Nora Jenny Vollmers, Uwe Gerstmann, and Wolf Gero Schmidt — Theoretische Physik, Universität Paderborn

Diamond has a lot of outstanding qualities but the lack of a suitable n-type donor has hindered this material to gain broad technological application. Nevertheless, nitrogen doping was already successfully used to improve the emission behavior of field emission devices based on a-C:H diamond thin films [1, 2, 3]. In this theoretical work we want to propose a possible way to n-type surface conductivity at the clean diamond (001) (2×1) reconstructed surface which consists of flat dimer rows. Using density functional theory together with the Quantum ESPRESSO PWscf package [4], we compare the electronic and magnetic properties for different N incorporation depths. Built-in directly at the surface, N gives rise to localized surface states similar to intrinsic carbon dangling bond-like states. Otherwise N is able to introduce surface conductivity as demonstrated by ab initio calculated effective mass tensors. In addition, the extreme anisotropy of the effective mass tensor comparable with those of metallic indium-chains on silicon substrates indicates the possibility to achieve n-type 1D surface-conductivity along the dimer-chains.

[1] R.S. Balmer et al., J. Phys.: Cond. Matt. 21, 364221 (2009).

[2] J. Xu et al., Appl. Phys. A 80, 123 (2005).

[3] M. Kaukkonen et al., Phys. Rev. Lett. 83, 5346 (1999).

[4] Ch.J. Pickard, F. Mauri, Phys. Rev. Lett. 88, 086403 (2002).

O 35.38 Tue 18:15 Poster B

Electronic spectrum of pure and doped Si(111)-(2x1) surfaces

— •M. Pötter[1], M. Rohlfing[1], K. Löser[2], M. Wenderoth[2], T.K.A. Spaeth[2], J.K. Garleff[2], and R.G. Ulbrich[2] — [1]Fachbereich Physik, Universität Osnabrück — [2]IV. Physikalisches Institut, Universität Göttingen

We discuss the electronic structure of the Pandey-chain terminated Si(111)-(2x1) surface, as resulting from density-functional theory and from the GW approximation of many-body perturbation theory. Our theoretical investigations are complemented by experimental scanning-tunneling microscopy and spectroscopy studies. We focus on two issues:

(i) The Pandey chain can be buckled in two possible configurations (positive and negative buckling). The corresponding electronic spectra show distinctively different fundamental gaps, that can be used to identify the buckling.

(ii) When Pandey-chain Si atoms are substituted by phosphorus (e.g. from n-type doping), the geometry and potential are modified, and the additional electron further changes the electronic structure of the system. We discuss the spatial and spectral signatures of this modification.

O 35.39 Tue 18:15 Poster B

Photo-induced tunneling current microscope setup for UHV

applications — •Uwe Schmitt, Andreas Englisch, and Uwe Hartmann — Institute of Experimental Physics, Universität des Saarlandes, P.O. Box 15 11 50, D-66041 Saarbrücken

In order to measure photo-induced tunneling currents on clean metal and semiconductor surfaces an UHV-STM-system was completed with suitable optical components which allows a simultaneous illumination of the sample with two wavelengths. The wavelengths can be modulated in the intensity with different modulation frequencies in order to detect the influence of both wavelengths with a lock-in-amplifier. The modulation deep can be chosen in a way that the DC-part of the light intensity determines the time independent photo conductivity and consequently the tunnel gap which is controlled by the feed-back-loop. In the original UHV-system (Omicron VT-STM) the Scala-electronic was replaced by a low cost controller from Soft dB.

O 35.40 Tue 18:15 Poster B

Cluster Models for Surface Reactions on Copper Oxide

— •Martin Schmeisser[1], Jörg Schuster[2], Stefan E. Schulz[1,2], Ulrich Biedermann[3], and Alexander Auer[1,3] — [1]Chemnitz University of Technology, Gemany — [2]Fraunhofer ENAS, Chemnitz, Germany — [3]Max-Planck Institute for Iron Research, Düsseldorf, Germany

Copper is the most widely used material in semiconductor interconnect technology. Atomic Layer Deposition has recently been proposed as a means to deposit copper oxide on nanostructured surfaces with high aspect ratio for possible integration in the metalization step of device fabrication. A reduction step is required to convert the deposited copper oxide film into metallic copper. Several reduction agents have been used but little experimental data is available on the reduction reaction pathways.

Thus, a theoretical investigation has been started to model reduction reactions on a copper oxide surface. As a starting point different cluster model systems of a Cu2O surface have been proposed and tested for consistency with system size and against similar slab models. Adsorption mechanisms of formic acid were investigated and stable adsorbed structures are reported. A few reactions of an adsorbed formic acid molecule were modeled within a synchronous transit scheme at the b-p/TZVP level of theory.

O 35.41 Tue 18:15 Poster B

Topographic deconvolution of molecular photoemission spectra

— •Serguei Soubatch[1], Peter Puschnig[2,3], Eva Reinisch[3], Thomas Ules[3], Georg Koller[3], Markus Ostler[4], Lorenz Romaner[2], Claudia Ambrosch-Draxl[2], Stefan Tautz[1], and Michael Ramsey[3] — [1]Peter Grünberg Institut, Forschungszentrum Jülich — [2]Chair of Atomistic Modeling and Design of Materials, Montanuniversität Leoben — [3]Institut für Physik, Karl-Franzens Universität Graz — [4]Lehrstuhl für Tech- nische Physik, Universität Erlangen-Nürnberg

We propose a method of photoemission spectra interpretation based on tomographic deconvolution of spectral features into individual orbitals suitable for cases when two or even several molecular orbitals overlap in the same energy interval. Suggested approach utilizes the earlier finding that the ARPES intensity distribution from a single molecular state is related to the Fourier transform of respective molecular orbital. Deconvoluting the entire experimental datacube of photoemission current recorded with toroidal electron analyzer into momentum dependent and energy dependent components and approximating the momentum dependent part by the Fourier transform of a chosen molecular orbital, one achieves the energy distribution of corresponding orbital. In the photoemission experiments on PTCDA/Ag(110), using tomographic deconvolution, four orbitals situated within an energy range of only 0.4 eV were successfully differentiated demonstrating applicability of the method even for strongly interacting molecule/metal interfaces.

O 35.42 Tue 18:15 Poster B

Spin-resolved photoemission experiments of Rashba-split quantum-well electron states

— •Sebastian Jakobs[1,2], Andreas Ruffing[1], Sabine Steil[1], Indranil Sarkar[1], Stefan Mathias[1], Mirko Cinchetti[1], and Martin Aeschlimann[1] — [1]Department of Physics and Research Center OPTIMAS, University of Kaiserslautern, 67663 Kaiserslautern, Germany — [2]Graduate School Materials Science in Mainz, University of Kaiserslautern, D-67663 Kaiserslautern, Germany

The Rashba-Bychkov effect in a two-dimensional electron gas originates from spin-orbit interaction and an asymmetric confinement of the electron gas. It can produce spin-split energy bands in nonmagnetic materials without the need of applying any external magnetic field. This effect has been shown on various surfaces, and the resulting spin-split surface-state bands show a high spin polarization directed in the surface plane, perpendicularly to the k-vector of the photoelectrons [1]. Recently, we reported on the observation of a giant Rashba spin-orbit splitting of quantum-well state bands in the unoccupied electronic structure of a Bi monolayer on Cu(111) [2]. In this poster we will present first spin-resolved photoemission experiments of both commensurate and incommensurate structure of the quantum-well system Bi/Cu(111), which confirm the Rashba-character of the splitting.

[1] J.H. Dil, J. Phys.: Condens. Matter 21, 403001 (2009)
[2] S. Mathias et al., Phys. Rev. Lett. 104, 066802 (2010)

O 35.43 Tue 18:15 Poster B

Spin Splitting Mechanism in Surface Alloys investigated by Circular Dichroism in the Angular Distribution of Photoelectrons

— •Carola Strasser, Isabella Gierz, Hadj-Mohamed Benia, Klaus Kern, and Christian R. Ast — MPI für Festkörperforschung, Stuttgart

Circular dichroism in the angular distribution (CDAD) of photoelectrons refers to the difference of the measured photocurrent for right and left circularly polarized light. The CDAD signal contains information about the photoemission process and is determined by the experimental geometry, the orbital composition of the initial state and also the relative phase between different final state partial waves.

We used an ARPES (angular resolved photoemission spectroscopy) setup with different light polarizations and applied this technique to the band structure of two surface alloys on the Ag(111) surface with different spin splitting. Both systems show a clear CDAD signal but variant features. To get more information about the spin splitting mechanism we combined tight binding calculations with general theoretical descriptions of CDAD to explain the characteristic patterns in the experimental data.

O 35.44 Tue 18:15 Poster B

Angular resolved photoemission study of a two-dimensional electron system induced by Cs adsorption on InSb(110).

— •Alexander Georgi[1], Carola Strasser[2], Isabella Gierz[3], Stefan Becker[1], Marcus Liebmann[1], Christian Ast[2], and Markus Morgenstern[1] — [1]II. Physikalisches Institut B and JARA-FIT, RWTH Aachen University, Aachen, Germany — [2]Max-Planck-Institut für Festkörperforschung, Stuttgart, Germany — [3]Max Planck Research Department for Structural Dynamics, University of Hamburg, Centre for Free Electron Laser Science, Hamburg, Germany

Using angular resolved photoemission (ARPES) at 70 K, we investigated the band structure of a two-dimensional electron system (2DES) created by Cs adsorption on p-type InSb(110). Cs induces a large band bending on the surface of p-type InSb(110) and creates a 2DES in the inversion layer. ARPES measurements reveal the parabola of the first 2DES subband exhibiting an effective mass of only $m^* = 0.022\,m_0$ in accordance with theory.

The large electric field within the 2DES leads to a large Rashba parameter estimated to be about $\alpha = 7\times10^{-11}$eVm. Scanning tunneling spectroscopy studies [1] indeed show a beating pattern in the Landau levels of the system which can be attributed to this Rashba spin splitting. Experiments to probe this spin splitting by ARPES are under way.

[1] S. Becker, Phys. Rev B 81, 155308 (2010)

O 35.45 Tue 18:15 Poster B

Phase behavior of chain molecules on surface: Monte Carlo simulation

— •Pritam Kumar Jana and Andreas Heuer — Institute of Physical Chemistry, University of Muenster, Corrensstr. 28/30, Muenster, Germany

Self assembled monolayers of organic molecules on solid substrate build well defined surfaces, which can be structured efficiently on a nanometer scale. Self assembled monolayers are formed by organic molecules which spontaneously chemisorb on solid substrate [1,2], e.g. alkanethiolates attaching to gold surfaces with their sulfur head groups. We have studied an idealized model of chain molecules adsorbed on a flat substrate by means of extensive Monte Carlo Simulations. Our study focuses on phase transitions within a monolayer rather than on self aggregation. We model the molecules as rigid chains of Lennard-Jones spheres with one head group. As chain molecules are considered as rigid rod, all intra molecular degrees of freedom have been neglected. The Monte Carlo dynamics involves translational move in 3D space and rotational moves in 2D space. In the course of the simulation the concentration of chain molecules is increased with a fixed flux. We determine the phase diagram in dependence of the different energetic and structural parameters (e.g. chain length) of the model.

[1] A. Ulman, Chem.Rev., 96, 1533, 1996. [2] G. E. Poirier, Chem. Rev., 97, 117, 1997.

O 35.46 Tue 18:15 Poster B

Atomistic Simulations of Pressure-Induced Structural Transformations in Ice Nanocrystals — •Konstantin Weber[1,2] and Carla Molteni[1] — [1]King's College, Physics Department, London, UK — [2]ICMM/CCC, University of Erlangen-Nürnberg, Germany

Ice has a very complex and widely studied phase diagram, which includes many crystalline phases (stable as, e.g., ice Ih, ice II, and ice III, and metastable ones as ice Ic) as well as amorphous phases. Pressure can be used to induce structural transitions between these phases, allowing the study of transition mechanisms and of phase dependent properties. Ice nanocrystals of variable size add an extra dimension to the phase diagram, and it is interesting to understand how size affects the phase transformations. We present the results of a series of simulations where we have modeled pressure-induced structural transformations in ice Ih nanocrystals using the classical TIP4P force field, a constant pressure molecular dynamics method for finite systems, and the metadynamics technique for accelerating rare events. Metadynamics allows us to study the phase transformations at realistic pressure conditions, without the need to overpressurize the systems as in conventional molecular dynamics because of time scale limitations.

O 35.47 Tue 18:15 Poster B

Depth profiling X-ray photoemission investigation and its impact into the field of Fusion Energy Materials — •Stephanie Rädel[1,2,3], Martin Köppen[3], Martin Oberkofler[3], Johann Riesch[3], Heike Löchel[1], Max Bauer[1], Antje Vollmer[1], and Christian Linsmeier[3] — [1]Helmholtz Zentrum Berlin für Materialien und Energie GmbH, Berlin, Germany — [2]TU Berlin, Berlin Germany — [3]Max-Planck-Institut für Plasmaphysik, Garching, Germany

The next step of the roadmap in fusion energy research is the construction of the experimental fusion reactor ITER. Due to particle collision and energy deposition in the reactor vessel, requirements for first wall materials are extremely high. Therefore it is crucial to gain knowledge on the interaction of the plasma and the surface of ITER. During operation, diffusion, erosion and re-deposition occur. For a successful operational scenario, these reactions need to be predicted. In this study we investigate selected surface processes by XPS measurements. By using synchrotron radiation, it is possible to tune photon energies (kinetic energy of photo-electrons) achieving different information depths. Following diffusion processes and chemical reactions by depth profing becomes feasible. Here we present the ternary system Be/W/C and its chemical and physical behaviour upon annealing. This understanding is a step towards predictions of the behaviour of the elements at the ITER first wall under different reaction conditions during operation.

O 35.48 Tue 18:15 Poster B

Patterning of the surface termination of ultrananocrystalline diamond films — •Mahsa Mozafari, Alexandra Voss, Cyril Popov, and Johann Peter Reithmaier — Universität Kassel, Institut für Nanostrukturtechnologie und Analytik, Heinrich-Plett-Straße 40, 34132 Kassel, Germany

Diamond and diamond films attract an ever increasing interest for different biotechnological applications due to their extraordinary properties, like excellent biocompatibility, high chemical stability, wide electrochemical window, high wear resistance and optical transparence, etc. Further advantage of the diamond surface is the possibility to tailor the surface termination and respectively the surface properties, including the wettability and conductivity. These properties are decisive for the interactions with any bioentity (cells, proteins, RNA, DNA). In the current work we present the results for the surface modification of ultrananocrystalline diamond/amorphous carbon (UNCD/a-C) composite films and its patterning. The surface of these films is H-terminated after growth, which determines the hydrophobic character and the p-type surface conductivity. Applying O_2-plasma, NH_3/N_2-plasma or UV/O_3 modifications it can be rendered hydrophilic and insulating due to the change of the surface termination. The modified surfaces were investigated by contact angle measurements, SEM, AFM, XPS and electrical measurements. Further, the possibility to pattern the surface termination by electron, ion and laser beams was also studied.

O 35.49 Tue 18:15 Poster B

Molecular beam studies of methane dissociation on Ru(0001) — •Harald Kirsch, Zefeng Ren, R. Kramer Campen, and Martin Wolf — Fritz-Haber-Institut , Abt. Physikalische Chemie, Faradayweg 4-6, 14195 Berlin

Understanding the dissociation of methane on transition metal surfaces is a challenge in heterogeneous catalysis. We have investigated the dissociation products of CH_4 and CD_4 on a Ru(0001) surface with vibrational sum-frequency spectroscopy (SFG) and temperature-programmed desorption(TPD). To overcome the dissociation barrier under UHV conditions, a supersonic molecular beam of CH_4/CD_4 seeded in He or H_2 has been used to generate adsorbed methyl radicals. The system was studied as function of surface temperature (300K - 500K) and coverage. Coverage was determined after each measurement by oxygen coadsorption and recombinative C + O desorption. High resolution ($<$5 cm^{-1}) vibrational sum-frequency generation spectroscopy has allowed the observation of new features in the C-H stretching region. For adsorption at surface temperatures below 350K just one resonance could be observed at 3000 cm^{-1}, which is identified as the CH stretching mode. At temperatures higher than 350K, two additional red shifted peaks appear. These observation could help to identify intermediates of the methane dehydrogenation and complement previously discovered decomposition pathways.

O 35.50 Tue 18:15 Poster B

Catalytic activity of free and graphene-supported transition metal clusters — •Sanjubala Sahoo, Markus E. Gruner, and Peter Entel — Faculty of Physics and Center for Nanointegration CeNIDE, University of Duisburg-Essen, Lother Str. 1, 47048 Duisburg

We have studied the CO oxidation reaction for CO adsorbed on a Pt_{13} cluster and for CO adsorbed on a graphene sheet. The reaction pathway is identified and the activation barrier is calculated. Our results show that the activation barrier in case of the Pt_{13} cluster is similar in magnitude to that of the Pt(111) surface. On the other hand, we find that the activation barrier for CO oxidation on graphene alone is lower compared to that of a free Pt cluster. In future, we also explore the reaction for Pt13 cluster is deposited on graphene. The studies are done with the nudged elastic band method [1] by employing the total energy calculations from density functional theory within generalized gradient approximation as implemented in Vienna ab-initio simulation package (VASP) [2].

[1] A. Eichler et al., Phys. Rev. B **59**, 5960 (1999).

[2] G. Kresse et al., Comput. Mater. Sci. **6**, 15 (1996).

O 35.51 Tue 18:15 Poster B

Flame-Synthesis of Tailored Metal-Oxide Nanoparticle Surfaces for Highly Selective and Reactive Gas Sensors — •Antonio Tricoli — Particle Technology Laboratory, Department of Mechanical and Process Engineering, ETH Zurich, 8092 Zurich, Switzerland

Metal-oxide nanoparticles such as SnO_2 and TiO_2 are state-of-the-art materials for the assembly of solid-state chemical gas sensors. The remarkable chemical and temperature stability of these wide band-gap semiconductors allows operation in very harsh environments as for exhaust oxygen sensors in modern fuel control feedback loop. The high reactivity of their surface with simple and complex gaseous compounds allows detection of important analytes down to particle per billion concentrations (ppb). However, this is usually achieved by exploitation of spill-over effects on noble-metal clusters post-deposited (e.g. by impregnation) on their surface. This drastically limits the stability of their sensing performance at the elevated operation temperatures ($250-600\,^{\circ}$C) of these metal-oxides and considerably increases the cost for their production. Additionally, such gas sensing metal-oxides suffer of very poor selectivity confining their application to relatively simple gas mixtures. This is a main limitation to their utilization as gas sensors in novel applications such as non-invasive medical diagnostics by breath analysis. Development of noble-metal-free metal-oxide nanoparticles with high selectivity to trace concentrations (ppb) of the target analyte is a key-step toward the fabrication of portable and wearable gas sensing technology with numerous applications. Here, the one-step flame-synthesis of tailored multi-oxide nanoparticles is presented as a tool for the production of very selective and sensitive gas sensors. In particular, the synthesis of highly reactive SnO_2-SiO_2 nanocomposites with limit of detection (LOD) in the ppb range is demonstrated as a valid alternative to the utilization of noble-metals leading to considerably higher sensitivity and stability. In particular, the thermal stabilization of very fine SnO_2 nanocrystals with size below twice their Debye length up to very high temperatures (900 °C) is shown as a reliable method for the synthesis of wide band-gap semiconductors with surface states-controlled conductivity and thus very high sensitivity. Additionally, the flame-synthesis of $SnO_2 - TiO_2$ solid solutions with rutile crystal structure is presented as a powerful approach to control the selectivity of such metal-oxide surfaces against disturbing agents such as water vapor, an omnipresent and varying component in gas sensing.

O 35.52 Tue 18:15 Poster B

Solar2Fuel: Spectroscopic and electrochemical characterization of functionalized semiconductor surfaces for photocatalytic reduction of CO_2 — •Florian Staier, Michael Grunze, and Michael Zharnikov — Angewandte Physikalische Chemie, Universität Heidelberg, Im Neuenheimer Feld 253, 69120 Heidelberg

The handling of CO_2 produced by industrial installations and power plants has become a very important environmental issue nowadays because of it's generally accepted impact on the green house effect. In this context, storage of CO_2 or its conversation to fuel or useful chemicals are highly desirable. Along these lines, the Solar2Fuel project, funded by German BMBF (13N11793), aims on photocatalytic conversion of CO_2 to methanol with a sufficient quantum efficiency to make an industrial realization of the process profitable. As the basic catalytic system, semiconductor nanoparticle powder coatings are used. These particles are functionalized with dye molecules to promote the photocatalytic reaction and to move the absorption spectrum from UV to the visible range. Here we present first results on the adsorption kinetics, absorption character, and photoactivity for a variety of the relevant systems. These properties were primary addressed by X-ray photoelectron spectroscopy and electrochemical methods.

O 35.53 Tue 18:15 Poster B

Solar2Fuel: ATR-IR-Spectroscopic characterization of functionalized semiconductor surfaces for photocatalytic reduction of CO_2 — •Leo Pöttinger[1] and Thomas Bürgi[2] — [1]Physikalisch-Chemisches Institut, Universität Heidelberg, Im Neuenheimer Feld 253, 69120 Heidelberg — [2]Département de Chimie Physique Université de Genève, 30 Quai Ernest-Ansermet CH-1211 Genève 4

The handling of CO_2 produced by industrial installations and power plants has become a very important environmental issue nowadays because of it's generally accepted impact on the green house effect. In this context, storage of CO_2 or its conversation to fuel or useful chemicals are highly desirable. Along these lines, the Solar2Fuel project, funded by German BMBF (13N11793), aims on photocatalytic conversion of CO_2 to methanol with a sufficient quantum efficiency to make an industrial realization of the process profitable. As the basic catalytic system, semiconductor nanoparticle powder coatings are used. These particles are functionalized with dye molecules to promote the photocatalytic reaction and to move the absorption spectrum from UV to the visible range. ATR-IR-Spectroscopy during adsorption of different dyes and CO_2 on the nanoparticles is performed, as well as the reaction upon visible light irradiation.

O 35.54 Tue 18:15 Poster B

Oxidation behavior of orientated brass surfaces investigated with STM, XPS and LEED — •Andreas Zychma, Renate Wansing, and Alexander Birkner — Lehrstuhl für Physikalische Chemie I, Ruhr-Universität Bochum

In heterogeneous catalysis, especially in methanol synthesis, the system Cu/ZnO plays an important role. Particularly the metal-substrate interaction of copper and zinc oxide is of great interest. While many groups therefore study the system copper on zinc oxide, we investigate the behavior of zinc oxide on copper, the so called 'inverse system'. For that we use brass single crystals with an amount of 15 percent zinc. After oxygen exposure in ultra high vacuum at different substrate temperatures the stepwise formation of zinc oxide and copper oxide can be observed with x-ray photoelectron spectroscopy (XPS). Additionally low energy electron diffraction (LEED) and scanning tunneling microscopy (STM) as well as spectroscopic measurements with the STM are performed to investigate the formation process of zinc oxide and copper oxide on brass surfaces with different crystal orientation.

O 35.55 Tue 18:15 Poster B

Reactivity of Acetylene on thin NiO films and on Pd(100) — •Oliver Höfert, Wei Zhao, Karin Gotterbarm, Andreas Bayer, Christian Papp, and Hans-Peter Steinrück — Lehrstuhl für Physikalische Chemie II, Universität Erlangen-Nürnberg, Egerlandstr. 3, 91058 Erlangen

NiO is an important material in heterogeneous photocatalysis for degradation of azodyes [1] or water splitting [2]. We studied different thin NiO films on Pd(100) and Pd (100) towards their reactivity with C_2H_2 by in situ XPS, applying synchrotron radiation at BESSY II. Our data shows that acetylene adsorbs molecularly on the substrate; the thermal evolution studies point to a reaction at 300 K leading to an intermediate that was shown to be CCH [3]. At higher reaction temperatures further decomposition and reaction is found. On thin, highly stressed NiO films acetylene adsorbs on many different adsorption sites leading to a broad peak in the C 1s photoelectron spectrum. Thermal treatment of C_2H_2 leads to an intermediate similar to the one on the clean substrate. At higher temperatures carbon is produced which reacts with the NiO to CO and desorbs.

This work was supported by BMBF (05 ES3XBA/5) and the DFG through the Cluster of Excellence "Engineering of Advanced Materials".

[1] Hu, X. et al, J. Chem. Tec. & Biotec., 85 (2010) 11
[2] Kato, H. et al, J. Phys. Chem. B, 105 (2001) 19
[3] Camplin, J. P. et al, Phys. Chem. Chem. Phys. 2 (2000) 4433

O 35.56 Tue 18:15 Poster B

Methanol synthesis on ZnO(000$\bar{1}$): CO reduction at oxygen vacancies. — •Johannes Frenzel, Nora Graf, and Dominik Marx — Lehrstuhl für Theoretische Chemie, Ruhr-Universität Bochum, 44780 Bochum, Germany

In the heterogeneous catalytic synthesis of methanol on the ZnO(000$\bar{1}$) surface with oxygen vacancies [1] gives rise to a complex free energy landscape[2] for the reduction of CO on this catalyst at high temperature and pressure conditions as required in the industrial process. Using *ab initio* metadynamics for computational heterogeneous catalysis the underlying complex reaction network from CO to methanol has been generated in the first place by exploring the global free energy, that allowed a subsequent refinement of individual reaction pathways.[2]

In the present study, the complex reduction process from CO to methanol is studied by exploring the electronic structure of reaction intermediates with density functional theory. After comparing the electronic bands and molecular orbitals involved we find the reduction state of surface and O vacancy bound adsorbates to be controlled by the charge states of the F–center, which is defined by the gas phase conditions.[1] Monitoring the reduction process of reaction paths obtained by metadynamics sampling of the free energy surface at the electronic structure level on snapshots reaction allows further mechanistic insight into the catalytic process.

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O 35.57 Tue 18:15 Poster B

The dynamic redox properties of MoV oxide catalysts for the selective oxidation of alkanes studied by in-situ microwave cavity perturbation — •Christian Heine, Maik Eichelbaum, Annette Trunschke, and Robert Schlögl — Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, Germany

The semiconducting M1 phase MoVNbTeOx is a selective catalyst for the direct oxidation of propane yielding about 50% acrylic acid. During the redox reaction a charge transfer between the catalyst and the chemisorbed reactants takes place. To study the interaction between the gas phase and the catalyst surface, we developed a method based on the microwave cavity perturbation technique enabling the investigation of (di)electric properties of powder catalysts under operation in a contact-free manner, thus completely avoiding contact resistance and electrode-related problems (Eichelbaum et al., PCCP, DOI 10.1039/C1CP23462E). This method offers the possibility to probe the electronic structure of the catalyst under reaction conditions. It is known from in-situ photoelectron spectroscopy studies that the surface of the M1 phase behaves dynamically and changes its electronic and geometric structure during the catalytic reaction, which is associated with a modification of the surface density of states. As a consequence, the equilibrium between surface and bulk states is shifted modifying the surface states-induced band bending. The impact of the surface electronic structure on the electrical conductivity of the catalyst will be discussed.

O 35.58 Tue 18:15 Poster B

Micro-flow tube reactor for investigations on the catalytic activity of model catalysts — Kwabena Offeh Gyimah, Matthias Roos, •Joachim Bansmann, and R. Jürgen Behm — Institute of Surface Chemistry and Catalysis, Ulm University, D-89069 Ulm

Here, we report on a newly developed glass reactor for investigating the catalytic activity of model catalysts which usually exhibit very small surface areas and, as a consequence, very low reactions rates. The design of the reactor is based on a reactor developed by Wong et al. [1], it is fabricated from glass, allows temperatures up to 400°C, and is connected to a quadrupole mass spectrometer. Due to its small reaction volume, it is only suitable for small samples (e.g., 3mm x 3mm). The reactor has been tested for the CO oxidation reaction on thin film based Au/TiO$_2$ catalysts [2] in the pressure regime of several mbars (CO and O$_2$). Due to its design, it allows fast measurements on the activation energy of catalysts. The properties of this reactor will be compared to other reactors, e.g. [1,3].

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O 35.59 Tue 18:15 Poster B

Low cost low noise amplifier for charged nanoparticle beam detection — •Sebastian Schleicher, Wolfgang Rosellen, and Mathias Getzlaff — Institute of Applied Physics,University Duesseldorf

For our investigations we generate nanoparticles in the gas phase by a UHV compatible Arc Ion Cluster Source (ACIS)[1]. Nearly 50% of the beam consists of charged nanoparticles with sizes between 5 nm and 15 nm. For beam positioning and controlling, the nanoparticles are detected by a very low noise current amplifier in an embedded system. The charged nanoparticle beam has an electrical current of a couple of pico-Ampere. By amplifying this signal by a magnitude of 10^{15}, it can be quantified. The main problem to overcome when amplifying a signal is to minimize the noise. There are four known noise sources, which need to be considered ($1/f$ noise, $1/f^2$ noise, Johnson-Nyquist Noise and Shot noise). We use a transimpedance amplifier. For this purpose the construction elements, like the power supply and the transimpedance amplifying circuit, were made by low-cost components. Each construction element was chosen by their highest possible noise suppression according to signal enhancement. The final signal will be converted by a 24-bit delta-sigma analog-to-digital converter. The system will be designed as an embedded microcontroller system.

[1] R.-P. Methling, V. Senz, E.-D. Klinkenberg, Th. Diederich, J. Tiggesbäumker, G. Holzhüter, J. Bansmann, K.-H. Meiwes-Broer, European Physical Journal D **16**, 173 (2001)

O 35.60 Tue 18:15 Poster B

Ag clusters on SiO$_2$ and in matrices: effects of cluster-structure and surroundings — •Sabrina Hoffmann[1], Stefanie Duffe[1], Kamil Latussek[1], David Engemann[1], Christoph J. Sahle[1], Christian Sternemann[1], Heinz Hövel[1], Ralph Wagner[2], and Pieter Glatzel[3] — [1]TU Dortmund, Experimentelle Physik I/DELTA, Dortmund, Germany — [2]BU Wuppertal, Fachgruppe Physik-Materialwissenschaften, Wuppertal, Germany — [3]ESRF, Grenoble, France

Embedding Ag clusters produced in a supersonic expansion using THECLA, a THErmal CLuster Apparatus [1,2] into a polydimethylsiloxane (PDMS) / SiO$_2$ aerogel matrix enables the investigation of a much higher amount of separated clusters [3] which on a SiO$_2$ substrate is limited by coalescence and electromagnetic coupling [2]. The plasmon resonances of Ag clusters on SiO$_2$ and in PDMS / SiO$_2$ aerogel before and after exposure to air were investigated by optical spectroscopy [4]. XANES measurements at the Ag L$_{1,2,3}$ absorption edges [5] carried out at the synchrotron radiation sources DELTA and ESRF were compared to ab initio multiple scattering calculations (FEFF) for different cluster sizes and structures.

[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 35.61 Tue 18:15 Poster B

Cluster aus fokussierten Ionenstrahlen - Massenspektroskopische Untersuchung von Flüssigmetall-Ionenquellen — •Martin Wortmann, Dirk Reuter und Andreas D. Wieck — Ruhr-Universität Bochum, Universitätsstr. 150, 44780 Bochum

Bei der Untersuchung der Cluster-Emission aus Flüssigmetall-Ionenquellen (LMIS) war man bisher durch die Auflösung der in herkömmlichen FIB-Systemen (focused ion beam) verwendeten $E \times B$ – Massenfilter limitiert. Die Auflösung nimmt mit zunehmender Masse der untersuchten Cluster rapide ab. Will man auch im Bereich größerer Cluster ($n > 10$) eine hinreichende Massenseparation erreichen, werden also hochauflösende Massenspektrometer benötigt.

Die durch die Verwendung von LMIS erreichbaren Clusterströme eröffnen außerdem die Möglichkeit, derartige Quellen zur Erzeugung monodisperser Cluster zu verwenden. Durch ein geeignetes elektrisches Potential können die Cluster abgebremst und auf Substraten deponiert werden.

In diesem Beitrag werden die Designüberlegungen für den in Bochum im Aufbau befindlichen hochauflösenden Massenfilter diskutiert. Die Massentrennung kann sowohl durch einen $E \times B$ – Filter als auch durch Time-of-Flight-Spektroskopie erreicht werden. Präsentiert werden Details des experimentellen Aufbaus, sowie Ergebnisse der ionenoptischen Berechnungen, die für die Planung einer solchen Anlage zwingend notwendig sind. Außerdem werden die Ergebnisse der bereits durchgeführten Messungen diskutiert.

O 35.62 Tue 18:15 Poster B

Mass selected copper clusters on graphite (HOPG): Photoelectron spectroscopy with ultraviolet light — •Christoph Schröder[1], David Engemann[1], Niklas Grönhagen[1], Natalie Miroslawski[1], Bernd von Issendroff[2], and Heinz Hövel[1] — [1]Technische Universität Dortmund, Experimentale Physik I, Germany — [2]Albert-Ludwigs-Universität Freiburg, Physikalisches Institut, Germany

We investigated mass selected copper clusters between 34 and 92 atoms deposited at 125 K on graphite (HOPG) using ultraviolet photoelectron spectroscopy (UPS). The clusters were softlanded with less then 0.1 eV per atom kinetic energy. Cluster were deposited with different coverage for each cluster size and measured at 125 K. For a better interpretation we subtracted normalized HOPG spectra from the measured cluster spectra to extract the d-band structure of the clusters. Afterwards we annealed the sample for 1 hour at RT and observed changes in the UPS spectra depending on the cluster coverage. For these investigations the source of exciting radiation was a He-gas discharge lamp (hν=21,2 eV). In order to get more information about the clusters we will use Ar (hν=11,6 eV) instead of He in our discharge lamp for future experiments. For this reason we have installed a heatable LiF-window.

O 35.63 Tue 18:15 Poster B

Catalytic activity of supported Pt clusters compared to Pt(111) — •Andrew S. Crampton, Claron. J. Ridge, Florian F. Schweinberger, and Ulrich Heiz — Technische Universität München, Catalysis Research Center, Chair of Physical Chemistry, Lichtenbergstr. 4, 85748 Garching, Germany.

Softlanding size-selected metal clusters, generated with a laser ablation source and mass selected with a QMS, onto a metal oxide support enables independent size and coverage control. These model systems then provide a direct path for the experimental chemist to probe electronic and geometric effects by changing the particle size by one single atom. The reactivity of these systems is investigated using a variety of surface science methods such as TPD/TPR, pMBRS, IRRAS, UPS and MIES. Recent studies on adsorbates have proven the potential of MIES to study adsorbate systems with a superior sensitivity compared to UPS. With these methods the kinetics and thermodynamics of reactions on clusters can be examined, as well as the electronic structure and vibrational properties of the adsorbates. Of particular interest are common model systems and demanding reactions, such as hydrogenation of olefins, on Pt clusters in the range from a single atom to nano crystallites (1-80 atoms). Comparing the results of measurements on the clusters with Pt(111) within the same experimental setup allows for a precise and comprehensive understanding of the effects on catalytic activity imparted by particle masses in the non-scalable size regime. The information obtained from these experiments contributes to deciphering fundamental catalytic mechanisms on the nanoscale.

O 35.64 Tue 18:15 Poster B

Linear and nonlinear spectroscopy of size selected metal clusters on surfaces — •Philipp Heister, Tobias Lünskens, Martin Tschurl und Uli Heiz — Technische Universität München, Lehrstuhl für physikalische Chemie

The catalytic activity of small metal clusters has been shown to vary by orders of magnitude upon addition of a single metal atom. A better understanding of the interplay between the electronic and geometrical structure and the catalytic activity of the clusters may be gained through a precise knowledge of the electronic structure and geometry from spectroscopic studies. Therefore we use different spectroscopic methods to investigate size selected and unselected metal clusters on surfaces under UHV conditions. We use highly sensitive techniques such as surface Cavity Ring-Down spectroscopy (s-CRD) and surface Second-Harmonic-Generation spectroscopy (s-SHG) for observing the obtical properties of these clusters. The interest mainly focuses on the size and shape dependent electronic structures and plasmon-like transitions of small deposited clusters. With these plasmon oscillations we are able to gain further information about oxidation and reduction of the supported size selected clusters. We also observe interesting cluster-plasmon size effects, for example a sudden increase in plasmon resonances (parallel to the surface normal) for increasing cluster size. It seems that these clusters need to be at least three atomic layers thick in order to show plasmon oscillations, whereas thinner clusters (one or two atomic layer) do not show any plasmon oscillations.

O 35.65 Tue 18:15 Poster B

Setup and characterisation of CRD and SHG spectrometer for measuring optical response of supported metal clusters and evaporated molecules under UHV conditions — •Tobias Lünskens, Philipp Heister, Martin Tschurl und Uli Heiz — Technische Universität München, Lehrstuhl für physikalische Chemie

Supported metal clusters have attracted considerable interest due to their special catalytic properties. Optical and catalytic properties of these metal clusters are determined by their electronic structure which can be studied by optical absorption spectroscopy as well as surface second harmonic generation (s-SHG) spectroscopy under UHV conditions. The interest mainly focuses on the size and shape dependent electronic structure of deposited cluster. Due to their low absorption cross-section and the low surface coverage that is necessary to avoid agglomeration of the clusters highly sensitive techniques such as surface cavity ring-down (s-CRD) spectroscopy and s-SHG-spectroscopy are needed. By s-CRD-spectroscopy we also investigate evaporated molecules and their interaction with different substrates und size selected metal clusters. We present the experimental setup which is composed of two main parts: A cluster deposition unit including laser vaporization cluster source, ion optics, and mass selection device and three different spectroscopic methods, including s-CRD spectroscopy in the UV-Vis- (from 400 nm to 900 nm) and in the IR-region (from 2500 nm to 3500 nm), and s-SHG-spectroscopy for measurements down to 200 nm. A transfer chamber allows fast change of support materials without breaking UHV.

O 35.66 Tue 18:15 Poster B

STM of size selected silver and copper clusters deposited on $Au(111)$ and $C_{60}/Au(111)$ — •David Engemann[1], Niklas Grönhagen[1], Natalie Miroslawski[1], Bernd von Issendorff[2], Tommi T. Järvi[3], Michael Moseler[2,3,4], and Heinz Hövel[1] — [1]Technische Universität Dortmund, Experimentelle Physik I — [2]Albert-Ludwigs-Universität Freiburg, Physikalisches Institut — [3]Fraunhofer-Institut fuer Werkstoffmechanik IWM, Freiburg — [4]Freiburger Materialforschungszentrum

Size selected silver and copper clusters with sizes in between 34 atoms to 147 atoms were soft landed on clean $Au(111)$ and $Au(111)$ covered with 1 and 2 ML C_{60} and measured with scanning tunneling microscopy (STM) at $77K$. We observed a deformation of the cluster shape due to the strong metallic interaction between the clusters and $Au(111)$. The silver clusters became epitaxial and developed a structure composed of several monolayers. The number of these monolayers depends on the number of atoms in the clusters and the deposition energy. The larger the cluster mass the more monolayers the clusters develops on $Au(111)$ and the larger the deposition energy the fewer monolayers occur. These results are compared with molecular dynamic simulations and other atomistic calculations. The clusters were annealed up to room temperature and afterwards measured with STM at $77K$. On 1 ML C_{60} all cluster heights became smaller after annealing. We compare these results for copper and silver clusters. Resulting differences may be explained with the fact that for the same number of atoms copper clusters are smaller than silver clusters.

O 35.67 Tue 18:15 Poster B

Photocatalysis with supported size-selected metal clusters — •Martin Tschurl[1], Josef Kiermaier[1], Andreas Winbauer[1], Friedrich Esch[1], Claude Henry[2], and Ulrich Heiz[1] — [1]TU München, Catalysis Research Center, Lichtenbergstr. 4, 85748 Garching, Germany — [2]CINaM-CNRS, Campus de Luminy, Case 913, 13288 Marseille Cedex 09, France

In this work we present a setup for the study of the photochemical properties of size-selected clusters softlanded on various support materials. The apparatus consists of a laser ablation cluster source with ion optics for guiding the cluster beam and a quadrupole for mass selection. The size-selected clusters are softlanded on a special temperature-adjustable sample holder and can then be further characterized.

To determine the photocatalytic activity of the clusters, reaction products will be monitored. For this purpose our setup is equipped with a standard quadrupole mass selector with electron ionization. In addition, we have developed a new type of time-of-flight mass spectrometer, which is used in combination with REMPI (Resonant Enhanced Multiphoton Ionization). This spectrometer is specially designed to study the formation of different isomers. In this case, discrimination can be achieved by selecting a wavelength, which is in resonance with the electronic states of just one of the reaction products. This resonant process will greatly enhance the ionization yield of this particular species, which can then be detected in the time-of-flight spectrometer with very high sensitivity.

O 35.68 Tue 18:15 Poster B

d^0 ferromagnetic interface between non-magnetic perovskites — •Riku Oja and Risto M. Nieminen — Aalto University, Helsinki, Finland

In perovskite oxides, oxygen p bands are narrow and have a high density of states just below the band gap. Also, oxygen p electrons have a strong exchange coupling. Hence, Stoner criterion for itinerant ferromagnetism is fulfilled in hole-doped d^0 perovskites, if the hole density is high enough. Obtaining high hole densities, moving the Fermi level to the oxygen p band, is easily done by so-called intrinsic doping by a charge-imbalanced interface between two d^0 perovskites. This introduces holes (for p type interface) or electrons (for n type interface) confined in the interface region.

We have performed DFT and DFT+U calculations with both LSDA and GGA for both types of $KTaO_3/SrTiO_3$ interfaces. The atomically sharp p type interface has been observed in experiments. The hole on oxygen $2p$ orbitals is localized on $SrTiO_3$ side of the interface and is spin-polarized. Very small values of on-site Hubbard interaction U on oxygen p orbitals cause complete spin-polarization and half-metallic, ferromagnetic holes. The antiferromagnetic solution has higher energy. For the n type interface, on the other hand, electrons on Ti d orbitals do not magnetize completely.

As the density of states at the top of the O p band is higher than at the bottom of the Ti d band, we conclude that p type interfaces between d^0 perovskites are good materials for interfacial ferromagnetism below ferroelectric thin films.

O 35.69 Tue 18:15 Poster B

A new mode of operation of electron energy loss spectrometers: Application to surface magnon and surface vibration spectra — •Rajeswari Jayaraman, Harald Ibach, and Claus Michael Schneider — Peter Grünberg Institut, Forschungszentrum Jülich, 52425 Jülich, Germany

Using advanced simulations of the electron optics we have found a new mode of operation for the lens system in electron energy loss spectrometers (EELS) in which the cardinal planes of the lenses are closer to the sample. The product of transmission and solid angle angle accepted by the analyzer thereby increases by a factor of 3-5, yielding a corresponding gain in the intensity. The effect is demonstrated for a recently developed high-intensity spectrometer [1] with spectra of surface spin waves on fcc cobalt. Using this new mode we have been able to obtain spin wave spectra with 7meV resolution. Commercially available EEL-spectrometers can likewise be operated in the new mode. We demonstrate this with vibration spectra of water on Ag(115). The electron optical calculations furthermore allow an absolute calibration of the cross section for inelastic electron scattering. [1] H. Ibach, J.

Rajeswari, C. M. Schneider, to be published.

O 35.70 Tue 18:15 Poster B

Investigation of ultrathin Fe films on Ag(001) using linear and nonlinear photoemission — •Thiago Peixoto[1], Mariusz Pazgan[1], Francesco Bisio[1,2], Aimo Winkelmann[1], Maciej Dabrowski[1], Marek Przybylski[1], and Jürgen Kirschner[1] — [1]MPI of Microstructure Physics, Halle-Saale, Germany — [2]CNR-SPIN, Genova, Italy

Investigations of iron films grown on silver surfaces have shown an intriguing thickness-dependent oscillatory magnetic anisotropy [1,2]. This behaviour was explained by the appearance of quantum well states (QWS) in the Fe film. In order to access the relevant electronic states, we investigated ultrathin Fe/Ag(001) films by angle- and spin-resolved one-photon (1PPE, $h\nu = 6\,eV$) and multi-photon photoemission (2PPE, 3PPE, $h\nu = 3\,eV$) at 150 K. Consistent with the observation of 5.6 ML oscillations of QWS in Fe/Ag(001) [2], we report periodic thickness- and energy-dependent intensity variations of electronic transitions in 1PPE and 2PPE spectra. Using different incident light polarizations, we identify the presence of specific unoccupied states in 2PPE. The Fe films show an average spin-polarization of about 30% near E_F in 2PPE and 10% in 1PPE. This difference is attributed to the influence of unoccupied states. By means of angle-dependent 3PPE, the $n = 1$ image-potential state of Fe/Ag(001) is identified, with an estimated electron effective mass of $m_{eff} = 0.75m_e$ and a binding energy of $E_B = 0.77$ eV with respect to the vacuum level.

[1] U. Bauer and M. Przybylski, Phys. Rev. B 81, 134428 (2010).

[2] J. Li *et al.*, IEEE Trans. Magn. 47, 1603 (2011).

O 35.71 Tue 18:15 Poster B

Twin-Photoemission Electron Microscopy System (Twin-PEEM) — •Alexander Krasyuk[1], Christian Tusche[1], Gerd Schönhense[2], and Jurgen Kirschner[1] — [1]Max-Planck-Institut für Mikrostrukturphysik, Weinberg 2, D-06120 Halle, Germany — [2]Johannes Gutenberg Universität Mainz, Staudinger Weg 7, D-55128 Mainz, Germany

We will present an innovative twin photoemission electron microscopy system (Twin-PEEM), which consists of two fully functionally crossed PEEMs. The Twin-PEEM was calculated with commercial software to design charged particle optics devices and constructed using professional 3D CAD software. The new design allows to place a single crystalline target directly after the cathode lens of the microscope in such a way that the low energy electrons diffracted on the single crystal can be imaged in a 90° mirror-like geometry. As was recently shown [1,2] such electron mirror can be used as a highly efficient spin-filter for 2D PEEM images. We characterize a few micro-structured samples obtained with Twin-PEEM using unpolarised deep ultraviolet light (discharge lamp) with the aim to demonstrate the potential of the novel electron microscope. We will discuss also the possibility of using the Twin-PEEM as tool for spin-resolved photoemission experiment.

[1] C. Tusche, M. Ellguth, A. A. Ünal, C.-T. Chiang, A. Winkelmann, A. Krasyuk, M. Hahn, G. Schönhense, and J. Kirschner, APL 99, 032505 (2011)

[2] M. Kolbe, P. Lushchyk, B. Petereit, H.J. Elmers, G. Schönhense, A. Oelsner, C. Tusche, and J. Kirschner. PRL 107, 207601 (2011)

O 35.72 Tue 18:15 Poster B

Time-resolved ARPES studies with high-oder harmonic radiation — •Björn Frietsch[1,2], Robert Carley[1,2], Martin Teichmann[1,2], Kristian Döbrich[1], Cornelius Gahl[2], and Martin Weinelt[2] — [1]Max-Born-Institut, Max-Born-Straße 2A, 12489 Berlin, Germany — [2]Freie Universität Berlin, Fachbereich Physik, Arnimallee 14,14195 Berlin, Germany

We present results from a high-order harmonics XUV source and beamline. The setup produces XUV photons between 20-65 eV, at an energy resolution of 150 meV and a pulse duration of 100 fs for time-resolved photoelectron spectroscopic studies of laser-driven dynamics in correlated systems. To create harmonics, 40-fs pulses from a commercial amplified Ti:Sapphire laser system running at 10 kHz repetition rate are focused into an argon-filled gas cell. The XUV wavelength and energy resolution are selected using a toroidal grating monochromator. We have used the instrument to study ultrafast magnetization of the lanthanide metals Gadolinium and Terbium, and to perform preliminary experiments on laser-driven phase transitions in VO2.

O 35.73 Tue 18:15 Poster B

$[\mathrm{Mn}_6^{\mathrm{III}}\mathrm{Cr}^{\mathrm{III}}]^{3+}$-SMMs and its counterions on HOPG analyzed by Means of FM-KPFM — •Aaron Gryzia[1], Natalie Frese[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 (SMM) consisting of two bowl-shaped fragments, each containing three Mn-atoms, which are bridged by a central Cr-complex. For charge neutrality, counterions have to be coupled to the SMM. The SMM creates different kinds of structures on HOPG such as flat islands consisting of one or two layers of **$[\mathrm{Mn}_6^{\mathrm{III}}\mathrm{Cr}^{\mathrm{III}}]^{3+}$** or agglomerations at step edges. Data is acquired by means of nc-AFM. The position of the counterions is not yet known exactly, neither can they, if visible, be discriminated from the SMM by AFM. We expect the counterions to have a big influence on how the SMM adsorbs onto the substrate. The SMM is triply positive charged and each counterion carries a negative charge therefore differences in the contact potentials occur. If these differences are strong enough we are able to observe them and identify the SMM and its counterions by means of FM-KPFM (Frequency Modulated - Kelvin Probe Force Microscopy). Most recent results of our KPFM-Data will be shown and discussed with respect to the counterions.

O 35.74 Tue 18:15 Poster B

Using a two-dimensional electron mirror for efficient spin-resolved bandstructure mapping — •Christian Tusche, Martin Ellguth, Aimo Winkelmann, Alexander Krasyuk, and Jürgen Kirschner — Max-Planck-Institut für Mikrostrukturphysik, 06120 Halle, Germany

We measure the spin-polarization of photoelectrons emitted from several atomic layers thick Co films grown on Cu(100) using a momentum microscope. This instrument, consisting of a photoemission electron microscope (PEEM) and an aberration corrected electrostatic energy analyzer directly records the parallel momentum component, $k_{||}$, of photoelectrons emitted from the sample. Spin-filtering is based on the diffraction of low energy electrons in the (00)-LEED spot of a W(100) crystal, installed at the exit of the energy filter. In the spatial imaging mode, PEEM images of the magnetic domain structure of the Co films showed that 3800 image points can be recorded simultaneously [1].

A series of constant-energy cuts through the Brillouin zone gives direct access to the valence band electronic structure of the ultra-thin Co-film. By inserting the W(100) electron mirror into the electron optical path, the spin-resolved distribution of photoelectrons as a function of $k_{||}$(x,y) is recorded simultaneously with unprecedented efficiency. By exploiting the energy dependent spin-sensitivity of the low energy diffraction process, the absolute value of the spin-polarization can be obtained without magnetization reversal of the sample.

[1] Tusche, Ellguth, Ünal, Chiang, Winkelmann, Krasyuk, Hahn, Schönhense and Kirschner, Appl. Phys. Lett. **99**, 032505 (2011)

O 35.75 Tue 18:15 Poster B

(001) and (011) 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 3*d* transition metal oxides (TMOs) MnO and NiO is given by an ideal rock-salt (*rs*) structure. Below their respective Néel temperature, however, they are 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 surface probing 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) and (011) surfaces of MnO and NiO. Exchange and correlation are treated within the generalized-gradient approximation (GGA) to DFT within the parametrization of Perdew, Burke, and Ernzerhof (PBE). For a proper treatment of the on-site Coulomb interaction, we correct with an effective interaction *U* according to Dudarev's approximation (GGA+*U*).

O 35.76 Tue 18:15 Poster B

Metal- Porphyrins on metallic and superconducting surfaces — •Nino R. Hatter, Benjamin W. Heinrich, Lukas Z. Braun, Tobias R. Umbach, Jose I. Pascual, and Katharina J. Franke — Institut für Experimentalphysik, Freie Universität Berlin, Germany

While magnetic properties of single magnetic molecules on metal surfaces have been vividly studied in the last years, only little research has been done on magnetic impurities on superconducting substrates. On metal surfaces spin-excitations or Kondo screening can be observed. On a superconductor exchange coupling to Cooper pairs adds another complex many-body interaction, which is competing with Kondo screening[1,2,3]. Here we present a comparative study of metal-porphyrins on Au(111) and on the type-I superconductor Pb(111) using Scanning Tunneling Microscopy/Spectroscopy (STM/STS).

[1] K.J. Franke, G. Schulze, J.I. Pascual, Science 332, 940 (2011), [2] A. Yazdani et al., Science 275, 1767 (1997), [3] H. Shiba, Prog. Theor. Phys. 40, 435 (1968)

O 35.77 Tue 18:15 Poster B

Magnetic and structural investigations of thin ferromagnetic CrSb layers on GaAs(110)/GaAs(001) — •Carsten Godde and Ulrich Köhler — Institut für Experimentalphysik IV, AG Oberfläche, Ruhr-Universität Bochum, Germany

Thin CrSb layers grow in the metastable zinc blende structure on III-V semiconductors and are predicted to be halfmetallic with a spin polarization of 100% at the Fermi-level. Thus, these systems are of great interest because of their possible use as spin aligning layers for spintronic devices. In this contribution we present structural and magnetic measurements of thin CrSb layers on the GaAs(110) and GaAs(001) surfaces for different coverages and annealing temperatures by STM and SQUID magnetometry. STM reveals for both surfaces a Volmer-Weber growth mode of the CrSb layers and atomic resolution show an ordering alongside the lattice structure of the substrate. Particularly with regard to the existence of different phases at the GaAs(001) surface, we investigate the influence of a Ga- and an As-terminated surface of the substrate for the film deposition. SQUID magnetometry measurements show ferromagnetic characteristics of the thin CrSb layers up to 4 ML thickness with a magnetic moment per Cr-atom of up to 5 μ_B.

O 35.78 Tue 18:15 Poster B

Susceptibility measurements of Ni clusters embedded in organic matrices — •Mariella Denk, Robert Mittermair, Daniel Queteschiner, Richard Denk, Michael Hohage, Lidong Sun, and Peter Zeppenfeld — Institut für Experimentalphysik, Johannes Kepler Universität Linz, A-4040 Linz, Austria

Reflectance Difference-Magneto Optic Kerr spectroscopy (RD-MOKE) and Atomic Force Microscopy (AFM) was used to study the morphologic and magnetic properties of organic magnetic molecules, namely, cobalt tetramethoxyphenylporphyrin (CoTMPP) on Cu(110)-(2x1)O. The magneto optic Kerr signal of the organic molecules strongly depends on the photon energy [1]. Thick layers (≈ 100 nm) of organic molecules were used as host material for subsequent Ni cluster growth. The size, shape and distribution of the Ni particles strongly influences their optical and magnetic properties. By using an embedding organic matrix, we try to tune the interparticle interactions as well as the coupling between the organic molecules and the metal clusters, which, for instance, will affect the superparamagnetic limit of the nanoparticles. In order to address superparamagnetic effects the experimental setup was upgraded to measure the magnetic susceptibility, directly, and over the whole spectral range from 1.5 to 5 eV.

[1] M. Fronk, B. Bräuer, J. Kortus, O. G. Schmidt, D. R. T. Zahn and G. Salvan, Phys. Rev. B 79, 235305 (2009)

O 35.79 Tue 18:15 Poster B

Electronic states on Si(111)-(5×2)-Au — •Kerstin Biedermann and Thomas Fauster — Lehrstuhl für Festkörperphysik, Universität Erlangen-Nürnberg, Staudtstr. 7, D-91058 Erlangen, Germany

Submonolayers of gold on vicinal Si(111) surfaces form a variety of atomic chain structures and hence serve as a model system for one-dimensional electronic systems. We concentrate here on the Si(111)-(5 × 2)-Au surface, which exhibits three gold chains per unit cell.

Angle- and time-resolved two-photon photoemission experiments were carried out using infrared (IR, E_{IR}=1.55 eV) and ultraviolet (UV, E_{UV}=4.65 eV) femtosecond laser pulses. For photoemission (UPS) experiments the fourth harmonic (IR+UV) provided a source of 6.2 eV photons. The polarization of all beams could be chosen independently. Using optical dipole-selection rules, at normal emission, we evaluated the parity of the electronic states, which is either even or odd with respect to the $(1\bar{1}0)$ mirror plane orthogonal to the gold chains.

Apart from bulk transitions we observed an even, short-lived ($\tau <$ 20 fs) $n = 1$ image-potential resonance and a long lived feature ($\tau >$ 600 fs) within the bulk band gap of silicon. States related to the gold chains were detected at high emission angles. We present here an analysis of our time-, angle- and energy-resolved measurements and compare our findings to the Si(557)-Au and Si(553)-Au surfaces.

O 35.80 Tue 18:15 Poster B

Photoemission study of occupied and unoccupied states on Si(553)-Au — •Stefan Regensburger[1], Kerstin Biedermann[1], Thomas Fauster[1], Franz J. Himpsel[2], and Steven C. Erwin[3] — [1]Lehrstuhl für Festkörperphysik, Universität Erlangen-Nürnberg, Staudtstraße 7, 91058 Erlangen, Germany — [2]Department of Physics, University of Wisconsin-Madison, 1150 University Avenue, Madison, WI 53706, USA — [3]Center for Computational Materials Science, Naval Research Laboratory, Washington, DC 20375, USA

Atomic gold chains on vicinal Si(111) surfaces serve as model system for one-dimensional electronic states. For the characterization of the electronic states near the $\bar{\Gamma}$-point we used angle- and time-resolved two-photon photoemission with photon energies of 1.55 eV and 4.65 eV, as well as photoemission with 6.2 eV photon energy. Information about the symmetry of the electronic states was obtained from the polarization dependence of the spectra.

In addition to bulk transitions, the Rasha-split gold bands [1] and the $n = 1$ image-potential resonance we find two states related to the step-edge atoms. We observe an unoccupied state with even symmetry in the bulk band gap of silicon with a lifetime of $\tau = 125$ fs. It is assigned to the spin-polarized step-edge atoms predicted by theory [2]. An occupied state located 0.42 eV below the Fermi level corresponds to non-magnetic step-edge atoms coupled in pairs.

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

[2] Erwin, S. C. and Himpsel, F. J., Nat. Commun. **1**, 58 (2010)

O 35.81 Tue 18:15 Poster B

Two-photon photoemission from Si(111) 7×7 — •Jens Güdde, Andreas Damm, Marcel Reutzel, Alexander Lerch, and Ulrich Höfer — Fachbereich Physik und Zentrum für Materialwissenschaften, Philipps-Universität, D-35032 Marburg

The dynamics of photoexcited electrons in unoccupied states of the Si(111) 7×7 surface has been investigated by time- and angle-resolved two-photon photoemission (2PPE) for different sample temperatures. Aside from non-resonant 2PPE from the occupied S_2 surface band and the valence band maximum we observe the population dynamics in the initially filled (S_1) and and empty (U_1) surface bands as well as in the X valley of Si close to the surface. The population in the conduction band (CB) shows a temperature-dependent delayed rise on the same time scale of several hundred femtoseconds as the electron thermalization in the U_1 band. The photoemission from the S_1/U_1 as well as from the CB is completely quenched by hydrogen adsorption. Together with the delayed population rise, this suggests that the CB is populated by electrons which were initially excited in the U_1 band. The investigation of the population dynamics for different parallel momenta along the $\bar{\Gamma}$-$\bar{\text{K}}$-direction reveals that the intraband relaxation within the CB proceeds on a time scale of few picoseconds while the population at the conduction band minimum decays with a time constant of several tens of picoseconds.

O 35.82 Tue 18:15 Poster B

Photoemission studies of graphene on Pt(111) — •David Nobis, Daniel Niesner, and Thomas Fauster — Lehrstuhl für Festkörperphysik, Universität Erlangen-Nürnberg, Staudtstr. 7, D-91058 Erlangen, Germany

Graphene can be grown on a variety of metal surfaces with different quality. On the Pt(111) surface graphene was prepared by decomposition of hydrocarbons. Ultraviolet photoelectron spectroscopy (UPS, 6.22 eV) and two-photon photoemission (2PPE, pump pulse 4.66 eV, probe pulse 1.55 eV) experiments were carried out on the graphene-covered surface.

The UPS experiments show a downward-dispersing state 260 meV below the Fermi level. This state fits well to a Shockley surface state from the bare Pt(111) surface calculated by the phase accumulation model. The graphene layer increases its binding energy.

By 2PPE the first two image-potential states with binding energies of 820 meV and 210 meV were observed. Lifetimes were determined to 13 fs and 79 fs and effective masses are close to the free-electron mass. Compared to the clean Pt(111) surface [1] the graphene layer enlarges the binding energy (mostly of n=1 image-potential state) and the lifetime of the image-potential states. This can be understood by the screening of the charge being dominated by the graphene. Angle-

resolved spectra show maximum intensity around $\mathbf{k}_{\parallel} = 0.1$ Å^{-1} which is attributed to a resonance with the Shockley surface state.
[1]Link, S. *et al.*, Phys. Rev. B **63** (2001) 115420

O 35.83 Tue 18:15 Poster B

Towards time- and angle-resolved photoemission at a free-electron laser with an angle-resolving ToF spectrometer — •Christian Sohrt[1], Michael Bauer[1], Wilfried Wurth[2], Lutz Kipp[1], and Kai Rossnagel[1] — [1]Institut f\"ur Experimentelle und Angewandte Physik, Kiel, Germany — [2]Institut f\"ur Experimentalphysik and Center for Free-Electron Laser Science, Hamburg, Germany

The Free-Electron Laser (FEL) in Hamburg (FLASH) generates highly brilliant, ultrashort pulsed radiation with pulse durations down to 50 fs and photon energies up to 1000 eV. This enables unique experiments, as for example time-resolved core-level photoelectron spectroscopy. However, to establish photoelectron spectroscopy as a completely viable technique at an FEL, one has to develop a detection scheme with maximum efficiency, because the pulse repetition rates of FELs are notoriously low and the available beam time is extremely scarce. Our proposed solution is a photoelectron spectroscopy experiment based on a novel angle-resolved time-of-flight spectrometer. Compared to traditional detection schemes the instrument is expected to enhance the detection efficiency by a factor of about 200–due to the larger acceptance angle–and the temporal resolution by a factor of seven to about 100 fs–due to single-pulse detection. Thus, it will become possible to correlate core-level dynamics which is sensitive to changes in the charge distribution around specific atomic sites, with the dynamics of electrons at the Fermi surface in a single experiment. Here we present the progress of this project. This work is supported by the BMBF (FSP 301 FLASH).

O 35.84 Tue 18:15 Poster B

Thickness dependence of ion induced eletron emission — •Kevin Kusmierek[1], Christian Haake[1], Andreas Wucher[1], Marika Schleberger[1], and Detlef Diesing[2] — [1]Universität Duisburg-Essen, Fakultät für Physik, 47057 Duisburg, Germany — [2]Universität Duisburg-Essen, Fakultät für Chemie, 45117 Essen, Germany

Ion bombardment of thin metal films leads to electronic excitations causing the well known secondary electron emission. When the film thickness is in the range of the excited carrier's mean free path, reflection of carriers at the back side of the film and subsequent passage through the front side to the vacuum may increase the secondary electron emission yield. This increase of the yield is influenced by the relaxation of the ion induced electronic excitation. Thus, we present a study on the thickness dependence of the secondary electron emission yield. Our metal films are evaporated on glass and AFM studies show a mean roughness of 3 nm. The films have thicknesses between 10 and 100 nm and are bombarded with keV Ar ions.

O 35.85 Tue 18:15 Poster B

Surface and Image-Potential States of Ni(111) Investigated with Spin- and Time-Resolved 2PPE — Thomas Odebrecht[1,2], •Beatrice Andres[1,2], Marko Wietstruk[1,2], Anke B. Schmidt[3], Markus Donath[3], and Martin Weinelt[1,2] — [1]Max-Born-Institut, 12489 Berlin — [2]Fachbereich Physik, Freie Universität Berlin, 14195 Berlin — [3]Physikalisches Institut, Westfälische Wilhelms-Universität Münster, 48149 Münster

The surface electronic structure of Ni(111) does not only exhibit occupied *sp*- and *d*-derived bulk states and surface resonances [1], but also a partially occupied Shockley-like surface state (SSS) as well as a Rydberg-series of image-potential states (IPS) close to the vacuum enegy. In two-photon photoemission experiments (2PPE) using the fundamental ($1h\nu = 1.6$ eV) and the third harmonic ($3h\nu = 4.8$ eV) of our Ti:Sa laser, we gain information on exchange splitting, spin polarization and spin-dependent lifetimes of these states.
We can either populate the unoccupied minority component of the SSS with a $1h\nu$ pulse and probe with $3h\nu$ or use a $3h\nu$-pump and $1h\nu$-probe pulse to reach the energetic region of the IPS. Populating the IPS out of the occupied components of the surface and bulk states we create a spin-polarized population in these unoccupied states which allows us to study their spin-dependent properties.

[1] Okuda *et. al.*, *Phys. Rev. B* **80**, 180404 (2009).

O 35.86 Tue 18:15 Poster B

Thermal desorption spectroscopy of interstellar relevant molecules on Forsterit and Olivine — •Robert Frigge, Tushar Suhasaria, Nadine Heming, Björn Siemer, and Helmut Zacharias — Physikalisches Institut, Universität Münster, Germany

Chemical surface reactions on dust grains are a possible way of molecule formation in the Interstellar Medium (ISM). These grains typically consists of carbonaceous and silicate particles embedded in icy mantles which are formed by molecules like CO, CO_2, H_2O or CH_4. Temperature programmed desorption (TPD) is used to investigate the binding energy and reaction order of several interstellar relevant molecules like D_2, CO, CO_2, CH_4, and D_2O on different interstellar silicate analogues like Forsterite (Mg_2SiO_4) and Olivine ($Mg_xFe_{1-x}SiO_4$). The experimental set-up consists of a quadrupole mass spectrometer, a dosing chamber and a liquid helium cooled sample holder. Due to this set-up it is possible to investigate the behavior of these molecules at very low temperatures (≈ 5 K) comparable to the ISM. Further due to the dosing chamber it is possible to prepare a sample with a precise and low coverage. We present desorption spectra, binding energies and their coverage dependence on both Olivine and single crystal Forsterite.

O 35.87 Tue 18:15 Poster B

On the relation between fluctuations in STM currents and diffusion coefficients of molecules on surfaces — •Susanne Hahne[1], Julian Ikonomov[2], Moritz Sokolowski[2], and Philipp Maass[1] — [1]Department of Physics, University of Osnabrück, Barbarastr. 7, 49076 Osnabrück, Germany — [2]Institute of Physical and Theoretical Chemistry, University of Bonn, Wegelerstr. 12, 53115 Bonn, Germany

A widely used method to measure surface diffusion coefficients is by tracking particles via STM, FEM or FIM. To obtain reliable data one needs a good statistic, which is generally quite extensive. Also these methods are limited to sufficiently small mobilities. An alternative experimental approach is the recording of the signal fluctuations in time from a locally fixed microscope [e.g. tunneling current in case of STM; frequency/height in case of AFM]. This procedure on the other hand needs a good theoretical description in order to obtain reliable results. Three different methods can be applied to analyze this signal fluctuations: (i) Determination of the autocorrelation-function or extraction of the peaks in the fluctuation, where either (ii) the distribution of peak widths is studied or (iii) the distribution of peak to peak distances. We critically discuss and extend analytical theories underlying these methods and evaluate their power by comparison to recent experiments [1].

[1] J. Ikonomov, P. Bach, R. Merkel, and M. Sokolowski, Phys. Rev. B 81, 161412(R) (2010).

O 35.88 Tue 18:15 Poster B

Surface and bulk states at Ge(100) - Binding energies, lifetimes and dispersions — •Jens Kopprasch[1,2], Kristof Zielke[1,2], Cornelius Gahl[1,2], Christian Eickhoff[1,2], Jörg Schäfer[3], and Martin Weinelt[1,2] — [1]Max-Born-Institut, Max-Born-Straße 2a, 12489 Berlin, Germany — [2]Freie Universität Berlin, Fachbereich Physik, Arnimallee 14, 14195 Berlin, Germany — [3]Universitat Würzburg, Fakultät für Physik und Astronomie, Am Hubland, 97074 Würzburg, Germany

Germanium (Ge) is a material of growing interest in semiconductor industry. Increased industrial engineering has opened a broad field of applications for Ge, e.g. solar cells, high-power transistors, infrared optics and X-ray detectors.

We observed band bending at n-doped samples and flat-band conditions on p-doped samples. In this way we determine the Ge(100) ionisation potential. A series of two-photon-photoemission measurements with variing photon energies allows us to identify the dangling-bond states D_{up}, D_{down} and the first image-potential state n=1. We determined the binding energies, lifetimes and dispersions of these states. Furthermore we observed bulk-band transitions at 90K which lead to carrier dynamics on a picosecond timescale. In addition we observe ultrafast interband scattering between the conduction band and Γ-valley.

O 35.89 Tue 18:15 Poster B

Electronic energy dissipation - obtain mechanisms and models from TDDFT — •Michael Grotemeyer and Eckhard Pehlke — Institut für Theoretische Physik und Astrophysik, Universität Kiel, Germany

Molecular dynamics simulations based on time-dependent density-functional theory to describe the electron dynamics and Ehrenfest dynamics for the motion of the nuclei have provided detailed information about the electronic energy dissipation of vibrationally highly excited HCl molecules in front of a metal surface. Inspection of the time development of the electronic excitation spectra reveals the energy transfer mechanism and helps to identify the diabatic states responsible for the dissipation. The striking asymmetry between the excitation spectra of the holes and the electrons pinpoints the importance of the energetical position of the molecular resonances in the energy range of the unoccupied states. This leaves us with the question how to produce simple tight-binding like models and whether there is a unifying description of the energy dissipation process that holds the potential to be generalized to arbitrary molecular trajectories. Already a one-dimensional tight-binding model including only the LUMO is capable of describing the energy transfer process and illustrates many effects of the *ab initio* TDDFT-MD simulations. By adding an additional unoccupied molecular orbital into the model we obtain an improved description of the excitation spectra at the maximum of the dissipation. We suggest the resonance width of the LUMO plays a decisive role for the nonaddiabatic effects.

O 35.90 Tue 18:15 Poster B

Dynamic space charge effects in time-resolved photoelectron spectroscopy — •Lars Oloff, Stefan Hellmann, Christian Sohrt, Ankatrin Stange, Timm Rohwer, Michael Bauer, Lutz Kipp, and Kai Rossnagel — Institut für Experimentelle und Angewandte Physik, Universität Kiel, 24118 Kiel, Germany

The development of fs-pulsed lightsources, e.g. Free-Electron Lasers or High Harmonic Generation sources (HHG), opened up a new field of photoelectron spectroscopy (PES) in terms of time-resolved pump-probe-experiments. The high intensity of these sources leads to the effect that the interaction beween the photoelectrons emitted in such an ultrashort time frame can not be neglected anymore. This phenomenon known as space charge effect results in general in non-negligible impact on kinetic energy and detected angle of the emittted electrons. Specifically in time-resolved pump-probe-PES in the high pump-power regime a further intensity-caused effect can be recognized: Via multi-photon-processes the low energy pump-pulse may lead to unwanted emission of electrons from the material. This pump electron cloud interacts via Coulomb forces with the electron cloud emitted through the probe pulse resulting in shifted and broadened photoelectron spectra. We investigated these dynamic space charge effects at a HHG source (42.66 eV, 27th Harmonic) on $TiSe_2$ and $Pt(111)$ demonstrating their dependency on material, intensity and chosen delay between the two pulses. The results can be interpreted via molecular dynamic simulations.

O 35.91 Tue 18:15 Poster B

Preparation and spectroscopic studies of benzo[ghi]perylene dye on SiC — •Nils Fabian Kleimeier[1], Deb Kumar Bhowmick[1], Nabi Aghdassi[1], Steffen Linden[1], André Devaux[1,2], Luisa De Cola[1,2], and Helmut Zacharias[1,2] — [1]Physikalisches Institut, Westfälische Wilhelms-Universität, Wilhelm-Klemm-Str. 10, 48149 Münster, Germany — [2]CeNTech GmbH, Center for Nanotechnology, Heisenbergstr. 11, 48149 Münster, Germany

Organic-inorganic hybrid systems have gained increasing interest due to their versatile applications, e.g., as organic solar cells, biosensors, light emitting devices, or molecular electronics. Our research focuses on polyaromatic hydrocarbons (PAHs) due to their characteristically high fluorescence yield and the possibility to tune their photophysical and electrochemical properties. SiC substrates are functionalized with aminopropyl triethoxysilane (APTES) molecules by a siloxane bond. The benzo[ghi]perylene-1,2-dicarboxylic anhydride is then bound covalently to the APTES via imide bonds. Covalent attachment of the dye to the surface is verified by X-ray photoemission spectroscopy and FT-IR spectroscopy. UV absorption and time-resolved fluorescence and two-photon photoemission spectroscopy (TR-2PPE) measurements have been performed, yielding lifetimes between τ_1=1.4 to 1.8 ns and τ_2=4.3 to 4.7 ns for the fluorescence and τ=84 fs for the TR-2PPE measurement.

O 35.92 Tue 18:15 Poster B

Real-time observation of electron propagation in condensed matter — •Stefan Neppl[1], Elisabeth M. Bothschafter[1,2], Ralph Ernstorfer[3], Adrian L. Cavalieri[4], Johannes V. Barth[1], Dietrich Menzel[1], Reinhard Kienberger[2], and Peter Feulner[1] — [1]TU München — [2]Max-Planck-Institut für Quantenoptik — [3]Fritz-Haber-Institut — [4]CFEL

Photo-ionization with isolated attosecond (1 asec = 10^{-18} s) XUV pulses simultaneously dressed by a precisely timed NIR electric field is envisaged as a tool for probing the ultrafast dynamics of electrons in condensed matter [1]. Here we demonstrate the ability of this streaking technique for real-time probing the motion of photo-excited electrons in thin metal films as they traverse single atomic layers. By growing epitaxial layers of magnesium on a W(110) substrate, we are able to follow the time evolution of the XUV-induced photoelectron wave packets originating from the W4f and Mg2p core states and the joint conduction band with a time resolution of only a few attoseconds. Depending on the initial state character of the released electrons, we measure relative time delays in their emission ranging from 10 to 200 asecs, with different dependencies on the thickness of the overlayer. The results will be compared to corresponding streaking experiments performed on magnesium and tungsten single crystals

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

O 35.93 Tue 18:15 Poster B

Nonequilibrium phonon gas in laser-excited solids — •Isabel Klett[1], Orkhan Osmani[1,2], and Bärbel Rethfeld[1] — [1]TU Kaiserslautern, 67663 Kaiserslautern, Germany — [2]Universität Duisburg-Essen, 47048 Duisburg, Germany

Irradiation of metals with a femtosecond laser pulse leads to a hot electron gas, while the lattice stays nearly cold. Due to the excitation, the electronic system is out of thermal equilibrium, so after laser irradiation, two main processes occur: The first is the electron thermalization, the second is the energy transfer from the electrons to the lattice due to the electron-phonon-coupling. Both processes have been described by assuming a thermalized distribution function for the phononic system. However, due to the fact that only longitudinal phonon modes can absorb the energy of the electrons, this assumption does not hold. Besides, with THz-Lasers [1], different phonon modes can be excited directly, leading to a thermal nonequilibrium within the phononic system. Furthermore, in thin films phonon confinement effects have been observed [2], which is also an indication for a nonequilibrium distribution of the phonons. We describe the phonon-phonon interaction and phonon thermalization with a Boltzmann collision integral. Our aim is to model nonequilibrium phonon distributions and the resulting observable effects after ultrashort laser-matter interaction.

[1] S. Kumar et al., Appl. Phys. Lett. 84, 2494*2496 (2004)

[2] B. Krenzer et al., Phys. Rev B 80, 024307 (2009)

O 35.94 Tue 18:15 Poster B

Time-resolved femtosecond Se 3d core level spectroscopy in the Mott insulator TiSe2 — •Hatem Dachraoui[1], Tobias Milde[1], Michael Porer[2], Norbert Müller[1], Recardo Manzke[3], Walter Pfeiffer[1], Rupert Huber[2], and Ulrich Heinzmann[1] — [1]Molecular and Surface Physics, Faculty of Physics, Bielefeld University, Germany — [2]Ultrafast Quantum Electronics and Photonics, Faculty of Physics, Regensburg University, Germany — [3]Elektronische Eigenschaften und Supraleitung, Faculty of Physics, Humboldt-University Berlin, Germany

Strongly correlated materials exhibit interesting dynamics and phase transitions for which the underlying mechanisms are still under debate. Fs-laser induced dynamics provide information about the phase transition mechanism. The recent progress in the creation of femtosecond EUV pulse generation (by means of high harmonic Generation HHG) offers the feasibility of time-resolved core level photoelectron spectroscopy which is capable of probing ultra-fast light driven processes at surfaces. Here we use 20 fs EUV-pulses to directly study the ultrafast dynamics of the charge density wave in TiSe2 after near-infrared excitation (1.5 eV). Structural transitions, evidenced by a dynamic shift of Se 3d core-levels, occurs before electrons lattice thermalization is established.

O 35.95 Tue 18:15 Poster B

2PPE-measurement on Cu(1 1 11) with an angle-resolving time-of-flight spectrometer — •Thomas Kunze[1,2], Jens Kopprasch[1,3], Martin Teichmann[1,3], Thorsten U. Kampen[2], and Martin Weinelt[1,3] — [1]Max Born Institut, Max-Born-Straße 2a, 12489 Berlin, Germany — [2]SPECS GmbH, Voltastr. 5, 13355 Berlin, Germany — [3]Freie Universitat Berlin, Fachbereich Physik, Arnimallee 14, 14195 Berlin, Germany

We aim at the implementation of an advanced concept for photoemission spectroscopy into a robust and reliable experiment for time-and energy-resolved photoemission with ultrahigh transmission. The basic idea is to combine a parallel imaging technique comprising ultimate $\vec{k}$-resolution with time-of-flight energy dispersion. Therefore we developed, in cooperation with SPECS GmbH, the angular-resolving Time-of-Flight spectrometer THEMIS. This instrument allows us to measure energy E over parallel momentum $k_{x\|}$ and $k_{y\|}$ without rotating the sample.

We present two-photon photoemission measurements on Cu(1 1 11), a vicinal copper surface with (001)-terraces. The dispersion of the image-potential states reveals back-folding and mini-gap opening with the periodicity of the step superlattice. The lifetimes of the image-potential states at Cu(1 1 11) depend on the parallel momentum of the photoemitted electrons.

O 35.96 Tue 18:15 Poster B

Charge-transfer collisions of H^+ with He using Time-Dependent Density Functional Theory — •Guillermo Avendano-Franco, Xavier Gonze, and Bernard Piraux — Université Catholique de Louvain, Louvain-la-Neuve, Belgium

We present a theoretical study of the Charge-transfer collisions of H^+ with He using Time-Dependent Density Functional Theory. The energies of the projectile were between 70 keV to 1.2MeV. We found some charge being transferred to the proton and we considered those results in relation to current theoretical descriptions of the collision processes.

O 35.97 Tue 18:15 Poster B

Investigations of the Patch Effect with a Scanning Kelvin Probe — •Gertrud Konrad[1,2], Stefan Baessler[3], Iain Baikie[4], Henry Bonner[3], Werner Heil[2], Rachel Hodges[3], Thorsten Lauer[2], Sean McGovern[3], and Xuying Tong[3] — [1]Atominstitut, TU Wien, Austria — [2]Universität Mainz, Germany — [3]University of Virginia, Charlottesville, USA — [4]KP Technology Ltd., Wick, UK

Precision measurements of observables in neutron beta decay address important open questions of particle physics and cosmology, and are generally complementary to direct searches for new physics beyond the Standard Model in high-energy physics.

The analysis of the decay protons is based on a precise energy measurement, by means of an electrostatic filter or by TOF measurement. Then the electric potential between the decay and filter regions has to be known with an accuracy of better than 10 mV. Possible inhomogeneities of the work function (WF) at the electrode surface vary the electric field distribution. On the inside of a cylindrical electrode, a spatial variation of order of 100 meV over a distance of several cm was found. A scanning Kelvin probe (SKP) has been used to map the WF, with a spatial resolution of 2 mm and a WF resolution of $1-3$ meV. To minimize the WF variations, different surface materials, treatments, and coatings are being investigated. A platinized surface yielded a RMS WF value of better than 10 meV. Coating adhesion and surface roughness have a significant influence on the measured WF values.

The physics motivation, the SKP technique as well as the status of the investigation will be presented in this talk.

O 35.98 Tue 18:15 Poster B

Dynamische Rasterreibungskraftmikroskopie: Bildkontrast bei höheren Moden auf HOPG — •Felix Mertens, Karsten Krischker, Thomas Göddenhenrich und André Schirmeisen — Institut für Angewandte Physik, Justus-Liebig-Universität Gießen, D-35392 Gießen

Es wird ein Modulations-Reibungsmikroskop präsentiert, das für Topographie- und Reibungsmessungen unter UHV Bedingungen geeignet ist [1]. Eine modifizierte Lock-In Technik regt die Probe zu Schwingungen entlang der Hebelarmlängsachse an [2]. Durch den Spitze-Probe Kontakt werden dem Hebelarm Oszillationen aufgeprägt, die durch ein Glasfaserinterferometer detektiert werden. Entspricht die Anregungsfrequenz der modulierten Probenschwingung einem ganzzahligen Bruchteil der Hebelarmbiegeresonanz, so setzt sich die Hebelarmoszillation sowohl aus niederfrequenten als auch aus hochfrequenten Schwingungsanteilen zusammen. Die niederfrequenten Schwingungsanteile korrespondieren mit der Topographie, die Anregung der hochfrequenten Schwingungsanteile wird durch den Reibungskontakt verursacht. Die Anwendung dieser Technik auf hochorientiertem Pyrographit ermöglicht Reibungsaufnahme, bei denen die Orientierung der Kornstruktur einen wesentlichen Kontrastmechanismus der Aufnahme darstellt. [1] T. Göddenhenrich, S. Müller, and C.Heiden, Rev. Sci. Instrum. 65, 2870 (1994) [2] A. Spychalski-Merle, K. Krischker, T. Göddenhenrich, and C. Heiden, Appl. Phys. Lett. 77, 501 (2000)

O 35.99 Tue 18:15 Poster B

Nanoparticle Manipulation With Combined AFM/SEM — •Michael Feldmann[1], Antoni Tekiel[2], Jessica Topple[2], Dirk Dietzel[1], Peter Grutter[2], and André Schirmeisen[1] — [1]Institut für Angewandte Physik, JLU Giessen, Germany — [2]Department of Physics, McGill University, Montréal, Canada

To understand friction on a fundamental level the investigation of friction with nanoparticles has presented itself as a very promising approach[1][2]: a nanoparticle is pushed by an AFM tip to measure the friction between the particle and a substrate. These experiments allow to study friction of extended single asperity nanocontacts. If this kind of experiment is executed with just a single AFM tip as a probing channel, the tip can either move the particle or image it, but not both at the same time. To gain a better understanding of the involved processes and to increase control over the manipulation, we performed nanoparticle manipulations with a combined AFM / SEM system. This setup enabled us to move the particles with the AFM, while simultaneously observing the particle translations with scanning electron microscopy. We observed that the AFM tip is not only able to push the particles, but also to pull the particles over the substrate due to the adhesion between tip and particle. On the other hand complete detachment of the particles from the substrate did never occur, consistent with the assumption of having very flat interfaces and thus high adhesion between particle and substrate.

[1] D. Dietzel et. al., Phys. Rev. Lett. 101, 125505 (2008)
[2] D. Dietzel et. al., Phys. Rev. B 82, 035401 (2010)

O 35.100 Tue 18:15 Poster B

Charge transport mesasurements performed with an ultra compact multi-tip STM — •Marcus Blab, Vasily Cherepanov, Peter Coenen, and Bert Voigtländer — Peter Grünberg Institut (PGI-3), Forschungszentrum Jülich, 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 through nanostructures. Examples for systems which can be studied with such a microscope include nanowires, graphene and nanoscale semiconductor devices. The instrument diameter of 50 mm leads to high mechanical stability and low thermal drift. The heart of this multi tip STM is the ultra compact Koala Drive nanopositioner. We will show the characteristics of this new machine like drift and noise. Furthermore first measurements at test samples and lithographic structured samples of nanowires will be presented.

O 35.101 Tue 18:15 Poster B

Radio frequency optimized STM for the use with pulsed tunneling voltages — •Christian Saunus, Marco Pratzer, and Markus Morgenstern — II. Physikalisches Institut, RWTH Aachen University, Aachen Germany

The measurement of fast surface dynamics with an STM suffers from the low readout bandwidth given by the high gain preamplifier. To overcome this limit, Sebastian Loth introduced an all electrical pump-probe measurement which enabeled him to measure electron spin relaxation at the order of 100 ns by a commercial standard STM [1]. To increase this time resolution even more we designed a very compact STM with an insitu tip exchange mechanism operating with high frequency voltage pulses. We have shown that a time resolution of 710 ps is achieved by using the non-linearity of the I(V) curve on HOPG. The microscope is designed to work in a 4 K UHV system with 7 T rotatable magnetic field.

[1] S. Loth, Science 329, 1628 (2010)

O 35.102 Tue 18:15 Poster B

Ion conduction in glass ceramics: Influence of nanoscopic boundary surfaces in experiment and simulation — •Marvin Stiefermann[1], Dirk Dietzel[2], André Schirmeisen[2], Harald Fuchs[1], and Bernhard Roling[3] — [1]Physikalisches Institut, University of Münster and CeNTech, Center for Nanotechnology, Münster — [2]Institut für Angwandte Physik, University of Gießen — [3]Department Chemie, Universität Marburg

The ongoing progress in miniaturization leads to a constantly increasing number of mobile electronic devices. The largest factor limiting the usability of the devices is the battery endurance. Hence further research is needed for a better understanding leading to higher battery performance. We analysed a solid electrolyte as found in modern batteries using a N2 cooled variable temperature atomic force microscope. Electrostatic force spectroscopy in the time domain (TDEFS) was employed to study the relaxation times of ions within nanoscopic subvolumes of a phase separated glass ceramic, consisting of a well conducting glassy phase and poorly conducting crystalline phase. An effect observed earlier in ion conduction studies was the decrease of relaxation time when increasing the fraction of weakly conducting crystalline phase[1]. To understand this phenomenon we compared the experimental TDEFS spectra with simulations based on a Comsol Multiphysics finite element simulation. The model built consists of 2500 elements allocated to well and poor conducting phases randomly. By varying the fraction of both phases, the trend of nanoscopic ion conduction can be reproduced and related to the amount of surface boundaries.

O 35.103 Tue 18:15 Poster B

Contact size effects for the β-relaxation of PMMA using friction force microscopy — •Johannes Sondhauss[1], Bernd Gotsmann[2], Mark A. Lantz[2], and André Schirmeisen[3] — [1]Institute of Physics, University of Münster, Germany — [2]IBM Zurich Research Laboratory, Rüschlikon, Switzerland — [3]Institute of Applied Physics, University of Giessen, Germany

The importance of polymer films for different technical applications brought increased attention to polymer surface studies. In addition polymers are an ideal model system for tribology due to their distinct modes of dissipation. The friction force microscope (FFM) has been recently proved useful to study surface processes in polymers. In this work we performed friction experiments using different Si-tips sliding on a PMMA film. We varied the applied load, the scan velocity and the sample temperature. In addition we used three different cantilevers with tip radii between 18 nm and 2.65 μm. Latter were produced by attaching a spherical Si-particle to the modified tip apex of a cantilever. Within the chosen parameter range we observed the β-relaxation as well as the onset of the α-relaxation and we were able to determine the activation energy of the β-relaxation for each of the data sets measured with the different tips. The observed activation energy increases for increasing tip radii.This trend seems to follow the Eyring model which describes the influence of the shear stress on the activation energy. Furthermore, a conversion of the scan velocity to frequency [1] allowed us to combine the individual data sets to one curve.

[1] Tocha et al., Soft Matter 5, 1489 – 1495 (2009)

O 35.104 Tue 18:15 Poster B

Nano-Raman Microscope with Novel Probe Design for High-Resolution Surface Investigations — •Christoph Zeh[1], Daria Kovalenko[1], Martin Küttner[1], Bernd Köhler[1], Jörg Opitz[1], and Lukas M. Eng[2] — [1]Fraunhofer Institut für Zerstörungsfreie Prüfverfahren, Institutsteil Dresden, Maria-Reiche-Str. 2, 01109 Dresden — [2]Institut für Angewandte Photophysik, TU Dresden, 01069 Dresen

Optical Raman signals contain a wealth of information about the physical and chemical properties of many different substances. In this work, we demonstrate our home-built Nano-Raman microscope (NRM) and special optical fiber probes. The NRM comprises a standard microscope as optical detection system and a scanning near-field optical (SNOM) head. It is intended for investigations of nano-structured materials for novel industrial applications. The probe acts as a nanoscale light source and locally illuminates the sample. In each examined point of the sample, light scattered from the surface is collected through the microscopes objective lens and sent to an optical detector, e.g. spectrometer. The smaller the light source is, the higher is the resolution. To achieve a small spot size and high light intensities at the same time, we use sharp optical fiber tips prepared from a special optical fiber. The fiber has a refractive index profile allowing better polarization control, especially for circular light distributions. These modes of the optical field allow for a higher efficiency of the fiber probe. We will present recent results on the fabrication of suitable fiber tips.

O 35.105 Tue 18:15 Poster B

Implementing a setup to detect ballistic and inelastic transport channels in an LT-STM experiment — •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

As low cost and easy to process alternatives to conventional inorganic semiconductors, organic molecules are already applied in a variety of electronic devices. For an improvement in speed, energy consumption and lifetime of these devices the understanding of the electronic transport through the molecules is essential. Electrons injected into a molecule by the tip of a scanning tunneling microscope (STM) may lead to an electronic excitation. The relaxation may follow different pathways, one of which is a radiative decay, i.e. the emission of photons [1]. The spectral analysis of these photons combined with the ultimate lateral resolution of the STM has been demonstrated to allow a mapping of dissipative channels within a single molecule [2]. Here, we present the implementation of a detection unit for light emission which is integrated into an existing home built low temperature STM experiment. As a complementary technique, ballistic electron emission microscopy (BEEM) can be used to identify ballistic transport channels [3]. The combination of both techniques will give further access to study transport phenomena on an atomic scale.

[1] R. Berndt et al., Science 262, 1425 (1993). [2] C. Chen et al., Phys. Rev,. Lett. 105, 217402 (2010). [3] A. Bannani et al., Science 315, 1824 (2007).

O 35.106 Tue 18:15 Poster B

STM characterization of self-assembled organic compounds on metallic surfaces — •Oscar Diaz Arado[1,3], Lars Jansen[1], Hendrik Wagner[2], Amido Studer[2], and Harald Fuchs[1] — [1]Physikalisches Institut and Center for Nanotechnology, Muenster — [2]Organisch-Chemisches Institut, Westfaelische Wilhelms-Universitaet, Muenster — [3]Centro de Estudios Avanzados de Cuba, CEAC, La Habana, Cuba.

Chemical reactions on surfaces (2D reactions) through the self-assembly of organic compounds have been an uprising field of research in the last years, being a promising alternative to construct covalent-linked organized structures, something thought to be impossible up to now [1]. Therefore, we investigate the possibility to initiate a chemical reaction between two organic compounds, 2,5-Dihexylterephthalaldehyde and Octanehydrazide, on Au (111), a simple geometry to study their possible 2D reactions [2]. These compounds were initially studied with a scanning tunneling microscope (STM) under a liquid environment, where no self-assembly process was observed. Organic molecular beam epitaxy is a method suitable to perform a controlled layer-by-layer deposition of organic compounds in the ultra high vacuum (UHV) regime. We present our preliminary results of the combination of the OMBE deposition technique with a room temperature STM under UHV conditions. The successful deposition and self-assembled structure formation of each compound is presented here. [1] D. F. Perepichka, F. Rosei, Science 2009, 323, 216 [2] T. R. Linderoth et. al., Angew. Chem. 2007, 119, 9387

O 35.107 Tue 18:15 Poster B

Thermal Scanning Probe Lithography: Progress and Applications — •Felix Holzner[1,2], Philip Paul[1], Cyrill Kuemin[1,2], Ute Drechsler[1], James L. Hedrick[3], Heiko Wolf[1], Nicholas Spencer[2], Urs Duerig[1], and Armin Knoll[1] — [1]IBM Research, Rueschlikon, Switzerland — [2]Laboratory of Surface Science and Technology, ETH Zurich, Switzerland — [3]BM Research, Almaden, USA

The presented poster summarizes our recent advances in Thermal Scanning Probe Lithography with polyphthalaldehyde (PPA) as resist material. The polymer responds to the presence of a hot tip by depolymerization and local desorption. Thereby arbitrarily shaped patterns in the form of topographic reliefs can be written.

Patterning speeds with up to 500000 pixels/s and a positioning error of less than 10 nm at 10 mm/s scan speed were achieved. The written reliefs were imaged with the same cantilever with similar scan speeds leading to short fabrication turn-around times. In addition, we show that it is possible to use the surface roughness of the polymer films as fingerprints for the alignment of subsequently written patterns. The method achieves a stitching accuracy of <5 nm.

First applications shown on the poster include ”Ultra long-term data preservation” and ”Removable templates for directed placement of gold nanorods”.

[1] Holzner et al., Nano Letters, 2011, 11, 3957-3962 [2] Paul et al., Nanotechnology, 2011, 22, 275-306 [3] Knoll et al., Advanced Materials, 2010, 22, 3361-3365 [4] Holzner et al., Appl. Phys. Lett., 2011, 99, 023110 [5] Pires et al., Science, 2010, 328, 732

O 35.108 Tue 18:15 Poster B

Electron induced dynamics of hepthathioether β-cyclodextrin molecules — •Avijit Kumar[1], René Heimbuch[1], Kim S. Wimbush[2], Hasan Atesci[1], Adil Acun[1], David N. Reinhoudt[2], Aldrik H. Velders[2,3], and Harold J W Zandvliet[1] — [1]Physics of Interfaces and Nanomaterials, MESA+ Institute for Nanotechnology — [2]Supramolecular Chemistry and Technology, MESA+ Institute for Nanotechnology — [3]Biomolecular Chemistry, MIRA Institute for Biomedical Technology and Technical Medicine, University of Twente, the Netherlands

Macroscopic junctions using Self Assembled Monolayers (SAMs) are prevalent in charge transport studies in molecular electronics. However, the macroscopic nature of metal-molecules contacts lead to an ensemble averaging of the transport events that occur across array of contacted molecules. Here, we have performed variable temperature scanning tunneling microscopy (STM) and spectroscopy (STS) measurements on hepthathioether β-cyclodextrin (β-CD) SAMs on Au to investigate dynamical behavior, which is not apparent in ensemble averaged studies. The dynamics is reflected in the tunneling current-time (I-t) traces, which were recorded with the STM feedback disabled. The dynamics is temperature independent, but increases with increasing tunneling current and sample bias, indicating that the conformational changes of the β-CD molecules are induced by electrons that tunnel inelastically. Even for sample biases as low as 10 mV we observe well-defined levels in the I-t traces. We attribute these jumps to the excitations of the molecular vibration of the macrocyclic β-CD molecule.

O 35.109 Tue 18:15 Poster B

Chromium Bulk Tips for Spin-Polarized Scanning Tunneling Microscopy — •Christian Hanneken, André Kubetzka, Kirsten von Bergmann, and Roland Wiesendanger — Institute of Applied Physics and Microstructure Research Center, University of Hamburg, Jungiusstrasse 11, D-20355 Hamburg, Germany

For the investigation of magnetic nanostructures using spin-polarized scanning tunneling microscopy (SP-STM), one would like to avoid uncontrolled magnetic interactions between tip and sample and the tip and an external magnetic field. Antiferromagnetic material features these properties, therefore being desirable as a tip material. In this work, a new method is presented for the production of antiferromagnetic chromium bulk tips. The electrochemically etched tips were characterized *ex situ* using scanning electron microscopy. In order to demonstrate the magnetic sensitivity of the produced tips, one tip was characterized *in situ* using SP-STM. The polar angle of the tip magnetization and its variation after different tip changes is determined and is found not to change significantly. In addition, it is shown that an external magnetic field has no effect on the tip magnetization up to $\mathrm{B} = \pm 2\,\mathrm{T}$. To conclude, this Chromium bulk tip is found to be similar to Cr coated W tips with the advantage of a nearly infinite amount of magnetic material.

O 35.110 Tue 18:15 Poster B

Conductive AFM for CNTs characterisation — •Marius Toader[1], Holger Fiedler[2], Stefan E. Schulz[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 Research Institute for Electronic Nano Systems, D-09126 Chemnitz, Germany

Within a continuous downscaling tendency, the remarkable mechanical and electrical properties of Carbon NanoTubes (CNTs) recommend them as suitable candidates for nanoscale electronics and interconnects. A versatile technique able to address simultaneously morphological and electrical measurements within such nanosystems is Conductive Atomic Force Microscopy (C-AFM). In this work, MWCNTs networks were vertically grown by chemical vapour deposition on a conductive bottom contact line as described in [1]. Using C-AFM, topographic information as well as current mapping of CNTs networks within distinct trenches were obtained. Current-voltage (I-V) characteristics were recorded down to single CNTs bundles. The corresponding reproducibility was checked over multiple measurements sets and distinct locations. Moreover, the sample bias used during the spectroscopy measurements was found to have no influence on the I-V response. The outcome I-V spectra were found to be highly reproducible and consistent with the voltage dependent current mapping of the CNTs networks. [1] Fiedler et al. online via DOI: 10.1109/IITC.2011.5940346

O 35.111 Tue 18:15 Poster B

Experiments on molecular heat transport — •Nils Könne, Ludwig Worbes, David Hellmann, Konstantin Kloppstech, Hanna Fedderwitz, and Achim Kittel — EHF, Fak. V, Physik, Carl von Ossietzky Universität Oldenburg

The aim of our research is the heat transfer through a single molecule a topic which has attracted a lot of interest in recent years [1]. We have developed a near field scanning thermal microscope (NSThM) to investigate heat transfer under ultra high vacuum conditions across distances ranging from fractions of a nanometer to a few nanometers. The microscope has a lateral resolution in the range of a few nanometers. In the present project we are using this instrument to investigate the molecular heat transfer. To address this we are using self assembled mono layers as a model system. For this purpose different thiols are arranged on a gold covered substrate to which the thiol group of the molecule is bound covalently. Firstly, we characterize the degree of coverage of the film by means of atomic force microscopy. The heat transfer is investigated under ultra high vacuum conditions by cooling (about 120K) or heating the sample (350K) and keeping the NSThM tip at room temperature. First result will be presented. [1] Yonatan Dubi and Massimiliano Di Ventra, Rev. Mod. Phys. 83, 131 (2011).

O 35.112 Tue 18:15 Poster B

A combined LT-STM/FIM for tip specific tunnelling experiments — •Ben Wortmann and Rolf Möller — Faculty of Physics, Center for 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 characterization of the tip is possible without transfer to a different position in the UHV system. This guarantees that the tip characterized by FIM is identical to the one used for the STM experiment. The geometry of the microscope resembles a cylinder with a height of only 13 cm and a diameter of 4 cm. 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 unit (*slider*) by a slip-stick motion. The tip is spot welded to the slider which can be easily exchanged in vacuum. The STM is screwed directly onto a commercially available continuous flow cryostat which allows cooling to about 5-7 K. Insulation from vibration is provided by a combination of springs and eddy current damping. An almost identical system already shows the performance of the STM setup[1]. The very compact design minimises helium consumption to about 1 litre/hour. [1] (H. Karacuban, M. Lange, J. Schaffert, O. Weingart, Th. Wagner and R. Möller, Surf. Sci. Lett., 603, Issue 5, L39 (2009).

O 35.113 Tue 18:15 Poster B

On the characterization of thermal properties of Near-field scanning thermal microscope (NSThM) thermocouple-sensors by means of 3-ω technique — •Konstantin Kloppstech, David Hellmann, Ludwig Worbes, Nils Könne, Hanna Fedderwitz, and Achim Kittel — EHF, Fak. V, Physik, Carl von Ossietzky Universität Oldenburg

The experimental analysis of near-field heat transfer from defined surfaces by a NSThM is founded on accurate knowledge of thermal properties of the thermocouple sensor, particularly the thermal resistance κ. The fact that the sensor consists of a multi-material system complicates common analysis methods. The 3ω method provides an alternative for determining κ and in addition to this the effective heat capacity c_p and the Seebeck-coefficient S. The method bases on a very small AC heating current at angular frequency ω which is sent through a wire, resulting in a temperature and thus in a resistance fluctuation at 2ω. This periodic change in resistance leads to an alternating voltage at 3ω angular frequency, from which κ, c_p, and S can be determined. In our approach we use a 5 μ thin glass fiber coated with 2 nm Pt and 80 nm Au whose thermal properties are determined with the 3-ω method in a first step. Held in UHV the glass fiber is approached with a NSThM sensor adding a second channel for heat drain, resulting in a measurable change in κ that gives access to κ of the sensor. As the 3-ω method relies on established theoretical formulation it gives access to a value of thermal resistance and an exact error estimation. In summary we show that this method is first class in characterizing NSThM-sensors.

O 35.114 Tue 18:15 Poster B

Scanning near-field optical microscopy with single color centers — •Thomas Oeckinghaus, Julia Tisler, Rainer Stöhr, Roman Kolesov, Rolf Reuter, Friedemann Reinhard, and Jörg Wrachtrup — Universität Stuttgart, 3. physikalisches Institut

We are using single color centers as a light source for apertureless scanning near-field optical microscopy. Specifically, we use a nanodiamond of a size below 10nm, containing only a single nitrogen-vacancy color center, which we attach to the tip of an AFM. Close to a sample, the fluorescence of the color center is modulated by fluorescence resonance energy transfer (FRET), a short ranged dipole-dipole interaction. This interaction quenches the fluorescence of the donor (color center), whenever it is approached to an acceptor (sample). Because of the short range of FRET, high resolution scanning images can be obtained in this way. We successfully acquired SNOM images of a graphene monolayer with a resolution of 20 nm.

Furthermore, we present a technical development, stroboscopic detection of an oscillating tapping-mode AFM tip. This allows to scan at a specific height above the sample or to reduce stress on the sample by avoiding contact mode scanning.

O 35.115 Tue 18:15 Poster B

A next-generation room-temperature AFM setup with optical access for NV-magnetometry — •Dominik Schmid-Lorch, Tobias Staudacher, Friedemann Reinhard, and Jörg Wrachtrup — 3. Physikalisches Institut und Forschungszentrum SCoPE, Universität Stuttgart, Germany

The nitrogen-vacancy (NV) color center in diamond can be used as a magnetic field sensor with sub-nanometer special resolution. This is due to the fact that its spin sublevels are sensitive to magnetic fields and that they can be monitored using optically detected magnetic resonance (ODMR). Using this center as a scanning probe in an AFM [1] the sensing and imaging of single spins under ambient conditions might be feasible.

We present a novel integrated design for such a scanning probe diamond nano-magnetometer as well as our planed experiments, such as single spin MRI and single molecule SNOM.

[1] G. Balasubramanian et al., Nature Vol 455 (2008)

O 35.116 Tue 18:15 Poster B

Recent progress on the open source software package GXSM — •Thorsten Wagner[1] and Percy Zahl[2] — [1]Johannes Kepler University Linz, Institute of Experimental Physics, Linz, Austria — [2]Brookhaven National Laboratory, Upton, USA

Since 1998 the open source software package GXSM has an increasing community of users and developers all over the world. [1] The linux based software packages provides in combination with a digital signal processor (DSP) a very flexible tools for acquiring and processing data of all kinds of scanning probe microscopes. [2] With the implementation of the vector probe engine [3], GXSM developed to a full spectroscopic system. Besides traditional point spectroscopy (STS) it acquires spectroscopic data on grids and does atom tracking and manipulation. Just recently new algorithm for the automatic drift correction and tip crash prevention (for force spectroscopy) were implemented. With intelligent over sampling it goes beyond the 16bit limit of the hardware. Up to four input channels, like tunnel current and oscillation frequency, can be used simultaneously and mixed for the Z feedback control. The new hardware platform "SR-MK3Pro" will also allow an internal PLL feedback to drive tuning fork and needle sensors.

[1] http://gxsm.sf.net and http://sranger.sf.net

[2] P. Zahl, M. Bierkandt, S. Schröder, and A. Klust, Rev. Sci. Instr. 74 (2003) 1222

[3] P. Zahl, T. Wagner, R. Möller, and A. Klust, J. Vac. Sci. Technol. B 28 (2010) C4E39

O 35.117 Tue 18:15 Poster B

Investigations by intermittent contact AFM on free-standing static and mechanically vibrating nanowires — •Moid Bhatti, Ivo Knittel, and Uwe Hartmann — Institut für Experimentalphysik, Uni Saarland

The scanning speed of the atomic force microscope (AFM) is mainly limited by the resonant frequency of the (conventionally micron-sized) cantilever (fc) and the feedback control loop for height control with piezo resonant frequency fz. A reduction of the cantilever size leads to a higher fc for instance a nano-sized cantilever has fc typically in MHz range. Scanning at such high speeds will require a correspondingly fast feedback control loop (high fz). Besides, an understanding of the interaction between a sample surface and a static or oscillating nanowire (NW) or "nanocantilever (NC)" is required.

We have been studying the contact mechanics of the cantilever-sample system in the context of dynamic mode AFM using NCs of various types: (1)Nanowires grown on a substrate. (2)Carbon nanotubes attached to an AFM cantilever. (3)Focused-Ion-Beam (FIB)-structured AFM cantilevers. (4)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 oscillating at its tip.

We will present distance-dependent resonance curves and show various oscillatory states of an AFM cantilever interacting with a static NW and of NCs tapping on a sample surface. NWs were excited piezoelectrically and electrostatically up to 100 MHz. The detection of such vibrations is discussed.

O 35.118 Tue 18:15 Poster B

Low noise, wide band current to voltage amplifier for low temperature scanning tunneling microscope operation — •Hanna Fedderwitz, David Hellmann, Ludwig Worbes, Konstantin Kloppstech, Nils Könne, and Achim Kittel — EHF, Fak.V Physik, Carl von Ossietzky Universität Oldenburg

We are interested in the heat transfer across a nanoscale vacuum gap between two surfaces mediated by evanescent electromagnetic fields [1]. The characteristic length scale depends on the temperature of the two opposing surfaces and increases drastically at low temperatures. To investigate this effect we are setting up a low temperature scanning tunneling microscope (LT-STM) which can be equipped with a coaxial thermocouple tip [2]. Therefore it is necessary to apply the tunnel voltage to the sample instead of the STM-tip as in most STM setups. We achieve this by choosing a two stage setup. The first stage features low-noise transimpedance amplification by using a commercial high performance FET operational amplifier together with a high-ohm feedback resistor. Giving access to the current which is drained into the tip at tunnel voltage level the amplifier has to be powered by a floating supply voltage. A second stage is employed to reference the output signal to ground needed by the feedback electronics. This stage makes use of a commercial instrumentation amplifier. The two-stage system shows a low inherent total current noise of 4pA and a stable frequency response up to 10kHz cutoff frequency. [1] Achim Kittel et al., Appl. Phys. Lett. 93, 193109 (2008). [2] Uli F. Wischnath et al., Rev. Sci. Instrum. 79, 073708 (2008).

O 35.119 Tue 18:15 Poster B

Investigations by intermittent contact AFM on free-standing static and mechanically vibrating nanowires — •Moid Bhatti, Ivo Knittel, and Uwe Hartmann — Institut für Experimentalphysik, Uni Saarland

The scanning speed of the atomic force microscope (AFM) is mainly limited by the resonant frequency of the (conventionally micron-sized))cantilever (fc) and the feedback control loop for height control with piezo resonant frequency fz. A reduction of the cantilever size leads to a higher fc for instance a nano-sized cantilever has fc typically in MHz range. Scanning at such high speeds will require a correspondingly fast feedback control loop (high fz). Besides, an understanding of the interaction between a sample surface and a static or oscillating nanowire (NW) or "nanocantilever (NC)" is required.

We have been studying the contact mechanics of the cantilever-sample system in the context of dynamic mode AFM using NCs of various types: (1)NWs grown on a substrate. (2)Carbon nanotubes attached to an AFM cantilever. (3)Focused-Ion-Beam(FIB) structured AFM cantilevers. (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 oscillating at its tip.

We will present distance-dependent resonance curves and show various oscillatory states of an AFM cantilever interacting with a static NW and of a NC tapping on a sample surface. Free-standing NWs were excited piezoelectrically by using LiNbO3 single crystal and electrostatically in an electron microscope using a microwave line.

O 35.120 Tue 18:15 Poster B

A low-temperature facility for spin-polarized scanning tunneling microscopy — •Lihui Zhou, Peter Löptien, Focko Meier, Jens Wiebe, and Roland Wiesendanger — Institute of Applied Physics, University of Hamburg, Germany

Spin-polarized scanning tunneling microscopy (SP-STM) is a well-established technique to give insights into magnetic properties [1]. To investigate atomic-scale magnetism of atomic-size nanostructures where the typical energy scale is on the order of sub-meV [2] a facility being able to conduct measurements at a temperature in the range of one Kelvin is a prerequisite. We have planned and constructed a low-temperature facility capable of SP-STM measurements. The commercial main chamber (SPECS, Berlin) contains a scanning tunneling microscope cooled by a Joule-Thomson cryostat resulting in a base temperature of 1.2 K using ^{4}He. The microscope integrates a lateral positioning stage enabling to perform cross-sectional STM investigations. This chamber also includes evaporators directing to the microscope's sample receptacle enabling to deposit single atoms onto cold surfaces. There are two additional home-built vacuum chambers for *in situ* magnetic sample and spin-polarized tip preparation. These chambers contain evaporators, a sample heating manipulator, an e-beam heater, and a sputter gun. We will present measurements demonstrating both the spatial and the energy resolutions, and SP-STM measurements of the Fe double layer on W(110).

[1] R. Wiesendanger, Rev. Mod. Phys. **81**, 1495 (2009)
[2] J. Wiebe et al., J. Phys. D: Appl. Phys. **44**, 464009 (2011)

O 35.121 Tue 18:15 Poster B

A scanning tunneling microscope control system based on a field programmable gate array

— •Peter-Jan Peters, Thomas Jürgens, and Richard Berndt — Institut für Experimentelle und Angewandte Physik, Christian-Albrechts-Universität zu Kiel, 24098 Kiel, Germany

A new scanning tunneling microscope control device based on a field programmable gate array (FGPA) and a real time computer is presented. Industry standard PXI data acquisition cards and custom design digital to analog converter circuits are used. The custom converters show a noise density of 950 nV/$\sqrt{Hz}$ in the relevant frequency range. New modes of measurement can be implemented in a flexible manner owing to the programmability of the FPGA. A layered software design is used to hide the detail of the FPGA programming from most users. Test measurements on Au(111) surfaces performed at ambient temperatures resolving the surface reconstruction show that state of the art performance is achieved.

O 35.122 Tue 18:15 Poster B

Setup and characterization of a new-built 300 mK ultra high vacuum scanning tunneling microscope

— •Danny Baumann[1], Torben Hanke[1], Christian Hess[1], Marko Kaiser[2], Ralf Voigtländer[2], Dirk Lindackers[2], and Bernd Büchner[1] — [1]Institut für Festkörperforschung, IFW Dresden — [2]Bereich Forschungstechnik, IFW Dresden

We present the setup and characterization measurements of a newly built ultra high vacuum (UHV) 300 mK scanning tunneling microscope (STM). The used cryostat is a bottom loading ^{3}He single shot system equipped with a 9T superconducting magnet and connected to a three-chamber UHV system. The UHV system gives the possibility to prepare, store and analyze tips and samples and mount them in the STM without breaking the UHV conditions.

Furthermore, we show the very high spatial resolution as well as the very high long-term stability of the STM system with measurements on standard samples and investigations on the iron pnictide superconductor LiFeAs.

Additionally, we have performed scanning tunneling spectroscopic measurements with a superconducting Niobium tip to show that the energy resolution of the STM at base temperature is close to the thermal limit.

O 35.123 Tue 18:15 Poster B

Investigations on nanowire-cantilever interactions

— •Moid Bhatti, Ivo Knittel, and Uwe Hartmann — Institut für Experimentalphysik, Universität des Saarland

High speed (video rate and beyond) atomic force microscopy (AFM) requires a height feedback with a bandwidth of 100 kHz and more, for which solutions are emerging. On the other hand, cantilevers with resonant frequencies (f) in the MHz range are required. Nano-sized cantilevers with f in the MHz range can fulfill this requirement. However, an understanding of the interaction between a sample and a static or oscillating nanowire (NW) or nanocantilever (NC) is needed.

We have been studying the contact mechanics of the cantilever-sample system in the context of dynamic mode AFM using NCs of various types: (1)NWs grown on a substrate (whose dynamic behavior 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 AFM cantilevers. (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 oscillating at its tip.

We will present distance-dependent resonance curves and show various oscillatory states of an AFM cantilever interacting with a static NW and of a NC tapping on a sample. A dedicated piezoelectric element was excited to vibrations of up to 100 MHz. The detection of such vibrations is discussed besides a technique for the electrostatic excitation of mechanical vibrations of free-standing NWs in MHz range.

O 35.124 Tue 18:15 Poster B

Development of a cryogenic scanning tunneling microscope with integrated optical lenses

— •Jeannette Kemmer, Jens Kügel, Pin-Jui Hsu, Paolo Sessi, and Matthias Bode — Institute of Experimental Physics II, University Würzburg, Am Hubland, 97074 Würzburg

We present the current status of a home-built low-temperature Scanning Tunneling Microscope (STM) with integrated lenses for in-situ optical excitation studies. The STM design includes an x-y-stage for sample positioning as well as lenses for back- and front-side focused laser illumination. It is integrated into a two-chamber UHV system equipped with a commercial LHe cryostat with a projected hold time of $t > 100$ h. Test measurements performed under ambient conditions (HOPG), UHV and at low-temperatures will be presented.

O 35.125 Tue 18:15 Poster B

An oxygen annealing chamber for the preparation of clean hard metal substrates

— •Johannes Friedlein, Andreas Sonntag, Benjamin Ehlers, Stefan Krause, and Roland Wiesendanger — University of Hamburg, Institute of Applied Physics, Jungiusstr. 11A, 20355 Hamburg, Germany

Reproducible measurements on the atomic scale require surfaces of high purity. The preparation of hard metal substrates like W and Mo crystals for scanning tunneling microscopy experiments involves creating a surface impurity depletion zone by annealing in oxygen atmosphere ($p \leq 1 \times 10^{-6}$ mbar) at high temperature ($T \leq 2000$ °C) [1-2].

We present the design and construction of a dedicated preparation chamber for clean W and Mo surfaces. It has a separate pumping system, consisting of turbo, ion getter and titanium sublimation pump. An ion gauge and a mass spectrometer allow for the control and analysis of vacuum conditions. The preparation process is conducted via remotely controlled O_2 leak valve and electron beam heating. During the annealing process the surroundings heat up leading to an increase of their degasing rates. To avoid this we implement a water cooling system for the chamber wall as well as for the heating stage.

[1] M. Bode, S. Krause, L. Berbil-Bautista, S. Heinze, R. Wiesendanger, Surface Science **601**, 3308 (2007).
[2] Kh. Zakeria, T.R.F. Peixotoa, Y. Zhanga, J. Prokopa, J. Kirschner, Surface Science **604**, L1 (2010).

O 35.126 Tue 18:15 Poster B

Advanced pulse-shaper design for simultaneous phase, amplitude, and polarization control of femtosecond laser pulses

— •Christoph Schwarz, Ole Hueter, Fabian Ebert, and Tobias Brixner — Institut für Physikalische und Theoretische Chemie, Universität Würzburg, Am Hubland, 97074 Würzburg

The technique of femtosecond pulse shaping is an essential tool for recent advances in the area of optical near-field control and spectroscopy. So far the commonly used pulse-shaper setups are restricted in terms of their degrees of freedom. Either the amplitude and phase of a single polarization state or the phases of two perpendicular polarizations can be modulated. In the latter case, shaping is limited to certain polarization states. To achieve shaping of the full vector field we introduce an improved pulse-shaper design. In contrast to other approaches a single dual-layer liquid-crystal spatial light modulator (LC-SLM) is employed in order to shape independently phase and amplitude of two mutually perpendicular polarization components. To maximize the number of usable pixels of the LC-SLM for both polarizations, it is important to achieve almost equal frequency distributions in the Fourier plane of the zero-dispersion compressor. Numerical calculations and ray-tracing simulations are employed to optimize these distributions. To realize the calculated parameters experimentally we use a tailor-made thin-film polarizer for generation of two perpendicularly polarized pulses and a volume phase holographic grating for the zero-dispersion compressor. By recombining the two polarizations in a common-path setup we achieve control over the complete vector field of the resulting pulse.

O 35.127 Tue 18:15 Poster B

Development of a System measuring Adhesion Forces in Powder Collectives

— •Stefanie Wanka[1], Michael Kappl[1], Markus Wolkenhauer[2], and Hans-Jürgen Butt[1] — [1]Max Planck Institute for Polymer Research, Mainz, Germany — [2]Boehringer Ingelheim Pharma GmbH & Co. KG, Ingelheim, Germany

Fine powders commonly have poor flow ability and dispersibility due to interparticle adhesion that leads to formation of agglomerates. Knowing about adhesion in particle collectives is indispensable to gain a deeper fundamental understanding of particle behavior in powders. Especially in pharmaceutical industry a control of adhesion forces in powders is mandatory to improve the performance of inhalation products. Typically the size of inhalable particles is in the range of 1-5 μm. To measure adhesion forces in fine powder collectives a new method was developed which is based on particle detachment from a surface caused by its inertia. To achieve detachment of particles in the relevant size range, accelerations in the order of 500 000g are necessary. Existing techniques for measurement of particle adhesion forces are experimentally demanding and time consuming. Therefore we aim to develop a system that will allow routine measurements of adhesion in particle collectives. The acceleration required for particle detachment is provided by a shock excitation system based on the Hopkinson bar principle (SPEKTRA GmbH Dresden) and measured via laser vibrometry. Particle detachment events are detected by optical video microscopy. First test measurements showed successful detachment of particles < 10 μm and thus a proof of concept.

O 35.128 Tue 18:15 Poster B

Soft Landing of Macromolecules using Electrospray Ionization — •Richard Steinacher, Seung Cheol Oh, Julian Lloyd, Hartmut Schlichting, and Johannes V. Barth — Physik Department, E20, TU München, Germany

Recent developments in research towards positioning macromolecules on surfaces, relevant for organic electronics or materials, made it desirable to deposit and investigate species that can not be sublimated by thermal evaporation techniques. We present a set-up with several stages, where an ion beam of macromolecules is produced by an electrospray ionization source, focused by electrodynamic funnels, and guided by electrostatic lenses. Furthermore, a quadrupole is used, to mass-selectively seperate the constituents of the ion beam. The apparatus allows to bring the molecules into a clean UHV environment and deposit them on a substrate, for the production of films with high purity. Beyond the generation and the guidance techniques of the ion current, the set-up is compact and thus very versatile. This will enable the usage of one instrument with multiple devices, such as scanning probe microscopes or for the production of hybrid organic-semiconductor components.

O 35.129 Tue 18:15 Poster B

Preparation and application of highly polarized Xe with variable ^{129}Xe content — •Alexander Potzuweit, Richard Kastelik, Hagen Allmrodt, Lars Kraft, Anuschka Schaffner, and Heinz Jänsch — Fachbereich Physik, Philipps-Universität Marburg, D-35032 Marburg

We employ NMR of hyperpolarized ^{129}Xe to investigate surface phenomena and diffusion. To increase the sensitivity towards structurally caused, local inhomogeneities a small line width is favorable. In solid Xe the line width is dominated by dipolar interaction with neighboring nuclear spins. This can be substantially reduced by diluting the NMR-active isotope ^{129}Xe in the NMR-inactive isotope ^{132}Xe. Thus we are able to investigate ordering effects like annealing. Dynamic processes at the bulk surfaces can be monitored by exchange spectroscopy (EXSY) of the bulk and surface atoms ($\Delta\nu \approx 100$ ppm). Here we present the technical development of the apparatus and discuss first results.

O 35.130 Tue 18:15 Poster B

High-Resolution Double-Photoelectron Spectroscopy from superconducting Surfaces — •Tobias Bauer, Robert Wallauer, Stefan Voss, and Reinhard Dörner — Institut für Kernphysik, Goethe Universität, 60486 Frankfurt am Main, Germany

It is theoretically predicted that the breakup of Cooperpairs by a single XUV photon leads to the emission of two electrons which formed the pair. First experiments which have been performed with a custom-build Time-of-Flight spectrometer, failed to show evidence for this process due to the low energy resolution.

With a new developed experimental setup which includes a new spectrometer (THEMIS1000 with an Wide Angle Lens - SPECS) and an especially for coincident measurements designed time- and position-sensitive detector (HEX90 - RoentDek), we will be able to measure coincident electrons with +/- 30° emission angle and a resolution comparable to state of the art hemispherical analyzers. The data analysis plays a crucial role in the experiment, since the electrons are expected to hit the detector at the same time. We present the results of a new method for pulse analysis and other experimental improvements in order to achieve nearly dead-time free detection efficiency.

O 35.131 Tue 18:15 Poster B

Towards NMR of buried interfaces — •Anuschka Schaffner, Hagen Allmrodt, Lars Kraft, Richard Kastelik, Alexander Potzuweit, and Heinz Jänsch — Fachbereich Physik, Philipps-Universität Marburg, D-35032 Marburg

We employ Xe-NMR to investigate surface phenomena by adsorbing hyperpolarized ^{129}Xe onto a helium-cooled single crystal and studying the electronic interactions of substrate and adsorbate. The high nuclear spin polarization of the adsorbed Xe-film could be transferred to buried interfaces within the substrate (which then would be accessible for further NMR experiments) via dipolar near distant-field transfer. The proposed distant-field transfer [1] will be discussed. As a test of the here proposed polarization transfer, we use a system of an absorbed hyperpolarized ^{129}Xe-film beneath a layer of unpolarized ^{129}Xe in a matrix of CO_2, geometrically and spectrally separated. Here, we present the experiments and discuss the transfer mechanism.

[1] Desvaux et al. Eur. Phys. J. Appl. Phys. Vol. 36, No. 1, 2006

O 35.132 Tue 18:15 Poster B

Construction of a Neural Network Potential-Energy Surface for R,R-Tartaric Acid — •Sinja Klees, Tobias Morawietz, and Jörg Behler — Lehrstuhl für Theoretische Chemie, Ruhr-Universität Bochum, D-44780 Bochum, Germany

The availability of accurate interatomic potentials is a necessary condition for studying complex systems for example by molecular dynamics simulations. Typically, a number of physical approximations are introduced to obtain potential-energy surfaces (PESs), which are sufficiently efficient to study large systems. Artificial Neural Networks (NN) offer a very general way to construct accurate PESs without the introduction of any constraint on the functional form. They are extremely flexible and allow to interpolate reference energies and forces obtained from first-principles calculations. To date, most NN potentials for molecules have been reported only for very small systems containing up to six atoms. Using R,R-tartaric acid as a benchmark system we show that also high-dimensional NN PESs for larger molecules can be constructed in a systematic way.

O 35.133 Tue 18:15 Poster B

Excitons of pure and functionalized carbon nanotubes studied by many-body perturbation theory — •Ferdinand Schulz and Michael Rohlfing — Fachbereich Physik, Universität Osnabrück

We discuss excitonic states in semiconducting carbon nanotubes from first principles. Based on structural data from density-functional theory, band structures and optical excitations are obtained from many-body perturbation theory (GW approximation and Bethe-Salpeter equation, BSE). We employ a simplified, perturbative LDA+GdW version of the theory, which is numerically much more efficient than conventional GW and BSE realizations. This enables us to discuss both pure and functionalized nanotubes, with functionalization given by point defects and adsorbates (like hydrogen).

O 35.134 Tue 18:15 Poster B

Method for solving the N-point Hedin equations — •Falk Tandetzky, Sangeeta Sharma, Kay Dewhurst, and Hardy Gross — Max-Planck-Institut für Mikrostrukturphysik (Theory Dep.), Weinberg 2, D-06120 Halle, Germany

The GW approximation is a state-of-the-art method for band structure calculations but there are still some cases for which GW fails [1]. Towards the goal of improving on this situation, we present a new method for solving the Hedin equations which, expressed perturbatively, includes an infinite subset of vertex corrections. We further provide conditions for guaranteeing convergence of the algorithm to a unique solution. This is an important point since it has recently been pointed out that there is danger of running into unphysical solutions, when using vertex corrections [2].

All these findings are supported by numerical calculations for $N = 1$ which compare the exact $\Sigma[G, W]$ to that obtained from our approximate algorithm as well as a Borel resummation of the linearised Hedin equations [2,3]. As our method has a favourable scaling with N we envisage that it can be applied to physical problems, albeit with discretized degrees of freedom and be useful for band structure calculations beyond the *GW* approximation.

[1] M. Guzzo, G. Lani, F. Sottile, P. Romaniello, M. Gatti, J. J. Kas, J. J. Rehr, M. G. Silly, F. Sirotti and L. Reining, Phys. Rev. Lett. 107, 166401 (2011). [2] G. Lani, P. Romaniello and L. Reining, arXiv:1103.1630v1 (2011). [3] Y. Pavlyukha and W. Hübner, J. Math. Phys. 48, 5 (2007).

O 35.135 Tue 18:15 Poster B

Electronic and optical properties of tin oxides computed from first principles with different levels of approximation — •Anna Miglio, Martin Stankovski, Matteo Giantomassi, and Xavier Gonze — NAPS-IMCN Université catholique de Louvain, Louvain la Neuve, Belgium

SnO2 is a wide-gap semiconductor of considerable industrial interest as a transparent conductor. Depending on deposition conditions a SnO phase might coexist with SnO2. In this work, we apply the standard DFT approach and the more accurate many-body formalism in the GW approximation to compute the electronic and optical properties of SnO2 and SnO. One-shot G0W0 calculations performed with the plasmon pole approximation[1]and the more accurate contour deformation technique[2] improves the agreement of the computed band gap with the experimental value. The effect of self-consistency in GW is then investigated by using two different methods: a one-shot G0W0 iteration performed on top of self-consistent COHSEX results[3] and the quasi particle self-consistent GW method proposed in [4]. Finally we analyze the importance of excitonic effects by comparing the absorption spectrum computed within the RPA with the results obtained by solving the Bethe Salpeter equation. [1] R. W. Godby and R.J. Needs, Phys. Rev. Lett. 62, 1169 (1989). [2] S. Lebegue et al. PRB 67, 155208 (2003). [3] F. Bruneval, N. Vast, and L. Reining, Phys. Rev. B 74, 045102 (2006). [4] T. Kotani, M. van Schilfgaarde, S. V. Faleev, Phys. Rev. B 76, 165106 (2007).

O 35.136 Tue 18:15 Poster B

Nucleation Growth: Occupation Probability Field Ansatz as an Approximation of a Lattice Monte Carlo Simulation — •Tanja Mues and Andreas Heuer — Institut für Physikalische Chemie, Westfälische Wilhelms-Universität Münster

Molecular nucleation growth on surfaces was studied numerically with different simulation models on microscopic and macroscopic scale. The adaption of a macroscopic method without loss of accuracy is the topic of this work. Regarding the occupation probability of a site by a molecule as the key observable we can simulate nucleation growth on larger time and length scales as compared to a Lattice Monte Carlo (LMC) simulation. To prevent loss of information on macroscopic scale, we import three main parameters: the diffusion constant, the critical nucleus size and a nucleation pre-factor from our LMC simulation. By means of the cluster density and their radial distribution we compare the results of both methods and find very good agreement.

O 35.137 Tue 18:15 Poster B

DFT-Calculations of NEXAFS spectra of small alkanes and alkanethiols — •Katharina Diller[1], Klaus Hermann[2], Florian Klappenberger[1], and Johannes V. Barth[1] — [1]Physik Department, E20, Technische Universität München, James- Franck-Str. 1, 85748 Garching, Germany — [2]Fritz-Haber-Institut der Max-Planck-Gesellschaft, Faradayweg 4-6, 14195 Berlin, Germany

We simulate near-edge x-ray absorption fine structure (NEXAFS) spectra of different small alkanes and alkanethiols in gas phase using the density functional theory (DFT) package StoBe. Since alkanethiols are widely used as building blocks for self-assembled monolayers (SAMs) their properties are of great interest. However, the interpretation of the experimental NEXAFS data, especially the peak assignment, can be challenging as vibrational features dominate the spectra of small alkane(thiol)s and are still present for larger molecules. In this work we examine the performance of StoBe using (i) the implemented transition potential method and (ii) ΔSCF calculations to determine the first transitions for the peak assignment and interpretation of NEXAFS spectra of saturated hydrocarbons. Additionally we address the problems arising when progressing from the analysis of small alkanes in gas phase to the examination of adsorbed long-chained alkanethiols.

O 35.138 Tue 18:15 Poster B

Systematic Construction of High-Dimensional Potential-Energy Surfaces by Neural Networks — Tobias Morawietz, Nongnuch Artrith, and •Jörg Behler — Lehrstuhl für Theoretische Chemie, Ruhr-Universität Bochum, D-44780 Bochum, Germany

Artificial neural networks (NNs) have become a promising method for the development of reliable potential-energy surfaces (PESs) for a wide range of systems including molecules, solids and surfaces [1,2]. Due to their high flexibility NNs are able to accurately represent energies and forces obtained from quantum chemical calculations, which makes them ideal tools to extend the length and time scale of molecular dynamics simulations. An important aspect for the constructing of high-dimensional NN PESs is the choice of the reference configurations. Here we present a systematic approach to build up NN potentials in an iterative fashion by identifying poorly represented parts of the configuration space.

[1] J. Behler, PCCP **13**, 17930 (2011).

[2] N. Artrith, T. Morawietz, and J. Behler, PRB **83**, 153101 (2011).

O 35.139 Tue 18:15 Poster B

Description of Rabi oscillations in density-functional theory: The effect of spin — •Jeiran Jokar and Nicole Helbig — Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, 52425 Jülich, Germany

Applying a monochromatic laser with a frequency close to resonance leads to Rabi oscillations between the initial and an excited state of the system. These oscillations are a prototype for the nonlinear interaction of light with matter and one of the few analytically solvable cases of nonlinear electron dynamics where the population of states changes dramatically in time. Due to these dramatic changes a description within density-functional theory needs to go beyond the use of adiabatic functionals. Here, we investigate the influence of the spin of the initial state as well as the polarization of the laser on the quality of a DFT description in order to gain more insight into how to construct non-adiabatic approximations. Through the exact solution of one and two-dimensional two-electron systems interacting with a monochromatic laser of either linear or circular polarization we are able to assess the quality of a local density approximation and the exact exchange approximation.

O 35.140 Tue 18:15 Poster B

Magnetism and unusual Cu valence in correlated perovskites — •Paola Alippi[1] and Vincenzo Fiorentini[2] — [1]CNR-ISM, Rome, Italy — [2]CNR-IOM and University of Cagliari, Italy

The interplay of the valence states of Cu and of the X cation determines the magnetic and conduction properties of the $A\mathrm{Cu_3X_4O_{12}}$ quadruple perovskites. $\mathrm{CaCu_3Ti_4O_{12}}$ (CCTO) should be a Mott-like insulator due to the nominal 4+ valence of Ti and 2+ valence of Cu. As Fe and Co prefer greatly a 3+ valence to a 4+ one, $\mathrm{LaCu_3Fe_4O_{12}}$ (LCFO) and $\mathrm{YCu_3Co_4O_{12}}$ (YCCO) will be insulating if Cu is 3+. It was suggested that the nominally 3+ Cu state may actually be a "Zhang-Rice singlet" bound state of a ligand hole and a native Cu hole, coupled antiferromagnetically. If however Cu is 3+ and unmagnetized along with its neighbors, neither Mott nor Zhang-Rice physics are at play.

Based on ab initio calculations using several beyond-local density-functional approaches (GGA+U, HSE hybrid, self-interaction correction, G_0W_0) we confirm the Mott-like nature of CCTO, and show that LCFO is an antiferromagnetic (on the Fe lattice) insulator, while Co adopts a low-spin state and produces a non-magnetic and insulating YCCO. Unexcitingly, neither LCFO or YCCO are Mott or Zhang-Rice-like systems, as Cu therein is strictly non-magnetic and effectively 3+ in valence. CCTO may instead exhibit Zhang-Rice type behavior upon hole doping, progressively emptying its flat Cu-like top valence band.

O 35.141 Tue 18:15 Poster B

Reversible switching process of spiropyran on Au(111) — F. Lorbeer[1], •P. Stoll[1], I. Fernandez Torrente[1], T. R. Umbach[1], C. Maity[2], S. Hecht[2], J.I. Pascual[1], and K.J. Franke[1] — [1]Institut für Experimentalphysik, Freie Universität Berlin, Berlin — [2]Department of Chemistry, Humboldt-Universität zu Berlin

The isomerisation process of molecules adsorbed on a metal surface can be very different from the one in solution or gas phase. The prototypical light induced ring-opening reaction of spiropyran (SP) to its isomer merocyonine (MC) and the thermally induced ring-closing back-reaction in gas phase is not easily reproduced on the surface due to the electronic coupling of molecular orbitals with the substrate states. We study 5',6,8 Tri-tertbutylindolinospirobenzopyran on Au(111) with low temperature scanning tunneling microscopy and spectroscopy. The molecule is functionalised with the three tertbutyl groups to reduce the interaction with the substrate and enable reversible switching. An ordered structure is obtained by mixing SP with thermally isomerised MC. In this ordered structure we can excite a ring-opening reaction of SP by electric field and illumination with 445nm laser light. This change is visible as an upward pointing tertbutyl group and is completely reversible by individually adressing the molecule with a voltage pulse. A complete unfolding into the MC form however does not take place due to steric hindrance in the ordered structure.

O 35.142 Tue 18:15 Poster B

In situ metalation of 2H-tetraphenylporphyrins with copper substrate atoms on Cu(111): a scanning tunneling microscopy study — •Martin Drost, Stefanie Ditze, Michael Stark, Florian Buchner, Hans-Peter Steinrück, and Hubertus Marbach — Lehrstuhl für Physikalische Chemie II, Universität Erlangen-Nürnberg, Egerlandstr. 3, D-91058

The development of functional nanostructures requires a detailed understanding of the physical and chemical properties of the involved species. In this regard porphyrinoids appear to be ideal candidates. They can bear various peripheral ligands, which enables control over molecule/molecule and molecule/substrate interactions, and their reactivity can be modified by inserting specific metal atoms at the center of the macrocycle. Herein, we studied the in situ coordination reaction of 2H-tetraphenylporphyrin molecules (2HTPP) with copper substrate atoms under ultra high vacuum conditions with scanning tunneling microscopy. The experiment reveals that 2HTPP molecules deposited on Cu(111) react to form metaloporphyrins (CuTPP) at 400K, by incorporation of substrate Cu atoms. While at room temperature, 2HTPP shows a specific 1D diffusion behavior of individual molecules, after partial metalation the coexistence with an ordered 2D CuTPP phase is found. To obtain detailed insight, a kinetic analysis of the metalation behavior as a function of time and temperature was performed.

This work has been funded by the DFG through Sonderforschungsbereich 583.

O 35.143 Tue 18:15 Poster B

DFT study of the attachment of silane linker molecules to hydroxylated Mg surfaces — •Steffen Seiler and Bernd Meyer — Interdisziplinäres Zentrum für Molekulare Materialien und Computer-Chemie-Centrum, Universität Erlangen-Nürnberg

The prospect of using magnesium and its alloys as biodegradable implants has triggered much interest in finding suitable processes for functionalization of their surfaces with biomolecules. In recent experimental work it was shown that by surface hydroxylation and the use of appropriate linker molecules (3-aminopropyltriethoxysilane, APTES) self-assembled monolayers of proteins can be formed on Mg surfaces [1].

DFT calculations have been used to explore the binding mode and the most favorable binding configuration of silane molecules on hydroxylated magnesium. Attachment of the silane molecules via hydrogen bonding or covalent bond formation have been considered. Special attention was given to the role of water recombination and association to the surface in the silane adsorption process. Also the influence of van der Waals contributions to the adsorption energy will be discussed.

[1] M.S. Killian, V. Wagener, P. Schmuki, S. Virtanen, *Langmuir* 26 (2010) 12044

O 35.144 Tue 18:15 Poster B

Probing gas ligation of surface anchored porphyrins through an experiment-theory IETS study — •Knud Seufert[1], Willi Auwärter[1], Shiri Burema[2], Marie-Laure Bocquet[2], Johannes V. Barth[1], David Écija[1], and Saranyan Vijayaraghavan[1] — [1]Physik Department E20, TU München, Germany — [2]CNRS, Université de Lyon, France

The response of metalloporphyrins towards small gas molecules is of fundamental interest as it plays a key role in both biological systems as the transport of respiratory gases and artificial nanostructures as sensors. STM and STS investigations combined with DFT-calculations turned out to be a good method to get insight into such systems. Here we present the ligation of NO to Co-TPP, immobilized onto a metallic substrate. The molecular interaction with the substrate is weakend by the binding of the bent NO radical to the metal-center. This results in a changed appearance and electronic structure. IETS spectra of this system were performed and the measured signal was assigned to an unique vibration mode on the NO-complex, namely the Co-N-O Rocking mode lying in a plane perpendicular to the metallic surface. Furthermore the experimental extension to other porphyrins and diatomic gases is shown.

O 35.145 Tue 18:15 Poster B

Switching of an industrial dye-molecule on Au(111) and Ag(111) — •Marcel Müller[1], Gerald Dräger[2], Konrad Boom[1], Friederike Matthaei[1], and Karina Morgenstern[1] — [1]Leibniz Universität Hannover, Institut für Festkörperphysik, Abteilung ATMOS, Appelstraße 2, 30167 Hannover — [2]Leibniz Universität Hannover, Institut für Organische Chemie, AK Dräger, Schneiderberg 1B, 30167 Hannover

Molecular switches are an essential part of future ideas in molecular electronics. We investigated a possible candidate, the cyanine astraphloxine, on Au(111) and Ag(111) with a low-temperature STM. We deposit a coverage of 0,022 molecules/nm^2 at a sample temperature of 113 K on Au(111) and 0,014 molecules/nm^2 at a sample temperature of 83 K on Ag(111). Astraphloxine exists in two different sizes on both surfaces. On Ag(111), the molecule forms smaller clusters while on Au(111) it adsorbs as single molecule. The molecule's size and shape are changed by manipulation via inelastic tunneling electrons. In this presentation we will show different switching processes and discuss possible interpretations of these processes, in particular which isomerisations are induced. Finally, we will discuss these results in light of a combustion analysis of the molecule.

O 35.146 Tue 18:15 Poster B

Tuning the interaction between carbon nanotubes and dipole switches: influence of the change of the nanotube-spiropyran distance — •Pascal Bluemmel[1], Antonio Setaro[1], Chandan Maity[2], Stefan Hecht[2], and Stephanie Reich[1] — [1]Department of Physics, Freie Universität Berlin, Arnimallee 14, 14195 Berlin — [2]Department of Chemistry, Humboldt Universität zu Berlin, Brook-Taylor-Str. 2, 12489 Berlin

The non-covalent functionalization of carbon nanotubes with spiropyran molecules, serving as optically addressable dipole switches, is reported. Two types of pyrene-spiropyran based dyads with spacers of different lengths resulting in different switch-tube distances were investigated. While both surfactants were able to form stable carbon nanotube suspensions, the different distances between the switch and the tube affect both of the components' optical properties. In the case of the shorter spacer, the nanotubes' luminescence as well as the merocyanine absorption band were red-shifted and furthermore, the rate of the merocyanine to spiropyran thermal back isomerization was decreased.

O 35.147 Tue 18:15 Poster B

Efficient energy transfer in perylene-nanotube complexes — •Friederike Ernst[1], Timm Heek[2], Antonio Setaro[1], Rainer Haag[2], and Stephanie Reich[1] — [1]Institut für Physik, Freie Universität Berlin — [2]Institut für Chemie, Freie Universität Berlin

Carbon nanotubes are interesting for biomedical applications because they emit in the IR part of the spectrum; establishing nanotube-adsorbant energy transfer complexes in aqueous solution is thus a key step towards the complex non-covalent functionalization of nanotubes in biocompatible environments. We demonstrate direct energy transfer in perylene-imido-diester nanotube complexes in water: upon excitation of the adsorbed perylene unit we observe an emission from the carbon nanotubes, which indicates a successful excitation transfer. The efficiency of the indirect excitation via the adsorbant is of the same order of magnitude as the direct excitation of the nanotubes. Furthermore the perylene-imido-diester compound simultaneously serves as a surfactant for the nanotubes with a strong chirality preference for tubes with a small E11 transition energy, obliterating the need for a supplementary surfactant. We thus created a self-sufficient excitation transfer complex which is stable in an aqueous medium over many months.

O 35.148 Tue 18:15 Poster B

Chirality Enrichment of Carbon Nanotubes by Amphiphile Replacement — •Marcus Ulf Witt, Antonio Setaro, Frederike Ernst, Pascal Bluemmel, Michael Gegg, and Stephanie Reich — Frei Universität Berlin, Institut für Experimentalphysik, Arnimallee 14,14195 Berlin

We present suspensions with selected enriched chiralities of carbon nanotubes. Such a suspension of selected chirality has well defined photoluminecence spectra and conductive properties. The chirality enrichment is achieved by the replacement of amphiphiles. The solvatochromic shift of the carbon nanotubes during the replacement was monitored with the photoluminescence excitation (PLE). From this PLE measurements we calculated the required concentration of the second amphiphile to replace the first one applying the Hill-model. The achieved enrichment was verified by the PLE. The use of amphiphiles with different morphologies leads to the enrichment of different chiralities depending on the coupling between amphiphiles and carbon nanotubes. This will help understanding the fundamental mechanisms of coupling between carbon nanotubes and aromatic moieties.

O 36: Invited talk (Joseph A. Stroscio)

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

Invited Talk O 36.1 Wed 9:30 HE 101

Exploring the Physics of Graphene with Local Probes — •Joseph A. Stroscio — Center for Nanoscale Science and Technology, NIST Gaithersburg, MD 20899

The recent ability to isolate and study the single atomic sheet of graphene has created a great deal of excitement in the scienctific community. Graphene is composed entirely of exposed surface atoms, which offers a unique opportunity to examine a 2-dimensional electron system with local probe measurements. In this talk I will describe our studies using scanning tunneling spectroscopy (STS) to examine interactions and disorder in various graphenes produced by different methods with varying degrees of disorder. Electron interactions are observed in tunneling spectroscopy measurements in high mobility graphene produced by thermal decomposition of SiC [1]. In these graphene samples Landau level (LL) degeneracies are lifted with energy scales that vary as function of magnetic field and filling factor. Additionally, enhanced energy splittings are measured when LL sublevels are emptied or filled as they cross the Fermi level. Using a back-gated exfoliated graphene device on SiO2 we observe a Landau level spectrum and charging resonances [2,3] that are completely different from the above STS measurements on weak disorder graphene systems. Applying a gating potential allows us to obtain *STS gate maps*, which allow a detailed examination of the transitions from compressible to incompressible electron systems.

[1] Y. Jae Song et al., Nature 467, 185 (2010). [2] S. Jung et al., Nature Physics 7, 245 (2011). [3] G. M. Rutter et al., Nature Physics 7, 649 (2011).

O 37: [MA] Joint Session "Topological Insulators II" (jointly with DS, HL, O, TT)

Time: Wednesday 9:30–13:00 Location: EB 301

O 37.1 Wed 9:30 EB 301

Topologically-related properties in presence of disorder. First-principle study — •Stanislav Chadov — Max-Planck-Institut für Chemische Physik fester Stoffe, Dresden

The presence of disorder is often seen as a destructive mechanism which must be reduced by any means. In present study we attempt to make it constructive due to the robustness of the spin current in topological insulators with respect to the time-reversal symmetric perturbations. Based on the first-principle calculations involving the Coherent Potential Approximation (CPA), we inspect the disorder-affected transport properties of the random alloys between topologically non-trivial and trivial materials. The subsequent analysis encounters few interesting aspects: the way how to increase the Hall angle by using random disorder and an indication for the topological Anderson insulator. In addition CPA provides an alternative recipe to validate the non-trivial topological state of the material based on a purely bulk information.

O 37.2 Wed 9:45 EB 301

Probing the topological states of Sb_2Te_3 by spin polarized photoemission spectroscopy — •Christian Pauly[1], Gustav Bihlmayer[2], Marcus Liebmann[1], Dinesh Subramaniam[1], Martin Grob[1], Alexander Georgi[1], Markus Scholz[3], Jaime Sanchez Barriga[3], Stefan Blügel[2], Oliver Rader[3], and Markus Morgenstern[1] — [1]II. Physikalisches Institut B, RWTH Aachen University and JARA-FIT, Germany — [2]Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich and JARA-FIT, Germany — [3]Helmholtz-Zentrum für Materialien und Energie, Berlin, Germany

Using high resolution spin- and angle-resolved photoemission spectroscopy, we map the electronic structure and spin texture of the surface states of the topological insulator Sb_2Te_3. Similar to the well explored Bi_2Te_3 and Bi_2Se_3 which possess TI properties with the most simple electronic structure [1], we directly show that Sb_2Te_3 exhibits Z_2 topological properties with a single spin-Dirac cone at the Γ-point. In addition, a strongly spin-orbit split surface state is observed at lower energy. In Γ-K direction, the band is located within a spin-orbit gap, governing the energy position of the state. In combination with DFT calculation, we provide direct evidence for an argument given by Pendry [2], that there must be at least one surface state inside a SO gap, if the gap is located in the zone. Thus, similar to the topological state, this state is protected by symmetry. [1] H. Zhang et al., Nature Phys. 5, 438 (2009) [2] J. B. Pendry et al., Surf. Sci. 49, 87 (1975)

O 37.3 Wed 10:00 EB 301

Electronic properties and magnetic anisotropy of individual Co adatoms adsorbed on topological insulator surfaces — •T. Eelbo[1], M. Sikora[2], M. Waśniowska[1], M. Dobrzański[2], M. Gyamfi[1], G. Bihlmayer[3], I. Miotkowski[4], A. Kozlowski[2], and R. Wiesendanger[1] — [1]Institute of Applied Physics, University of Hamburg, Jungiusstr. 11, Hamburg, Germany — [2]Department of Solid State Physics, AGH University of Science and Technology, Aleja Mickiewicza 30, Kraków, Poland — [3]Peter Grünberg Institute and Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, Jülich, Germany — [4]Department of Physics, Purdue University, West Lafayette, USA

The interaction of magnetic impurities adsorbed on topological insulator surfaces causes changes of the electronic properties of the surfaces or the adatoms themselves. In addition the adatoms can present different magnetic properties due to interaction with the host. For this reason we studied the electronic properties and magnetic anisotropy of individual Co atoms adsorbed on Bi_2Se_3 by means of scanning tunneling microscopy/spectroscopy (STM/STS) and x-ray magnetic circular dichroism (XMCD) at low temperatures. After the deposition onto the cold surface STM measurements reveal two different adsorption sites for Co adatoms. Two resonances in the occupied states for both species of adatoms are found using STS. Moreover, XMCD measurements reveal a magnetic anisotropy with the easy axis being aligned out-of-plane. The experimental findings are compared to results of ab-initio calculations.

O 37.4 Wed 10:15 EB 301

Theoretical study on the reactive chemical doping of the Bi_2Se_3 surface — •Janos Kiss[1,2], Stanislav Chadov[1,2], and Claudia Felser[1,2] — [1]Institute of Inorganic Chemistry and Analytical Chemistry, Johannes Gutenberg University, Mainz — [2]Max Planck Institute for Chemical Physics of Solids, Dresden, Germany

Recent experimental results have shown that the surface of Bi_2Se_3 exposed to air will become *n*-type doped. Furthermore, the surface gradually undergoes an oxidation reaction leading to a degradation of the surface transport properties, where the contribution of the topological surface states are consequently decreasing. This is expected to be caused by Se vacancies. However, the formation mechanism of this vacancies and the interaction of moisture -i.e. water- with Bi_2Se_3 is still not clarified. Therefore, we will present the results of our large scale ab-initio calculations and molecular dynamics simulations in order to investigate the effect of Se vacancies and the reactivity of water upon the electronic and atomic structure of the surface.

O 37.5 Wed 10:30 EB 301

Heusler topological insulators: Electronic structure and transport properties — •C. Shekhar[1], S. Ouardi[2], G. H. Fecher[1,2], A. K. Nayak[1], A. Gloskovskii[2], E. Ikenaga[3], S. Ueda[4], K. Kobayashi[4], and C. Felser[1,2] — [1]Max Planck Institute for Chemical Physics of Solids, Dresden — [2]Institute of Inorganic Chemistry and Analytical Chemistry, Johannes Gutenberg - University, Mainz — [3]Japan Synchrotron Radiation Research Institute, SPring-8, Hyogo, Japan — [4]National Institute for Materials Science, SPring-8, Hyogo, Japan

Topological insulators have a high potential for spintronics devices and quantum computation. Various Heusler compounds crystallize in a fcc structure of the $C1_b$ type and consist of 2 transition metals and a main group element. If the compounds contain heavy metals and a lanthanide element then they exhibit extraordinary physical properties including superconductivity, half-metallic, semiconducting-like behavior, giant magnetoresistivity, heavy fermion state and zero band gap. The density of states of XMZ Heusler compounds (M = Gd, Lu, X= Au, Pt, Pd and Z= Pb, Sb, Bi) were investigated by hard X-ray photoelectron spectroscopy. The comparison of the experimental results to calculations gives evidence for the zero band gap state of the compounds. Further, the temperature dependence of electrical conductivity, magneto resistance, Hall mobility, Seebeck coefficient and thermal conductivity were investigated. The compounds exhibit a high Hall mobility and a linear magnetoresistance (MR). The observed linear MR is a quantum MR and due to the topological insulator state.

O 37.6 Wed 10:45 EB 301

Topological phase transitions in Bi(111) bilayer by breaking time-reversal symmetry — •Hongbin Zhang, Frank Freimuth, Gustav Bihlmayer, Stefan Blügel, and Yuriy Mokrousov — Peter Grünberg Institut & Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, 52425 Jülich, Germany

Time-reversal breaking brings forth many novel phenomena in topological insulators [1]. In this work, using the first principles FLAPW method combined with the Wannier functions technique [2], we investigated topological phase transitions with respect to exchange fields of a two-dimensional topological insulator – Bi(111) bilayer [3]. Numerical evaluation of the spin Chern number [4] for different magnitudes of exchange fields reveals that when the time reversal symmetry is broken by a small exchange field, the system keeps the properties of a topological insulator. After a metallic phase in the intermediate region, the quantum anomalous Hall phase with the non-zero Chern number occurs at sufficiently large enough exchange fields. We analyzed the relation between the spin Chern number, the Z_2 number and the Chern number, and also the phase diagram from the viewpoint of the evolution of the electronic structure, edge states and transport properties in this system. We acknowledge funding under HGF-YIG Programme VH-NG-513.

[1] X. Qi, *et al.*, Phys. Rev. B. **78**, 195424 (2008).
[2] www.flapw.de; F. Freimuth, *et al.*, Phys. Rev. B. **78**, 035120 (2008).
[3] M. Wada, *et al.*, Phys. Rev. B **83**, 121310(R) (2011).
[4] E. Prodan, *et al.*, Phys. Rev. B **80**, 125327 (2009).

O 37.7 Wed 11:00 EB 301

Predicting surface states from the bulk embedding self-energy — •Daniel Wortmann, Gustav Bihlmayer, and Stefan Blügel — Institute for Advanced Simulation & Peter Grünberg Institut, Forschungszentrum Jülich und JARA, 52425 Jülich, Germany

The protected states localized at surfaces and interfaces of topological insulators are a consequence of the electronic structure of the bulk. Their peculiar features like the typical spin-structure makes them an interesting field of basic research with possible applications in spintronics.

We demonstrate how these states can be efficiently simulated by means of the embedding self-energy as obtained in the Green function embedding technique[1]. The embedding self-energy, which can be understood as a generalized logarithmic derivative, is a property of the bulk crystal only and contains all information required to analyze the consequences of the bulk topology on the surface bandstructure. Using the FLAPW implementation of the embedding method as provided in the FLEUR-code[2], we show how the surface states of prototypical topological insulators like Bi_2Se_3 can be studied efficiently with an easy and direct access to effects for example due to electric fields applied to the surface.

[1] D. Wortmann, H. Ishida, S. Blügel. Phys. Rev. B **66**, 075113(02)
[2] http://www.flapw.de

15 min. break

O 37.8 Wed 11:30 EB 301

Influence of magnetic impurities on doping and scattering properties of topological surface states: Fe on $\mathbf{Bi_2X_3}$ (X=Te, Se) — •Markus R. Scholz[1], J. Sánchez-Barriga[1], D. Marchenko[1], A. Varykhalov[1], E. Rienks[1], A. Volykhov[2], L. V. Yashina[2], and O. Rader[1] — [1]Helmholtz-Zentrum Berlin — [2]Moscow State University

We study the effect of Fe impurities deposited on the surface of the topological insulators $\mathrm{Bi_2Se_3}$ and $\mathrm{Bi_2Te_3}$ by means of photoelectron spectroscopy. The topological surface state reveals surface electron doping when the Fe is deposited at room temperature and hole doping when deposited at low temperture ($\sim$ 10 K). We show that in both cases the topological surface state remains intact and gapless. We analyze the line broadening for pure $\mathrm{Bi_2X_3}$ (X=Se, Te) and after deposition of Fe. We observe that the constant broadening in the bulk band gap range increases by a factor of 2 upon deposition of Fe. Because we deposit the Fe without electron doping, this result is not due to a gain in warping as was recently suggested. We discuss the results based on different types of scattering mechanisms.

O 37.9 Wed 11:45 EB 301

Origin of the strong circular dichroism of the topological surface state of $\mathbf{Bi_2Te_3}$ — •Jaime Sánchez-Barriga[1], M. R. Scholz[1], D. Marchenko[1], A. Varykhalov[1], O. Rader[1], A. Volykhov[2], L. V. Yashina[2], J. Braun[3], J. Minár[3], and H. Ebert[3] — [1]Helmholtz-Zentrum Berlin — [2]Moscow State University — [3]Ludwig-Maximilians-Universität München

We have recently reported a strong circular dichroism effect in angle-resolved photoemission of the spin polarized topological surface state of $\mathrm{Bi_2Te_3}$ [1]. The effect has been observed recently also for $\mathrm{Bi_2Se_3}$ and the origin is controversial [2-4]. An initial-state model has been employed to determine the spin orientation directly [3]. We present a series of photoemission measurements and density functional calculations coupled to one-step photoemission theory. Both experiment and theory reveal that the dichroism effect changes sign as a function of photon energy which excludes the initial-state model.

[1] M. R. Scholz, J. Sánchez-Barriga, D. Marchenko, A. Varykhalov, A. Volykhov, L. V. Yashina, O. Rader, submitted to Phys. Rev. Lett. (2010), arXiv:1108.1053
[2] S. R. Park et al., arXiv:1103.0805
[3] Y. H. Wang, D. Hsieh, D. Pilon, L. Fu, D. R. Gardner,Y. S. Lee, N. Gedik, arXiv:1101.5636
[4] Y. Ishida et al., Phys. Rev. Lett. 107, 077601 (2011)

O 37.10 Wed 12:00 EB 301

Prediction of topological insulators in TlBiSe2 family of chalcogenides — •binghai yan — BCCMS, University of Bremen, Bremen

In this work, we predicted several new topological insulator materials in thallium (Tl) based ternary chalcogenides from first-principles calculations, including TlBiQ2 and TlSbQ2 (Q=Te, Se and S). TlBiSe2 and TlSbSe2 are found to be strong TIs with a large energy gap (˜ 0.2 eV), while TlBiTe2 is a topological semimetal. A simple Dirac-type dispersion of topological surface states is observed, similar to the Bi2Se3 type of materials. On the other hand, TlBiS2, TlSbTe2 and TlSbS2 are small gap insulators near the topological trivial-nontrivial transition boundary. Particularly TlBiTe2 can be a good candidate in the seeking of Majorana fermions for its co-existing superconductivity property. The topological feature of TlBiSe2 and TlBiTe2 has already been confirmed by recent experiments. References: 1. B.H. Yan, C.X. Liu, H.J. Zhang, C.Y. Yam, X.L. Qi, Th. Frauenheim and S.C. Zhang, Europhys. Lett. 90, 37002 (2010). 2. Y. L. Chen, Z. K. Liu, J. G. Analytis, J.-H. Chu, H. J. Zhang, B. H. Yan, S.-K. Mo, R. G. Moore, D. H. Lu, I. R. Fisher, S. C. Zhang, Z. Hussain, and Z.-X. Shen, Phys. Rev. Lett. 105, 266401(2011).

O 37.11 Wed 12:15 EB 301

A recipe for new Topological Insulators based on bonds, bands, symmetry andheavy atoms — •L. Müchler[1], B. Yan[2,3], S. Chadov[1,4], F. Casper[1], S-C. Zhang[2], and C. Felser[1,4] — [1]Institute of Inorganic Chemistry and Analytical Chemistry, Johannes

Gutenberg - University, Mainz — [2]Department of Physics, McCullough Building,Stanford University,Stanford, CA 94305-4045, USA — [3]Bremen Center for Computational Materials Science, Universität Bremen, Am Fallturm 1, 28359 Bremen, Germany — [4]Max Planck Institute for Chemical Physics of Solids, Dresden, Germany.

In this work we will present a recipe to find new Topological Insulators (TIs) based on bonds, bands, symmetry and heavy atoms. A big issue concerning the compounds known up to now is the control of the bulk carrier density to produce truly insulating samples in the bulk. Using concepts from chemistry and supported by density-functional calculations, we want to motivate an extended search for new compounds with tunable bulk properties.

O 37.12 Wed 12:30 EB 301

Graphene nanoribbons with Au induced spin-orbit effects: a DFT study — •Gustav Bihlmayer and Stefan Blügel — Peter Grünberg Institut & Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, 52425 Jülich, Germany

Historically, the prediction of a topological protection of the edge state of a zig-zag graphene nanoribbon (ZGNR) was at the beginning of the field of topological insulators. Unfortunately, a realization of this system is prevented by (i) the extremely small spin-orbit coupling (SOC) in graphene and (ii) the tendency towards formation of antiferromagnetically coupled edge states in ZGNRs.

New experimental and theoretical results show that SOC effects can be enhanced by substrates and/or adatoms with a large atomic number, so that up to 100 meV spin-splitting can be realized in the graphene. Additionally, hybridization with the substrate changes also the localization of the edge state and its tendency towards antiferromagnetic ordering. Density functional theory calculations of Au supported graphene (with and without adatoms) and ZGNRs will illustrate these effects and point the way towards a realization of a ZNGR with a topologically protected edge state.

O 37.13 Wed 12:45 EB 301

Collision dominated scattering in 3D topological insulators — •Peter Lemmens[1], Vladimir Gnezdilov[2], Dirk Wulferding[1], Yurii Pashkevich[3], Ekaterina Pomjakushina[4], Kazimierz Conder[4], and Helmuth Berger[5] — [1]IPKM, TU-BS, Braunschweig, Germany — [2]ILTPE NAS, Ukraine — [3]DonFTI, Donetsk, Ukraine — [4]PSI, Villigen, Switzerland — [5]EPFL, Lausanne, Switzerland

Despite topological protection in 3D topological insulators there exist scattering processes induced by a resonant excitation from a bulk valence band to Dirac states. This signal in Raman scattering has a Lorentzian lineshape and spin-helical symmetry with a scattering rate of 40 cm^{-1}. A comparison of different compounds (Bi$_2$Se$_3$, Bi$_2$Te$_3$), substitution experiments as well as first results on BiTeI with giant Rashba spin splitting are presented. Work supported by DFG and NTH.

O 38: [DS] Organic electronics and photovoltaics: electronic properties I (jointly with CPP, HL, O)

Time: Wednesday 9:30–11:15 Location: H 2032

O 38.1 Wed 9:30 H 2032

Design of novel dielectric surface modifications for perylene thin-film transistors — •Christian Effertz[1], Ingolf Segger[1], Philip Schulz[1], Arno Classen[2], Carsten Bolm[2], and Matthias Wuttig[1,3] — [1]I. Physikalisches Institut (IA), RWTH Aachen, 52056 Aachen — [2]Institut für Organische Chemie (IOC), RWTH Aachen, 52056 Aachen — [3]JARA FIT, Forschungszentrum Jülich, 52425 Jülich

Dielectric surface modifications (DSMs) can improve the performance of organic thin-film transistors (OTFTs) significantly. To gain a deeper understanding of this performance enhancement and to facilitate high mobility transistors, perylene based OTFTs utilizing novel dielectric surface modifications have been produced. Novel DSMs, which are based on derivates of tridecyltrichlorosilane (TTS) with different functional end-groups have been applied to tailor the adhesion energy of perylene. The resulting samples were characterized by electronic transport measurements, scanning probe microscopy and x-ray diffraction (XRD). Measurements of the surface free energy of the modified dielectric enabled the calculation of the adhesion energy of perylene upon these novel DSMs by the equation-of-state approach. These calculations demonstrate the successful tailoring of the adhesion energy. The insight gained in this study was used to carefully choose further novel DSMs based on polymers. Utilizing these novel DSMs, perylene thin-films and TFTs with a superior film quality, in terms of crystallinity and morphology, as well as performance, in terms of mobility, have been produced[1]. [1]: Effertz, C., et. al. (2011), Adv. Func. Mater. doi: 10.1002/adfm.201101299

O 38.2 Wed 9:45 H 2032

Intermolecular hybridization governs molecular electrical doping — •Ingo Salzmann[1], Georg Heimel[1], Steffen Duhm[2], Martin Oehzelt[3], Patrick Pingel[4], Benjamin George[3], Alexander Schnegg[3], Klaus Lips[3], Ralf-Peter Blum[1], Antje Vollmer[3], and Norbert Koch[1,3] — [1]Humboldt Universität zu Berlin, Germany — [2]Chiba University, Japan — [3]Helmholtz Zentrum Berlin, Germany — [4]Universität Potsdam, Germany

Strong molecular acceptors in organic semiconductor (OSC) films are typically used for molecular electrical p-type doping assuming electron transfer from OSC to dopant. Positive polarons in the fundamental OSC gap are thus expected and could be observable in ultraviolet photoelectron spectroscopy (UPS) as emission feature at, or close to the Fermi Energy (E$_F$) with *reduced* ionization energy (IE), which, however, has not been observed to date. We present a study on the prototypical OSC/p-dopant pair pentacene (PEN) and tetrafluorotetracyano-quinodimethane (F4-TCNQ) up to 1:1 ratio [1]. The IE of 1:1 mixed (amorphous) films is *increased* and larger than possible for pure PEN, while all states occur well below E$_F$ in UPS. We suggest OSC/dopant frontier molecular orbital hybridization forming a doubly occupied bonding and an empty anti-bonding supramolecular hybrid orbital with reduced fundamental gap, which is in fact found by optical absorption measurements and corroborated by density-functional theory (DFT) calculations. Based on similar results for various OSCs, common doping-related observations are discussed within this framework. [1] I. Salzmann, G. Heimel et al., *Phys. Rev. Lett.*, in press.

O 38.3 Wed 10:00 H 2032

Effect of molecular p-doping on hole density and mobility in P3HT and MEH-PPV — •Patrick Pingel and Dieter Neher — Institute of Physics and Astronomy, University of Potsdam, D-14476 Potsdam

Molecularly doped semiconducting polymers can exhibit exceptionally high electrical conductivity, making them suitable for use in solution-processed organic circuitry. Recently, p-doping of conjugated polymers with the strong molecular acceptor tetrafluorotetracyanoquinodimethane, F$_4$TCNQ, has been introduced.

Here, we present a detailed study of the doping efficiency and carrier mobility in thin layers of poly(3-hexylthiophene), P3HT, and poly(2-methoxy-5-(2'-ethylhexyloxy)-p-phenylene vinylene), MEH-PPV, doped with F$_4$TCNQ over a wide range of concentrations. Investigation of these layers with impedance spectroscopy in a metal-insulator-semiconductor (MIS) geometry allowed us to determine both charge carrier density and mobility as a function of doping ratio.

We show that the density of mobile holes increases strictly linearly with increasing F$_4$TCNQ concentration, but the mobilities in P3HT and MEH-PPV exhibit non-monotonic dependencies on doping concentration. This behavior can be fully explained by a model originally developed by Arkhipov et al. [Phys. Rev. B **72**, 235202 (2005)], which predicts that the Coulomb potential of a doping-induced negative counterion acts as a trapping center for holes. Thus, energetical disorder in the polymer layer is effectively increased upon chemical doping.

O 38.4 Wed 10:15 H 2032

Investigation of the degradation processes in small molecule solar cells using impedance spectroscopy — •André Döring, Lorenzo Burtone, Martin Hermenau, Karl Leo, and Moritz

Riede — Institut für Angewandte Photophysik, Technische Universität Dresden, 01062 Dresden, Germany

The purpose of this work is to correlate the impedance spectra (IS) of different solar cell structures - composed of small molecules - with the degradation processes that take place under different aging conditions.

The materials chosen for the optically active bulk-heterojunction layer are ZnPc as donor and C_{60} as acceptor, often used in small-molecule solar cells. In addition to the bulk-heterojunction, doped electron and hole transport layers forming a p-i-n structure are used. Concomitant with the measurement of the IS, the characteristic parameters of the device (i.e. j_{SC}, V_{OC}, FF, PCE, EQE) are monitored during the degradation and correlated to the changes in the IS.

Analyzing the IS gives the possibility to identify different electrical processes that take place in the device. At the beginning of the aging process, we observe an initial improvement of the solar cell parameters, in conjunction with a decreasing trap response in the IS spectra. To investigate in more details the role of trap states for the solar cell performance, simplified structures are prepared. We identify in this way the trap location, type and density inside the solar cell structure. The devices are also exposed to controlled atmospheric conditions to investigate whether oxygen or water vapor is more responsible for the observed change in the electrical properties of the solar cell.

O 38.5 Wed 10:30 H 2032

IR spectroscopic investigation of the MoO_3 doping efficiency in CBP — •Tobias Glaser[1,4], Sven Tengeler[1,4], Sebastian Beck[1,4], Daniela Donhauser[2,4], Bernd Lunkenheimer[3,4], Andreas Köhn[3,4], and Annemarie Pucci[1,4] — [1]Universität Heidelberg, Kirchhoff-Institut für Physik, INF 227, 69120 Heidelberg — [2]Technische Universität Braunschweig, Institut für Hochfrequenztechnik, Schleinitzstraße 22, 38106 Braunschweig — [3]Universität Mainz, Institut für Physikalische Chemie, Jakob-Welder-Weg 11, 55128 Mainz — [4]InnovationLab GmbH, Speyerer Str. 4, 69115 Heidelberg

A major challenge towards high-efficiency and low-voltage organic electronic devices such as OLEDs is to overcome the low bulk conductivity of the organic films. P-type doping with transition-metal oxides like tungsten oxide and molybdenum oxide has proven to increase the charge carrier concentration in hole transporting materials. But the doping efficiency of only a few percent is rather low and the reason for the low efficiency is not fully understood yet. We investigated doping of the ambipolar charge transport material 4,4'-Bis(N-carbazolyl)-1,1'-biphenyl (CBP) with MoO_3 using FTIR-spectroscopy in ultrahigh-vacuum. Comparison of the measured spectra of films with different MoO_3-concentration to DFT-calculations reveals the amount of charge transfer from CBP to MoO_3 but also shows that most of the CBP molecules are still in the neutral state. Also the impact of substrate temperature during the evaporation process is investigated.

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

O 38.6 Wed 10:45 H 2032

Agglomeration of MoO_3 doped into organic thin films studied by TEM-spectroscopy and Tomography — •Daniela Donhauser[1,2], Katrin Schultheiss[1,2], Levin Dieterle[1,2], Martin Pfannmöller[3], Rasmus R. Schröder[3], Tobias Glaser[4,2], Bernd Lunkenheimer[5,2], Michael Kröger[1,2], and Wolfgang Kowalsky[1,2] — [1]Institut für Hochfrequenztechnik, Technische Universität Braunschweig — [2]InnovationLab GmbH, Heidelberg — [3]CellNetworks, Universität Heidelberg — [4]Kirchhoff-Institut für Physik, Universität Heidelberg — [5]Institut für Physikalische Chemie, Johannes Gutenberg-Universität Mainz

Electrochemical doping is essential to overcome limitations in organic devices imposed by low intrinsic conductivity and high injection barriers at the contacts. Materials with very deep lying HOMO-levels like CBP (4,4'-Bis(N-carbazolyl)-1,1'-biphenyl) can be doped with transition metal oxides, e.g. MoO_3. In such systems a very low doping efficiency has been found for which the physical origin is not understood. With TEM spectroscopy we could show that agglomeration of MoO_3 in the CBP-matrix is most likely the reason for the low doping efficiency. Using TEM tomography we observed that MoO_3 forms filament-like structures perpendicular to the substrate. Combining our results with FTIR-measurements, which indicate a charge carrier localization at single molecules, we can model the charge transport to occur at the interface of the MoO_3 filaments and the organic matrix.

O 38.7 Wed 11:00 H 2032

Depth Profiling of Organic Electronic Materials by Gas Cluster Ion Beam — •Andrey Lyapin — Physical Electronics GmbH, Fraunhoferstr. 4, D-85737, Ismaning, Germany

The development of new electronic devices incorporating organic materials, such as Organic Light Diodes (OLED) and Organic Photovoltaics (OPV) is rapidly increasing. To control quality, performance and lifetime of these devices, it is necessary to characterize the layered structures and the dopant distributions in the thin organic materials. Conventional surface analysis techniques such as XPS and ToF-SIMS, combined with mono-atomic ion beam sputtering, have been widely used for chemical depth profiling of inorganic thin films. However, this approach has not been successful for the depth profiling of organic materials due to the loss of chemical information during the sputtering process. Recent cluster ion beam developments utilizing C_{60}^{+} ions have also had limited success for the depth profiling of OLED and OPV structures due to similar modification of chemical and molecular information as a function of sputter depth. The use of surface-sensitive techniques will be discussed for chemical and molecular characterization of OLED and OPV materials in combination with newly developed Gas Cluster Ion Beam (GCIB) source to achieve non-destructive chemical/molecular characterization beyond the surface and through the device. The GCIB source with an average of 2500 Ar atoms per single charged ion has shown dramatic results that both simplify and improve upon the analysis of OLED and OPV materials with a C_{60}^{+} cluster ion beam.

O 39: Focussed session: Frontiers of electronic structure theory: Strong correlations from first principles III (jointly with TT)

Time: Wednesday 10:30–13:15 Location: HE 101

O 39.1 Wed 10:30 HE 101

Reduced effective spin-orbital degeneracy and spin-orbital ordering in paramagnetic transition metal oxides: Sr_2IrO_4 vs. Sr_2RhO_4 — •Cyril Martins[1,2], Markus Aichhorn[1,3], Loïg Vaugier[1], and Silke Biermann[1,2] — [1]Centre de Physique Théorique, Ecole Polytechnique, CNRS, 91128 Palaiseau Cedex, France. — [2]Japan Science and Technology Agency, CREST, Kawaguchi 332-0012, Japan. — [3]Institute of Theoretical and Computational Physics, TU Graz, Petersgasse 16, Graz, Austria.

We discuss the notions of spin-orbital polarization and ordering in paramagnetic materials, and address their consequences in transition metal oxides. Extending the combined density functional and dynamical mean field theory scheme to the case of materials with large spin-orbit interactions, we investigate the electronic excitations of the paramagnetic phases of Sr_2IrO_4 and Sr_2RhO_4. We show that the interplay of spin-orbit interactions, structural distortions and Coulomb interactions suppresses spin-orbital fluctuations. As a result, the room temperature phase of Sr_2IrO_4 is a paramagnetic spin-orbitally ordered Mott insulator. In Sr_2RhO_4, the effective spin-orbital degeneracy is reduced, but the material remains metallic, due to both, smaller spin-orbit and smaller Coulomb interactions. We find excellent agreement of our *ab-initio* calculations for Sr_2RhO_4 with angle-resolved photoemission, and make predictions for spectra of the paramagnetic phase of Sr_2IrO_4.

O 39.2 Wed 10:45 HE 101

***Ab initio* determination of excitation energies and magnetic couplings in correlated, quasi two-dimensional iridates** — •Vamshi Katukuri[1], Hermann Stoll[2], Jeroen van den Brink[1], and Liviu Hozoi[1] — [1]Institute for Theoretical Solid State Physics, IFW Dresden, Helmholtzstrasse 20, 01069 Dresden, Germany — [2]Institute for Theoretical Chemistry, Universität Stuttgart, Pfaffenwaldring 57, 70550 Stuttgart, Germany

Using many-body quantum-chemical techniques, we compare the electronic structure of two layered j=1/2 Ir 5d^5 oxides, Sr_2IrO_4 and Ba_2IrO_4. Multi-orbital and multiplet physics, spin-orbit interactions and O 2p to Ir 5d charge-transfer effects are all treated on equal footing, fully *ab initio*. Our calculations provide valuable complementary information to hybrid schemes based on density-functional theory and dynamical mean-field theory. In particular, for Sr_2IrO_4, the computed magnetic constant (J), d-d and charge-transfer excitation energies show good agreement with recent resonant inelastic x-ray scattering and optical measurements. For Ba_2IrO_4, we find a J that is even somewhat larger, which renders it roughly a factor 2-3 lower than the J's in typical quasi 2D cuprates. This might in itself be encouraging for a scenario of magnetic mediated super-conductivity in doped iridates.

O 39.3 Wed 11:00 HE 101

First-principles study of electronic structure and magnetism of CaIrO$_3$ — •Alaska Subedi — Max Planck Institute for Solid State Research, Stuttgart, Germany

Recent experiments by Ohgushi and co-workers show that post-perovskite $CaIrO_3$ is a Mott insulator in a $J_{\mathrm{eff}} = 1/2$ state.[1,2] I study the electronic structure and magnetism of post-perovskite $CaIrO_3$ using first principles calculations. The density functional calculations within the local density approximation without the combined effect of spin-orbit coupling and on-site Coulomb repulsion show the system to be metallic, which is in disagreement with the experimental evidences. However, when spin-orbit coupling is taken into account, the Ir t_{2g} bands split into fully-filled $J_{\mathrm{eff}} = 3/2$ bands and half-filled $J_{\mathrm{eff}} = 1/2$ bands. I find that spin-orbit coupling along with a modest on-site Coulomb repulsion opens a gap leading to a Mott insulating state. The ordering is antiferromagnetic along the c-axis with total moments aligned antiparallel along the c-axis and canted along the b-axis.

[1] K. Ohgushi, J.-I. Yamaura, H. Ohsumi, K. Sugimoto, S. Takeshita, A. Tokuda, H. Takagi, M. Takata, and T.-H. Arima, arXiv:1108.4523.

[2] K. Ohgushi, H. Gotou, T. Yagi, Y. Kiuchi, F. Sakai, and Y. Ueda, Phys. Rev. B **74**, 241104(R) (2006).

O 39.4 Wed 11:15 HE 101

Interplay of Coulomb interactions and spin-orbit coupling in the bilayer Ruthenate $Sr_3Ru_2O_7$ — •Malte Behrmann, Christoph Piefke, and Frank Lechermann — 1. Institut für Theoretische Physik, Universität Hamburg

The combination of the local-density approximation to density functional theory with explicit many-body approaches has proven to be a powerful tool to investigate the problem of strong electronic correlations on a realistic level. The complex interplay of the effective dimensionality and the symmetry of the underlying crystal structure with the competition between the localized and the itinerant character of electrons is indeed giving rise to highly interesting physical phenomena in many modern materials, especially within the family of transition-metal oxides.

Here we want to discuss the intriguing interplay between rotational-invariant local Coulomb interactions and spin-orbit coupling for the case of the bilayer Ruthenate $Sr_3Ru_2O_7$. New results based on a generic realistic modeling of the correlated electronic structure will be presented. In this respect, also the intriguing metamagnetic behavior of $Sr_3Ru_2O_7$ will be addressed.

O 39.5 Wed 11:30 HE 101

Strong correlations enhanced by charge-ordering in highly doped cobaltates — •Oleg Peil[1], Antoine Georges[2,3,4], and Frank Lechermann[1] — [1]I. Institut für Theoretische Physik, Universität Hamburg, D-20355 Hamburg, Germany — [2]Centre de Physique Théorique, École Polytechnique, CNRS, 91128 Palaiseau Cedex, France — [3]Collège de France, 11 place Marcelin Berthelot, 75005 Paris, France — [4]DPMC, Université de Genève, 24 Quai Ernest Ansermet, 1211 Genève 4, Suiss

Layered cobaltates represent a family of strongly correlated systems with quite unusual properties. In particular, they exhibit the strong mass and low-temperature-conductivity renormalization in the high-doping regime. We present an explanation for the puzzling spectral and transport properties of layered cobaltates close to the band-insulator limit, which relies on the key effect of charge ordering. Blocking a significant fraction of the lattice sites deeply modifies the electronic structure in a way that is shown to be quantitatively consistent with photoemission experiments. It also makes the system highly sensitive to interactions (especially to intersite ones), hence accounting for the strong correlations effects observed in this regime, such as the high effective mass and quasiparticle scattering rate. These conclusions are supported by a theoretical study of an extended Hubbard model with a realistic band structure on an effective kagome lattice.

O 39.6 Wed 11:45 HE 101

Magnetic charge-ordered bad-metal ground state of nickelate superlattices — Danilo Puggioni, Alessio Filippetti, and •Vincenzo Fiorentini — Dept of Physics, U of Cagliari and CNR-IOM, Cagliari, Italy

Short-period strained $LaNiO_3/LaAlO_3$ superlattices undergo paramagnetic–antiferromagnetic metal–"insulator" transitions at low temperature, with charge ordering signaled by spectral weight transfer and XAS line splitting. Further, DMFT calculations suggest that the Fermi surface may become a single hole-like cylinder similar to optimally-doped cuprates, quite unlike that of bulk $LaNiO_3$.

We report ab initio self-interaction-corrected density functional calculations showing that these superlattices are antiferromagnetic and charge-ordered. Although not gap-insulating, they show a sharp pseudo-gap at the Fermi energy, a dc conductivity 2 orders of magnitude lower than in the paramagnetic phase, and a joint density of states for vertical transitions kicking in near the experimental charge gap. While the paramagnetic state has a cuprate-like Fermi surface, the ground-state antiferromagnetic phase has a reconstructed, underdoped-cuprate-like Fermi surface with both electron and hole-like small pockets, at points known as "nodal" and "antinodal" in cuprates. We thus predict that these superlattices should exhibit quantum oscillations in magnetic field.

O 39.7 Wed 12:00 HE 101

Computing the magneto-electric coupling between atoms with numerous open-shells to experimental accuracy : $YMnO_3$ — •Marie-Bernadette Lepetit — CRISMAT UMR6508 CNRS-ENSICAEN, 6 bd Maréchal Juin, 14050 Caen, FRANCE

In strongly correlated systems the electron-electron repulsion between the Fermi level electrons is of larger magnitude than the kinetic energy. It results that the nature of the ground and the low-lying excited-states is thus fundamentally multi-configurational and single-determinant based methods (such as density functional theory) encounter difficulties in properly describing their electronic structure and more specifically their magnetic properties.

The multireference CAS+DDCI [1] and related LCAS+S [2] methods proved their high reliability and efficiency for accessing the local physics such as the magnetic exchange within experimental accuracy, however they cannot be used for systems involving more than one or two unpaired electrons per magnetic center. We will use a simple physical criterion in order to propose a new ab initio approach that overcomes this problem [3].

We used this new method to study the magneto-electric coupling in a prototypal magneto-electric system $YMnO_3$ [4]. Indeed we were able to computed the magnetic exchange as a function of an applied electric field within experimntal accuracy. The importance of the different microscopic contributions (piezzo-magnetic effects, spin-orbit couplign etc…) on the magneto-electric coupling will be discussed from he ab-initio results.

[1] J. Miralles, J. P. Daudey and R. Caballol, *Chem. Phys. Lett.* **198**, (1992) 555 ; V. M. García *et al.*, *Chem. Phys. Lett.* **238**, (1995) 222 ; V. M. García, M. Reguero and R. Caballol, *Theor. Chem. Acc.* **98**, (1997) 50.

[2] A. Gellé, M. L. Munzarová, M.B. Lepetit and F. Illas, *Phys. Rev.* **B 68**, 125103 (2003) ; C J. Calzado, J. F. Sanz and J. P. Malrieu, *J. Chem. Phys.* **112**, 5158 (2002).

[3] A. Gellé, J. Varignon et M.-B. Lepetit, *EPL* **88** 37003 (2009).

[4] J. Varignon and M.-B. Lepetit, in preparation.

O 39.8 Wed 12:15 HE 101

Electron conductivity of Li2O2 in Li-air batteries — •Juan María García Lastra and Kristian Thygesen — Center for Atomic-scal Design. Technical University of Denmark.

The development of non-aqueous Li-air batteries in the late 90s and the rapidly growing demands for better and more sustainable methods for energy storage, have recently spurred a great deal of interest in the material Li2O2. The main limiting factor in the performance of reversible Li-air batteries, namely the large potential losses at realistic current densities, is believed to be related to poor intrinsic transport properties of Li2O2 and/or the carbon- Li2O2 interface. Li2O2 is a wide-gap insulator material (4.9 eV gap) and thus is only able to transport electrons if it contains some kind of defect. Li+ ion vacancies have been detected by means of X-ray diffraction (XRD) and X-Ray Absorption Near Edge Spectroscopy (XANES) in Li2O2 during the discharge of the Li-air batteries. These defects are believed to be the responsible for the electronic transport in Li2O2. Nevertheless, the transport mechanism is not yet clear. In a previous paper from our group it was proposed that Li+ vacancies create electron holes in the valence band of Li2O2, which gives rise to the electronic conduction. However, recent optical absorption experiments have revealed strong excitonic effects in Li2O2 , which point towards to the creation of Li+-Superoxide pairs, instead of holes in the valence band. In this work I will present confirmation of the last hypothesis through DFT+U calculations and propose possible routes for improving Li2O2 electron conductivity through doping.

O 39.9 Wed 12:30 HE 101

Signatures of Electronic Correlations in the Narrow Gap Semiconductor FeSi — •Jan M. Tomczak, Kristjan Haule, and Gabriel Kotliar — Department of Physics and Astronomy, Rutgers University, Piscataway, New Jersey 08854, USA

Correlated semiconductors have been studied intensively over the years, because they exhibit an unusual metallization process which is poorly understood. At low temperatures FeSi behaves as an ordinary semiconductor, while at high temperatures the system is a bad metal with a Curie like susceptibility. Analogies with heavy fermion Kondo insulators and mixed valence compounds, and an anomalous electron-phonon coupling have been invoked to account for this behavior, but lacking quantitative methodologies applied to this problem, a consensus remained elusive to date. Here, we use realistic many-body calculation methods to elucidate the metallization mechanism of FeSi. Our methodology accounts for all substantial anomalies observed in FeSi : lack of conservation of spectral weight in optics, Curie susceptibility and, in particular, an anomalous thermoelectric power. Having quantitatively validated our methodology for this system, we propose a new scenario for FeSi : Unlike in conventional semiconductors the metallization in correlated insulators such as FeSi is induced by the emergence of non-quasiparticle incoherent states in the gap. This temperature induced coherence-incoherence crossover is accompanied by a massive reorganization of the spin excitation spectrum. Besides the fundamental interest, our work is relevant to the design of thermoelectric materials based on correlated insulators.

O 39.10 Wed 12:45 HE 101

Point defect calculations in $CuInSe_2$ and $CuGaSe_2$ using a screened-exchange hybrid functional — •Johan Pohl, Andreas Klein, and Karsten Albe — Institut für Materialwissenschaft, Petersenstr. 32, D-64287 Darmstadt

We present point defect calculations in $CuInSe_2$ and $CuGaSe_2$ (CIGS) using the screened-exchange hybrid functional HSE06 with adapted screening. The use of a functional that gives a correct band gap is important for this material, which is used as absorber material in solar cells. The resulting formation enthalpies, charge transition levels and migration barriers of native defects are presented and their implications for solar cell performance are discussed. We focus on the properties of the copper vacancy [1], which is responsible for Fermi-level pinning at the buffer-absorber interface in CIGS solar cells, and the copper interstitial [2], whose fast diffusion has been proposed to play a role for the metastable behaviour of CIGS solar cells. The results for other native antisite and vacancy defects are also presented and discussed. Finally, we compare the different pictures of the defect physics of CIGS obtained by the adapted HSE06 functional versus the local generalized gradient functional in order to point out general issues with local functionals for point defect calculations in semiconductors. [1] J. Pohl, K. Albe, J. Appl. Phys., 108, 023509, (2010). [2] J. Pohl, A. Klein, K. Albe, Phys. Rev. B, 84, 121201(R), (2011).

O 39.11 Wed 13:00 HE 101

Entanglement of electron-ion motion and decoherence in trans-polyacetylene oligomers — •Heiko Appel — {Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin

Describing decoherence and energy transfer, which is arising after optical excitation in coupled electron-ion systems, is central for the understanding of physical processes appearing in photosynthesis, vision, or in solar-cell applications. As prototypical system for these applications, we investigate in this work the coupled electron-ion dynamics in trans-polyacetylene oligomers which are described by Su-Schrieffer-Heeger Hamiltonians. By tracing the density operator of the combined quantum electron-ion system over either electronic or ionic coordinates, we quantify decoherence, energy transfer and the mutual entanglement in the system after optical excitation.

O 40: Focussed session: Coherence and coherent control in nanophotonics and plasmonics I

Time: Wednesday 10:30–12:45 Location: MA 005

Topical Talk O 40.1 Wed 10:30 MA 005

Active control of light propagation in nanophotonic structures — •Kobus Kuipers — FOM Institute AMOLF, Science Park 104, 1098 XG Amsterdam, The Netherlands

With recent advances in nanofabrication it has become possible to control the flow and/or concentration of light at the nanoscale with proper combinations of geometry and materials. This has led to the unprecedented concentration of light in hot spots of only a fraction of a wavelength cubed and the controlled propagation of light at group velocities several orders of magnitude smaller than c. However, in the majority of cases the control over the light is "static", i.e., for a given choice of geometry and materials, the resulting light control is what it is. This lecture will present our latest progress in gaining active control of light fields at the nanoscale. For example, by using amplitude and phase control obtained through spatial light modulators we are able to position plasmonic "hot spots" at arbitrary positions in a "plasmonic arena". Active control of the photonic bandstructure allows changing the "color" of slow light, control over its group velocity and spectral compression. Through a combination of active control and fixed geometry we are able to achieve an "indirect" transition between photonic eigenstates that can be expoited to control the timing of individual ultrashort pulses originally separated in time by mere picoseconds.

Topical Talk O 40.2 Wed 11:00 MA 005

Coherent exciton-plasmon coupling in metal-dye hybrid nanostructures — •Erich Runge — Technische Universität Ilmenau, 98693 Ilmenau, Germany

At nano-structured metal surfaces, light can be localized to spatial regions well below the diffraction limit by the excitation of surface plasmon polaritons (SPPs). A major challenge for future devices employing SPPs is the fact that SPPs travel only over very short distances, since they are strongly damped in the metal. One approach to overcome this problem is to compensate the damping by coupling of the SPPs to active media, e.g., dyes or quantum wells [P. Vasa et al., Phys. Rev. Lett. 110 (2008) 116801].

Based on recent experiments in the Lienau group at Oldenburg University, I discuss in detail the coupling of quantum mechanical excitations in a j-aggregated dye with the SPP excitation at a metal grating [P. Vasa et al., ACS Nano, 4 (2010), pp. 7559]. The strong coupling (energy transfer) of the SPP and the excitonic dye resonance manifests itself as avoided crossing in the dispersion relation. At resonance, the coupled eigenmodes show excitonic as well as plasmonic features. They inherit a ultrafast strongly non-linear response (saturation and induced biexcitonic absorption) from their excitonic parent, i.e., from the organic dye. If the dye is saturated, its excitonic polarizability vanishes and so does its coupling to the plasmon. The hybridization gap in the mixed-mode dispersion relation closes. This allows for reflectivity changes by about 40% on and off in less than a picoseconds, arguably making the sample the fastest switchable metallic mirror ever made.

Topical Talk O 40.3 Wed 11:30 MA 005

Control and spectroscopy of plasmonic systems using ultrafast pulse shaping — •Tobias Brixner[1], Martin Aeschlimann[2], and Walter Pfeiffer[3] — [1]Institut für Physikalische und Theoretische Chemie, Universität Würzburg, Am Hubland, 97074 Würzburg — [2]Fachbereich Physik and Research Center OPTIMAS, TU Kaiserslautern, Erwin-Schrödinger-Str. 46, 67663 Kaiserslautern — [3]Fakultät für Physik, Universität Bielefeld, Universitätsstr. 25, 33615 Bielefeld

Coherent control concepts using shaped femtosecond laser pulses have originally been developed for controlling the dynamics of molecular systems, and coherent two-dimensional spectroscopy provides insight into molecular electronic couplings. Recently, these principles have been extended to the realm of nano-optics. This adds new degrees of freedom through the control of spatial properties of electromagnetic near-fields in the vicinity of nanostructures. It is now possible to manipulate spatial-temporal and transport phenomena as well as to measure electronic coherences, both on a subdiffraction length scale. This talk provides a comparison between molecular and plasmonic implementations of coherent control and coherent multidimensional spectroscopies, discussing analogies and differences and showing exemplary realizations.

O 40.4 Wed 12:00 MA 005

Monitoring strong light-molecule coupling at field level — •Wei Wang[1], Parinda Vasa[1,2], Robert Pomraenke[1], and Christoph Lienau[1] — [1]Institut für Physik, Carl von Ossietzky Universität Oldenburg, Germany — [2]Department of Physics, Indian Institute of Technology Bombay, Mumbai 400076, India

The radiative coupling between quantum emitters and surface plasmon polaritons (SPPs) plays a key rule in designing hybrid plasmonic devices with active functionalities such as ultrafast all-optical switching, lasing as well as energy transfer and storage. We investigate the strong coupling between surface plasmon polaritons and excitons in metal-molecular aggregate hybrid nanostructures by linear spectroscopy combined with spectral interferometry. The spectral amplitude and phase information are used to reconstruct the response function of the hybrid system which provides an effective way to monitor the polarization response on the field level and gives a complete picture and accurate evaluation of the optical property of the strongly radiatively coupled exciton-SPP system. Model calculations confirm our experimental results and reveal novel features of these interactions such as the formation of sub- and superradiant states. Our field-level investigation of such coupled hybrid systems is expected to be of importance for understanding and manipulating the light-molecule interaction as well as for future implementations of active plasmonic devices.

O 40.5 Wed 12:15 MA 005

Time-domain simulation of quantum systems coupled to plasmonic nano-structures — Richard Ciesielski, •Andreas Hille, René Kullock, Stefan Grafström, and Lukas M. Eng — TU Dresden, Institut für Angewandte Photophysik, 01062 Dresden

Plasmonic nanostructures deserved an increased attention for the last 20 years due to their appealing optical properties such as high field concentration, enhanced optical transmission or negative refraction. Nevertheless, the most severe drawback of these (mostly metallic) nanostructures are their very high Ohmic losses, which for instance prevent bulk plasmonic applications, e.g. in metamaterials. In 2003, Bergman and Stockman proposed the so-called SPASER concept which compensates losses using optical gain media. This approach is very appealing; however, to date no clear proof of really (over-) compensating these losses in bulk plasmonic materials has been shown. We contribute here to this question by theoretically calculating how gain media couple to plasmonic nanostructures on the quantum mechanical (QM) level using the Discontinuous Galerkin (DG) method. DG is a relatively novel but very powerful numerical tool to model optical nanostructures with linear or non-linear optical properties, especially when combined with curved elements. By using time-dependent DG calculations, we study here QM emitters as the gain medium that couple to plasmonic nanoantennas. The nanoantenna is formed by spherical nanoparticles with a diameter of 40 - 100 nm while the QM emitters were chosen to be standard dye molecules.

O 40.6 Wed 12:30 MA 005

Combining spatiotemporal controlled optical excitations with coherent spectroscopy for coupled quantum dots — •Felix Schlosser[1], Mario Schoth[1], Sven Burger[2], Frank Schmidt[2], Andreas Knorr[1], Shaul Mukamel[3], and Marten Richter[1] — [1]Institut für Theoretische Physik, Technische Universität Berlin, Germany — [2]Zuse-Institut Berlin, Germany — [3]Department of Chemistry, University of California, Irvine, USA

Combining pulse shaping techniques for ultrashort laser pulses with nanoplasmonics enables spatiotemporal control of electronic excitations with subwavelength precision [1].

We investigate the quality of different structures to achieve controlled localizations of electric excitations. For one selected setup we present our simulation methods: Field distributions are calculated by a Maxwell solver (JCMsuite) in frequency domain and are composed to simulate time resolved distributions of shaped pulses. The pulse shapes needed to localize the electric field on a nanometer scale are found using a genetic algorithm [2].

We take advantage of this method to examine the excited states of coupled quantum dots: Extending a coherent spectroscopy method [3] (double quantum coherence) by the additional spatial control reveals more information about the system than without spatial control.

[1] M. Aeschlimann et al., Nature 446 (7133), 301-304 (2007)
[2] M. Reichelt and T. Meier, Opt. Lett. 34 (19), 2900-2902 (2009)
[3] L. Yang and S. Mukamel, Phys. Rev. Lett. 100, 057402 (2008)

O 41: Graphene III

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

O 41.1 Wed 10:30 MA 041

Morphology dependent kinetics of oxygen intercalation into graphene/Ir(111) — •Ulrike Schröder[1], Elin Grånäs[2], Timm Gerber[1], Jan Knudsen[2], Mohammad Arman[2], Karina Schulte[3], Jesper Andersen[2], and Thomas Michely[1] — [1]II. Phys. Institut, Universität zu Köln — [2]Division of Synchrotron Radiation Research, Lund University — [3]MAX-Lab, Lund University

Stability of graphene in the presence of gases and at elevated temperatures is of crucial importance for various applications, including its use as a template for well-ordered cluster growth [1].

We investigate the morphology and temperature dependence of oxygen intercalation into graphene/Ir(111) by STM measurements, complementary to our XPS results. A full monolayer of graphene grown with the TPG+CVD method [2] is remarkably stable against O_2 exposure. No intercalation takes place and etching of graphene is only observed at temperatures above 700 K. In STM the onset of etching is visible by hexagonal etch holes in the graphene after O_2 exposure at 740 K. In contrast, O intercalates readily at 400 K under large graphene flakes that cover only 50% of the surface. Surprisingly, smaller flakes resist intercalation at 400 K. Details of the intercalation kinetics can be distinguished by analyzing differences in moiré contrast and apparent graphene heights that are due to oxygen intercalation. Decoupling of graphene from the metal substrate is directly investigated through the effect intercalation has on the formation of metal cluster lattices. [1] N'Diaye et al.; NJP 2009, 11, 103045. [2] van Gastel et al.; APL 2009, 95, 121901.

O 41.2 Wed 10:45 MA 041

Intercalation of O_2 and CO on graphene grown on Ir(111) — •Elin Grånäs[1], Jan Knudsen[1], Timm Gerber[2], Ulrike Schröder[2], Mohammad Arman[1], Karina Schulte[3], Thomas Michely[2], and Jesper Andersen[1] — [1]Division of Synchrotron Radiation Research, Lund University, Sweden — [2]II. Physikalisches Institut, Universität zu Köln, Germany — [3]MAX IV Laboratory, Lund University, Sweden

Graphene is a potential support material for catalytic model systems since it is chemically inert at room temperature and has a high thermal stability in ultra-high vacuum (UHV). The stability in a controlled gas environment at slightly elevated temperatures (300 - 500 K), typical for many catalytic processes, is however virtually unexplored. In this contribution we will discuss the stability of graphene supported on Ir(111) in common gases such as O_2 and CO in the pressure interval from 10^{-8} to 0.1 mbar.

We find that both CO and O_2 intercalate when holes are present in the graphene film, and with the use of X-ray photoemission spectroscopy movies we follow the intercalation process in real time. Surprisingly our studies reveal that intercalation of O_2 and CO starts already close to room temperature. One important consequence of this is that graphene grown on transition metals often is converted to graphene floating on a layer of adsorbates when it is exposed to either

O_2 or CO at slightly elevated temperatures. Finally we will discuss scanning tunneling microscopy studies of the partly intercalated films, that reveal how the intercalation proceeds.

O 41.3 Wed 11:00 MA 041

Intercalation of transition metals underneath graphene on Rh(111) and Ir(111) — •Mikhail Fonin[1], Philipp Leicht[1], Konstantin Krausert[1], Lukas Zielke[1], Muriel Sicot[1], and Yuriy Dedkov[2] — [1]Fachbereich Physik, Universität Konstanz, Konstanz, Germany — [2]SPECS Surface Nano Analysis GmbH, Berlin, Germany

Structure and electronic properties of atomically sharp interfaces between graphene and transition metal surfaces are both of fundamental and technological interest in view of possible device applications. Intercalation of other metals between graphene and metallic substrate can be used to controllably modify the electronic properties of the graphene/metal interfaces.

In this work we report on the intercalation of transition metals (Fe, Co, Ni, Au) underneath a graphene monolayer on Rh(111) and Ir(111). Scanning tunneling microscopy (STM) and photoemission spectroscopy (PES) are implemented to study the atomic structure as well as the electronic properties of the intercalation systems. We show that intercalation starts already at temperatures as low as 400°C and can be efficiently performed up to 600°C without any visible damage of the graphene overlayer. Atomically-resolved imaging of the graphene surface after intercalation shows considerable changes of the moire structure on top of intercalated metal patches due to the changing of the bonding strength. The corresponding changes in the electronic structure of graphene are reflected in the PES spectra.

O 41.4 Wed 11:15 MA 041

Induced magnetism in transition metal intercalated graphitic systems — •Mousumi Upadhyay Kahaly, Thaneshwor Kaloni, and Udo Schwingenschlögl — KAUST, PSE Division, 23955-6900 Thuwal, Kingdom of Saudi Arabia

Inducing spin-polarization in graphene by doping transition metal (TM) atoms is interesting because it can modify the electronic states locally. Precise knowledge of the TM-C interaction is important for understanding carbon nanotube growth, fuel cells, and the role of implanted magnetic atoms, such as Fe, for the magnetic order. For these reasons, we will discuss first-principles results on the structure, chemical bonding, electronic properties, and the spin-polarization induced by Mn, Fe, Co, Ni, and Cu atoms intercalated between adjacent C layers in a three-dimensional graphitic network in aba and aaa stacking. Our results point to a strong preferential bonding of the transition metal atoms in specific lattice sites. The moment induced by Mn, Fe, and Co turns out to vary from 1.38 μ_B to 4.10 μ_B, whereas intercalation of Ni and Cu does not lead to a magnetic state. Overcoming the fundamental problem of the high mobility of transition metal atoms in graphene, this preferential bonding and the selective induction of spin-polarization opens up a way to graphitic Kondo systems. Intercalated graphitic materials are likely to provide new possibilities for applications in spintronics and nanoelectronics.

O 41.5 Wed 11:30 MA 041

Intercalation of Ni underneath graphene on Ir(111) — •Philipp Leicht, Konstantin Krausert, Lukas Zielke, and Mikhail Fonin — Fachbereich Physik, Universität Konstanz, Germany

Interfaces of ferromagnetic materials and graphene have been reported as candidates with potential spin filtering capabilities [1]. Apart from direct growth of graphene on ferromagnetic Ni substrates, ferromagnetic metals can be intercalated between graphene and the substrate interface for many graphene/metal systems [2]. Thereby pre-deposited metals can penetrate graphene upon thermal annealing at moderate temperatures.

In this work we present the investigation of Ni intercalation underneath a graphene monolayer on Ir(111). We use scanning tunneling microscopy (STM) to determine the structure of the prepared samples with the intercalated Ni amount ranging from a submonolayer to few monolayers. Intercalation preferentially occurs at step edges forming areas with strongly increased moiré corrugation and decreased average distance of graphene from the intercalant compared to graphene/Ir(111). The stronger corrugation in conjunction with a shift of the C 1s core level observed in x-ray photo-electron spectroscopy suggests a strong bonding between graphene and Ni.

[1] Karpan, V. M. et al. Phys. Rev. B 78, 195419 (2008) [2] Huang, Li et al. Appl. Phys. Lett. 99, 163107 (2011)

O 41.6 Wed 11:45 MA 041

Spin-polarized STM of cobalt intercalated graphene/Ir(111) — •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-20355 Hamburg — [2]Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich, D-52425 Jülich

It has been shown that graphite intercalation compounds present peculiar characteristics such as dramatic changes in the transport, optical and catalytic properties compared to bulk graphite, or even superconductivity. The intercalation of elements between graphene and its substrate can also influence the properties of graphene. In particular, this approach opens a new route to explore the behavior of graphene on a magnetic substrate.

Here, using the spin-polarized STM technique, we are able to study the structure, as well as the local electronic and magnetic properties of graphene on a magnetic substrate, where the magnetic substrate is obtained by the intercalation of a cobalt layer between graphene and an Ir(111) surface. The experimental results are compared to DFT calculations.

O 41.7 Wed 12:00 MA 041

Structural and electronic properties of the graphene/Al/Ni(111) intercalation system — •Elena Voloshina[1], Martin Weser[2], Stefan Böttcher[2], Karsten Horn[2], and Yuriy Dedkov[2,3,4] — [1]Physikalische und Theoretische Chemie, Freie Universität Berlin, Germany — [2]Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, Germany — [3]Institut für Festkörperphysik, Technische Universität Dresden, Germany — [4]SPECS Surface Nano Analysis GmbH, Germany

The atomic and electronic structure of the graphene/Al/Ni(111) system is studied via combination of experimental methods and density functional theory calculations. It has been demonstrated, that the graphene layer can be effectively decoupled from the ferromagnetic substrate via intercalation of the *sp* metal [1]. Despite the symmetry in the graphene lattice is broken in the trilayer under consideration, there is no sizable energy gap for the π states around the K point of Brillouin zone. In this talk, properties of graphene/Ni(111) and graphene/Al/Ni(111) are compared. The perspectives of application of the Al-based intercalation-like systems are discussed.

[1] E. N. Voloshina, A. Generalov, M. Weser, S. Boettcher, K. Horn, Yu. S. Dedkov, arXiv:1108.3002 (2011); New. J. Phys. (accepted).

O 41.8 Wed 12:15 MA 041

DFT study of the electronic structure of graphene/Ag(111)/Re(0001) — •Jörg Doppler, Florian Mittendorfer, and Josef Redinger — Inst. of Applied Physics, Vienna University of Technology, Vienna, Austria

Data from ARPES experiments on graphene/Re and graphene/Ag/Re(0001), which features an additional intercalated Ag monolayer, demonstrate that the strong interaction of Gr/Re is significantly lowered as soon as Ag is introduced. It is also found that the Ag atoms grow epitactically, and we have evidence of a hybridization of the Ag bands with graphene's π-state. We study the electronic structure of Gr/Ag(111)/Re(0001) by means of numerical ab-initio DFT calculations employing the program VASP. The properties of gr/Ag/Re were determined in a simplified approach by examining a (1x1) cell for the two equilibrium lattice constants of Re and Gr, i.e. either stretching Gr or compressing the underlying Ag/Re substrate, respectively. Different interface models and graphene-substrate distances were tested to determine the energetically most favourable placement of the carbon atoms relative to the substrate surface, yielding the top-fcc arrangement as the structure featuring the lowest energy. Due to interaction with the Ag/Re substrate, the electronic structure of graphene is modified, showing qualitative agreement with above mentioned ARPES experiments. We observe a downward shift of the Dirac point with respect to the Fermi energy as well as hybridization of the graphene π-band with the Ag d-bands. The strength of both phenomena depends on the graphene-substrate distance.

O 41.9 Wed 12:30 MA 041

Electronic spectrum and structure of an epitaxial graphene superlattice on SiC — •Konstantin Emtsev[1], Stiven Forti[1], Camilla Coletti[2], and Ulrich Starke[1] — [1]Max Planck Institute for Solid State Research, Stuttgart, Germany — [2]Center for Nanotechnology Innovation @ NEST, Istituto Italiano di Tecnologia, Pisa, Italy

The electronic spectrum of graphene can be altered profoundly by the presence of an external potential that is periodic on an atomic scale [1]. Experimentally, such perturbations are sought after in graphene grown epitaxially on a crystalline substrate with commensurate or incommensurate lattice arrangements. In the present work we address the electronic and structural properties of such a graphene superlattice realized on a SiC substrate. We utilize the atomic intercalation phenomenon established earlier [2, 3] in order to create a new heterointerface graphene/copper/SiC. The samples were characterized by high resolution ARPES, XPS and LEED. As observed by LEED, the modified interface imposes a new long range reconstruction on graphene as opposed to as-grown epitaxial graphene on SiC. Changes in the electronic valence band spectrum of the graphene film detected by ARPES are related to a structural transformation of the graphene layer that we derive from XPS core level spectra. We compare our data to other epitaxial graphene systems and theoretical predictions.

[1] C.H. Park et al., Nat. Physics, 4, 213 (2008) [2] I. Gierz et al., Phys. Rev. B, 81, 235408 (2010) [3] K.Emtsev et al., Phys. Rev. B, 84, 125423 (2011)

O 41.10 Wed 12:45 MA 041

Interaction of hydrogen with graphene on Silicon carbide: unraveling the interface structure — •Francois C. Bocquet[1,2,4], Regis Bisson[3], Thierry Angot[3], and Jean-Marc Themlin[1,2] — [1]Aix-Marseille Université, IM2NP, France — [2]CNRS, IM2NP (UMR 6242) F-13397 Marseille CEDEX 20, France — [3]PIIM, UMR 6633 CNRS-Université de Provence, F-13397 Marseille CEDEX 20, France — [4]Peter Grünberg Institut (PGI-3), Forschungszentrum Jülich, 52425 Jülich, Germany and JARA Fundamentals of Future Information Technology, 52425 Jülich, Germany

Since the stability of a single graphene layer has been discovered, much effort was devoted to the thermal growth of graphene over SiC. Recently, the reversible adsorption of atomic hydrogen on graphene was shown to induce drastic changes in electronic properties between clean, low [1] and high coverages [2]. Also, at high temperature, hydrogen penetrate beneath the buffer layer resulting in free-standing graphene [3]. We studied the buffer layer forming prior to graphene growth on SiC(0001) as well as a single-layer of free standing graphene obtained by hydrogen intercalation. By a subtle tuning of graphene electronic properties with hydrogen adsorption, High Resolution Electron Energy Loss Spectroscopy (HREELS) is allowed to probe below the graphene sheet. This reveals unambiguously the nature of the covalent bond between SiC and the buffer layer.

References [1] Bostwick, Phys. Rev. Lett., 103 (2009) 056404 [2] Elias, Science, 323 (2009) 610 [3] Riedl, Phys. Rev. Lett., 103 (2009) 246804

O 42: Nanostructures at surfaces I

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

O 42.1 Wed 10:30 MA 042

Synthesize and characterization of the properties of intrinsic defects in size-controlled surface ZnO nanowires by multiple spectroscopic techniques — •Kin Mun Wong[1,2], Yaoguo Fang[1,2], André Devaux[3], Liaoyong Wen[1,2], Luisa De Cola[3], and Yong Lei[1,2] — [1]Fachgebiet 3D-Nanostrukturierung, Institut für Physik & Zentrum für Mikro- und Nanotechnologien (ZIK MacroNano), Technische Universität Ilmenau, 98693 Ilmenau, Germany. — [2]Institut für Materialphysik, Westfälische Wilhelms-Universität Münster, 48149 Münster, Germany. — [3]Physikalisches Institut, Westfälische Wilhelms-Universität, 48149 Münster, Germany.

Arrays of regular and size-controlled ZnO nanowires with different length and diameter were synthesized by chemical vapour deposition and hydrothermal method. Quantitative information about the concentration of intrinsic defects such as oxygen vacancies and zinc interstitials as well as their luminescence lifetimes was obtained by a number of different spectroscopic techniques. From the correlation between the different sets of experimental data, some important relationships were observed between the concentration and spatial distribution of the intrinsic defects with regards to the size and surface to volume ratio of the ZnO nanowires. This connection between the defects and the size of the nanowires is essential for the fine tuning and optimatization of the defect related properties in ZnO nanowires. Furthermore, an analytical formula was derived for obtaining the donor concentration in the ZnO nanowires directly from the conductive atomic force microscopy measurements without prior need of depositing a metal electrode layer.

O 42.2 Wed 10:45 MA 042

Pulsed laser deposition of ZnO nanostructures for hybrid solar cells — •Sven Käbisch[1,2], Marc A. Gluba[2], Norbert H. Nickel[2], and Norbert Koch[1,2] — [1]Institut für Physik, Humboldt-Universität zu Berlin — [2]Helmholtz-Zentrum Berlin für Materialien und Energie GmbH

Hybrid solar cells benefit from the large optical absorption cross section of organic chromophores while effective charge transport is achieved through high mobility inorganic materials. Since exciton diffusion lengths in organic materials are typically shorter than ca. 10 nm, organic/inorganic interfaces with a nanoscale interdigitation are required. Zinc oxide (ZnO) readily forms nanostructures on various substrates. Pulsed laser deposition (PLD) of ZnO nanostructures is studied in detail with respect to process parameters like laser fluence, partial pressure of the oxygen process gas, substrate temperature and type of substrate. The laser fluence and the deposition temperature determine the density of nanostructures due to the control of nucleation and diffusion of particles on the surface. The substrate type and morphology determine the shape of the nanostructures, while the deposition pressure changes their alignment. Nanostructures with optimized morphology and density are fabricated and used as electron acceptor in hybrid solar cells. A light sensitive p-n-junction is demonstrated.

O 42.3 Wed 11:00 MA 042

Structured growth of ZnO on self-assembled monolayers — •Nivedita Yumnam, Miriam Schwarz, and Veit Wagner — School of Engineering and Science, Jacobs University Bremen, Campusring 1, D-28759 Bremen (Germany)

The architecture of ZnO nanostructures grown by electrochemical deposition coupled with its enhanced light trapping mechanism can be used as a semiconductor in hybrid solar cells. We focus on the structured electrochemical growth of ZnO nanorods through self-assembled monolayers of alkanethiols adsorbed on gold. The densely packed self-assembled monolayer of alkanethiol adsorbed on gold hinders the formation of ZnO crystals. We tune the number density and the size of the ZnO nanorods by varying the adsorption time of alkanethiol monolayers on gold and the electrochemical growth time of ZnO. In order to allow for laterally structured growth of ZnO on monolayer covered gold, we employed microcontact printing of alkanethiol on gold. Depending on deposition method and parameters our results indicate a varying degree of pinholes in the self-assembled monolayer on gold. With these pinholes the ZnO rod size and the average distance between ZnO rods can be controlled. This pinhole density is correlated to the leakage current through the self-assembled monolayer of alkanethiol determined by impedance measurements.

O 42.4 Wed 11:15 MA 042

Directed placement of gold nanorods using removable assembly guiding structures — •Felix Holzner[1,2], Cyrill Kuemin[1,2], Philip Paul[1,2], James L. Hedrick[3], Heiko Wolf[1], Nicholas D. Spencer[2], Urs Duerig[1], and Armin Knoll[1] — [1]IBM Research, Rueschlikon, Switzerland — [2]Laboratory of Surface Science and Technology, ETH Zurich, Switzerland — [3]IBM Research, Almaden, USA

We present a new assembly and transfer process, where we have used a temperature- sensitive, nanopatterned polymer film as a removable template to position and align gold nanorods onto an underlying target substrate with 10 nm precision [1]. Shape-matching guiding structures have been written by thermal scanning probe lithography with polyphthalaldehyde (PPA) as resist material. The patterns were written using a heated tip to decompose and evaporate the PPA locally pixel by pixel. This can be done with high speed (500000 pixels per second, 20 mm/s scan speed), high accuracy (<10 nm) and excellent control of the patterning depth [2],[3]. Capillary Assembly was used to trap gold nanorods of size 80 nm x 25 nm in the PPA shape-matching guiding structures. Measured standard deviations from the targeted orientation and position were 25.2° and 10.3 nm, respectively. Heating the sample to 215°C leads to a complete evaporation of the PPA and a transfer of the nanorods onto the underlying substrate without affecting the integrity and the placement accuracy of the nanorods.

[1] Holzner et al., Nano Letters, 2011, 11, 3957-3962 [2] Paul et al., Nanotechnology, 2011, 22, 275-306 [3] Knoll et al., Advanced Materials, 2010, 22, 3361-3365

O 42.5 Wed 11:30 MA 042

Surface optical and vibrational properties of Ge(001) at 300 K/40 K before and after Au nanowire deposition — •Jochen Räthel[1], Eugen Speiser[1], Christoph Cobet[1], Karsten Hinrichs[1], Utz Bass[2], Jean Geurts[2], 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

The interest in self organized 1-dimensional metallic nanowires on semiconductor surfaces is driven by their extraordinary electronic properties, like Luttinger liquid behaviour for Au nanowires on Ge(001) as shown recently. Therefore, the aims of our study comprise (i) the vibrational properties and the underlying surface structure and dynamics, and (ii) the anisotropic optical properties, arising from surface electronic transitions. For these purposes, we employed in-situ Raman spectroscopy as well as reflectance anisotropy spectroscopy (RAS) on self-organized Au nanowires, grown under UHV conditions on a flash-prepared Ge(001) c(4×2)/(2×1) surface. The Au chain order was identified by the expected c(8×2) LEED symmetry, with two orthogonal domain orientations. The clean Ge(001) shows surface vibration modes, whose energy values agree well with calculated mode patterns found in literature. These surface phonons vanish partly upon cooling to 40 K and completely upon Au deposition, indicating for both cases surface structure changes. RAS spectra in the range from 0.5 to 5 eV show several characteristic features before and after the Au deposition, assigned to electronic surface transitions.

O 42.6 Wed 11:45 MA 042

Structural Elements of Gold-Induced Atomic Chains on Ge(001) — •Sebastian Meyer[1], Jörg Schäfer[1], Christoph Loho[1], Christian Blumenstein[1], Simeon Sauer[2], Friedhelm Bechstedt[3], Phil Willmott[4], and Ralph Claessen[1] — [1]Physikalisches Institut, Universität Würzburg — [2]Institut für Physik, nivserität Freiburg — [3]Inst. f. Festkörpertheorie u. -optik, Universität Jena — [4]Paul Scherrer Institut, Villigen CH

Self-organized nanowires of gold on Ge(001) are outstanding among all previously reported atom chains because their electronic states are found to deviate from the common Fermi liquid picture. In contrast, the exotic many-body state of a Tomonaga-Luttinger liquid applies. Characteristic features are observed in terms of power-law suppression of the density of states towards the chemical potential in scanning tunneling spectroscopy and angle-resolved photoemission [1]. For a detailed understanding an atomistic model is highly desirable, enabling band structure calculations within density functional theory (DFT). Thus, we have performed surface x-ray diffraction (SXRD) at the Swiss Light Source. The Patterson map resulting from in-plane scattering data yields interatomic distances which are required for structural modeling. Comparison of SXRD with recent STM data reveals essential structural building blocks which are compatible with present DFT calculations.

[1] C. Blumenstein et al., Nat. Phys. 7, 776 (2011).

O 42.7 Wed 12:00 MA 042

Pb nanowire induced facetting of Si(557) surfaces — •Sebastian Gevers[1], Thomas Weisemoeller[1], Christoph Tegenkamp[2], and Joachim Wollschläger[1] — [1]Fachbereich Physik, Universitaet Osnabrueck, Barbarastr. 7, 49069 Osnabrueck — [2]Institut für Festkörperphysik, Leibniz Universität Hannover, Appelstraße 2, 30167 Hannover

Nanowires are of fundamental interest to study electronic correlations in low-dimensional systems which cause strong deviations from simple Fermi-liquid behavior. Here, the possibility to manipulate and to characterize these structures with a variety of techniques offer a wide field for scientific research. In particular anisotropic surface transport is interesting since it directly probes inherent electronic instabilities in these low-dimensional structures.

Since long-range ordering is required to perform transport measurements, Si(557) surfaces with high step stiffness are used as a substrate to grow arrays of crystalline Pb nanowires. Furthermore, it has been reported that the system switches from 2D to 1D conductivity which is correlated with structure phase transitions. In the present work, the surface structure and morphology of substrate and nanowires is investigated by grazing incidence x-ray diffraction (GIXRD) and spot profile low energy electron diffraction (SPALEED). It is shown that a layer by layer growth of Pb can be obtained and that refacetting of the Si(557) substrate occurs at elevated substrate temperatures. In particular we take advantage of the high precision of the GIXRD experiment to characterize the refacetting.

O 42.8 Wed 12:15 MA 042

Reconstruction of Atomic-Scale Wires on Si(553)-Au: Observation of Current-Dependent Periodicity — •S. Polei[1], I. Barke[1], P.C. Snijders[2], F.J. Himpsel[3], S.C. Erwin[4], and K.-H. Meiwes-Broer[1] — [1]Inst. für Physik, Uni Rostock, Rostock, Germany — [2]Materials Science & Technology Division, Oak Ridge Nat. Lab., Oak Ridge, Tennessee, USA — [3]Physics Dept., University of Wisconsin Madison, Madison, Wisconsin, USA — [4]Center for Computational Materials Science, Naval Research Lab., Washington, DC, USA

Quasi one-dimensional metallic chains on silicon have received considerable attention in the last few years, primarily because they possess unusual electronic properties [1]. In particular, the Au-induced reconstruction of the Si(553) surface is of great interest because recent theoretical findings predict that it has a magnetic ground state [4]. We present STM and STS measurements to investigate the nature of the phase transition to a reconstructed Si step edge at low temperature and the possible development of non-zero Si spin-polarization. Different periodicities are observed at the Si step-edge chains depending on the tunneling current. When the tunneling current is increased at 51 K the reconstruction along the chains changes gradually from 1x3 to 1x2. As a result, the STM topography has 1x6 periodicity in the transition regime. Findings are discussed in the context of a possible magnetic state [2].

[1] J. N. Crain et al., PRB 69, 125401 (2004); P. C. Snijders et al., PRL 96, 076801 (2006); I. Barke et al., PRL 97, 226405 (2006) [2] S. C. Erwin, F. J. Himpsel, Nat. Commun. 1, 58 (2010)

O 42.9 Wed 12:30 MA 042

Quasi-1D metallic Ag-wires grown on vicinal Silicon surfaces — •Christian Brand, Jędrzej Schmeidel, Christoph Tegenkamp, and Herbert Pfnür — Institut für Festkörperphysik, Leibniz Universität Hannover, Germany

A prototype system of a nearly free 2D electron gas system is the Ag-$(\sqrt{3} \times \sqrt{3})$ reconstruction on a Si(111)-(7×7) surface. Consequently, a promising route to fabricate a 1D electron gas system might be the self assembly of Ag wetting structures on uniaxial Si(557) surfaces.

The Si(557) surface consists of (111) terraces and triple steps with a periodicity of 5.73 nm. By adsorption of sub-monolayer amounts of Ag at 770 K several types of quasi-1D structures are formed, accompanied by locally varying refacetting of the surface. Besides insulating chains of monatomic width (α-, β- and γ-type) also metallic wires with $(\sqrt{3} \times \sqrt{3})$ reconstruction are formed, as deduced from our LEED- and STM/STS-study.

In many cases metallic monolayer species are decoupled electronically from the Si-surfaces by forming Schottky barriers, which limit the applicability of STS to measure the electronic structure of the wires themselves at low bias voltages. In order to contact the wires electrically, a shadow mask technique on the basis of a Si_3N_4 membrane has been developed. First results will be presented.

O 42.10 Wed 12:45 MA 042

Growth phenomena of Ge nanowires grown by MBE — •Roman Bansen, Jan Schmidtbauer, Robert Heimburger, Thomas Teubner, and Torsten Boeck — Leibniz Institute for Crystal Growth, 12489 Berlin, Germany

Advances in nanotechnology with its significantly lower material consumption and quantum effects-related new semiconductor properties have led to a renewed interest in germanium, with its advantageous properties for numerous possible applications in photovoltaics, thermoelectrics and electronics.

The presentation concentrates on growth as well as in-detail characterization of Ge nanowires with a focus on basic growth characteristics and their dependencies on surface preparation methods. The nanowires were grown by MBE on Ge substrates using the VLS mechanism with Au as catalyst metal.

A range of different surface passivations was tested for their effect on nanowire growth. The unexpected results reveal that very clean and smooth surfaces make the catalyst droplets preferentially form "in-plane" nanowires, instead of growing "conventional" (out-of-plane) nanowires. Depending on the respective types of passivation, changes of the in-plane wires' growth directions can be observed. It is possible to explain the directions with the help of SEM and TEM images for the most part, and a model will be presented for the effect itself.

O 43: Clean surfaces III

Time: Wednesday 10:30–13:00 Location: MA 043

O 43.1 Wed 10:30 MA 043

STM and STS study of $SrRuO_3(001)$ thin films on $SrTiO_3(001)$ — •Martin Trautmann[1], Dietrich Hesse[2], Ionela Vrejoiu[2], and Wolf Widdra[1,2] — [1]Institut für Physik, Martin-Luther-Universität Halle-Wittenberg — [2]MPI für Mikrostrukturphysik, Halle/S.

For applications in oxide-based electronic devices such as ferroelectric heterostructures and non-volatile ferroelectric random access memories the electrode material plays an important role. In this context $SrRuO_3$ has drawn significant attention due to its high conductivity and low lattice misfit with many functional perovskites. In this study a 40 nm thick PLD grown film of orthorhombic $SrRuO_3$ on $SrTiO_3(001)$ has been characterized by LEED, AFM, STM and STS. Upon heating to 400°C in 10^{-5} mbar of oxygen the film exhibits a well-ordered pseudocubic $SrRuO_3(001)$-(1x1) LEED pattern. The observed surface morphology as determined by STM is characterized by small vacancy islands as has been reported also earlier [1]. Annealing to higher temperatures in an increased O_2 atmosphere leads to a rearrangement of the vacancy islands in the high symmetry directions. STS on this $SrRuO_3(001)$ surface is dominated by a well-resolved unoccupied density-of-states feature at 2.5 eV above E_F which is assigned to an unoccupied Ru 4d state on the basis of DFT calculations [2].

[1] H. N. Lee, H. M. Christen, M. F. Chisholm, C. M. Rouleau, and D. H. Lowndes, Appl. Phys. Lett. **84**, 4107 (2004)

[2] J. M. Rondinelli, N. M. Caffrey, S. Sanvito, and N. A. Spaldin, Phys. Rev. B **78**, 155107 (2008)

O 43.2 Wed 10:45 MA 043

Ultrathin zirconia films on Pt_3Zr — Moritz Antlanger, Jiří Pavelec, Peter Varga, Ulrike Diebold, and •Michael Schmid — TU Wien, Austria

Zirconium dioxide (ZrO_2) has numerous applications, from high-performance ceramics for engineering and dentistry to gas sensors and solid-oxide fuel cells (SOFC). Its performance in sensors and SOFCs is based on its high bandgap (≈ 6 eV), which implies a low electronic conductivity even at high temperatures where it becomes an ionic conductor. This excludes many charged-particle techniques such as scanning tunneling microscopy (STM) for the study of bulk ZrO_2. We have therefore produced ultrathin zirconia films by oxidation of a Pt_3Zr alloy single crystal and determined their surface structure and properties by STM. The ultrathin film consists of a single O-Zr-O trilayer, exhibits a bandgap, and is remarkably stable. The interface structure between the ultrathin oxide and the substrate is analyzed from STM measurements and shows a reconstructed Pt layer. The surface is oxygen-terminated and almost defect-free, yet the surface diffusivity of Pd on the ZrO_2 film is much lower than on oxygen-terminated alumina surfaces.

This work was supported by the Austrian Science Fund (FWF; project F45).

O 43.3 Wed 11:00 MA 043

Electronic structure and formation energies of neutral and charged O vacancies at MgO (100) and (111) surfaces: Exchange-correlation effects — •Norina A. Richter, Sergey V. Levchenko, and Matthias Scheffler — Fritz Haber Institute of the Max Planck Society, 14195 Berlin, Germany

Surface O vacancies (F-centers) can strongly influence catalytic properties of MgO and metal clusters supported on MgO, but the experimental determination of their concentration at catalytic conditions is difficult. We employ density-functional theory and the *ab initio* atomistic thermodynamics approach to determine concentration and charge states of F-centers at (111) and flat and stepped (100) surfaces of MgO at realistic (T, p) conditions. Slab models and the virtual-crystal approximation [1] are used to model charged defects at surfaces. We find a strong dependence of F^{+} and F^{2+} formation energy on the exchange-correlation (XC) functional. Varying the amount of screening and fraction of exact exchange within the HSE functional, we find a linear correlation between defect formation energies and calculated valence-band width of the host material, in line with recent results for bulk systems [2]. Using this correlation and extrapolating to experimental band width, we conclude that only F^{2+} centers can be present in significant concentrations at the (100) terraces at realistic conditions. — [1] L. Vegard, Z. Phys. **5**, 17 (1921); M. Scheffler, Physica **146B**, 176 (1987); [2] R. Ramprasad, H. Zhu, P. Rinke, and M. Scheffler, subm. to Phys. Rev. Lett.

O 43.4 Wed 11:15 MA 043

Structure and polarity of step edges on (111) surfaces of fluorite type crystals — •Hans Hermann Pieper[1], Michael Reichling[1], and Clemens Barth[2] — [1]Universität Osnabrück, Germany — [2]CINaM-CNRS, Marseille, France

The morphology and polarity of step edges found on CaF_2 and CeO_2 (111) is investigated by non-contact atomic force microscopy (NC-AFM) and Kelvin probe force microscopy (KPFM). The macroscopic shape of step edges strongly depends on sample preparation, however both materials exhibit type I and II facets at the nanoscale.

While type I steps are neutral, KPFM reveals a positive local charge at type II steps. Different models for the origin and the compensation of the charge are suggested. On CaF_2 the positive charge is compensated by subsurface fluorine ions on interstitial sites while for CeO_2 oxygen is released leaving behind Ce^{3+} sites located on step edges.

O 43.5 Wed 11:30 MA 043

Fe-rich terminations and the role of subsurface charge order at the $Fe_3O_4(001)$ surface — •Zbynek Novotny, Gareth S. Parkinson, Zoltan Edes, Michael Schmid, and Urlike Diebold — Institute of Applied Physics, TU Wien, Vienna, Austria

Magnetite, Fe_3O_4, crystallizes in the inverse spinel structure with an fcc oxygen sublattice and Fe cations in tetrahedral (A) and octahedral (B) sites. The (001) surface exhibits undulating rows of Fe(B) atoms with two unoccupied Fe(A) bulk continuation sites in the 'narrow' and 'wide' regions of the unit cell, related to Fe^{2+}/Fe^{3+} subsurface charge ordering [1,2]. We present a route to produce a reduced, well-ordered $Fe_3O_4(001)$ surface by evaporating Fe on the distorted Fe(B) surface at room temperature. STM shows that this surface contains Fe(A) monomers and Fe clusters. Mild annealing of the sample leads to a surface containing Fe(A) monomers and, with increasing Fe coverage, dimers of 5-fold coordinated Fe. Both surfaces contain Fe adatoms located at the 'narrow' position within the unit cell, indicating a strong preference for sites located above Fe^{2+} cations in the subsurface layer.

This material is based upon work supported as part of the Center for Atomic-Level Catalyst Design, an Energy Frontier Research Center funded by the U.S. Department of Energy, Office of Science, Office of Basic Energy Sciences under Award Number #DE-SC0001058.

[1] R. Pentcheva et al., Phys. Rev. Lett. 94, 126101 (2005).

[2] Z. Łodziana, Phys. Rev. Lett. 99, 206402 (2007).

O 43.6 Wed 11:45 MA 043

2D Scanning Force Spectroscopy on Organic Layer Crystals — •Mathias Schulzendorf[1], Gregor Fessler[1], Shigeki Kawai[1], Thilo Glatzel[1], Shi-Xia Liu[2], and Silvio Decurtins[2] — [1]Department of Physics, University of Basel, Klingelbergstrasse 82, 4056 Basel, Switzerland — [2]Department of Chemistry and Biochemistry, University of Bern, Freiestrasse 3, 3012 Bern, Switzerland

Bis(benzylammonium)bis(oxalato)cuprate(II) is a layered organic bulk crystal. Previous work on this crystal compound indicated that the crystal exhibits a friction anisotropy depending on the molecular structure. To further study the dependence of surface features and molecular composition the crystal was probed by non contact scanning probe microscopy in ultra high vacuum at room temperature. By means of molecular tracking, multiple series of 2D force maps were performed along the [100] crystal axis. The background of a second minimum in the extracted interaction force curves, revealed by our measurements, will be analyzed and discussed.

O 43.7 Wed 12:00 MA 043

Structure of V_2O_3 films on Au(111) — •Eric Meyer, Jan Seifert, and Helmut Winter — Humboldt-Universität zu Berlin, Institut für Physik, Newtonstr. 15, 12489 Berlin

In recent studies Window et al. [1] have reported on the surface termination of thin V_2O_3 films grown on Au(111). Measurements reveal a reconstructed trilayer with O_3-termination in accord with DFT-calculations. This is in conflict with a complete monolayer of vanadyl species found by other groups [2].

In this work we present studies on the V_2O_3 surface via scattering of fast atoms under grazing angles of incidence. The measurements are compared with trajectory computer simulations in which electron emission is incorporated for both structual models.

We find clear evidence for the reconstructed trilayer structure. Excellent agreement between experiment and simulation is found so that we can confirm a O_3 termination with slightly modified positions of topmost O atoms compared to [1].

[1] Window et al., Phys. Rev. Lett. 107, 016105 (2011)

[2] Dupuis et al., Surf. Sci. 539, 99 (2003)

O 43.8 Wed 12:15 MA 043

Exploring highly correlated materials via electron pair emission — •Lucie Behnke, Frank O. Schumann, Chang-Hui Li, and Jürgen Kirschner — Max-Planck-Institut für Mikrostrukturphysik, Weinberg 2, 06120 Halle

Metal oxides like NiO are usually termed "highly correlated", because the material properties are decisively determined by the electron-electron interaction. This makes them interesting candidates for electron pair spectroscopy which is particularly sensitive to the electron correlation. We have prepared ultrathin NiO/Ag(100) films and studied the electron pair emission upon electron impact. Compared to metallic Ni we observe an increase of the coincidence intensity by a factor 8-10 for NiO. Thickness dependent measurements prove that this enhancement is an intrinsic effect rather than due to an increased mean free path for NiO. The Neel temperature T_N of NiO films is thickness dependent which allows to tune T_N. We performed temperature dependent measurements for various thicknesses and observed no temperature variation of the coincidence intensity. This proves that the electron pair emission probes the local correlation rather than long-range order. We discuss the prospect of a quantitative characterization of the electron correlation via pair emission spectroscopy.

O 43.9 Wed 12:30 MA 043

Atomistic modeling of electromechanical coupling at metal surfaces — •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 Mechanics, Helmholtz Zentrum Geesthacht, Geesthacht, Germany — [3]Institute of Materials Physics, Hamburg University of Technology, Hamburg, Germany

Designing functional materials with well-defined catalytic properties requires understanding of the relation between surface structure and reactivity. Electrochemical experiments on pseudomorphic Pd monolayers have revealed the importance of strain for the catalytic activity of metal surfaces. Although the strain response of the electrode potential $\delta E/\delta e$ has been measured for several materials, fundamental understanding of the underlying microscopic processes is far from complete. The variation of the potential of zero charge of an electrode surface in electrolyte is closely linked to the variation of the work function W in vacuum. In order to get further insight, we focus on simple s-p-bonded metals as they connect most readily to theory. We present density functional theory calculations of W for aluminum surfaces for varying tangential strain e which allow the determinination of $\delta W/\delta e$ from first-principles. Interestingly, the response parameter is found to be positive in contrast to the negative values reported for e.g. Au experimentally and theoretically. We decompose the work function into a volume and a surface contribution and discuss the response of these contributions in the framework of the Jellium model.

O 43.10 Wed 12:45 MA 043

Dichroism in double photoemission from a Cu surface — Zheng Wei[1], •Frank O. Schumann[1], Gianluca Difilippo[2], Giovanni Stefani[2], and Jürgen Kirschner[1] — [1]Max-Planck-Institut für Mikrostrukturphysik, 06120 Halle, Germany — [2]Dipartimento di Fisica, Università Roma Tre, Rome, Italy

We performed a double photoemission (DPE) experiment with circular polarized light on a Cu(001) surface. The photon energy was chosen to be 125 eV leading to comparable kinetic energies of the 3p photo electron and related Auger electron. We find that the coincidence spectra display circular dichroism while the singles spectra are helicity independent. Usually the emergence of an Auger electron is explained via a two-step process in which the relaxation leading to the Auger emission is preceded by the emission of a photoelectron. This is at odds with a continuous energy sharing [1] and the observation of dichroism in the coincidence spectra only. Our observation can only be explained within a single-step process.

[1] G. van Riessen, Z. Wei, R. S. Dhaka, C. Winkler, F. O. Schumann and J. Kirschner, J. Phys.:Condens. Matter **22**, 092201 (2010).

O 44: Focussed session: Functional molecules at surfaces II

Time: Wednesday 10:30–13:30 Location: A 053

Topical Talk O 44.1 Wed 10:30 A 053

Scanning Tunneling Spectroscopy and Atomic Force Microscopy of Functional Molecules on Thin Insulating Films — •Jascha Repp — Institute of Experimental and Applied Physics, University of Regensburg, 93053 Regensburg, Germany

Ultrathin insulating films on metal substrates facilitate the use of the scanning tunneling microscope (STM) to study the electronic properties of single atoms and molecules, which are electronically decoupled from the metallic substrate. The ionic relaxations in a polar insulator lead to a charge bistability of some adsorbed atoms and molecules. It is shown that control over the charge-state of individual molecules in such systems can be obtained by choosing a substrate system with an appropriate work function. The distribution of the additional charge is studied using difference images. These images show marked intra-molecular contrast. In addition, we investigated $C_{20}S_2H_{12}$ molecules adsorbed on ultrathin layers of NaCl using a combined low-temperature scanning tunneling and atomic force microscope. These non-planar molecules exist in two stable conformations. By means of excitations from inelastic tunneling electrons we can switch between both conformations. We present atomic force microscopy (AFM) measurements with submolecular resolution directly revealing the conformational changes. From AFM data and taking the chirality of the molecules into account, we could unambiguously determine the pathway of the conformational change. Hence, the AFM channel reveals additional information that is truly complementary to the STM data set.

Topical Talk O 44.2 Wed 11:00 A 053

Conductance switching and quantum interference in molecular junctions — •Sense Jan van der Molen — Kamerlingh Onnes Laboratorium, Leiden University, Leiden, The Netherlands

A fascinating prospect in nanoscience is to externally manipulate the conductance of molecular junctions. For this, an impressive set of (switchable) molecules has been synthesized in organic chemistry. However, once contacted, switchable molecules may easily lose their functionality, e.g. due to quenching of molecular excitations. Surprisingly, the opposite is possible too: junctions containing passive molecules may become switchable. I will give examples from our research, with a special focus on (arrays) of molecular junctions containing light-sensitive diarylethene molecules. The conductance properties of these devices can be switched reversibly by illumination, although the on/off ratio is limited. Next, I will deviate a bit from molecular switching and focus on the quantum aspects of charge transport through organic molecules. In some cross-conjugated molecules, destructive interference of electron waves can take place, leading to a dramatically low conductance. I will present experimental evidence for destructive quantum interference in (anthraquinone-based) molecular junctions. Remarkably, the large energy level spacing allows this interference phenomenon to be observed at room temperature, unlike the traditional case of Aharanov-Bohm rings. By turning quantum interference on and off, switchable molecular junctions with very high on/off ratios are anticipated shortly.

O 44.3 Wed 11:30 A 053

Direct observation of molecular switching at and close to room temperature by scanning tunneling microscopy — •Stefanie Ditze, Florian Buchner, Michael Stark, 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

An ultimate goal of nanotechnology is the usage of individual molecules as functional entities. One important example is the application of switchable molecular building blocks in information storage. Herein, we report the observation of a supramolecular ordered phase of 2H-5,10,15,20-Tetrakis(3,5-di-tert-butyl)-phenylporphyrin (2HTTBPP) on Cu(111) by scanning tunneling microscopy (STM) in ultrahigh vacuum around room temperature (RT). In this phase, the 2HTTBPP molecules are arranged in alternating rows with intrinsically different intramolecular conformations, i.e. a concave and a convex appearance in STM. Interestingly, it was found that individual 2HTTBPP molecules spontaneously switch between these two conformations at RT. Detailed analysis of the temperature dependence of the switching behavior allows to extract the activation energies and the prefactors for the molecular switching process. In addition, we demonstrate tip-induced switching of individual molecules at 200 K.

This work has been funded by the Deutsche Forschungsgemeinschaft (DFG) through Sonderforschungsbereich 583.

O 44.4 Wed 11:45 A 053

Thermally induced switching of azobenzene at coinage metal surfaces? A DFT perspective — •Reinhard J. Maurer and Karsten Reuter — TU München

Stimulating a controlled isomerization of functional molecules stabilized at a solid surface is a central step en route to a future molecular nanotechnology. Central questions particularly at metal substrates concern the detailed excitation mechanism and in how much established gas-phase isomerization pathways are modified by the presence of the surface. Building the basis for a detailed understanding of photoinduced isomerization we use dispersion-corrected density-functional theory to investigate the thermal switching of the prototypical molecular switch azobenzene at Au(111). For this we compute energy profiles for isomerization mechanisms predominantly discussed in gas-phase and analyze the electronic structure along the way. We find that the interaction with the surface selectively favors the rotational against the inversion pathway, and thereby reverses the ordering established in gas-phase or solution. Extending our calculations to Ag(111) surfaces as well as to tetra-tert-butyl-azobenzene (TBA) we specifically target the role of the substrate d-band and the influence of functional groups.

O 44.5 Wed 12:00 A 053

Photoswitching of Molecular Platform Adlayers — •Ulrich Jung[1], Sonja Kuhn[1], Mathias Müller[1], Sandra Ulrich[2], Jens Kubitschke[2], Rainer Herges[2] und Olaf Magnussen[1] — [1]Institut für Experimentelle und Angewandte Physik, Christian-Albrechts-Universität zu Kiel, Leibnizstr. 19, 24118 Kiel, Germany — [2]Otto-Diels-Institut für Organische Chemie, Christian-Albrechts-Universität zu Kiel, Otto-Hahn-Platz 4, 24098 Kiel, Germany

We have recently introduced a novel approach for preparation of adlayers with freestanding functional groups on metal surfaces based on customizable molecular platforms and characterized the structure of these adlayers by scanning tunneling microscopy [1,2,3] and various spectroscopies [4]. The adlayers were found to exhibit a high degree of order with the functionalities oriented in a defined way with respect to the surface and precisely controlable vertical and lateral distances.

Here, we will focus on photoswitching properties of platform adlayers exhibiting azobenzene functionalities. Generally, photoswitching is preserved upon formation of such adlayers, the according reactions follow first-order kinetics with high quantum efficiencies of $\approx 10^{-4}$. In addition, thermal backswitching is found to proceed several orders of magnitude faster in the adlayers than in solution, which can be attributed to pronounced electronic coupling of the azobenzene functionalities with the metal substrate.

[1] Baisch et al., J. Am. Chem. Soc. (2009), 131, 442, [2] Kuhn et al. PCCP (2010), 12, 4481, [3] Kuhn et al, Chem. Commun. (2011), 47, 8880, [4] Jung et al., Langmuir (2011), 27, 5899

O 44.6 Wed 12:15 A 053

Manipulation and spectroscopy of individual phthalocyanine molecules on InAs(111)A with a low-temperature scanning tunneling microscope — •Christophe Nacci[1], Kiyoshi Kanisawa[2], and Stefan Fölsch[1] — [1]Paul Drude Institute for Solid State Electronics, Berlin (Germany) — [2]NTT Basic Research Laboratories, NTT Corporation, Atsugi (Japan)

Phthalocyanine (Pc) is a promising class of organic molecules to develop functionality concepts based on hybrid organic-semiconductor systems. We report a low-temperature scanning tunneling microscopy (STM) study of single naphthalocyanine (NPc) and tin phthalocyanine (SnPc) molecules adsorbed on the InAs(111)A surface. InAs(111)A is In-terminated and characterized by completely saturated dangling bonds due to its (2x2) In-vacancy reconstruction. We found that NPc is in a physisorbed state, preserving the electronic molecular structure to a large extent. This indicates that the molecule is only weakly coupled to the InAs(111)A template. The non-planar SnPc adsorbs in two different configurations with the central Sn atom either above or below the molecular plane (SnPc_{up} and SnPc_{down}). We achieved the reversible switching between the two conformers by means of STM tip-induced excitation. It is revealed that SnPc_{up} is characterized by a weaker surface bonding compared to SnPc_{down}. This enables to reposition SnPc_{up} by STM-based lateral manipulation, whereas this is not possible for SnPc_{down}. The reversible switching can thus be utilized to either move the molecule or to pin it down to the surface. We acknowledge support by the Deutsche Forschungsgemeinschaft (SFB658).

O 44.7 Wed 12:30 A 053

First-principles study of redox-molecular switch above a polar thinfilm: a van der Waals + U description — •John Sharp, Felix Hanke, and Mats Persson — University of Liverpool, Liverpool, UK

A redox-type molecular switch functions by coupling the charging and discharging of a molecule to an obvious change in conformation. Such a switch was recently demonstrated experimentally, by investigating the molecule bis-dibenzoylmethanato-copper(II) ($\mathrm{Cu(dbm)_2}$) adsorbed on an ultra-thin insulating layer above a Cu substrate[1]. Here we aim to understand the molecular adsorption and switching properties using a first principles density functional approach to investigate the electronic structure of the complex. This investigation is challenging due to the van der Waals dominated adsorption and the presence of highly-correlated *d*-electrons in $\mathrm{Cu(dbm)_2}$. Here we use a van der Waals density functional [2] and a 'GGA+U' term to properly address these issues. Crystal field splitting of the *d*-orbitals underlies the conformational change that occurs upon charging, and the magnitude of the splitting is affected by the value of 'U' used. The experimentally observed changes in conformation upon charging the adsorbate are only reproduced with a self-consistently determined value of U. Moreover without inclusion of the U term a spontaneous charging of the adsorbate is observed even for the experimentally neutral configuration. Finally, we present scanning tunnelling microscopy simulations and compare the results with the experimentally available data.

[1] PRL **106** 216103 (2011); [2] PRB **83** 195131 (2011)

O 44.8 Wed 12:45 A 053

Quantum chemical calculations and open-system density matrix simulations for arrays of molecular switches on surfaces — Gereon Floss, Manuel Utecht, •Tillmann Klamroth, and Peter Saalfrank — Theoretische Chemie, Universität Potsdam, Germany

In this work different models are investigated to describe the absorption spectra and excitonic coupling in self-assembled monolayers of azobenzenes, on the (TD-) B3LYP/6-31G* level of theory [1]. The calculated blue shifts in optical absorption spectra account for the experimental observations made for azobenzene/gold SAMs, and hint to the fact that they can indeed be responsible for reduced switching probability in densely packed self-assembled structures [2].

Furthermore, using a quite general open-system density matrix model, we demonstrate that nevertheless controlled and complete switching should be possible in arrays of molecular switches on surfaces by analytical and optimal control pulses and the concept of "laser distillation" [3]. The parameters for this dynamics model are chosen to roughly resemble the all-trans → all-cis isomerization of an array of azobenzene molecules on a surface.

[1] M. Utecht, T. Klamroth, P. Saalfrank, Phys. Chem. Chem. Phys. **13**, 21608 (2011).
[2] C. Gahl, R. Schmidt, D. Brete, E. McNellis, W. Freyer, R. Carley, K. Reuter, M. Weinelt, J. Am. Chem. Soc., **132**, 1831 (2010).
[3] G. Floß, T. Klamroth, P. Saalfrank, Phys. Rev. B **83**, 104301 (2011).

O 44.9 Wed 13:00 A 053

Role of the electronic structure of adsorbate/substrate complexes on the photoisomerization ability — •Michael Schulze, Christopher Bronner, Sebastian Hagen, and Petra Tegeder — Freie Universität Berlin, Fachbereich Physik, Arnimallee 14, 14195 Berlin

We use two-photon photoemission to study two molecular photoswitches at the Au(111) surface, namely azobenzene and its derivative tetra-tert-butyl- azobenzene (TBA). Electronic states at the substrate-adsorbate interface are found to be a sensitive probe for the isomerization state of TBA while azobenzene loses its switching ability at the surface. We partly attribute the latter to a shift of the highest occupied molecular orbital (HOMO) with respect to the gold d-bands which quenches the hole transfer involved in the switching mechanism of TBA.

O 44.10 Wed 13:15 A 053

Adsorption height of benzene and azobenzene on Ag(111) and Cu(111) — •Martin Willenbockel[1], Giuseppe Mercurio[1], Erik R. McNellis[2], Christopher Bronner[3], Benjamin Stadtmüller[1], Stephan Meyer[3], Erwan Varene[3], Michael Schulze[3], Isabel Martin[3], Sebastian Hagen[3], Felix Leyssner[3], Jörg Meyer[2], Serguei Soubatch[1], Martin Wolf[2,3], Karsten Reuter[4], Petra Tegeder[3], and F. Stefan Tautz[1] — [1]Peter Grünberg Institut 3, Forschungszentrum Jülich and JARA, Jülich, Germany — [2]Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, Germany — [3]Fachbereich Physik, Freie Universität Berlin, Berlin, Germany — [4]Technische Universität München, Garching, Germany

Research focused on the interactions at organic/metal interfaces revealed that weak long-range van-der-Waals (vdW) forces play a significant role in the bonding mechanism. However, a clear experimental gauge is needed to judge to which extent the vdW interactions influence the adsorption strength. For molecules at surfaces the height of adsorption is known to satisfy this need.

Here we report the normal-incidence x-ray standing waves data on the adsorption height of the classical aromatic molecule benzene on Ag(111) and Cu(111) surfaces. In these systems the contribution of vdW interactions to the bonding is meant to be dominant. To identify the effect of additional chemical interaction channels, we furthermore studied the adsorption of azobenzene, a molecule containing two benzene rings linked by a diazo-bridge. Achieved experimental results are compared to density functional theory calculations.

O 45: Solid / liquid interfaces I

Time: Wednesday 10:30–12:30 Location: A 060

O 45.1 Wed 10:30 A 060

Structure of water layers on hydrogen-covered Pt electrodes — •Tanglaw Roman and Axel Gross — Institut für Theoretische Chemie, Universität Ulm, D-89069 Ulm

Recently, we have seen a growing number of theoretical studies addressing structures and processes at electrochemical solid/liquid interfaces from first principles. Still it is fair to say that up to now little attention has been paid to the fact that as a function of the electrochemical conditions (electrode potential, pH, electrolyte) in equilibrium electrochemical electrodes are typically covered by adsorbed species such as hydrogen. It is very likely that the presence of these adsorbed species has a severe influence on the structure of the electrochemical electrode-electrolyte interfaces and on the processes occurring at these interfaces. In this light, we have examined the structure of water layers at hydrogen-covered Pt(111) surfaces at room temperature by ab initio molecular dynamics simulations based on periodic density functional theory calculations. The resulting structures have been analyzed in detail as a function of hydrogen coverage. In particular, the thermal disorder in the water layer is examined in terms of deviations from the ice lattice, orientational inhomogeneity within the bilayers, as well as the onset of water dissociation.

O 45.2 Wed 10:45 A 060

Ab-initio derived force-field parameters for molecular dynamics simulations of deprotonated amorphous-SiO_2/water interfaces — •Anke Butenuth[1], Gianpietro Moras[1], and Lucio Colombi Ciacchi[2,3] — [1]Fraunhofer Institute for Mechanics of Materials IWM, Freiburg — [2]Hybrid Materials Interfaces Group, BCCMS, Bremen — [3]Fraunhofer Institute for Manufacturing Technology and Advanced Materials IFAM, Bremen

Due to its importance for many technologically relevant materials, a large research effort has been devoted to the SiO_2/water interface, where work on the theoretical side is based on both quantum-mechanical and classical atomistic methods. However, most of theses studies consider neutral silica surfaces and are, due to the low isoelectric point of silica, only valid under strong acidic conditions.

We present a force field for molecular dynamics simulations of interfaces between natively deprotonated amorphous SiO_2 surfaces and liquid water, to be used in combination with standard biomolecular force fields. The extent of negative charge delocalisation in the solid that follows the deprotonation of terminal silanol groups is revealed by extensive Bader analysis of electronic densities computed by Density Functional Theory (DFT). The absolute charge values in our force field are determined from best-fitting to the electrostatic potential computed ab-initio (ESP charges).

Our proposed parameter set is found to reproduce the energy landscape of single water molecules over neutral and deprotonated amorphous SiO_2 surfaces.

O 45.3 Wed 11:00 A 060

Atomistic simulations of the ZnO(1-210)/water interface: A comparison between first-principles, tight-binding and empirical methods — •Svea Sauer[1], Susan Köppen[2], Thomas Frauenheim[1], and Lucio Colombi Ciacchi[2] — [1]University of Bremen, Faculty of Physics, Computational Material Science and BCCMS — [2]University if Bremen, Faculty of Production Engineering, Hybrid Materials Interfaces and BCCMS

Owing to the prevalent role of zinc oxide in processing reactions involving water, the zinc oxide water interface is an ongoing field of research. Our study focuses on the (1-210) surface of zinc oxide. Thereby the adsorption starting from a single water molecule up to a full monolayer is investigated. Calculations are performed using ab initio DFT, the DFTB+ code and a reactive forcefield. A comparison of the results obtained by these three methods yields differences especially regarding the number of dissociated water. To study how the monolayer configurations change under the influence of bulk water and how well this is described by the three methods, the vacuum region of the systems is filled up with water. Three different initial monolayer configurations were taken into account: One fully dissociated, one half dissociated and one with a monolayer of molecular adsorbed water. Different trends, already observed for the monolayer could be observed for DFT, DFTB and the reactive forcefield regarding the fraction of dissolved water.

O 45.4 Wed 11:15 A 060

First-principles study of the water structure on flat and stepped gold surfaces — •Xiaohang Lin and Axel Gross — Institute of Theoretical Chemistry, Ulm University, D-89069 Ulm/Germany

The geometric structure and electronic properties of a water layer on flat and stepped gold surfaces have been addressed by periodic density functional theory (DFT) calculations. This work was motivated by a recent electron energy loss spectroscopy study [H. Ibach, Surf. Sci. 604 (2010) 377] indicating that the structure of a water layer on stepped Au(511) differs significantly from the one on Au(100). Based on ab initio molecular dynamics simulations, the measured spectra of H_2O/Au(511) have been reproduced and linked to the geometric arrangement of the water molecules. Furthermore, the electronic structure has been analyzed yielding a strong polarization of the water layers.

O 45.5 Wed 11:30 A 060

On the accuracy of ion hydration energies - an ab-initio study — •Mira Todorova and Jörg Neugebauer — Department for Computational Materials Design, Max-Planck-Institut für Eisenforschung GmbH, Düsseldorf, Germany

An accurate prediction of hydration free energies of ions and molecules is crucial for modelling chemical, electrochemical and biochemical reactions in water and at water/material interfaces. Experimental measurements are performed on neutral solutions and the extraction of individual ion solvation free energies relies on assumptions, such as the tetraphenylarsonium tetraphenylborate (TATB) extrathermodynamic assumption [1]. This severely hinders the assessment of theoretical approaches to compute such data.

Extending an approach originally derived to describe charged defects and their concentration in semiconductors [2], revealed that the TATB extrathermodynamic assumption employed to obtain experimental free energies is incorrect, and provided criteria to judge the accuracy of calculated ion-hydration energies. Focusing on the hydration energy of H^+(aq) and OH^-(aq) individual free energy contributions to calculated ion hydration energies will be discussed.

[1] Y. Marcus, J. Chem. Soc., Faraday Trans. 1, **83**, 339 (1987).

[2] C.G. Van de Walle and J. Neugebauer, J. Appl. Phys. **95**, 3851 (2004).

O 45.6 Wed 11:45 A 060

Self-assembly of solvent molecules adsorbed on HOPG (0001) controlled by sonication time of the liquid — •Nguyen Thi Ngoc Ha[1], Thiruvancheril G. Gopakumar[2], and Michael Hietschold[1] — [1]Institute of Physics, Solid Surfaces Analysis Group, Chemnitz University of Technology, D-09107 Chemnitz, Germany. — [2]Institut für Experimentelle und Angewandte Physik der Universität Kiel, Olshausenstr.40, D-24098 Kiel, Germany

Self-assembly at the liquid-solid interface depends on several experimental parameters such as temperature, chemical nature of the solvent, functional groups of the solute molecule, etc. which can influence on the interactions between adsorbate, substrate and solvent. The molecular concentration in a solvent has been shown to be a useful control parameter for self-asssembled molecular pattern formation out of these solutions on a crystalline substrate[1,2]. Sonication treatment of the solutions has been demonstrated to be an efficient method to change these concentrations. The adsorption of TMA-alcohol mixture on a HOPG substrate has been investigated which reveals an adsorption pattern consisting of alternating stripes made of of TMA and alcohol solvent molecules which changes in dependence on sonication time[3]. Sonication of the pure alcohol solvent without any other molecules solved within also changes the assembled pattern of the solvent molecules in dependenc of sonication time as we have observed.[1]N.T.N.Ha,etal.J.Phys.Chem.C, 2010,114,3531-3536.[2]N.T.N.Ha,etal.J.Phys.Chem.C,2011,115(44),21743-21749.[3]N.T.N.Ha,e
of TMA-alcohol controlled by concentration going to be submitted.

O 45.7 Wed 12:00 A 060

dI/dV imaging and spectroscopy of single molecules at solid-liquid interfaces — •Jose D. Cojal[1], Carlos A. Palma[2], Klaus Müllen[3], and Jürgen P. Rabe[1] — [1]Institute of Physics, Humboldt-Universität zu Berlin, Berlin — [2]Physik Department E20, Technische Universität München, Garching — [3]Max Planck Institute for Polymer Research, Mainz

Scanning tunneling spectroscopy (STS), i.e. superimposing a small high-frequency modulation voltage on the bias and recording the AC current component using a phase sensitive detector (PSD) to obtain the differential of the tunneling current, dI/dV, allows to measure the local density of states (LDOS) at surfaces. This has been widely used at low temperatures and under UHV conditions for metals, semiconductors, organic molecules, carbon nanotubes and graphene. In order to measure both topography and differential tunneling images at solid-liquid interfaces we have modified our home-built STM, and obtained dI/dV maps of single molecules of a monolayer of a hexa-peri-hexabenzocoronene (HBC) derivative, self-assembled at the interface between highly oriented pyrolytic graphite (HOPG) and a molecular solution. This allowed us to better localize HOMO and LUMO of the molecules than previously reported direct measurements of current voltage characteristics [1].

[1] K. Müllen, J. P. Rabe, Acc. Chem. Res. 41 (2008) 511

O 45.8 Wed 12:15 A 060

Adsorption of P123 at the solid-liquid Interface — •Stefan Gerth[1], Michael Klimczak[1], Andrew Nelson[2], Hans-Georg Steinrück[1], and Andreas Magerl[1] — [1]Chair of Crystallography and Structural Physics, Staudtstraße 3, Erlangen — [2]The Australian Nuclear Science and Technology Organization, Australia

Aqueous solutions of tri-block copolymers offer an excellent model system for the study of crystallization in soft matter. Further, these surfactants are well-known for the reduction of surface tension and to reduce friction at the interface. We investigate, as sample, the tri-block copolymer Pluronic P123 consisting of a central part of 70 propylene oxide (PO) units terminated by two end groups of 20 ethylene oxide (EO) units (EO_{20}–PO_{70}–EO_{20}).

Our interest is in the near surface crystallization of a diluted Pluronic P123 system, below the temperature and concentration for crystallization in the bulk. In particular we are interested in the effect of shear for these agglomerated polymers.

The recovery of an adsorbed micellar layer was observed in dependence of the previously applied shear rate and polymer concentration. It has to be stressed that in this concentration and temperature regime no bulk crystallization occurs as investigated in small angle X-ray scattering measurements and rheometry data. Therefore, the ordering is only induced from the interface.

O 46: [DS] Organic electronics and photovoltaics: electronic properties II (jointly with CPP, HL, O)

Time: Wednesday 11:30–13:00 Location: H 2032

O 46.1 Wed 11:30 H 2032

Point of inflection in IV curves due to degradation of cathode-organic interface — •Sidhant Bom, Nivedita Yumnam, and Veit Wagner — Jacobs University Bremen, School of Engineering and Science, Campus Ring 1, 28759 Bremen, Germany

The formation of point of inflection in IV curves is very well known in the field of organic photovoltaics. However, the opinion on this matter is diverse and conflicting. In an attempt to understand this phenomenon, we carried out series of experiments in which we were able to emulate the s-shape in the IV curve. In this study P3HT:PCBM bulk heterojunction solar cells were fabricated in between ITO/PEDOT:PSS and aluminum electrodes. Storing a completely fabricated cell in different environments resulted in a remarkable difference in the degradation of device parameters. Storing in vacuum completely stopped the degradation process while storing in an air tight container with nitrogen ambient showed extreme degradation within 24 hours with a severe s-shape in the IV curve. Interface modification at the cathode by inserting an additional thin C_{60} layer resulted in a similar s-shaped curve in contrast to the standard device. The data are explained by a model introducing a variable potential barrier at the aluminum cathode.

O 46.2 Wed 11:45 H 2032

Dye Sensitised Solar Cells with Carotenoid Molecules — •Gino Günzburger[1], Res Jöhr[1], Biljana Bozic Weber[2], Catherine Housecroft[2], Edwin Constable[2], Hubert Hug[3], Petra Buchwald Hunziker[3], Ernst Meyer[1], and Thilo Glatzel[1] — [1]University of Basel, Department of Physics, Switzerland — [2]University of Basel, Department of Chemistry, Switzerland — [3]DSM Nutritional Products Ltd., NRD CH, Kaiseraugst, Switzerland

We report the analysis of long time stable dye sensitized solar cells using organic carotenoid-based dyes (crocetin, torularhodin and bixin). The particular properties of natural dyes require sensitisation in anhydrous solvents as well as cell assembly under inert gas atmosphere.

Furthermore, the exposure to UV light, and the heat-transfer to the sensitised layers was minimized. However, a standard KI based electrolyte was still employed.

The cells were prepared and characterised by IV- and QE-measurements without any anti-reflective or light incoupling foils, or additional light-scattering titania layers. In contrast to the expectations the present cells yield relatively high efficiencies and stability (colour and efficiency was unchanged over a period of days or even weeks). The measured efficiencies under 100 mW/cm^2 AM1.5 simulated sun light at 25°C were 1.23%, 0.40% and 0.75% for the crocetin, torularhodin and bixin cells, respectively. Comparable literature values for crocetin dyes are 0.56% and thus lower by a factor of more than 2. [1].

[1]Yamakazi et al. Solar Energy 81 (2007)

O 46.3 Wed 12:00 H 2032

High Performance Organic Transistors and Circuits with Patterned Polypyrrole Electrodes — •Liqiang Li, Harald Fuchs, and Lifeng Chi — Physikalisches Institut, Universität Münster, Münster, Germany

Electronic circuits based on organic transistors have sparkled considerable research interests due to their unique applications. One of the key prerequisites to convert the high potential to real applications is the preparation and patterning of appropriate electrode materials. Until now, a variety of electrode materials have been utilized for organic devices, among which conducting polymer electrodes have been proposed to be a promising alternative to replace metal electrodes, as they are endowed with unique features which may embody some advantages of organic circuits. However, high performance and stable devices with pure polypyrrole electrodes, especially n-type transistors and complementary circuits, are not reported.

Here we demonstrate the high performance p-/n-type organic transistors and complementary inverter circuits by using patterned PPY as pure electrode. Remarkably, both transistors and inverters with PPY electrodes show good stability under continuous operation and long-term storage conditions. Furthermore, PPY electrodes also exhibit good applicability in solution-processed and flexible devices. All these results indicate the great potential of PPY electrodes in solution-processed, all-organic, flexible, transparent, and low-power electronics.

O 46.4 Wed 12:15 H 2032

Design rules for charge-transport efficient host materials for OLEDs — •Falk May[1], Björn Baumeier[1], Denis Andrienko[1], and Christian Lennartz[2] — [1]Max Planck Institute for Polymer Research, Mainz, Germany — [2]BASF SE, GVC/E - B009, Ludwigshafen, Germany

The use of blue phosphorescent emitters in organic light emitting diodes (OLEDs) imposes demanding requirements on a host material. Among these are large triplet energies, the alignment of levels with respect to the emitter, the ability to form and sustain amorphous order, material processability, and an adequate charge carrier mobility. A possible design strategy is to choose a pi-conjugated core with a high triplet level and to fulfill the other requirements by using suitable substituents. Bulky substituents, however, induce large spatial separations between conjugated cores, can substantially reduce intermolecular electronic couplings, and decrease the charge mobility of the host. In this work we analyze charge transport in amorphous bis(triphenylsilyl)dibenzofuran, a typical deep-blue OLED host material, and show that mesomeric effects delocalize the frontier orbitals over the substituents recovering strong electronic couplings without inducing significant variations of local dipole moments, which otherwise would lead to additional energetic disorder, site energy correlations, and undesirable current filaments. By linking electronic structure, molecular packing, and mobility we provide a pathway to the rational design of hosts with high charge mobilities.

O 46.5 Wed 12:30 H 2032

Octithiophene on Au(111): Coverage dependent adsorption geometry and exciton dynamics — •Lea Bogner[1], Erwan Varene[1], Yan Pennec[2], and Petra Tegeder[1] — [1]Freie Universität Berlin, Fachbereich Physik, Arnimallee 14, 14195 Berlin, Germany — [2]University of British Columbia, department of Chemistry and Physics, Vancouver, B.C. V6T 1Z4, Canada

Semiconducting organic molecules exhibit promising properties for applications in optoelectronic devices such as organic photovoltaic cells or organic light emitting diodes. In order to fully understand and improve the functionalities of organic semiconductors the investigation of adsorption properties, electronic structure and charge carrier dynamics at their interfaces with inorganic substrates plays a crucial role.

Octithiophene (8T) is the longest unsubstituted oligothiophene synthesized up to now and possesses the highest carrier mobility. Whereas several surface science studies on sexithiophene interfaces may be found in literature, little is known so far about 8T.

The adsorption geometry, electronic structure and exciton dynamics as function of 8T coverage have been investigated by means of scanning tunnelling microscopy (STM), high-resolution electron energy loss spectroscopy (HREELS) and time-resolved two-photon photoemission (2PPE). We found that 8T undergoes a change in the adsorption geometry from flat-lying in the sub-monolayer regime to a tilted configuration for the mono- and bilayer coverage. The photoemission intensities of the HOMO and HOMO-1 features as well as the exciton decay dynamics exhibit a strongly coverage dependent behavior.

O 46.6 Wed 12:45 H 2032

Local Investigations on Air-stable n-Channel Perylene Diimide Based OFETs on Surface Modified SiO_x Dielectric — •Franziska Lüttich[1], Daniel Lehmann[1], Harald Graaf[1,2], Christian von Borczyskowski[1], and Dietrich R. T. Zahn[1] — [1]Chemnitz University of Technology, Institute of Physics, Germany — [2]Now at University Kassel, Institute of Chemistry, Germany

Organic semiconducting materials are interesting for low-cost and flexible applications like organic light-emitting diodes, organic solar cells, and organic field-effect transistors (OFETs). Stability and low mobilities are the most limiting properties for these applications. Surface modifications changing the surface energy of the dielectric in OFETs influences the orientation of the organic molecules and therefore the mobilities. The surface energy can be determined by water contact angle measurements.

In order to investigate the influence of the surface energy we used OFET substrates from Fraunhofer IPMS and varied the water contact angle of the 100 nm thick dielectric of thermal silicon dioxide in the range from 20° to 55°. Thereafter the air-stable Polyera ActivInk$^{\text{TM}}$ N1200 (PDI8-CN_2) was deposited by spin coating. The topography was determined using an Atomic Force Microscope (AFM). The electrical characterization was performed by DC measurements and additionally locally resolved by Kelvin Probe Force Microscopy (KPFM) to obtain an insight in the local surface potential and the contact resistances. The determined electron mobility were found to change with varying water contact angle.

O 47: [DS] Micro- and nanopatterning (jointly with O)

Time: Wednesday 11:45–13:45 Location: H 0111

O 47.1 Wed 11:45 H 0111

Investigation of the Fe incorporation in ion-beam induced patterning on Si (100) — •behnam khanbabaee[1], andreas biermanns[1], marina cornejo[2], dietmar hirsch[2], frank frost[2], and ullrich pietsch[1] — [1]Universität Siegen, Festkörperphysik,Siegen, Germany — [2]Leibniz-Institut für Oberflächenmodifizierung e. V. (IOM), Leipzig, Germany

Ion beam erosion of semiconductor surfaces can modify the surface and depends on main sputtering parameters; different surface topographies such as ripple or dot like pattern are fabricated on the surface. Recent experiments have shown that the incorporation of foreign metallic atoms during the sputtering process plays a crucial role in pattern formation on surfaces. In the result of investigation we report on the depth profile of Fe atoms incorporated in sputtering process on Si (100) with low energy Kr ion beam. X-ray reflectivity (XRR) measurements determine the concentration profile of Fe atoms. X-ray absorption near edge spectroscopy (XANES) at the Fe K-edge (7112 eV) shows the formation of Fe rich silicide near surface region. X-ray photoelectron spectroscopy (XPS) shows a shift in the binding energy of Si2p levels at the surface compared top bulk confirming the formation of different phases of Fe-silicide on top and below the surface. The depth profiles obtained by XRR are compared to results obtained by complementary secondary-ion mass spectrometry (SIMS).

O 47.2 Wed 12:00 H 0111

Threshold sputter depth for nanopattern formation and "zero" sputter yield ion beam irradiation of amorphous carbon — •Omar Bobes, Kun Zhang, and Hans Hofsäss — II. Phys. Institut, Uni Göttingen, Friedrich-Hund-Platz 1, 37077 Göttingen, Germany

The question whether sputtering is actually needed for pattern formation by ion beam erosion is still under debate. Therefore, we investigate the minimal required sputter depth which corresponds to the transition from a flat surface to a nanostructured surface for ion energies up to 10 keV. Especially, we chose ion beam irradiation under conditions where the sputter yield approaches zero. This can be achieved by using a light substrate materials such as carbon and heavy ions with energies not exceeding 100 eV, e.g., for 100 eV Xe^+-ions at 60° angle of incidence the sputter yield is to 0.002. In order to distinguish between sputter effect and the effect of displacement of recoil atoms for the pattern formation, low energy He^+-ion irradiation has been used and compared with Xe^+-ion irradiation. He^+-ions are unique, because they provide a small and almost constant sputter yield in the energy region between 500 eV and 1200 eV for amorphous carbon, but the displacement yield changes by a factor of two. One can choose the energies of Xe^+- and He^+-ions in such a way, either resulting in similar sputter yields or in similar displacement yield. The first results of such experiments will be presented.

O 47.3 Wed 12:15 H 0111

Is silicide formation the decisive factor in impurity induced ion beam pattern formation? — Sven Müller[1], •Martin Engler[1], Frank Frost[2], and Thomas Michely[1] — [1]II. Physikalisches Institut, Universität zu Köln, Cologne, Germany — [2]Leibniz-Institut für Oberflächenmodifizierung e.V., Leipzig, Germany

Metal co-deposition during ion beam erosion of Si induces nanoscale patterns. Here we present the results of a comparative study of Pd and Ag co-deposition during 2 keV Kr^+ ion irradition of Si(001) at normal incidence. Co-deposition was conducted by e-beam evaporation and by sputter deposition from an adjacent target, which was hit by the eroding ion beam simultaneously with the Si surface.

The collision kinetics of Ag and Pd are almost identical due to their similar atomic masses (Ag: 107.9 amu, Pd: 106.4 amu) and nuclear charges (Ag: Z = 47, Pd: Z = 46). There should be differences in pattern formation If chemistry is of relevance it, since Ag is almost insoluble in Si and forms no silicides, while Pd forms a number of silicides with substantial enthalpy of formation.

We find that for Ag co-deposition no patterns are formed while a sequence of patterns forms for Pd co-deposition which depends strongly on the flux ratio of arriving Pd atoms to Kr^+ ions.

Most surprising, pattern formation with Pd not only ceases for low, but also for high flux ratios. We therefore speculate that under the conditions used, phase separation through spinodal decomposition triggers the formation of the most pronounced patterns.

O 47.4 Wed 12:30 H 0111

Innovative FIB specific Nanopatterning Strategies for Optimized Photonic Crystal Nanofabrication — •Frank Nouvertne and Achim Nadzeyka — Raith GmbH, Konrad Adenauer Allee 8, D-44263 Dortmund, Germany

The physical interactions underlying ion beam lithography (IBL) are quite complex as it brings in both sputtering and redeposition effects. Sputtering, the key mechanism for focused ion beam milling, is a complex process that depends on several factors, such as crystal orientation, surface topography, surface diffusion, ion implantation, and the stoichiometry of the solid. Redeposition is a less desirable mechanism that is ubiquitous in focused ion beam milling and has a similar complexity as sputtering. These additional physical complexities associated with the IBL technique call for more flexible beam deflection strategies than are typically available for EBL.

This talk will focus on the optimization of a photonic crystal fabricated by a FIB milling process, controlled by ELPHY MultiBeam, a new generation of nanofabrication pattern generators (PG). This newly developed PG allows for a huge variety of different directional and repetitive patterning strategies, which - in combination with a dedicated automatic drift compensation functionality - enables the required, most precise pattern placement accuracy and highest stability for this long term photonic crystal nanofabrication process over several hours.

O 47.5 Wed 12:45 H 0111

Photonic Crystal Gratings for High-Speed Energy-Efficient Laser Sources — •Philip Wolf[1], Werner Hofmann[1], Norbert Grote[2], and Dieter Bimberg[1] — [1]IFKP & Center of Nanophotonics, TU Berlin — [2]Heinrich Hertz Institute, Fraunhofer, Berlin

Recently, VCSELs with highest modulation speeds [1] and highest energy efficiencies have been demonstrated [2]. Furthermore, a novel nano-photonic element, the so-called sub-wavelength or high-contrast grating (HCG) has been successfully applied in various VCSEL structures [3-5]. This special photonic crystal can be understood as a multi-mode Fabry-Pérot interferometer being able to replace a thick distributed Bragg-mirror [3]. It has been demonstrated that a HCG can improve the modal behavior of this type of lasers [4]. We expect that this technology will enable us to demonstrate VCSEL of superior bandwidth and energy efficiency. The challenge is to implement this technology into cutting-edge high-speed device designs. Here, we like to show our new concept and present recent breakthroughs in fabrication of these photonic crystals using electron beam lithography and dry-etching with our ICP-reactor.

[1] Hofmann, W. et al.: ”44 Gb/s VCSEL for optical interconnects,” OFC 2011, PDPC5, 2011. [2] Moser, P. et al.: ”81 fJ/bit energy-to-data ratio of 850 nm VCSEL for optical interconnects,” APL, 98, 2011. [3] Chang-Hasnain, C.J. et al.: ”High-Contrast Grating VCSELs,” IEEE J. Sel. Top. Quantum Electron., 15, 2009. [4] Hofmann, W. et al.: ”Long-Wavelength High-Contrast Grating VCSEL,” IEEE Photon. J., 2, 2010. [5] Il-Sung Chung et al., IEEE PTL, 20, pp. 105, 2008.

O 47.6 Wed 13:00 H 0111

Nanopatterning by molecular polygons — •Stefan-Sven Jester, Eva Sigmund, Natalia Shabelina, Stephan M. Le Blanc, and Sigurd Höger — Rheinische Friedrich-Wilhelms-Universität Bonn, Kekulé-Institut für Organische Chemie und Biochemie, Gerhard-Domagk-Str. 1, 53121 Bonn, Germany

Self-assembly of rigid molecules at the solution/solid interface interface allows an efficient approach towards two-dimensional supramolecular crystalline surface patterns. In-situ 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 depends on the symmetry and dimensions of the molecular building blocks and their substituents. One approach to tailored adlayers is based on the adsorption of shape-persistent arylene-alkynylene macrocycles at the interface of 1,2,4-trichlorobenzene and HOPG. The molecules are accessible from organic synthesis and can be widely substituted with functional groups. Recent work has focused on macrocycles involving dithiophene corner building blocks connected via linear phenylene-ethynylene-butadiynylene units that can be viewed as molecular polygons of distinct symmetry (i.e. triangles, squares, pentagons, and hexagons), so that concepts of discrete geometry can be applied to design tailorable nanoscale surface patterns. The results gain insight into the 2D crystallization of nanoscale pentagons, binary mixtures of triangles and hexagons, and how large periodicities of several 10 nm may become accessible.

O 47.7 Wed 13:15 H 0111

Rapid Prototyping of Hierarchical Gecko-Mimicking Nano- and Microstructures using Multiphoton Absorption — •Michael Röhrig[1], Michael Thiel[2], Matthias Worgull[1], and Hendrik Hölscher[1] — [1]Karlsruhe Institute of Technology, P.O. Box 3640, 76021 Karlsruhe, Germany — [2]Nanoscribe GmbH, Hermann-von-Helmholtz-Platz 1, 76344 Eggenstein-Leopolds., Germany

Applying 3D direct laser writing, we designed hierarchical gecko-type structures which match the elastic modulus and the relevant length scale of the gecko’s setae very closely. These setae, delicate hairs covering the gecko’s toes, originate the famous ability of geckos to climb effortlessly walls and ceilings. The setae are consisting of beta-keratine, a stiff material with Young’s modulus of around 1 - 4 GPa. Due to their hierarchical design, they are very compliant and can achieve a very high real contact area even to rough substrates. Thus, the van der Waals forces cause high adhesion that enables geckos to stick to nearly every surface. Mimicking the gecko-effect is therefore pursued by groups all over the world. However, such structures are mostly based on soft materials that usually have some drawbacks, like degradation or rapid contamination. Hence, we used 3D direct laser writing to structure stiff materials. 3D direct laser writing is a rapid prototyping method based on multiphoton absorption that allows for the fabrication of arbitrary three-dimensional structures down to the nanometer scale. Measuring the adhesion by using atomic force microscopy, we could show that hierarchy is indeed favorable for artificial gecko-inspired structures made of stiff materials on the nanometer scale.

O 47.8 Wed 13:30 H 0111

Time and space resolved pump-probe investigations on induced ablation of thin films with femtosecond laser pulses — •Stephan Rapp, Matthias Domke, and Heinz P. Huber — Munich University of Applied Sciences

An about 500 nm thin molybdenum film acts as p-contact for CIGS thin film solar cells, which has to be separated to serially interconnect the sub cells of a solar panel. The Mo can be structured either by irradiating the Mo from the front side or from the glass substrate side, resulting in a selective removal or a lift-off of an intact Mo cap, respectively. To investigate the underlying physical effects, a pump-probe setup is used for time- and space resolved microscopy. Several series of pictures are taken with time delays between femto- and microseconds, showing the complete temporal evolution of laser ablation (lift-off). The front side irradiation with fluences up to 5.0 J/cm^2 leads to thermal effects after a few picoseconds and after 100 ps ring systems appear. This suggests a bulging of the material. After 3 ns a shock wave crosses the sample with velocities from 675 to 3950 m/s. The substrate side irradiation with fluences up to 1.0 J/cm^2 initiates a decrease of the sample reflectivity due to heating for delay times up to 10 ps. Ring systems are formed after 4 ns and a model was created to determine the bulging height by analyzing these Newton′s rings. After the bulging a lift-off of an intact Mo cap can be observed at times between 10 and 40 ns for fluences above the ablation threshold which was determined to 0,6 J/cm^2.

O 48: Invited talk (Ruslan Temirov)

Time: Wednesday 15:00–15:45 Location: HE 101

Invited Talk O 48.1 Wed 15:00 HE 101

Extending the scanning probe toolbox in a molecular playground — •Ruslan Temirov — Peter Grünberg Institute (PGI-3),Forschungszentrum Jülich, Germany — JARA-Fundamentals of Future Information Technology, Germany

Invented only a couple of decades ago, scanning tunnelling microscopy (STM) plays a prominent role in surface science today. One of the research fields in which the STM has spurred considerable progress is experiments with large organic molecules on surfaces. The complexity and versatility of the organic adsorption promises rich functionalities for future applications, but at the same time it generates tough challenges for the employed experimental techniques. In this talk, several examples will be considered which demonstrate the potential of the STM applied to the studies of molecular structures down to the level of a single molecule. Used in conjunction with complimentary surface science techniques and theory, the STM conveys a detailed bonding picture of a large multifunctional organic molecule on a metal surface. It will be shown how the methodology of the STM can be extended towards resolving chemically complex structures as well as transport studies on molecular wire junctions with controlled geometry.

O 49: Invited talk (Timo Jacob)

Time: Wednesday 15:45–16:30 Location: HE 101

Invited Talk O 49.1 Wed 15:45 HE 101

Analogies between surface science and electrochemistry — •Timo Jacob — Institut für Elektrochemie, Universität Ulm — Helmholtz-Institut Ulm

Batteries, fuel cells, photocells and many other applications are powered by fundamental electrochemistry. Compared to surface science under UHV conditions, electrochemical systems combine a whole variety of additional effects. These range from the presence of an electrolyte and a multi-component environment to reaction conditions such as finite temperature, pressure, and electrode potential. Due to this complexity our knowledge of the ongoing processes is mostly limited to the macroscopic regime. However, nowadays theoretical methods are able to provide deeper insight into structures and processes at the atomic level, which together with experiments could lead to a better understanding.

We compare the concepts of surface science and electrochemistry, addressing their similarities and differences. Using the oxygen reduction (ORR) on Pt as a model reaction, theoretical studies of the exact mechanism will be described, where, starting with the gas-phase system, effects from the reactive surrounding as well as environmental parameters are successively included. We find that the pure, perfect surface models, typically used to study this reaction, are insufficient.

Nanofaceting of Ir(210) provides another example of a phenomenon showing how analogies can be made between surface science and electrochemistry. Here pyramidal-like nanostructures that were first observed under UHV conditions were later produced electrochemically.

O 50: [MA] Joint Session "Surface Magnetism I" (jointly with O)

Time: Wednesday 16:00–19:00 Location: BH 243

O 50.1 Wed 16:00 BH 243

Observation and quantitative evaluation of superparamagnetic behavior utilizing magnetic exchange force microscopy and spectroscopy — •Schwarz Alexander, Schmidt Rene, and Wiesendanger Roland — Institute of Applied Physics, University of Hamburg, Jungiusstr. 11, 20355 Hamburg, Germany

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]. Here we show that the distance dependence of the magnetic exchange interaction can be utilized to modify the barrier height between two magnetization directions in a well-controlled manner. Contrast reversals observed with magnetically coated tips during imaging an antiferromagnetic surface show that tips can switch their magnetization direction by 180°. Since the magnetic exchange interaction is distance dependent, switching rate, lifetimes and the barrier height between the two states are distance dependent as well. Modeling the tip apex as superparamagnetic cluster with uniaxial anisotropy but otherwise independent of the rest of the tip, allows quantifying the energy barrier between both states as well as the zero field anisotropy. Moreover, the influence of a magnetic field via the additional Zeeman energy can be measured. Our study demonstrates the feasibility to observe dynamic magnetic processes utilizing magnetic exchange force microscopy and spectroscopy with atomic resolution.

[1] U. Kaiser et al., Nature 446, 522 (2007).

[2] R. Schmidt et al., Phys. Rev. Lett. 106, 257202 (2011).

O 50.2 Wed 16:15 BH 243

Possible detection of spin contrast on NiO(001) by AFM using a qPlus sensor with a bulk iron tip — •Florian Pielmeier and Franz J. Giessibl — Institute of Experimental and Applied Physics, University of Regensburg, 93040 Regensburg, Germany

Magnetic exchange force microscopy was first demonstrated with atomic resolution on the (001) surface of the antiferromagnetic insulator nickel oxide at low temperatures [1]. In order to detect spin contrast on NiO(001), the tips had to be magnetically polarized by an external field of 5 T [1-3].

Here, we observe spin contrast on NiO(001) at 4.3 K without an external field, using a bulk iron tip mounted on a qPlus sensor. However, magnetic contrast is only observed at a distance of about 10 pm further away than the distance where optimal chemical contrast is observed.

[1] U. Kaiser, A. Schwarz, R. Wiesendanger, Nature 446, 522 (2007)
[2] U. Kaiser, A. Schwarz, R. Wiesendanger, Phys. Rev. B 78, 104418 (2008)
[3] A. Schwarz, U. Kaiser, R. Wiesendanger, Nanotechnology 20, 264017 (2009)

O 50.3 Wed 16:30 BH 243

First-principles study of the magnetic exchange interaction across a vacuum gap — •Cesar Lazo and Stefan Heinze — Institute of Theoretical Physics and Astrophysics, University of Kiel, Germany

The miniaturization of spintronic devices towards the limit of single atoms calls for a quantification and understanding of the magnetic exchange interaction in atomic-scale junctions. Such a situation can be realized experimentally using a magnetic tip in an atomic force or scanning tunneling microscope. Here, we apply density functional theory to study the exchange interaction between tip and sample, i.e. across a vacuum gap. In particular, we choose the antiferromagnetic monolayer of Fe on W(001) as the sample system and consider different tips composed of Cr, Fe, and Cr/Fe alloys. We calculate the magnetic exchange energies and forces as a function of tip-sample distance. Our calculations are in good agreement with experiments [1]. We analyze the electronic structure of the tip and sample system and explain the origin and nature of the magnetic exchange interaction in this system [2].

[1] R. Schmidt, C. Lazo, U. Kaiser, A. Schwarz, S. Heinze, and R. Wiesendanger, Phys. Rev. Lett. **106**, 257202 (2011).

[2] C. Lazo and S. Heinze, Phys. Rev. B **84**, 144428 (2011).

O 50.4 Wed 16:45 BH 243

Micromagnetic simulations of the spin spiral state in bi-atomic Fe chains on Ir(001) — •Matthias Menzel[1], Yuriy Mokrousov[2], Robert Wieser[1], Jessica Bickel[1], Elena Vedmedenko[1], Stefan Blügel[2], Stefan Heinze[3], Kirsten von Bergmann[1], André Kubetzka[1], and Roland Wiesendanger[1] — [1]Institut für Angewandte Physik, Universität Hamburg — [2]Institut für Festkörperforschung, Forschungszentrum Jülich — [3]Institut für Theoretische Physik und Astrophysik, Universität Kiel

Recent spin-polarized scanning tunneling microscopy (SP-STM) measurements in combination with *ab initio* calculations reveal a 120° spin spiral ground state in bi-atomic Fe chains on (5×1)-Ir(001) [1]. Monte-Carlo simulations have shown that thermally induced switching of this magnetic state leads to a time-averaged signal in the SP-STM measurements.

We performed time-resolved and temperature dependent simulations using the Object Oriented MicroMagnetic Framework (OOMMF) [2] to investigate the thermal fluctuations and the stabilization mechanism. Due to their reduced coordination the chain's end atoms are more susceptible to an external magnetic field and the magnetocrystalline anisotropy and play a crucial role for the observability of the spin spiral. The three atom periodicity of the spin spiral leads to three symmetry classes for chains of different lengths, and we show how this affects the stability of the spin spiral.

[1] M. Menzel *et al.*, submitted.
[2] `http://math.nist.gov/oommf/`

15 min. break

O 50.5 Wed 17:15 BH 243

Dzyaloshinskii-Moriya driven spin spiral in Mn chains on Pt(664) — •Benedikt Schweflinghaus[1], Bernd Zimmermann[1], Marcus Heide[2], Gustav Bihlmayer[1], and Stefan Blügel[1] — [1]Peter Grünberg Institut (PGI-1) & Institute for Advanced Simulation (IAS-1), Forschungszentrum Jülich and JARA, 52425 Jülich, Germany — [2]Department of Precision Science and Technology, Osaka University, Suita, Osaka 565-0871, Japan

Ferromagnetic Co chains decorating the step edges of Pt(997) are historically the prime example of a one-dimensional metallic magnet [1]. We investigate this system in the light of the recently discovered Dzyaloshinskii-Moriya interaction (DMI) for ultrathin films [2], which can induce spiral magnetic structures of unique rotational sense. Besides Co, the research was extended to Fe and Mn chains.

In this contribution we investigate these structures applying density functional theory (DFT) by means of the full-potential linearized augmented plane-wave (FLAPW) method as implemented in the FLEUR code [3]. Using a micromagnetic model that includes the spin stiffness, magnetic anisotropy energy (MAE) and the DMI, we study possible magnetic phases such as homogeneous and inhomogeneous spin spirals. While the DMI induces for Mn chains a large-period spiral magnetic state superimposed on an antiferromagnetic order, the MAE prevents such a noncollinear structure for Co and Fe chains, respectively.

[1] P. Gambardella et al., Nature 416, 301 (2002)
[2] M. Bode et al., Nature 447, 190 (2007)
[3] http://www.flapw.de

O 50.6 Wed 17:30 BH 243

Competing interactions and chiral magnetism in Mn$_1$/X(111), X = Pd, Pt, Ag and Au — •Manuel dos Santos Dias[1,3], Julie Staunton[1], Andras Deak[2], and Laszlo Szunyogh[2] — [1]Department of Physics, University of Warwick, Coventry CV4 7AL, United Kingdom — [2]Department of Theoretical Physics, Budapest University of Technology and Economics, H-1111 Budapest, Hungary — [3]Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich, D-52425 Jülich, Germany

The magnetism of Mn monolayers on X(111), with X = Pd, Pt, Ag and Au, is analysed, using our Relativistic Disordered Local Moment Theory, based on DFT and the KKR Green function method [1]. The substrates control the antiferromagnetism, favouring either a collinear row–by–row state or a triangular Néel state. The latter is shown to possess a well–defined chirality pattern, originating from the Dzyaloshinksy–Moriya interactions. The anisotropic interactions are governed not only by the atomic number of the substrate but also by the extent of its hybridisation with the magnetic monolayer. Comparison with the experimental results for Mn$_1$/Ag(111) [2] is also given.

We acknowledge funding from Portugal (SFRH/BD/35738/2007) and Hungary (contract OTKA K77771 and project TAMOP-4.2.1/B-09/1/KMR-2010-0002).

[1] M. dos Santos Dias, J. B. Staunton, A. Deak and L. Szunyogh, Phys. Rev. B **83**, 054435 (2011)
[2] C. L. Gao, W. Wulfhekel and J. Kirschner, Phys. Rev. Lett. **101**, 267205 (2008)

O 50.7 Wed 17:45 BH 243

Tunneling anisotropic magnetoresistance on the atomic scale — •Kirsten von Bergmann[1], Matthias Menzel[1], David Serrate[1], Yasuo Yoshida[1], André Kubetzka[1], Roland Wiesendanger[1], and Stefan Heinze[2] — [1]Institute of Applied Physics, University of Hamburg, Germany — [2]Institute of Theoretical Physics and Astrophysics, University of Kiel, Germany

In non-collinear magnetic structures such as spin spirals, which have recently been found to occur at surfaces due to the Dzyaloshinskii-Moriya interaction [1,2], the spin quantization axis changes from atom to atom. In such a magnetic state the electronic structure of adjacent atoms is not equivalent due to spin-orbit coupling. We demonstrate that this effect leads to a tunneling anisotropic magnetoresistance on the atomic scale which can be detected using scanning tunneling microscopy (STM). This allows to image non-collinear magnetic structures at surfaces by STM with non-magnetic tips. We apply a simple model to relate the changes of the local density of states at the atoms with the tunnel current [3]. Thereby, we can explain the experimentally observed STM and spin-polarized STM images for spin-spirals observed for Mn/W [1,2] and for the atomic-scale magnetic skyrmion lattice found for Fe/Ir(111) [4].

[1] M. Bode et al., Nature 447, 190 (2007).
[2] P. Ferriani et al., Phys. Rev. Lett. 101, 27201 (2008).
[3] S. Heinze, Appl. Phys. A 85, 407 (2006).
[4] S. Heinze et al., Nature Phys. 7, 713 (2011).

O 50.8 Wed 18:00 BH 243

The spin structure of Mn on Co/Cu(001) studied by spin-polarized STM with bulk Cr tips and bulk Fe ring probes — •Chii-Bin Wu, Jiaming Song, and Wolfgang Kuch — Arnimallee 14, 14195 Berlin

Spin-polarized scanning tunneling microscopy with bulk Cr tips and bulk Fe ring probes was used to study the antiferromagnetic (AFM) domains of Mn on Co/Cu(001) at room temperature. Layerwise spin contrast was observed, as well as spin frustration along the overgrown steps of the underlying Co film. Besides, comparison of shape and size of additional small scattered areas with opposite spin contrast on flat terraces to islands at the surface of the Co layer indicates the importance of interface roughness on the spin structure of AFM layers in exchange bias systems.

O 50.9 Wed 18:15 BH 243

Exchange interactions in Fe clusters on Rh(111) and Ru(0001) from first principles — •Fabian Otte, Paolo Ferriani, and Stefan Heinze — Institute of Theoretical Physics and Astrophysics, University of Kiel, Leibnizstr. 15, 24098 Kiel, Germany

In the last few years it has been found that a non magnetic substrate can dramatically affect the magnetic properties of an adsorbed magnetic monolayer. For example, the nearest neighbor exchange of a Fe monolayer, which is the prototypical ferromagnetic material, becomes antiferromagnetic on W(001) [1] and Ru(0001) [2], while complex noncollinear magnetic order has been observed on Fe/Ir(111) [3].

Motivated by XMCD experiments [4] that found a surprisingly small dichroism in Fe clusters on Rh(111) and Ru(0001), we studied the magnetic properties of these systems by means of density functional theory calculations, using the projector augmented planewave method as implemented in the VASP-code. We considered collinear magnetic states and cluster sizes up to five atoms with different geometries and mapped total energy calculations onto an effective Heisenberg model. We found a complex trend of the magnetic exchange interaction which alternate between ferro- and antiferromagnetic depending on cluster size, geometry and interatomic distance.

[1] P. Ferriani *et al.*, Phys. Rev. Lett. **94**, 087204 (2005). [2] B. Hardrat *et al.*, Phys. Rev. B, **79**, 094411 (2009). [3] S. Heinze *et al.*, Nature Physics **7**, 524-526 (2011). [4] V. Sessi, S. Krotzky, M. Wasnioska, C. Tieg, J. Honolka and K. Kern, private communication

O 50.10 Wed 18:30 BH 243

SP-STM study of individual Co atoms on Pd/Co/Ir(111) — •Liudmila Dzemiantsova, André Kubetzka, Kirsten von Bergmann, and Roland Wiesendanger — Institut für Angewandte Physik, Universität Hamburg, Germany

Magnetic atoms adsorbed on nonmagnetic surfaces have become an active research topic in the last few years due to their importance in the fundamental understanding of magnetism and practical applications for spin-based computing schemes. In particular, the knowledge about the magnetic interactions on the atomic scale is crucial for the tailoring of magnetic devices in reduced dimensions and the tuning of their properties [1].

In this study we designed a system consisting of two atomic-scale magnets decoupled by a metallic layer. Magnetic monolayer Co islands on Ir(111) covered with a single atomic Pd layer were used as a substrate and a decoupling spacer, respectively. Individual Co atoms were deposited on the Pd surface and studied by spin-polarized STM (SP-STM). We observe that Pd grows in two stackings on Co/Ir(111) and gets spin-polarized by the underlying magnetic Co layer. We show that the spin polarization of the Co adatoms at the Fermi level is reversed with respect to Pd. This suggests that the spin moments of Co adatom and Co film are antiferromagnetically coupled [2] or the inversion is unique for single adsorbates on atomically flat surfaces [3].

[1] A. A. Khajetoorians et al., Science, 332, 1062 (2011).
[2] Y. Yayon et al., Phys. Rev. Lett., 99, 067202 (2007).
[3] L. Zhou et al., Phys. Rev. B, 82, 012409 (2010).

O 50.11 Wed 18:45 BH 243

How the local environment affects the magnetic anisotropy and Kondo Screening of a high-spin atom — •Jenny C. Oberg[1,2], Reyes M. Calvo[1], and Cyrus F. Hirjibehedin[1,2,3] — [1]London Centre for Nanotechnology, UCL, UK — [2]Department of Physics and Astronomy, UCL, UK — [3]Department of Chemistry, UCL, UK

We study the magnetic anisotropy and the Kondo screening of the spin of Co atoms on Cu2N using STM-based tunneling spectroscopy. We find that variations of the surface close to the edges of both small (ca 25nm^2) and large (ca 400 nm^2) Cu$_2$N islands result in changes in both anisotropy and Kondo screening. For small Cu$_2$N islands, we find that when the Co atoms are placed very close to the edges the Kondo screening weakens while the anisotropy increases in magnitude and changes its symmetry. Surprisingly, on larger Cu$_2$N islands formed on supersaturated Cu$_2$N surfaces, we find that a similar behavior occurs as the Co atoms move away from the edge of the islands: at the center of these large islands, Kondo screening is completely suppressed while the anisotropy energy is twice as large as at the edge of the islands. We examine possible causes for these dramatic changes in the Kondo screening and magnetic anisotropy, including a possible interaction with a quantum-confined surface state below the Cu$_2$N.

O 51: Oxides and insulators: Epitaxy and growth

Time: Wednesday 16:45–19:15 Location: HE 101

O 51.1 Wed 16:45 HE 101

The wurtzite termination of epitaxial CoO(111) films - implications for electronic structure and growth — •Lutz Hammer[1], Pascal Ferstl[1], Matthias Gubo[1], Markus Ostler[2], Thomas Seyller[2], M. Alexander Schneider[1], and Klaus Heinz[1] — [1]Ls. f. Festkörperphysik, Univ. Erlangen-Nürnberg — [2]Ls. f. Techn. Physik, Univ. Erlangen-Nürnberg

Cobalt monoxide films are found to grow on Ir(100) in the polar [111] direction, whereby the outermost subsurface Co layer exhibits a stacking fault altering the local structure from rocksalt- to wurtzite-type [1]. This structural switch renders the surface metallic which is proved both by photoelectron and scanning tunneling spectroscopy (as well as indicated by DFT calculations from the literature [2]). The metallic surface layer allows for the compensation of the film's dipole moment. In contrast, non-polar CoO(100) films, which can be grown on the same substrate via chemical modification of the interface, remain insulating also at the very surface. The latter films are bulk-like terminated and thus can be grown layer by layer, while this is prohibited by the structural switch in case of the (111) oriented films, which can only be produced via re-crystallisation of initially amorphous films.

[1] W. Meyer et al., PRL 101 (2008) 016103; [2] T. Archer et al., PRB 78 (2008) 014431.

O 51.2 Wed 17:00 HE 101

Tuning the growth orientation of epitaxial films by the interface chemistry — •Florian Mittendorfer[1], Josef Redinger[1], Matthias Gubo[2], Christina Ebensperger[2], Wolfgang Meyer[2], Lutz Hammer[2], and Klaus Heinz[2] — [1]TU Vienna, Austria — [2]Univ. Erlangen-Nürnberg, Germany

The support of epitaxial films frequently determines their crystallographic orientation, which is of crucial importance for their electronic and catalytic properties. We have investigated the growth of CoO films on Ir(100) with density functional theory (DFT) calculations, using the Vienna Ab-initio Simulations Package (VASP), in combination with scanning tunneling microscopy (STM) and low-energy electron diffraction (LEED) experiments.

The measurements show that the oxide film grows in the (111) orientation on the bare substrate, but the orientation switches to (100) by introducing a single layer of metallic Co between the oxide and substrate. On the basis of the DFT calculations, we find that these different growth modes are triggered by an oxide precursor structure, which is only stable on the Co/Ir(100) surface. The calculations demonstrate that the stabilization of the precursor is not driven by the surface stress, but rather by the chemical modification of the interface. Therefore, this approach offers a new way to change the film orientation without changing the substrate.

O 51.3 Wed 17:15 HE 101

Oxide growth on zinc in different atmospheres — •Ying

Chen[1,2], Juan Zuo[3], Paul Schneider[1], and Andreas Erbe[1] — [1]Max-Planck-Institut für Eisenforschung GmbH, Max-Planck-Str. 1, 40237, Düsseldorf, Germany — [2]Center for Electrochemical Sciences, Ruhr-Universität Bochum, Bochum, Germany — [3]Department of Mechanical Engineering, Xiamen University of Technology, Xiamen, China

The oxide layer formed on Zn surface in oxidising and non-oxidising humid and dry atmospheres was investigated by spectroscopic ellipsometry (SE) and X-ray photoelectron spectroscopy (XPS). XPS sputter profiles, analysis of the Auger LMM peaks, as well as SE analysis provide strong evidence for the presence of metallic Zn inside the oxide layer [1]. The growth kinetics of the oxide films were measured in a specially designed optical cell. By controlling the growth conditions, such as gas atmosphere (air, argon, oxygen) and humidity, the growth of the oxide layer was studied by in-situ SE measurements over 72 h. It was found that a two-stage growth process of the film is present. Overall growth rate increases in the increasing of the concentration of oxygen in the atmosphere, with a further effect of the presence of humidity. Furthermore, changes in the absorption coefficient indicate changes in electronic structure of the films in the initial phase of the growth, but much faster than the first phase of the thickness increase [2]. REFERENCE: [1] J. Zuo, A. Erbe, Phys. Chem. Chem. Phys., 12 (2010) 11467-11476. [2] Y. Chen, P. Schneider, A. Erbe, Phys. Stat. Solidi C, submitted.

O 51.4 Wed 17:30 HE 101

LEEM/LEED investigation of Fe3O4 thin film growth on a Pt(111) substrate — •Thomas Schmidt, Alessandro Sala, Helder Marchetto, Hagen Klemm, Francesca Genuzio, Shamil Shaikhutdinov, and Hans-Joachim Freund — Fritz-Haber-Institut, Abt. CP, 14195 Berlin

The formation of the Fe3O4 film has been observed in-situ and in real-time by LEEM and LEED, with preparation conditions that differs respect to the established recipe [1]. It has been revealed that an oxidation temperature of 1000 K leads to a dewetting of the magnetite film and the formation of FeO domains upon the step bunches of the Pt(111) surface. A new recipe has been tested for the formation of the thin film: by using a closed magnetite film formed with the canonical recipe as a template, the deposition of Fe at high temperature (above 850 K) and in an O2 atmosphere allows the formation of a more flat and regular thin film, that shows also particular surface structures. By changing in real-time the deposition and oxidation conditions, the film shows different surface structures and reconstructions, detected both in LEEM and LEED. The characterization of these surface phases is discussed. [1] W. Weiss and M. Ritter, Phys. Rev. B 59, 5201 (1999)

O 51.5 Wed 17:45 HE 101

Growth and characterization of hexagonal boron nitride on Cu(111) — •Sushobhan Joshi[1], Willi Auwärter[1], Felix Bischoff[1], David Ecija[1], Saranyan Vijayaraghavan[1], Hermann Sachdev[2], and Johannes V. Barth[1] — [1]Physik Department E20, Technische Universität München, James-Franck Str. 1, D-85748 Garching, Germany — [2]Max Planck Institut für Polymerforschung, Ackermannweg 10, D-55128 Mainz, Germany

Monolayer systems as hexagonal boron nitride (h-BN) or graphene can be epitaxially grown on various metal supports and recently attract considerable interest. Here we present a scanning tunneling microscopy (STM) and spectroscopy (STS) study characterizing hexagonal boron nitride (sub)monolayers grown on a Cu(111) surface by thermal decomposition of a borazine precursor. While no h-BN related contrast is observed in topographic images recorded at low bias, Moire patterns emerge at a voltage of about 4 V. Independent on the preparation procedure, we observe the coexistence of such patterns exhibiting different periodicities and orientations. This evidences the formation of various h-BN domains on the surface and thus points to a weak interaction of the h-BN sheet with the underlying Cu(111) lattice. Electronically, the h-BN/Cu(111) system is characterized by an interface state emerging from the Cu(111) surface state. Additionally, ST spectra recorded in the field emission regime indicate a spatially modulated workfunction on h-BN that is reduced in comparison to bare Cu(111). Such local variations of the surface electronic structure influence the formation of molecular assemblies as outlined for the case of porphines.

O 51.6 Wed 18:00 HE 101

In-situ XRD and XRR investigations of the oxidation process in ultra thin praseodymia films on Si(111) — •Henrik Wilkens[1], Sebastian Gevers[1], Marvin H. Zoellner[2], Thomas Schroeder[2], and Joachim Wollschläger[1] — [1]Fachbereich Physik, Universität Osnabrück, Barbarastr. 7, 49069 Osnabrück, Germany — [2]IHP, Im Technologiepark 25, 15236 Frankfurt (Oder), Germany

Due to its high dielectric constant and lattice constant between Ge and Si, praseodymia is an interesting buffer material for system on chip solutions (SOC). To build these praseodymia based systems, a detailed analysis of the various oxidation states and reaction kinetics in thin films is necessary.

Therefore, time-resolved in-situ x-ray diffraction (XRD) and x-ray reflection (XRR) measurements with an in-house built pressure cell were performed at the synchrotron beamlines W1 and P08 at HASYLAB, DESY. The oxidation and reduction process in oxygen atmosphere were studied over a wide pressure range from $1 \cdot 10^{-6}$ mbar to 1 bar and temperatures up to 500° C.

As a first result additional oxidation states in the region between cub-Pr_2O_3 and cub-Pr_6O_{11} were found, which haven't been observed in thin films up to now. Furthermore, the oxygen partial pressure seems to have larger impact on the reached oxidation state than the temperature.

O 51.7 Wed 18:15 HE 101

STM and LEED investigation of a quasicrystalline thin film phase of $BaTiO_3$ on Pt(111) — •Stefan Förster[1], Klaus Meinel[1], Karl-Michael Schindler[1], and Wolf Widdra[1,2] — [1]Institute of Physics, Martin-Luther-Universität Halle-Wittenberg, Halle, Germany — [2]Max Planck Institute of Microstructure Physics, Halle, Germany

$BaTiO_3$ is the most studied ferroelectric perowskite which has an easily accessible ferroelectric to paraelectric phase transition at about 400 K. It can be grown epitaxially on Pt(100) and Pt(111) due to its small lattice mismatch of only 2% relative to the substrate. Upon annealing in an oxygen atmosphere well-ordered $BaTiO_3$(100) and $BaTiO_3$(111) thin film phases have been reported [1]. However, here we report on a surprising thin film phase upon annealing in UHV. For 4 ML $BaTiO_3$ on Pt(111), annealing at 1250 K leads to the formation of large three-dimensional islands of bulk-like $BaTiO_3$. Between these islands, the Pt terraces are covered by a remaining $BaTiO_3$ wetting layer.

By means of low-energy electron diffraction (LEED) and scanning tunnelling microscopy (STM) the structure of this wetting layer has been identified to be a 2D quasicrystalline phase of $BaTiO_3$. In LEED this structure shows bright and sharp spots with dodecagonal symmetry. STM reveals that the surface structure is composed by an arrangement of quadratic and triangular building blocks which can explain the 2D quasicrystalline lattice with dodecagonal symmetry.

[1] S. Förster, M. Huth, K.-M. Schindler, and W. Widdra, *J. Chem. Phys. 135*, 104701 **2011**.

O 51.8 Wed 18:30 HE 101

Atomic-scale optimization of homoepitaxial growth of $SrTiO_3$(110) thin film — •Zhiming Wang[1,2], Lin Gu[2], Yuan Yao[2], Jiandong Guo[2], Michael Schmid[1], and Ulrike Diebold[1] — [1]Institut für Angewandte Physik, Technische Universität Wien, Wien 1040, Austria — [2]Institute of Physics, Chinese Academy of Sciences, Beijing 100190, China

Oxide multilayers display a rich diversity of properties that are different from their constituent materials. To understand the underlying physical mechanisms, it is essential to construct the oxide heterostructures with atomic-scale precision. We study homoepitaxial growth of $SrTiO_3$(110) with oxide molecular beam epitaxy and use scanning tunneling microscopy and transmission electron microscopy for characterization of the films. The $SrTiO_3$(110) surface exhibits a series of reconstructions, (n×1) and (m×8) (with n=4-6, m=2,6), which can be changed reversibly by deposition of Ti or Sr, These reconstructions are clearly observed by high energy electron diffraction at thin film growth temperature. This was used to optimize the Sr to Ti flux ratio in real time. We realized layer-by-layer growth of thin films with a deviation of cation stoichiometry of $< 0.5\%$ revealed by energy dispersive spectroscopy. The surface is always reconstructed and the buried layers transform into stochiometric $SrTiO_3$ during growth. Films prefer to grow along $[1\bar{1}0]$ on (n×1) (n=4-6) surfaces, and along [001] on the (2×8) surface. This leads to the formation of nanoscale trenches on surfaces with mixed terminations. This work was supported by the Austrian Science Fund (FWF project F45).

O 51.9 Wed 18:45 HE 101

Morphology and optical properties of Cr-doped MgO films — •Fernando Stavale, Niklas Nilius, and Hans-Joachim Freund — Fritz-Haber-Institut der MPG, Faradayweg 4-6, 14195 Berlin, Germany

MgO thin films doped with varying amounts of Cr have been analyzed from a structural, morphological and optical point of view, using cathodo- and photo-luminescence spectroscopy performed in an STM setup. Whereas at low Cr concentration, the MgO rocksalt structure is maintained, transition to a spinel-like magnesium chromate occurs at higher doping level. Depending on the Cr concentration, several zero-phonon and phonon-mediated emission lines are detected at around 700 nm in the optical spectra, originating from transition within the d-state manifold of the Cr ions. Their wavelength position and intensity provides insight into the local environment of the Cr centers. The development of the phonon sidebands, on the other hand, is governed by the excitation scheme, and the bands become particularly strong for an electronic stimulation of the system. The role of the Stark effect on the band positions is quantified by comparing photo- and cathodoluminescence spectra performed at different tip-electric fields.

O 51.10 Wed 19:00 HE 101

Density Functional Theory study of ZrO_2 bulk phases and Pt_3Zr-ZrO_2 interfaces — •Wernfried Mayr-Schmölzer, Florian Mittendorfer, and Josef Redinger — IAP and Center of Computational Materials Science, TU Vienna

Zirconium dioxide is a material with many interesting properties, which make it useful for example as a solid electrolyte in solid-oxide fuel-cells or as an oxygen gas sensor.

We present results of DFT calculations with the Vienna Ab-initio Simulation Package of four ZrO_2 bulk modifications and Pt_3Zr-ZrO_2 interfaces using different functionals, namely LDA, PBE, PBEsol and hybrid functionals (HSE). The ZrO_2 phases we studied were the monoclinic $P2_1/c$, the tetragonal $P4_2/nmc$, the cubic $Fm\bar{3}m$ and the orthorhombic $Pnma$ phase. For each functional a structural relaxation of the bulk crystal was done and compared to both earlier calculations and experiments.

To determine the correct interface between a Pt_3Zr substrate and a thin film of zirconium oxide we first had to identify the stacking order of the Pt_3Zr surface termination. A Pt_3Zr crystal forms a hexagonal lattice with an ABAC stacking order. It is known from experiments that steps on the surface are two layers high, but using STM it is not possible to measure whether there is an A-A or a B-C step. Using DFT calculations we were able to identify the termination layer of the crystal. These results were then used to study the interface between a Pt_3Zr substrate and a thin film of zirconium oxide.

O 52: Focussed session: Coherence and coherent control in nanophotonics and plasmonics II

Time: Wednesday 16:45–19:15 Location: MA 005

Topical Talk O 52.1 Wed 16:45 MA 005

Spatio-temporal focusing of ultrashort pulses through scattering media — •Yaron Silberberg — Weizmann Institute of Science, Rehovot, Israel

When a short pulse is passed through an inhomogeneous medium, such as a biological tissue, it gets randomly scattered, resulting in a diffuse smeared-up light pattern in space and time. Scattering-induced distortions pose one of the major limitations in many applications, ranging from astronomy to microscopy. We have recently shown [1] that one can engineer an ultrashort optical pulse such that it will focus in both space and time inside a scattering medium. Moreover, we have discovered that one can correct both spatial and temporal distortions by manipulating only the spatial degrees of freedom of the incident wavefront using a spatial light modulator.

[1] O. Katz, E. Small, Y. Bromberg and Y. Silberberg, Nature Photonics 5, 372 (2011).

Topical Talk O 52.2 Wed 17:15 MA 005

Attosecond control of electrons laser-emitted from a nanoscale metal tip — •Peter Hommelhoff[1], Michael Krüger[1], Markus Schenk[1], Michael Förster[1], Georg Wachter[2], Christoph Lemell[2], and Joachim Burgdörfer[2] — [1]MPI of Quantum Optics, Garching, Germany — [2]Technical University of Vienna, Vienna, Austria

With carrier-envelope phase stable few-cycle laser pulses we demonstrate steering of electrons photo-emitted from a nanoscale metal tip with the optical electric field of the laser pulses. In spectrally resolved measurements we have observed strong-field effects such as peak shifting and peak suppression already at moderate laser intensities of less than 10^{12} W/cm^2, owing to field enhancement [1]. The formation of interference fringes in the photoelectron energy spectrum as function of the carrier-envelope phase points at electronic matter wave interference in the time-domain. We explain our results with the classical three-step model, including rescattering [2]. A detailed simulation based on time-dependent density functional theory corroborates our findings and can be used to determine the effective laser field at the metal tip [3]. Based on our experimental and theoretical findings we could show that we coherently control the dynamics of the liberated electronic matter wave with the laser field on sub-cycle, i.e., attosecond time scales.

[1] M. Schenk, M. Krüger, P. Hommelhoff, PRL 105, 257601 (2010)

[2] M. Krüger, M. Schenk, P. Hommelhoff, Nature 475, 78 (2011)

[3] G. Wachter, Chr. Lemell, J. Burgdörfer, M. Schenk, M. Krüger, P. Hommelhoff, to be published

Topical Talk O 52.3 Wed 17:45 MA 005

Theory of quantum control of semiconductor quantum dots in complex environments — Andreas Knorr, •Julia Kabuss, Alexander Carmele, Sverre Theuerholz, and Marten Richter — Institut für Theoretische Physik, Technische Universität Berlin

This talk is focused on the control of the statistics of coupled quantum fields (electrons, phonons and photons) in nanostructured materials, composed of quantum dots, cavities and metal nanoparticles. Addressing the full quantum statistics of the fields within a microscopic theory we discuss:

- the phonon statistics in acoustic cavities externally driven by a Raman process,
- the manipulation of the photon statistics in optical cavities by feedback control, and
- the Förster transfer processes between quantum dots in the presence of metal nanoparticles and the disentanglement of intrinsic interaction by local spectroscopy.

O 52.4 Wed 18:15 MA 005

Control of second-harmonic generation in metal nanoparticles and nanowires — •Giovanni Piredda[1], Zhimin Shi[2], Nina Rauhut[1], Regina de Vivie-Riedle[1], and Achim Hartschuh[1] — [1]Physikalische Chemie, Department Chemie, Ludwig-Maximilians-Universität München — [2]The Institute of Optics, University of Rochester, Rochester, NY 14620, USA

The goal of ultrafast nanooptics is shaping the electric field at the nanometer spatial scale and the femtosecond temporal scale through the controlled excitation of optical resonances in metallic nanostructures [1]. Experiments on nanoparticles and nanowires allow one to consider in a separate way two different types of resonances: localized resonances that are based on dipolar response and Fabry-Perot resonances that are based on propagation effects. Accordingly, we excite nanoparticles with chirped femtosecond pulses, and nanowires with pulse trains; we observe second-harmonic generation from the metal structures [2] as a function of pulse parameters in the two cases and demonstrate that the coherent control of harmonic generation reflects the characteristics of the resonance.

[1] M.I. Stockman, S.V. Faleev, and D.J. Bergman; Coherent control of femtosecond energy localization in nanosystems; Phys. Rev. Lett., **88**, 067402 (2002).

[2] M. Zavelani-Rossi et al.; Near-field second-harmonic generation in single gold nanoparticles; Appl. Phys. Lett., **92**, 093119 (2008).

O 52.5 Wed 18:30 MA 005

Classical Analog of Electromagnetically Induced Absorption in Plasmonics — •Richard Taubert[1], Mario Hentschel[1,2], Jürgen Kästel[3], and Harald Giessen[1] — [1]4th Physics Institute and Research Center SCoPE, University of Stuttgart, 70550 Stuttgart, Germany — [2]Max-Planck-Institut für Festkörperforschung, Heisenbergstraße 1, D-70569 Stuttgart, Germany — [3]Deutsches Zentrum für Luft- und Raumfahrt, Institut für Technische Physik, D-70569 Stuttgart, Germany

The ability to manipulate the phase shift between two coupled plasmonic resonances in a controlled fashion has been unavailable up to now. Here we present a strategy to overcome this limitation by employing the benefits of near-field coupling on the one hand and retardation effects due to far-field coupling on the other hand. We theoretically and experimentally demonstrate that in the intermediate regime the coupling of a broad dipolar to a narrow dark quadrupolar plasmon resonance is possible while simultaneously allowing for a retardation-induced phase shift. This leads to constructive interference and enhanced absorption. The observed phenomena can thus be termed classical analog of electromagnetically induced absorption.

O 52.6 Wed 18:45 MA 005

Hybridization of dark & bright modes leading to longlived plasmonic coherences on a corrugated silver surface — Martin Aeschlimann[1], Tobias Brixner[2], Alexander Fischer[1], Christian Kramer[2], Pascal Melchior[1], Walter Pfeiffer[3], Christian Schneider[1], •Christian Strüber[3], Philip Tuchscherer[2], and Dmitri V. Voronine[4] — [1]Technische Universität Kaiserslautern, Germany — [2]Universität Würzburg, Germany — [3]Universität Bielefeld, Germany — [4]Texas A&M University, College Station, USA

The hybridization of dark and bright plasmonic modes leads to Fano resonances and electronically induced transparency phenomena. So far these effects have been observed only in engineered nanostructures. Coherent 2D nanoscopy, a combination of coherent 2D spectroscopy and time-resolved photoemission electron microscopy (PEEM), reveals longlived plasmonic coherences and quantum beats on a randomly structured silver surface [1]. The unexpectedly long coherence lifetime of about 100 femtoseconds is explained by hybridization of dark and bright modes, formed by multiply scattered surface plasmon polaritons (SPPs) and localized SPPs, respectively. Fitting the measured spectra using either a two mode hybridization model or unconstrained parameters reveals sharp Fano-like resonances in the local response. The results emphasize that dark modes, i.e. modes coupled weakly to the radiation field, support longlived coherent states even in highly scattering environment.

[1] M. Aeschlimann et al., Science 333, 1723-1726 (2011)

O 52.7 Wed 19:00 MA 005

Strong field acceleration of attosecond electron pulses emitted by a nanometer-sized gold taper — •Björn Piglosiewicz, Slawa Schmidt, Doojae Park, and Christoph Lienau — Ultraschnelle Nano-Optik, Institut für Physik, Fakultät V, Universität Oldenburg, 26111 Oldenburg, Deutschland

When few-cycle near-IR femtosecond pulses in the range of 1 - 2 microns and with nJ energy are focused onto the nanometer-sized tip of a conical metallic taper, the strong laser field induces the tunneling of electrons out of the very apex of this tip. The ejected electrons are then strongly accelerated within the field gradient near the tip apex and this acceleration results in unusual, plateau-like kinetic energy spectra of the ejected electrons. Here, we analyze for the first time the angle-resolved kinetic energy spectra generated by strong-field photoemission from single gold tips. We show that their dependence on dc-bias and laser wavelength allows us to deduced details of the light-driven electron dynamics on attosecond time and nanometer length scale. Our results might be interesting for electron microscopy with attosecond time resolution.

O 53: Graphene IV

Time: Wednesday 16:45–18:30 Location: MA 041

O 53.1 Wed 16:45 MA 041

Rotated / Scaled Overlayers and Moiré Patterns: a theoretical approach — •Klaus Hermann — Abt. Theorie, Fritz-Haber-Institut, Berlin

Rotated and/or scaled overlayers at regular single crystal surfaces, such as graphene on Ru(0001) [1] or silver on Ni(100) substrate [2], are found to show long-range order expressed by approximate 2-dimensional surface periodicity with very large lattice constants. This phenomenon can be described geometrically analogous to interference effects resulting in periodic Moiré patterns which are characterized by 2-dimensional superlattices. Here we discuss in detail the mathematical formalism of determining such Moiré patterns based on concepts of coincidence lattices. The formalism provides simple relations that allow to calculate 2-dimensional Moiré lattices in their depencence on layer rotation angles α and and scaling factors p for general Bravais lattices.

[1] D. Martoccia, P.R. Willmott, T. Brugger, M. Björck, S. Günther, C.M. Schlepütz, A. Cervellino, S.A. Pauli, B.D. Patterson, S. Marchini, J. Wintterlin, W. Moritz, and T. Greber, Phys. Rev. Lett. 101 (2008) 126102.

[2] C. Chambon, J. Creuze, A. Coati, M. Sauvage-Simkin, and Y. Garreau, Phys. Rev. B 79 (2009) 125412.

O 53.2 Wed 17:00 MA 041

Graphene and hexagonal Boron Nitride 2D Super Structures Analysed by Scanning Probe Spectroscopy — •Thilo Glatzel[1], Sascha Koch[1], Shigeki Kawai[1], Ernst Meyer[1], Sara Barja[2], and Enrico Gnecco[2] — [1]Department of Physics, University of Basel, Klingelbergstr. 82, 4056 Basel, Switzerland — [2]Instituto Madrileño de Estudios Avanzados en Nanociencia n (IMDEA Nanociencia), Cantoblanco, 28049 Madrid, Spain

By high temperature exposure of ethylene or borazine [(HBNH)3] on transition metals between 500-1000°C under UHV conditions leads to the formation of graphene or a boron nitride monolayer, respectively. A lattice mismatch between the layers and the metal surfaces cause a hexagonal superstructure but while graphene is electrically conducting the boron nitride layer is insulating.

STM measurements showed various imaging contrasts arising from the complicated surface geometry and electronic properties. In our nc-AFM and KPFM experiments the complexity of the superstructures is also frequently observed in the topography as well as in the local contact potential difference. We thoroughgoing investigate the tip-sample interaction by 2D dynamic force spectroscopy at room temperature. From the variations in the resonance frequency of the probing tip in close proximity to the sample and the low dissipation accompanying the tip vibrations an elastic nature of the graphene and boron nitride elevations is concluded.

O 53.3 Wed 17:15 MA 041

Theory of graphene-boron nitride heterostructures — •Burkhard Sachs[1], Tim Wehling[1], Mikhail Katsnelson[2], and Alexander Lichtenstein[1] — [1]1. Institut für Theoretische Physik, Universität Hamburg, Jungiusstraße 9, D-20355 Hamburg, Germany — [2]Institute for Molecules and Materials, Radboud University Nijmegen, NL-6525 AJ Nijmegen, The Netherlands

We report theoretical investigations of graphene-boron nitride heterostructures [1]. In detail, we investigate the adsorption of graphene sheets on hexagonal boron nitride substrates by means of first-principles calculations in the framework of adiabatic connection fluctuation-dissipation theory in the random-phase approximation. We obtain adhesion energies for different crystallographic stacking configurations and show that the interlayer bonding is due to long-range van der Waals forces. The interplay of elastic and adhesion energies is shown to lead to stacking disorder and moiré structures. Bandstructure calculations reveal substrate induced mass terms in graphene, which change their sign with the stacking configuration. The dispersion, absolute band gaps, and the real-space shape of the low-energy electronic states in the moiré structures are discussed. We find that the absolute band gaps in the moiré structures are at least an order of magnitude smaller than the maximum local values of the mass term. Our results are in agreement with recent scanning tunneling microscopy experiments.

[1] B. Sachs, T. O. Wehling, M. I. Katsnelson, and A. I. Lichtenstein, Phys. Rev. B 84, 195414 (2011)

O 53.4 Wed 17:30 MA 041

Graphene on 3C-SiC(111): *Ab initio* study of structure and stability including van der Waals effects — •Lydia Nemec, Volker Blum, Patrick Rinke, and Matthias Scheffler — Fritz-

Haber-Institut der Max-Planck-Gesellschaft, D-14195 Berlin

SiC is a widely used substrate for the growth of mono- and few-layer graphene. By Si sublimation, large ordered areas of graphene form on the Si side as $(6\sqrt{3}\times 6\sqrt{3})$-R30° ("$6\sqrt{3}$") commensurate periodic films [1]. In experiment, a first, partially covalently attached "buffer layer" (BL) $6\sqrt{3}$ carbon layer can be grown in a small temperature window, followed by a quasi-freestanding $6\sqrt{3}$ monolayer of graphene (GBL) at higher temperatures, and finally, few-layer graphene. What is not *a priori* clear is whether the BL and GBL phases are the result of some (narrow) *thermodynamic* equilibrium condition, and how the substrate affects the structure (monolayer graphene corrugation). Both are natural questions for theory, but a challenge for two reasons: (1) system size (up to ~ 2000 atoms in this work) and (2) van der Waals interactions, not accounted for by most standard density functionals. We show that the BL and GBL phases are in fact equilibrium phases within all-electron density functional theory (DFT) including van der Waals effects (PBE+vdW [2]). The equilibrium geometry emerges as a direct prediction, including the significant graphene layer corrugation. We also show that smaller-cell approximants may miss some geometric features, and could erroneously stabilize buffer layer defects due to artificially induced strain. [1] K. V. Emtsev *et al.*, Nature Materials **8**, 203 (2009). [2] A. Tkatchenko, M. Scheffler, PRL **102**, 073005 (2009).

O 53.5 Wed 17:45 MA 041

Graphene sublattice symmetry and isospin determined by ARPES using circularly polarized light — Isabella Gierz[1], Matti Lindroos[2], Hartmut Höchst[3], •Christian R. Ast[1], and Klaus Kern[1] — [1]MPI für Festkörperforschung, Stuttgart — [2]Tampere University of Technology, Tampere, Finland — [3]Synchrotron Radiation Center, Stoughton, WI, USA

The origin of the Dirac-like electronic structure of graphene can be traced back to the symmetry properties of the honeycomb lattice characterized by the equivalence of the two carbon atoms within the unit cell (the sublattice symmetry) as well as their relative phase (the isospin). We determine these parameters using angle-resolved photoemission spectroscopy (ARPES) in combination with circularly polarized synchrotron radiation. We developed a simple theoretical model which shows that the photocurrent can be written as the product of a well known sublattice interference term containing the relevant information about the initial state and a — previously neglected — matrix element accounting for the influence of the geometry of the experimental setup as well as final state effects. We will show that for a photon energy of $h\nu = 52\,\mathrm{eV}$ matrix element effects actually can be neglected which allows us to determine the sublattice symmetry parameter as well as the isospin with high accuracy.

O 53.6 Wed 18:00 MA 041

Nitrogen doped graphene on Ni(111) — •Roland J. Koch[1], Martin Weser[2], Markus Ostler[1], Julian Gebhardt[3], Francesc Vines[3], Wei Zhao[4], Christian Papp[4], Andreas Görling[3], Hans-Peter Steinrück[4], Karsten Horn[2], and Thomas Seyller[1] — [1]Lehrstuhl für Technische Physik, Universität Erlangen-Nürnberg, 91058 Erlangen — [2]Fritz-Haber-Institut der Max-Planck-Gesellschaft, 14195 Berlin — [3]Lehrstuhl für Theoretische Chemie, Universität Erlangen-Nürnberg, 91058 Erlangen — [4]Lehrstuhl für Physikalische Chemie II, Universität Erlangen-Nürnberg, 91058 Erlangen

We report on the N doping of CVD-grown graphene on Ni(111) using a N-containing precursor. After in-situ growth, the graphene film was investigated using ARPES to study the valence band structure, and XPS was used to determine the N content and bonding situation. The results from PES were supplemented by DFT calculations for various slab models that mimic different possible doping situations. The valence band spectra show a broadening of the photoemission features as well as a shift of the bands with respect to the Fermi level. In order to decouple the N doped graphene film from the strongly interacting Ni substrate and to recover the Dirac cone, Au was intercalated. The XPS spectra show that the N doping is present in two different configurations. The majority of the N atoms are present in a pyridinic configuration, which involves a carbon vacancy. The minority of the N atoms is occupying a substitutional site. The observed variation of the electronic structure of N doped graphene compared to pristine graphene depends on the ratio of pyridinic to substitutional N.

O 53.7 Wed 18:15 MA 041

Phonons in single-layer and few-layer $\mathbf{MoS_2}$ — •Alejandro Molina-Sanchez and Ludger Wirtz — Institute for Electronics, Microelectronics, and Nanotechnology (IEMN), Lille, France

In recent experiments, the single-layer dichalcogenide MoS_2 has exhibited a direct band-gap of 1.75 eV and a electron mobility close to that of graphene, becoming an appealing material in the area of optoelectronic devices [1].

Recent Raman measurements have revealed unexpected trends in the vibrational properties of MoS_2 when the number of layers changes, as a frequency decreasing of the phonon mode E^1_{2g} with increasing numbers of layers, that contradicts the expectation that the weak interlayer forces between neighbour layers should increase the effective restoring forces acting on atoms [2].

The purpose of our work is the clarification of this issue by a detailed *ab initio* study of the phonons, and comparing afterwards with experimental results. We explain this decrease by an enhancement of the dielectric screening of the long-range Coulomb interaction between the effective charges with a growing number of layers [3].

[1] B. Radisavljevic et. al., Nat. Nano. 6, 147 (2011). [2] C. Lee et. al., ACS Nano 4 2695 (2010). [3] A. Molina-Sanchez and L. Wirtz, Phys. Rev. 84, 155413 (2011).

O 54: Nanostructures at surfaces II

Time: Wednesday 16:45–19:15 Location: MA 042

O 54.1 Wed 16:45 MA 042

Dynamic AFM with reduced contact stiffness by the employment of nanowires — •Ivo Knittel, Moid Bhatti, and Uwe Hartmann — Fachrichtung Experimentalphysik, Universität des Saarlandes, 66123 Saarbrücken

Nanowire tips for atomic force microscopy, employing a nanowire or a "supertip" on top of a conventional AFM tip, have been found advantageous in many respects. Nanowire tips are employed for high-resolution imaging of high-aspect ratio sample features, but also in order to obtain well-defined and enhanced local fields. However, in many cases a nanowire at the tip is flexible, reducing the contact stiffness to extremely low values. The resulting effective tip-sample force-distance relation is characteristic and leads to an unusual dynamics in intermittent-contact AFM.

Nanocantilever-on-cantilever AFM tips were produced by modification of conventional silicon AFM tips by means of a focused ion beam. A second type of probes were multiwalled carbon nanotube AFM tips. In addition, the intermittent-contact interaction between a conventional AFM tip and several types of nanowires on substrates was investigated. Nanowires were freely standing with resonant frequencies between 10Mhz and 1GHz and lengths between 5μm and 300nm.

Experimental and simulated intermittent-contact distance-dependent resonance curves were compared. We show the existence of a third state of intermittent-contact cantilever dynamics besides the well-known "low-amplitude" and the "high-amplitude" states. The particular role of adhesion and dissipation is also discussed.

O 54.2 Wed 17:00 MA 042

Evaluation of the Growth Mechanism of Ag-TCNQ for Morphology Control — •Benedikt Rösner, Andreas Späth, Stephan Wenzel, and Rainer H. Fink — Department Chemistry and Pharmacy, University Erlangen-Nürnberg, Egerlandstr. 3, 91058 Erlangen

Silver-(7,7*,8,8*)-tetracyanoquinodimethane (Ag-TCNQ) represents a form of charge transfer salts which can be described as needle-shaped crystals. This material features interesting properties regarding optical, electrical and magnetic behaviour and is therefore an interesting candidate for use in field emission devices, opto-electric storage devices and boards based on organic components. The control of the morphology, which is strongly dependent on the growth mechanism, is an essential precondition for the production of nanostructured devices. Two bottom-up growth mechanisms have been described so far. [1,2] However, these mechanism lag to describe phenomena observed by various microscopic methods growing this material in different reaction environments. We therefore evolve a diffusion-controlled reaction mechanism based on the first approaches mentioned above and discuss the influence of different parameters on the behaviour of silver and TCNQ on the molecular scale. 1.*Cao, G.-Y., et al., Micron, 2005. 36: p. 285-290. 2.*Ye, C.-N., et al., Chin. Phys. Lett., 2004. 21: p. 1787-1790.

O 54.3 Wed 17:15 MA 042

Ordered Supramolecular Nanowires on a Neutral Substrate — •Roozbeh Shokri[1,2], Françoise Serein-Spirau[3], Jean M. Sotiropoulos[4], Günter Reiter[1], and Laurent Simon[2] — [1]Physikalisches Institut, Universität Freiburg, Germany — [2]Institut de Science des Matériaux de Mulhouse (IS2M), France — [3]Institut Charles Gerhardt de Montpellier, France — [4]Institut Pluridisciplinaire de Recherche sur l'Environnement et les Matériaux, Pau, France

Here we present a scanning tunneling microscopy study on a well-defined organic oligomer composed of three thiophene-benzene-thiophene units deposited onto graphene. Mono-layer graphene can be considered as a neutral substrate which only weakly interacts with the molecules and thus allows observing molecular organization processes dominated by molecule-molecule interactions. Our studies exhibit well-ordered 2D domains of these molecules consisting of long supramolecular wires formed by a pi-stacking arrangement between the thiophene endgroups. The precise molecular arrangement and measurements of the HOMO-LUMO gap and spatial mapping of the electronic states reveal the possibility of transporting charges through a hoping mechanism. Scanning tunneling spectroscopy in combination with DFT calculations manifest that the electronic states of the molecules are not perturbed by the underlying graphene layer, i.e. decoupled from the substrate. Such weak interaction between molecules and graphene provides the possibility to image and "see" all molecular orbitals in detail, and to distinguish unambiguously individual molecular segments.

O 54.4 Wed 17:30 MA 042

Oxygen adatoms on the MoO$_2$/Mo(110) surface: from nanoscale writing to oxide nanowires — •Olaf Lübben[1], Sergey A. Krasnikov[1], Sergey I. Bozhko[1,2], Barry E. Murphy[1], and Igor V. Shvets[1] — [1]School of Physics, Trinity College Dublin, Dublin, Ireland — [2]Institute of Solid State Physics, Russian Academy of Sciences, Chernogolovka, Russian Federation

Nanoscale writing using oxygen adatoms on the MoO$_2$/Mo(110) surface is demonstrated by scanning tunneling microscopy (STM). Oxidation of metal surfaces can produce a variety of ordered oxide nanostructures and two-dimensional surface oxides, which are of great significance for heterogeneous catalysis. High-temperature oxidation of the Mo(110) surface forms well-ordered molybdenum oxide nanorows separated by 2.5 nm. Further oxidation results in perfectly-aligned double rows of oxygen adatoms, imaged by STM as bright protrusions. These adatoms can be removed from the surface in a controlled fashion by the STM tip. Tip movement along the surface can be used for controlled lithography, with a minimum feature size of just 5 nm. Finally, deposition of Fe on the oxygen-rich MoO$_2$/Mo(110) surface leads to the formation of well-ordered Fe oxide nanowires with a zig-zag structure.

O 54.5 Wed 17:45 MA 042

2D-Quantum confinement in nanoporous networks — •Nenad Kepčija[1], Florian Klappenberger[1], Wolfgang Krenner[1], Javier García de Abajo[2], and Johannes Barth[1] — [1]Physik Department E20, Technische Universität München, James-Franck Straße, 85748 Garching, Germany — [2]Instituto de Optica - CSIC, Serrano 121, 28006 Madrid, Spain

Quantum confinement of a 2D electron gas in supramolecular nanoporous networks is investigated using the Boundary Elements Method (BEM) based on Green's functions for finite geometries and electron plane wave expansion (EPW) for periodic systems. The "particle in a box" picture was analyzed for cases with selected symmetries that model previously reported architectures constructed from purely organic and metal-organic scattering centers. The networks can be seen as arrays of coupled quantum dots. By varying the appropriate parameters we demonstrate how the scattering properties affect the electronic characteristics. For the reported features of the local density of states (LDOS) we were able to separate lifetime broadening from splitting of quantum dot states due to nearest-neighbour interaction. For each system we analyze the local electron density distribution and relate it with the corresponding band structure. Thereby, we connect the complementary information typically obtained by local scanning tunneling spectroscopy and $\vec{k}$-sensitive angle-resolved photoemission spectroscopy.

O 54.6 Wed 18:00 MA 042

Reactivity of Co-alloy clusters — •Ivan Baev, Torben Beeck, Michael Martins, and Wilfried Wurth — Universität Hamburg, Institut für Experimentalphysik

The chemical reactivity of small particles such as clusters strongly varies as a function of size in the Nano scale. Understanding the nature of chemical reactions at this small size limit is crucial for a further development of Nano catalysts. With our source "ICARUS" we can create a perfectly size selected cluster beam in the size range of 20 atoms per cluster. This beam is used to deposit clusters onto metallic substrates or thin oxide films. Clusters are deposited using the "soft-landing" technique to avoid fragmentation, agglomeration or implantation of the clusters into the substrate combined with a low surface coverage of less than 5% of a monolayer. Using core-level photoelectron spectroscopy at the BESSY U49-2PGM1 beamline the metallic core levels are measured as a function of cluster size and composition. The core level spectra are very sensitive to the chemical environment of the cluster so that chemical processes can be directly traced back to the cluster sites. Combined with the measurement of oxygen and carbon 1s core levels a stoichiometric interpretation of the surface reactions can be given. This work is supported by the DFG through the collaborative research center SFB 668.

O 54.7 Wed 18:15 MA 042

Behavior of Co, Fe and FeCo alloy nanoparticles deposited on W(110) — •Wolfgang Rosellen, Hendrik Bettermann, Torsten Veltum, and Mathias Getzlaff — Institute of Applied Physics,University Duesseldorf

In contrast to free nanoparticles, deposited clusters and particles become more and more interesting from a technological point of view due to their size dependent electronic and magnetic properties. Therefore, it is important to have access to the structure of the particles after deposition. In this contribution we will discuss different aspects of mass and therefore size selected magnetic 3d-nanoparticles deposited on W(110). The deposited nanoparticles, mainly Fe, Co and their alloys are investigated by means of Scanning Tunneling Microscopy in-situ under UHV conditions. For our investigations we assemble the nanoparticles in the gas phase by a UHV compatible Arc Ion Cluster Source (ACIS)[1] being developed for softlanding condition. At this regime, a kinetic energy below 1 eV/atom, nanoparticles could be deposited without deformation. We will discuss the properties of individual particles as well as statistically appreciable particle ensembles. Therefore, we will report on size dependent structural properties including crystallographic structure, height and size, shape, the influence of substrate etc. We will additionally focus on the melting behavior of nanoparticles. Finally, we demonstrate a method for the spontaneous orientation of Fe, Co and alloy nanoparticles deposited on W(110).

[1] R.-P. Methling et al., European Physical Journal D **16**, 173 (2001)

O 54.8 Wed 18:30 MA 042

Transition metal adatoms on Rh(111) supported monolayer boron nitride — •Fabian Donat Natterer, François Patthey, and Harald Brune — Institute of Condensed Matter Physics (ICMP), Ecole Polytechnique Fédérale de Lausanne (EPFL), Switzerland

The low temperature adsorption of transition metal (TM) adatoms (Ti, Cr, Mn, Fe and Co) onto Rh(111) supported boron nitride (BN) monolayers leads to different behaviors. A bistable adsorption complex is found for Mn, Fe and Co. One of its states strongly weakens the boron nitride substrate binding of more than 100 boron and nitrogen atoms. In consequence, the BN layer locally acts as a soft membrane that is elastically deformed in the presence of the scanning tunneling microscope tip. For Ti and Cr, different spectral features are observed depending on the hydrogen exposure, showing a concomitant modification of the TM adatom electronic structure.

O 54.9 Wed 18:45 MA 042

RHEED Study of Ag Nanoparticles for catalytic reactions — •Stephan Bartling[1], Hannes Hartmann[1], Vladimir Popok[2], I. Barke[1], and Karl-Heinz Meiwes-Broer[1] — [1]Institut für Physik, Universität Rostock, 18051 Rostock, Germany — [2]Department of Physics and Nanotechnology, Aalborg University, 9220 Aalborg, Denmark

Size-selected silver clusters deposited on amorphous alumina films can act as high performance nanocatalysts for the partial oxidation of propylene [1].

This contribution focuses on *in situ* reflection high energy electron diffraction (RHEED) investigations of deposited Ag clusters on amorphous alumina films. For randomly oriented particles a ring structure, similarly to the Debye-Scherrer rings in conventional X-ray powder diffraction is expected [2]. Diffraction patterns after different sample treatments (heating, varying ambient environment) are presented. The cluster structure and orientation with respect to the substrate is discussed. The analysis is supported by height distributions obtained from *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 54.10 Wed 19:00 MA 042

Study of collective efforts of catalytic activity and photoactivation phenomenon for an enhanced response of SnO2 based thin film sensors towards methane gas — •Divya Haridas[1] and Vinay Gupta[2] — [1]Department of Physics, Keshav Mahavidyalaya, University of Delhi, Pitampura, delhi, India-110034 — [2]Department of Physics and Astrophysics, University of Delhi, Delhi, India110007

Detection of methane is always a great cause of concern for safety productions in mines and chemical factories. The present study investigates the twin effect of UV illumination and catalytic activity on methane sensing characteristics of SnO2 sensors. The sensitivity and selectivity of pure SnO2 thin film sensors are improved by loading it with different catalyst (Pd, Pt, Ni, Au) clusters (8 nm). Palladium clusters catalyst showed an enhanced sensor response (97.6%) towards 200 ppm of methane detection at an operating temperature of 220oC. Further, optimizing the thickness of Pd clusters leads to an enhanced sensing response of 97% to 99% over a wider temperature range (160oC to 240oC) for 10 nm thick Pd clusters. The room temperature response of the same sensor increases to 99.7% under UV illumination which is attributed to the efficient catalytic dissociation of methane molecules besides the spillover process at room temperature. Results indicate the possibility of utilizing the sensor structure with novel dispersal of Pd catalyst clusters on SnO2 film surface for efficient detection of methane at room temperature under the illumination of UV radiations.

O 55: Theoretical methods II

Time: Wednesday 16:45–19:15 Location: MA 043

O 55.1 Wed 16:45 MA 043

Interacting electrons in a quantum dot: A wave packet approach — •Johannes Eiglsperger[1], Susmita Roy[1], Christian Bracher[2], and Tobias Kramer[1] — [1]Institut für theoretische Physik, Universität Regensburg, Germany — [2]Physics Program, Bard College, Annandale-on-Hudson, USA

Solving quantum systems with interacting electrons is a complicated task: The antisymmetrization postulate renders calculations more and more cumbersome with increasing particle number n. The interaction between electrons entangles their dynamics, and the ensuing correlations leads to a full n-body wave function dependent upon $n \cdot d$ variables, where d is the dimensionality of the system, instead of simpler product states of single particle wave functions.

(TD)DFT is a popular and versatile method to describe the properties of these systems in terms of the electron density only, a function of d variables. However, the quality of the results depends critically on the sophistication of the employed exchange correlation functionals.

Semiclassical techniques based on wave packets offer a complementary approach. In our method, the system is modeled using complex coherent Gaussian states which populate a classical trajectory in phase space. The evolution of the trajectory is governed by Hamilton's equations. We employ this coherent state dynamics model to study n-electron quantum dots in a magnetic field.

O 55.2 Wed 17:00 MA 043

DFT based tight-binding with environment-dependent crystal field splittings — •Alexander Urban[1], Matous Mrovec[2,3], Christian Elsässer[2,3], and Bernd Meyer[1] — [1]ICMM/CCC, University of Erlangen-Nürnberg — [2]Fraunhofer IWM, Freiburg — [3]IAM-ZBS, Karlsruhe Institute of Technology

In traditional tight-binding (TB) models the intra-atomic (on-site) matrix elements of the Hamiltonian are approximated by constant atomic values and crystal field splittings are neglected. Using our recently developed scheme for deriving TB bond and overlap integrals from DFT calculations of arbitrary reference configurations it is, however, easy to analyze also the on-site integrals [1]. We find that the values of these matrix elements may depend strongly on the atomic environment, and neglecting the crystal field splittings introduces significant errors in the electronic structure. A new crystal field TB (CF-TB) scheme will be presented which allows to take the environmental dependence of the on-site terms into account [2]. The parameters for this straightforward extension of the Slater-Koster rules are readily accessible using our projection framework [1]. Comparisons of the CF-TB band structures and densities of states for a representative set of benchmark cases with DFT reference results demonstrate an enhanced transferability of the CF-TB parametrization.

[1] A. Urban, M. Reese, M. Mrovec, C. Elsässer, B. Meyer, *Phys. Rev. B* 84 (2011) 155119

[2] A. Urban, M. Mrovec, C. Elsässer, B. Meyer, *in preparation*

O 55.3 Wed 17:15 MA 043

Ferrocene-Peptide Charge Transfer on Gold Surface: a First Principles Study — •Filipe C. D. A. Lima[1], Arrigo Calzolari[2], and Helena M. Petrilli[1] — [1]Universidade de São Paulo, Instituto de Física - Brasil — [2]CNR-NANO Istituto Nanoscienze, Centro S3-Italia

Ferrocene-peptide self-assembled layers are one of the most studied redox-active assemblies on metal surfaces as prototypical models to probe heterogeneous electron transfer at hybrid interfaces. Recent experimental investigations have shown that the electron transfer in peptides can occur across long distances, by separating the donor from the acceptor.From the experimental point of view, it is not clear which charge transfer mechanism occurs in this type of system. We study the interaction of an oligo-peptide chain Fc-Gly-CSA (Ferrocene, Glycine and Cystamine) on the Au(111) from first principles calculations to evaluate its electron transfer mechanism. The method employed is based on the KS-DFT as implemented in the Quantum-ESPRESSO suit of codes, using ultrasoft pseudopotentials and the GGA-PBE exchange correlation functional to evaluate the ground-state atomic and electronic structure of the system. By analyzing the KS orbital at the Fermi Energy we see a high electronic density at the Ferrocene and minor contributions from the solvent and counter ion. On the other hand, higher energy states mainly contributes to the gold surface. We infer the considered models are able to simulate heterogeneous electron transfer and the results indicates an electron tunneling mechanism from the Ferrocene to the Surface.

O 55.4 Wed 17:30 MA 043

Redshift of excitons in carbon nanotubes caused by the environment polarizability: A BSE study — •Michael Rohlfing — Fachbereich Physik, Universität Osnabrück

Optical excitations of molecular systems can be modified by their physical environment. We analyze the underlying mechanisms within many-body perturbation theory (GW approximation and Bethe-Salpeter equation, BSE), which is particularly suited to study nonlocal polarizability effects on the electronic structure. Here we focus on the example of a semiconducting carbon nanotube, which observes redshifts of its excitons when the tube is touched by another nanotube or other physisorbates. We show that the redshifts mostly result from the polarizability of the attached ad-system. Electronic coupling may enhance the redshifts, but depends very sensitively on the structural details of the contact.

O 55.5 Wed 17:45 MA 043

xcitons in solids captured with bootstrap approximation for the exchange-correlation kernel of time-dependent density functional theory — •Sangeeta Sharma, J. K. Dewhurst, A. Sanna, and E. K. U. Gross — Max-Planck-Institut fur Mikrostrukturphysik, Weinberg 2, D-06120 Halle, Germany

The ab-initio calculation of optical absorption spectra of nanostructures and solids is a formidable task. The current state-of-the-art is based on many-body perturbation theory: one solves the Bethe-Salpeter equation (BSE). Unfortunately, solving the BSE involves diagonalizing a large matrix making this method computationally very expensive.

Time-dependent density functional theory (TDDFT) is another method able to determine neutral excitations of a system. Although formally exact, the predictions of TDDFT are only as good as the approximation of the exchange-correlation (xc) kernel. There are only a few xc-kernels which correctly reproduce the excitonic effect, but these kernels suffer from either being computationally as expensive as solving BSE or depend upon external parameters.

In our latest work we propose a new approximation[1] for xc-kernel, and demonstrate that this kernel is nearly as accurate as BSE and has the correct $1/q^2$ behavior. The computation cost for the bootstrap kernel is minimal and no system-dependent external parameter is required.

1. S. Sharma, J. K. Dewhurst, A. Sanna, E. K. U. Gross, Phys. Rev. Lett., 107, 186401 (2011).

O 55.6 Wed 18:00 MA 043

One-particle excitation energies and optical spectra of alkali-metal fluorides, oxides and nitrides

— •Christoph Sommer, Peter Krüger, and Johannes Pollmann — Institut für Festkörpertheorie, Universität Münster, D-48149 Münster, Germany

We present a comparative study of one-particle excitation energies and excitonic properties of the alkali-metal fluorides LiF, NaF and KF, oxides Li_2O, Na_2O and K_2O as well as nitrides Li_3N and Na_3N. To this end, we have calculated band structures based on self-interaction corrected (SIC) pseudopotentials as well as quasiparticle energies within the GW approximation. It turns out that DFT-SIC improves the band gaps of the alkali compounds considerably in comparision to the results of standard density-functional calculations. For the alkali fluorides and oxides, the SIC band gaps are very close to those of the quasiparticle bands while somewhat larger deviations occur for the nitrides. In particular, we find for Na_3N band gaps of 0.8 and 1.6 eV in SIC and GW, respectively. In LDA, on the other hand, Na_3N turns out to be metallic in contradiction to experiment. We have evaluated the optical spectra of the alkali compounds by solving the Bethe-Salpeter equation for a thorough comparison with experimental results that have been derived mainly from optical data for these materials. The influence of going towards self-consistency in the screened interaction W or using SIC as a starting point for GW is also discussed. On this basis, the experimental electronic band gaps available in the literature are examined closely.

O 55.7 Wed 18:15 MA 043

The Role of van der Waals Interactions for Non-Metallic Solids

— •Guo-Xu Zhang, Alexandre Tkatchenko, and Matthias Scheffler — Fritz-Haber-Institut der MPG, Faradayweg 4-6, 14195 Berlin, Germany

Cohesion in non-metallic solids arises mainly from covalent bonding and/or electrostatic interactions, and it is typically assumed that van der Waals (vdW) forces play a minor role. Nevertheless, the qualitative and quantitative role of vdW interactions has been a matter of discussion for quite some time. In particular, most state-of-the-art functionals, based on the generalized gradient approximation (GGA), meta-GGA, or (screened) hybrid functionals yield systematic deviations for the lattice constants, cohesive energies, and bulk moduli for a wide range of solid-state systems. We recently demonstrated that vdW interactions play an important role for the quantitative description of cohesive properties of benchmark semiconductors and ionic solids [1]. Here we extend our study to a wide range of materials including ionic crystals, semiconductors, and insulators. The vdW energy is computed using our recently developed DFT+MBD method [2], which includes short- and long-range Coulomb screening effects, and computes the many-body vdW energy to infinite order in the dipole approximation. We show that many-body vdW interactions play a significant role for cohesive properties of non-metallic solids.

[1] G.-X. Zhang *et al.*, Phys. Rev. Lett., in print (2011); [2] A. Tkatchenko, R. A. DiStasio Jr., R. Car, and M. Scheffler, submitted.

O 55.8 Wed 18:30 MA 043

Dispersion corrected DFT studies of molecule-surface interactions

— •Katrin Tonigold and Axel Gross — Institute of Theoretical Chemistry, Ulm University, D-89069 Ulm/Germany

The interfaces between soft and condensed matter are of vital importance for technological applications as well as in biological systems. Thus, a thorough description of both the substrate-adsorbate and the adsorbate-adsorbate interactions occuring at the interface is needed. In many cases these interactions are dominated by dispersion. Unfortunately, commonly used GGA density functionals are not able to describe these long-range correlation effects and more sophisticated methods are often computationally too demanding to be applied to extended surfaces.

Therefore, we employ and try to validate DFT-GGA calculations with semiempirical corrections for dispersion effects (DFT-D) regarding the adsorption of different kinds of molecules on (metallic) surfaces. Not only for the physisorption of aromatic molecules [1] or the interactions of the rest groups of chemisorbed thiolate molecules, but also for the adsorption of rather small inorganic molecules, such as water bilayers on metallic surfaces, dispersive interactions were found to be important [2].

[1] K. Tonigold and A. Groß, J. Chem. Phys. **132**, 224701 (2010).

[2] K. Tonigold and A. Groß, J. Comput. Chem., *accepted.*

O 55.9 Wed 18:45 MA 043

A High-Dimensional Neural Network Potential for Water: First Applications to Water Clusters

— •Tobias Morawietz, Vikas Sharma, and Jörg Behler — Lehrstuhl für Theoretische Chemie, Ruhr-Universität Bochum, D-44780 Bochum, Germany

Large-scale atomistic simulations using molecular dynamics or Monte Carlo methods require a reliable but efficient representation of the interatomic potential. In recent years, artificial neural networks (NNs) have been shown to provide accurate potential-energy surfaces (PESs) for complex systems. NNs are flexible functions, which allow to interpolate a set of energies and forces obtained from electronic structure data but can be evaluated several orders of magnitude faster. Here we present an application of our generalized NN scheme for high-dimensional systems [1], which incorporates long-range electrostatic interactions based on environment-dependent atomic charges [2], to water clusters [3]. We show that binding energies and vibrational frequencies for several stationary points on the NN-PES are in excellent agreement with reference DFT data.

[1] J. Behler, and M. Parrinello, PRL **98**, 146401 (2007).

[2] N. Artrith, T. Morawietz, and J. Behler, PRB **83**, 153101 (2011).

[3] T. Morawietz, V. Sharma, and J. Behler, submitted (2011).

O 55.10 Wed 19:00 MA 043

Static and Frequency Dependent Dipole Polarizabilities from the Ground-State Electron Density

— •Vivekanand Gobre[1], Robert DiStasio Jr.[2], Matthias Scheffler[1], and Alexandre Tkatchenko[1] — [1]Fritz-Haber-Institut der MPG, Berlin, Germany — [2]Princeton University, Princeton, NJ, USA

Molecular polarizability is an essential observable, and its accurate determination is important, e.g., for calculation of van der Waals interactions. Accurate polarizability calculations in principle require computationally expensive electronic structure methods with an explicit treatment of many-electron excitations. These methods can only be applied to systems with less than about 100 atoms. However, one is often faced with the problem of computing polarizabilities for large systems with thousands of atoms. We present a parameter-free computationally efficient approach to calculate accurate static and frequency dependent polarizabilities for molecules and non-metallic solids. Specifically, we link the TS-vdW [1] method, which accurately treats hybridization effects, with the self-consistent screening equation from classical electrodynamics [2]. Using only the electron density and reference data for the free atoms, we obtain an accuracy of about 7% for both static polarizabilities and van der Waals coefficients for a wide variety of systems. We illustrate the interplay of hybridization and long-range electrostatic screening effects for the polarizability of large proteins and condensed-matter systems. [1] A. Tkatchenko and M. Scheffler, PRL 102, 073005 (2009); [2] B. U. Felderhof, Physica 76, 486 (1974).

O 56: Metal substrates: Adsorption of organic / bio molecules III

Time: Wednesday 16:45–19:15 Location: A 053

O 56.1 Wed 16:45 A 053

Ruthenium dyes on Au(111) and Ag(111) investigated by scanning tunneling microscopy — •Nadine Hauptmann[1], Christian Hamann[1], Felix Köhler[2], Rainer Herges[2], Hao Tang[3], and Richard Berndt[1] — [1]Institut für Experimentelle und Angewandte Physik, Christian-Albrechts-Universität zu Kiel, 24098 Kiel, Germany — [2]Otto-Diels-Institut für Organische Chemie, Christian-Albrechts-Universität zu Kiel, 24098 Kiel, Germany — [3]CEMES/CNRS, 31055 Toulouse Cedex, France

Ruthenium dyes are promising candidates for sensitizers in dye-sensitized solar cells. We used electrospray ionization to deposit the dyes on Ag(111) and Au(111) surfaces in ultra high vacuum. The structure of the adsorbed molecules was analyzed with low-temperature scanning tunneling microscopy. In addition, scanning tunneling spectroscopy was used to investigate the electronic properties of the ruthenium dyes revealing sharp features in the differential conductance in addition to the HOMO-LUMO gap. Financial support by the Deutsche Forschungsgemeinschaft via the SFB 677 is acknowledged.

O 56.2 Wed 17:00 A 053

Organometallic opto-electronically active magnetic molecules on metallic surfaces — •Cormac Toher, Jörg Meyer, Anja Nickel, Robin Ohmann, Francesca Moresco, and Gianaurelio Cuniberti — Institute for Materials Science and Max Bergmann Center of Biomaterials, TU Dresden, 01062 Dresden, Germany.

Opto-electronically active organic molecules offer several advantages over traditional solid-state semiconductor materials in the fabrication of solar cells, including their low-cost, low weight, and flexibility. Here, we present the results of combined STM and DFT investigations of organometallic optoelectronically active magnetic molecules which are based on aza-BODIPY derivatives. Aza-BODIPY molecules have a tunable infra-red absorption and function as electron donors in organic solar cells [1, 2]. By switching between different central metal atoms such as Co or Zn, both magnetic and non-magnetic examples of this molecule can be synthesized. STS conductance measurements on the magnetic molecules suggest evidence of changes in their spin configuration when an electric field is applied. DFT calculations indicate that this may be due to the electrostatic spin-crossover effect [3].

[1]J. Meyer et. al, Phys. Chem. Chem. Phys. 13, 14421 (2011).
[2]R.Gresser et. al., Chem.-Eur. J. 17, 2939 (2011).
[3]N. Baadji et. al., Nature Materials 8, 813 (2009).

O 56.3 Wed 17:15 A 053

Cysteine on Ag(111) – Chiral self-assembly and temperature-dependant phase-transitions — •Sybille Fischer[1], Anthoula C. Papageorgiou[1], Matthias Marschall[1], Joachim Reichert[1], Katharina Diller[1], Florian Klappenberger[1], Francesco Allegretti[1], Alexei Nefedov[2], Christof Wöll[2], and Johannes V. Barth[1] — [1]Physik Department E20, Technische Universität München, 85748 Garching, Germany — [2]Institut für Funktionelle Grenzflächen, Karlsruher Institut für Technologie, Hermann-von-Helmholtz-Platz, 76344 Eggenstein-Leopoldshafen, Germany

Understanding the interactions between the chiral amino acid cysteine and metal surfaces is an important step towards creating tailored biofunctionalized surfaces using the molecule's chemical functionalities and medical properties. L-cysteine is involved in the pathogenetic mechanism of HIV [1] as well as in metal interaction centers of many proteins [2]. Being the only proteinogenic amino acid containing a thiol group, cysteine is also used to anchor longer peptides on metal surfaces.

Here a combined STM and XPS study on cysteine is presented. STM measurements at room temperature were carried out on both enantiopure cyteine compounds showing distinctive self-assembly patterns. A phase transformation was discovered after annealing to 400 K. XPS was employed to elucidate the driving force of this transformation. A strong chemical shift of the nitrogen 1s core level revealed a concomitant change of the molecule from a zwitterionic to an anionic state.

[1] Eck, H.-P. et al, *Biol. Chem. Hoppe-Seyler* **1989**, *370*, 101–108
[2] Barnham, K.J. et al, *Nat. Rev. Drug Discovery* **2004**, *3*, 205–214

O 56.4 Wed 17:30 A 053

Orientation-dependent electronic structure of a molecule investigated by STM and DFT with dispersion corrections — •Maya Lukas[1], Karin Fink[1], Kerrin Dössel[1], Alexandrina Stuparu[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

In recent years it has become obvious that the exact orientation and bond of a molecular wire to its connecting electrodes has a crucial influence on the molecular conductance. Determining the exact bond configuration as well as the electronic properties within the same experiment is hardly ever acchieved, if possible at all.

We investigated a molecule which consists of several identical molecular wires connected in a rigid conformation. Due to the form of the molecule, some of the wires protrude freely from the surface, while others are attached to it. The influence of the coupling to the surface electrode on the position and electronic properties of the molecule is investigated by scanning tunneling microscopy and density functional theory with dispersion corrections. Within the same molecular conformation, chemically identical parts of the molecule with different orientations towards the surface show strong variations of the electronic structure in the experiment as well as in the calculations.

O 56.5 Wed 17:45 A 053

Perylene derivative on Au(111): Influence of a large built-in dipole on molecular assembly and work function — •Jens Niederhausen[1], Heith Kersell[2], Henrike Wonneberger[3], Saw-Wai Hla[2], Jürgen P. Rabe[1], Klaus Müllen[3], and Norbert Koch[1] — [1]Humboldt- Universität, Institut für Physik, Berlin, Germany — [2]Ohio University, Physics & Astronomy Department, Athens, USA — [3]Max Planck Institut für Polymerforschung, Mainz, Germany

The anhydride- and diphenylamine-functionalized perylene derivative 9-(bis-p-tert-octylphenyl)-amino-perylene-3, 4-dicarboxy anhydride (ID28) is expected to exhibit a dipole moment as large as 12.2 Debye [1]. When evaporated on Au(111) in ultrahigh vacuum, ID28 molecules adopt a flat-lying conformation in the monolayer regime, as evident by room temperature scanning tunneling microscopy. We analyze the observed packing structures by involving molecule-substrate and molecule-molecule interactions, and the influence of the molecular dipole moment.

The macroscopic surface-normal electrostatic effect of the molecular dipole moment is investigated by ultraviolet photoelectron spectroscopy. The dipole of a monolayer of ID28 molecules shows no significant contribution to the sample work function. However, when going from monolayer to multilayer coverage we find a continuous work function decrease of up to about 1 eV. This is attributed to a preferred orientation of the molecules in multilayers, resulting in a macroscopic dipole pointing away from the sample surface.

[1] T. Edvinsson et al., J. Phys. Chem. C Letters 2007, 111, 15137

O 56.6 Wed 18:00 A 053

Charge state of a donor-acceptor complex on the surface of a metal — •Isabel Fernandez-Torrente, Tobias R. Umbach, Adrian Olivera, Jose Ignacio Pascual, and Katharina J. Franke — Institut für Experimentalphysik, Freie Universität Berlin, Berlin, Germany

The charge state of a molecule has a strong impact on its reactivity and transport properties. We investigate by means of scanning tunneling microscopy (STM) and spectroscopy (STS) the electronic properties of the electron-acceptor 2,3,5,6-Tetrafluoro-7,7,8,8-tetracyanoquinodimethane (F4TCNQ) adsorbed on Au(111), and its mixture with the electron-donor tetrathiafulvalene (TTF). Highly ordered pure F4TCNQ islands leave the underlying herringbone reconstruction unaffected. The charge state of the molecule depends strongly on the adsorption site: only the molecules located on the hcp regions are single charged, as demonstrated by the presence of a Kondo resonance in STS experiments. Combined deposition of TTF and F4TCNQ results in the formation of two mixed, ordered phases with 1:1 and 5(F4TCNQ):4(TTF) stoichiometries that destroy the reconstruction of the surface. The F4TCNQ within each unit cell are not homogeneously coupled to the surface due to the lateral interaction with TTF and, consequently, they exhibit different charge states. Furthermore, STS displays extremely sharp features on the F4TCNQ molecules of this mixed phases that are associated to charging/discharging events in a double barrier tunnelling junction mediated by the electric field of the STM tip.

O 56.7 Wed 18:15 A 053

Site-specific adsorption and reversible switching of C60 on porphyrin double-decker complexes — •Saranyan Vijayaraghavan, David Écija, Sushobhan Joshi, Willi Auwärter, and Johannes Barth — Physik Department E20, Technische Universität München, D-85748 Garching, Germany

Organic solar cells based on donor-acceptor architectures are the next paradigm in photovoltaics taking into account that they are flexible, easier to process than the inorganic counterparts and environmental friendly. . Accordingly, a fundamental understanding of molecular donor-acceptor systems is of immense interest for related applications. Here, we report a scanning tunneling microscopy (STM) and spectroscopy (STS) study characterizing C60 molecules on CeTPP2 arrays on a Ag(111) substrate. At low coverage and temperature, the C60s adsorb on the center of the top porphyrin of the CeTPP2, thus forming non-covalent porphyrin-C60 dyads. The STS measurements indicate a weak coupling of the C60 to the Ag substrate, as evidenced by a large HOMO-LUMO gap and a negative differential resistance regime. High-resolution images resolve three distinct orientations of the C60 on CeTPP2. By applying a current pulse with the STM tip, it is possible to switch individual C60s between these three configurations without changing the lateral registry. A plot of tunneling current vs. time reveals three levels of conductance. Each level corresponds to one of the distinct C60 orientations and thus represents a specific intra-dyad coupling

O 56.8 Wed 18:30 A 053

Tuning the electronic and magnetic properties of adsorbed Co porphyrin molecules by NO as an axial ligand — •Christian Felix Hermanns, Matthias Bernien, Alex Krüger, Jorge Miguel, and Wolfgang Kuch — Freie Universität Berlin, Arnimallee 14, 14195 Berlin, Germany

Metalloporphyrin molecules consist of a metal ion, surrounded by a planar porphyrin ligand and two axial coordination sites, which can be occupied by additional ligands like small molecules or a metal surface. This allows to tune the electronic and magnetic properties of the ion.

Here, we report on X-ray absorption spectroscopy (XAS) measurements of submonolayers of Co octaethylporphyrin (CoOEP) molecules and NO-CoOEP nitrosyl complexes on bare and oxygen-covered Ni films grown on Cu(100). Angle-dependent N K edge XAS measurements reveal a quasi-flat adsorption of CoOEP on both substrates.

By means of Co $L_{3,2}$ X-ray magnetic circular dichroism (XMCD) spectra we demonstrate, how the ferromagnetic substrate, as an additional ligand to the CoOEP molecules, induces a magnetic ordering on the spins of the Co ions, which are on both substrates parallel aligned to the Ni magnetization. The adsorption and thermal desorption of NO, as second axial ligand to CoOEP enables the reversible switching of the electronic properties of the Co ions on the oxygen-covered Ni films. On both substrates, angle-dependent Co $L_{2,3}$ XAS measurements reveal different oxidation states of the Co ions of CoOEP and NO-CoOEP.

This work is supported by the DFG (Sfb 658).

O 56.9 Wed 18:45 A 053

Free-base porphine on Ag(111): Repulsive interaction and substrate mediated phase transitions. — •Felix Bischoff, Willi Auwärter, David Écija, Saranyan Vijayaraghavan, Sushobhan Joshi, Knud Seufert, and Johannes V. Barth — Physik Department, E20, TU München, Germany

Motivated by nature, porphyrins have been established as useful building blocks in functional nano-architectures. A key issue is the tailoring of porphyrin building blocks with desired properties, yet a detailed understanding of the influences of different constituents, such as meso-substituents and central metal ions, is still lacking. To advance the control of surface-confined porphyrins, we studied the simplest molecule - the porphine - that is the basic macrocyclic body of all porphyrins. We present systematic low-temperature STM experiments of free-base porphines (2H-P) on Ag(111). At low coverages, porphines exhibit a disordered phase, indicating repulsive electrostatic interactions that could arise from charge-transfer bonds with the metal substrate. The molecules are selectively chemisorbed at specific adsorption sites. This also causes substrate-mediated phase transitions with increasing coverage from a disordered lattice gas, to a liquid-like phase, to a regular solid and finally to a glassy layer that shows an average positional, but no orientational order.

O 56.10 Wed 19:00 A 053

2D glassy crystals from flexible molecular modules — •David Ecija[1], Saranyan Viyagaravhan[1], Willi Auwärter[1], Sushobhan Joshi[1], Knud Seufert[1], Claudia Aurisicchio[2], Davide Bonifazi[2], and Johannes V. Barth[1] — [1]Physik Department E20, Technische Universität München, D-85748 Garching, Germany — [2]University of Namur, Department of Chemistry, B-5000 Namur, Belgium

Molecular glassy crystals are materials where the constituents are positioned in registry with a periodic crystalline lattice, but the molecular units are disordered regarding their orientational degrees of freedom. Here, to our knowledge, we present for the first time a two-dimensional (2D) analogue of the three-dimensional glassy crystal state of matter, i.e, a 2D glassy crystal. In particular, the deposition of a flexible molecular module on Cu(111) gives rise to distinct phases whose characteristics have been examined in real space by scanning tunneling microscopy: a hitherto unrecognized 2D conformational glassy crystal and a 2D orientational glassy crystal, respectively. Herein, the 2D conformational glassy crystalline phase constitutes a novel organization of matter, which combines local conformational disorder and translational symmetry. Both phases are porous and exhibit an arrangement of nanopores that are stabilized by the simultaneous presence of pyridyl-Cu-pyridyl links and C-H***N interactions. In the 2D conformational glassy crystal the framework displayed unprecedented flexibility as probed by the STM tip that modifies the pore shape, a prerequisite for adaptive behavior in host-guest processes.

O 57: Solid / liquid interfaces II

Time: Wednesday 16:45–18:45 Location: A 060

O 57.1 Wed 16:45 A 060

Two-Dimensional Colloidal Alloys — •Adam Law[1], Martin Buzza[2], and Tommy Horozov[3] — [1]Max Planck Institute for Intelligent Systems, 70569 Stuttgart, Germany — [2]Surfactant and Colloid Group, Department of Physics, The University of Hull, England, HU6 7RX — [3]Surfactant and Colloid Group, Department of Chemistry, The University of Hull, England, HU6 7RX

We study both experimentally and theoretically the structure of mixed monolayers of large (3 μm) and small (1μm) very hydrophobic silica particles at an octane/water interface as a function of the number fraction of small particles. We find that a rich variety of two-dimensional hexagonal superlattices of large and small particles can be obtained in this system experimentally due to strong and long-range electrostatic repulsions through the nonpolar oil phase. These represent the first experimental results for long-range order in a 2D binary colloid system. The structures obtained for the different compositions are in good agreement with zero temperature lattice sum calculations and finite temperature Monte Carlo simulations. Our theoretical analysis also reveals that the melting behaviour of the superlattice structures is very rich, proceeding via a multi-stage process, with melting temperatures that have a very strong and non-monotonic dependence on composition.

O 57.2 Wed 17:00 A 060

Photoelectrochemical Characterization of Bimodal *ZnO* Nanostructures as Photoanodes in Dye-sensitized Solar Cells — •Christoph Richter[1], Michael Schröder[2], Melanie Rudolph[1], Max Beu[1], Bernd Smarsly[2], and Derck Schlettwein[1] — [1]Justus-Liebig-Universität Gießen, Institut für

Angewandte Physik, Heinrich-Buff-Ring 16, D-35392 Gießen — [2]Justus-Liebig-Universität Gießen, Physiklaisch-Chemisches Institut, Heinrich-Buff-Ring 58, D-35392 Gießen

Bimodal *ZnO* nanostructures were fabricated by electrochemical deposition from aqueous solution. A layer of monodisperse polystyrene spheres obtained by mini-emulsion polymerization acts as a template for the electrodeposition. *EosinY* serves as a structure-directing agent towards formation of a mesoporous *ZnO/EosinY* hybrid material. *EosinY* can easily be removed by soaking in an aqueous solution of sodium hydroxide. The polystyrene spheres are chemically decomposed and a meso-macroporous network of *ZnO* is obtained. Following sensitization by a dye monolayer, these films were characterized by intensity modulated photocurrent spectroscopy (IMPS), intensity modulated photo voltage spectroscopy (IMVS), open circuit voltage decay (OCVD) and electrochemical impedance spectroscopy (EIS). Charge transport, recombination and photovoltaic properties are discussed.

O 57.3 Wed 17:15 A 060

Electrocatalytic activity of small Pt nanoparticles on monolayer graphene supported by Ru(0001) — •Christoph U. Lorenz, Otavio B. Alves, and R. Jürgen Behm — Ulm University, D-89069 Ulm, Germany

With their characteristic Moiré-type nm-scale superstructure, graphene monolayers supported on metal single crystals [1,2] can serve as ideal, chemically inert template for the growth of ordered arrays of very small nano-sized metallic (electro-)catalyst particles. For Pt deposition on gr/Ru(0001), particles fabricated by metal vapor deposition under ultrahigh vacuum conditions, displayed heights of a few layers and lateral diameters in the range of 1-2 nm as measured by STM [3,4]. Based on their narrow size distribution and their regular arrangement, these Pt nanoparticles appear as interesting and promising system for (electro-)catalytic model studies. Cluster arrays with different Pt coverages and cluster size distributions, which were determined by STM, were tested as electrodes for elementary reactions such as hydrogen evolution/oxidation, CO oxidation, and O2 reduction. Potential-dependent reaction rates were measured in a wall-jet type flow cell located in an electrochemical pre-chamber attached to the main UHV system. The electrochemical behavior of the Pt cluster arrays will be discussed in comparison to bulk Pt and realistic carbon supported Pt catalysts. [1] C. Oshima et al., J. Phys. Condens. Matter 9, 1 (1997). [2] S. Marchini et al., Phys. Rev. B 76, 075429 (2007). [3] N'Diaye et al., New J. Phys. 11, 103045 (2009). [4] K. Donner & P. Jakob, J. Chem. Phys. 131,164701 (2009).

O 57.4 Wed 17:30 A 060

EC-STM study of bulk Cu(1 1 1) and Cu covered Au(1 1 1) electrodes in a phosphate buffer solution — •Christian Schlaup and Sebastian Horch — Center for Individual Nanoparticle Functionality (CINF), Department of Physics, Technical University of Denmark (DTU), DK–2800 Kongens Lyngby, Denmark

Copper is known to have an outstanding catalytic activity for the electroreduction of carbon dioxide. For a deeper insight into the involved sites as well as their dynamics under reaction conditions well defined single crystalline copper surfaces can be used as an adequate model system.

In a first step the fundamental interaction of both, a bulk Cu(1 1 1) surface and a laterally expanded Cu surface, i.e. an ultrathin Cu film on a Au(1 1 1) electrode, in contact with neutral phosphate buffer electrolyte has been studied using in-situ STM. Thereby, depended on the actual sample treatment, several phases, e.g. phosphate adsorbate or copper oxide film, were found and characterized.

O 57.5 Wed 17:45 A 060

Analyzing the hydrodynamic boundary condition at solid-liquid interfaces with fluorescence correlation spectroscopy — Stoyan Yordanov, David Schäffel, Roman Schmitz, Burkhard Dünweg, Kaloian Koynov, and •Hans-Jürgen Butt — Max-Planck-Institut für Polymerforschung, Mainz, Deutschland

An important step towards an understanding of hydrodynamics is determining the correct boundary conditions. A new method for direct studies of flows in the close proximity of a solid surface has been developed. It is based on total internal reflection fluorescence cross-correlation spectroscopy (TIR-FCCS).

The effect of TIR is used to create an evanescent optical field that excites fluorescent tracer particles flowing with the liquid. A high numerical aperture microscope objective is employed to monitor simultaneously the fluorescent light from two small and laterally shifted (in flow direction) observation volumes. A cross-correlation of the fluorescent signals from these volumes yields the tracers and hence the flow velocity. By tuning the TIR conditions and therefore the evanesced wave penetration depth we can determine flow velocity profiles in the range 0-300 nm from the interface.

O 57.6 Wed 18:00 A 060

Dynamic Electro-Chemo-Mechanical Analysis — •Qibo Deng[1], Maxim Smetanin[1], and Jörg Weissmüller[1,2] — [1]Institut für Werkstoffphysik und -Technologie, Technische Universität Hamburg-Harburg, Hamburg — [2]Institut für Werkstoffforschung, Werkstoffmechanik, Helmholtz-Zentrum Geesthacht, Geesthacht

In various instances in surface science it is of relevance to study coupling between mechanical stress or strain of surface and its thermodynamic or electrochemical properties. Experiments use alternatively cantilever bending measurements of the variation of surface stress f, with charge density q, during electrochemical cycles or Dynamic Electro-Chemo-Mechanical Analysis(DECMA), which detects the coupling between electrode potential E, and strain e. At equilibrium, a Maxwell relation equates relevant response parameters,$\zeta_E = \zeta_f$ where $\zeta_f = \mathrm{d}f/\mathrm{d}q|e$ and $\zeta_E = \mathrm{d}E/\mathrm{d}e|q$. The surfaces under study are not perfect single crystals. They contain defects such as step edges and terraces. Indeed ζ_E or ζ_f vary significantly between as-prepared and annealed states of electrode. A recent analysis of surface stress measurements on rough electrode surfaces finds corrugation has an important effect on the way in which f is transferred into the substrate. The action of f can even invert its sign; this appears at moderate values of roughness. We adopt theory to correct DECMA data. Our analysis shows the variation of ζ_E between different states of surface is indeed controlled by mechanics and can be precisely corrected. The finding has implications for reported values of ζ and for the design of commercial cantilever arrays exploiting surface stress changes for sensing.

O 57.7 Wed 18:15 A 060

Diffuse scattering of Hg-electrolyte interface — •Benjamin Runge[1], Annika Elsen[1], Sven Festersen[1], Moshe Deutsch[2], Oliver H. Seeck[3], Olaf M. Magnussen[1], and Bridget M. Murphy[1] — [1]Institute for Experimental and Applied Physics, CAU, Kiel, Germany — [2]PETRA III, DESY, Hamburg, Germany — [3]PD, Bar-Ilan University, Ramat-Gan, Israel

Surface x-ray scattering methods belong to the very few experimental approaches that allow access to data on the nano-scale structure of liquid surfaces and in particular liquid-liquid interfaces. Here first x-ray diffuse scattering studies of a liquid-liquid interface are presented for the case of an interface between liquid Hg and electrolyte solutions. By these studies the lateral correlations caused by surface capillary waves were investigated. The measurements were carried out at the new liquid interface scattering apparatus (LISA) at the high resolution X-ray diffraction beam line P08 at the PETRA III synchrotron radiation source. Previous x-ray reflectivity studies [1] revealed a dependence of the interface width on the applied potential, not consistent with capillary wave theory. The diffuse scattering studies focus on obtaining further insight into the origin of this dependence and on the effect of the potential on the capillary waves.

[1] A. Elsen, et al., Phys. Rev. Lett., 104. 105501 (2010)

O 57.8 Wed 18:30 A 060

Development of an electrochemical flow-through cell for *in situ* characterization of UHV-fabricated model surfaces — •Otavio B. Alves and R. Jürgen Behm — Ulm University, Institute of Surface Chemistry and Catalysis, 89069 Ulm, Germany

We report on the assembly of a wall-jet type electrochemical flow cell for electrochemical and electrocatalytic characterization under controlled and continuous electrolyte flow, which is connected to an ultrahigh vacuum scanning tunneling microscopy (UHV-STM) system via a sample transfer system. The electrochemical set-up exhibits a "true" wall-jet hydrodynamic characteristics [1-2]; and offers a high sensitivity, low solution hold-up and reproducible mass-transfer conditions when coupled to a closed loop miniature flow controller. We will discuss the experimental verification of the theoretical predictions for the limiting diffusion current [2] at UHV prepared single crystalline electrodes. It will also be examined in how far the Frumkin-Tedoradze [3] or an analogous treatment [4-5] is suitable for describing the measured kinetic data.

[1] M. B. Glauert, *J. Flui Mech.* 1, **1956**, 625.
[2] J. Yamada et al., *J. Electroanal. Chem.* 148, **1983**, 201.
[3] A. N. Frumkin et al., *Z. Elektrochem.* 62, **1958**, 252.
[4] W. J. Albery, *J. Electroanal. Chem.* 191, **1985**, 1.
[5] R. G. Compton et al., *J.Appl. Eletrochem.* 21, **1991**, 295.

O 58: Poster Session III (Solid/liquid interfaces; Metals; Semiconductors; Oxides and insulators)

Time: Wednesday 18:15–21:45 Location: Poster B

O 58.1 Wed 18:15 Poster B

Dye-sensitized Zinc Oxide on Tungsten Wire Electrodes — •Tim Helbig, Melanie Rudolph, and Derck Schlettwein — Justus-Liebig-Universität Gießen, Institut für Angewandte Physik, Heinrich-Buff-Ring 16, D-35392 Gießen

Thin films of Zinc Oxide/Eosin Y were deposited on tungsten wires via electrochemical deposition from aqueous solutions by using the dye Eosin Y as a structure-directing agent (SDA). After deposition the SDA was removed by an aqueous alkaline solution, leaving behind a porous zinc oxide film. As a sensitizer, the dye D149 was adsorbed to the surface of the porous zinc oxide. The films were studied as photo anodes in dye-sensitized solar cells (DSC) using the tungsten wire as back contact. The photoelectrochemical performance was measured in an iodide-containing electrolyte and a platinum wire as counter electrode. As light source a xenon arc lamp with an energy output of $100mW/cm^2$ was used. A photovoltaic efficiency of such cells of up to 1.4 % was reached but the films could not be stabilized under the present conditions. Degradation mechanisms and optimization strategies will be discussed.

O 58.2 Wed 18:15 Poster B

Measuring hydrodynamic force on soft materials — •Farzaneh Kaveh, Michael Kappl, and Hans-Jürgen Butt — Max-Planck Institute for Polymer Research, Mainz, Germany.

Hydrodynamic drainage occurs when two surfaces approach each other in liquid. When the distance between the surfaces becomes small, the confined liquid in the gap is squeezed out. At high approaching velocity, the shear rate is high, causing a hydrodynamic force. Recent measurements have shown that at such a high shear rate, the no slip boundary condition may break down, even in the case of complete wetting. Hydrodynamic force at the nanometre scale has been measured on hard substrates and on bubbles in other works [1]. We aim to measure hydrodynamic force on soft substrates and apply a model which has been developed for deformable interfaces [2]. The goal is to understand the influence of soft substrates on hydrodynamic boundary condition at different velocities. The measurements are carried out by atomic force microscopy (AFM) using fresh cured polydimethylsiloxane (PDMS) as a soft substrate and 10 μm borosilicate glass spheres attached to a tip-less cantilever (colloidal probe technique). We record forces at approaching velocities of 0.5-120 μm/s. At low velocities, i.e., low shear rates no slip will occur. At high approaching velocities, slip may occur and should be visible in the hydrodynamic force.

[1] Bonaccurso E., Butt H.-J., Craig V.S., *Phys. Rev. Lett.* **90**, 144501 (2003).

[2] Carnie S.L., Chan D.Y.C., Lewis C., Manica R., Dagastine R.R., *Langmuir* **21** (7), 2912 (2005).

O 58.3 Wed 18:15 Poster B

GIXD and X-ray reflectivity studies on the mercury-electrolyte interface under potential control — •Sven Festersen[1], Annika Elsen[1], Benjamin Runge[1], Oliver H. Seeck[2], Moshe Deutsch[3], Olaf M. Magnussen[1], and Bridget M. Murphy[1] — [1]Institute for Experimental and Applied Physics, Christian-Albrechts-Universität, Kiel, Germany — [2]PETRA III, DESY, Hamburg, Germany — [3]PD, Bar-Ilan University, Ramat-Gan, Israel

The interface between mercury and electrolyte solutions has been subject of extensive electrochemical studies, but structural information is largely lacking up to now. To investigate the interface structure on atomic scales, in situ GIXD and X-ray reflectivity measurements on a mercury electrode in aqueous solution, containing NaF, NaBr and $PbBr_2$, have been performed. Experiments were carried out at different potentials applied using the LISA liquid surface diffractometer at PETRA III (DESY, Hamburg). Using in situ x-ray reflectivity studies a potential dependent reversible adlayer formation at the mercury-electrolyte interface has been observed. Additional peaks in the reflectivity data also suggested electrochemical growth of 3D crystallites at the interface. The existence of the latter was confirmed by grazing incidence diffraction. The existence of partial powder rings indicates a preferred orientation of these crystallites with respect to the interface.

O 58.4 Wed 18:15 Poster B

Charge transfer processes in platinum-silicon-diodes induced by electrochemical surface reactions at the platinum-sulfuric acid interface — •Damian Bürstel and Detlef Diesing — Fakultät für Chemie, Universität Duisburg-Essen, D-45117 Essen, Germany

Schottky diodes consisting of a 16 nm platinum film as electrochemical working electrode and a n-doped Si<111>-substrate as back electrode are used to study the energy dissipation and charging effects of the platinum film induced by electrochemical surface reactions. For this purpose cyclovoltammetric experiments are carried out in 1 M sulfuric acid and the charge transfer processes between the platinum and the silicon back electrode is measured as a current j_{dev} during this experiments. Furthermore these processes are studied as a function of the internal barrier height varied by applying a bias U_{bias} at the silicon back electrode. The current j_{dev} may monitor excitations and also heating effects of the platinum film since diodes with a low internal barrier are sensitive for excitations with very small energies. It is shown that j_{dev} depends significantly on U_{bias} which is comparable with results from photo excitation experiments for these devices. An additional current in j_{dev} is measured in the H_{upd} region. This effect can be explained by a modification of the internal field of the diode due to a shift in the chemical potential caused by the adsorption of hydrogen. This shift can achieve values of 20 mV for the whole H_{upd} region. Sulfate and oxygen adsorption have a much smaller effect on the chemical potential of the film.

O 58.5 Wed 18:15 Poster B

Variations in backbone morphology of MnO_x infiltrated carbon xerogels — •Christian Weber[1], Volker Lorrmann[1], Gudrun Reichenauer[1], and Jens Pflaum[1,2] — [1]Bavarian Center for Applied Energy Research e.V. (ZAE Bayern), D-97074 Würzburg — [2]Julius-Maximilians-University of Würzburg, Institute of Physics, Experimental Physics VI, D-97074 Würzburg

Electrochemical capacitors (EC) bridge the gap between conventional capacitors with high power but low energy density and batteries with high specific energy density but rather low power density. In this contribution we analyzed hybrid capacitor structures relying on charge storage by the electrochemical double-layer between electrolyte and porous carbon electrode and an additional pseudocapacitance caused by redox processes of manganese oxide (MnO_x) with the electrolyte's ions. Variations in the structure of the carbon xerogel backbone and the amount of deposited MnO_x were characterized electrochemically and structurally. From MnO_x-mass uptake and its correlation with carbon particle size, we can conclude that the deposition of MnO_x preferably takes place on the external surface area of the carbon particles. As the amount of deposited MnO_x scales with the external surface area, a thinner layer will provide a more efficient use of the active material and lead to better electrode performance.

Financial support by Deutsche Bundesstifung Umwelt is thankfully acknowledged.

O 58.6 Wed 18:15 Poster B

Dilatation measurements of porous carbon electrodes during charging — •Anja Keckeisen[1], Christian Weber[1], Volker Lorrmann[1], Gudrun Reichenauer[1], and Jens Pflaum[1,2] — [1]Bavarian Center for Applied Energy Research e.V. (ZAE Bayern), D-97074 Würzburg — [2]Julius-Maximilians-University of Würzburg, Institute of Physics, Experimental Physics VI, D-97074 Würzburg

Electrochemical double layer capacitors, also known as “supercapacitors“ are high power energy storage devices. Due to purely electrostatic charge storage, they achieve very long cycle lifetimes. A suited model system for investigating porous electrodes are carbon xerogels since their properties like particle size or micropore distribution can be tuned in a controlled fashion. We present a method to measure the length variation of supercapacitor carbon electrodes upon charging. While performing cyclic voltammetry measurements we observe changes of the electrode dimensions as a consequence of ion loading into the carbon micropores. By varying the ratio between pore and ion size as well as the particle size of the carbon xerogel backbone we can draw conclusions on the influence of the carbon structure on the charging process, which provides a microscopic model of charging with respect to anions and cations.

O 58.7 Wed 18:15 Poster B

Shape-persistent linear oligomers. — •Robert May, Stefan-Sven Jester, and Sigurd Höger — Rheinische Friedrich-Wilhelms-Universität Bonn, Kekulé-Institut für Organische Chemie und Biochemie, Gerhard-Domagk-Str. 1, 53121 Bonn, Germany

Conjugated shape-persistent arylene-alkynylene oligomers are discussed as one-dimensional molecular wires and as building blocks for supramolecular materials as well as for two-dimensional adlayers on surfaces. Oligomerization reactions and subsequent recycling gel permeation chromatography for separation of the crude products allow an efficient acces to monodisperse oligomers of distinct oligomerization degree in sufficient quantities. Here we present an approach towards monodisperse shape-persistent oligo(phenylene-butadiynylene)s of up to 38 nm length. Self-assembled monolayers of these molecules at the liquid/solid interface (here: 1,2,4-trichlorobenzene/HOPG) are investigated by scanning tunneling microscopy.

O 58.8 Wed 18:15 Poster B

The crystal-fluid interface in a hard sphere system — •Andreas Härtel[1], Mohammad Hossein Yamanai[2], Martin Oettel[2], Roberto E. Rozas[1], Jürgen Horbach[1], Kirill Sandomirski[3], Stefan U. Egelhaaf[3], and Hartmut Löwen[1] — [1]Theoretische Physik II: Weiche Materie, Heinrich-Heine-Universität Düsseldorf, Germany — [2]Institut für Physik, WA 331, Johannes-Gutenberg-Universität Mainz, Germany — [3]Condensed Matter Physics Laboratory, Heinrich-Heine-Universität Düsseldorf, Germany

Properties of bulk crystals and the crystal-fluid interface in a system of hard spheres are studied by density functional theory using unconstrained minimization [1] of accurate fundamental measure functionals [2]. Results for free energies, density distributions and vacancy concentrations of bulk crystals compare very well to data from Monte Carlo simulations [3]. For the equilibrium hard-sphere crystal-fluid interface we combine fundamental measure density functional theory, Monte-Carlo computer simulation [4] and confocal microscopy experiments [5] on sterically-stabilized colloids to determine the orientation-resolved interfacial tension and stiffness.

[1] R. Ohnesorge et al, Phys. Rev. E **50**, 4801 (1994)
[2] H. Hansen-Goos and R. Roth, JPCM **18**, 8413 (2006)
[3] M. Oettel et al, Phys. Rev. E **82**, 051404 (2010)
[4] R. E. Rozas and J. Horbach, Europhys. Lett. **93**, 26006 (2011)
[5] K. Sandomirski et al, Soft Matter **7**, 8050 (2011)

O 58.9 Wed 18:15 Poster B

Molecular Scale Structure of Ionic Liquids near Electrodes — •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, Germany — [2]Technical University of Denmark and Risø National Lab, Roskilde, Denmark — [3]European Synchrotron Radiation Facility, Grenoble, France

To understand and optimize electrochemical processes in ionic liquids (ILs), information on their molecular-scale structure near electrodes is essential. Recent high-energy x-ray reflectivity experiments on dielectric substrates revealed interfacial layering comprised of alternating anion and cation enriched regions with this modulation decaying into the bulk liquid. To investigate the molecular-scale arrangement of ions near electrodes under electrochemical control, a novel sample chamber was developed. For the in-situ experiments at the High-Energy Micro Diffraction instrument at ID15, ESRF we selected two hydrophobic ILs based on butyl-1-methylpyrolidonium and tetrabutylammonium cations with the tris(pentafluoroethyl)trifluorophosphate anion that exhibit an exceptional wide electrochemical window. The solid-liquid interface between the ILs and a boron doped diamond substrate was studied at electrochemical potentials between -2.5 V and +1.6 V vs. platinum quasi reference electrode. Quantitative analysis of the experimental x-ray reflectivity data revealed distinct changes in the ion distribution near the interface, induced by the applied potentials.

O 58.10 Wed 18:15 Poster B

Determination of single crystal emissivity by comparison with black-body radiation — •Fabian Scheepers, Sara Wanjelik, and Mathias Getzlaff — Institute of Applied Physics, University Duesseldorf

Contactless determination of temperature provides advantages towards traditional thermometers. Pyrometers allow a quick measurement up to several thousand degrees Celsius even in physically and chemically aggressive environment. Based on Planck’s law, nowadays used devices are mostly limited by the knowledge of surface conditions. Ecspecially high reflective metals are the actual challenge. Their emissivity can vary over a large range. Therefore, the temperature and surface dependent correction coefficient must be known. Here we report concerning this correction for a tungsten surface; it was obtained by a spot infrared pyrometer that compared the apparent and their associated black-body radiation.The black-body was realised in the form of a cylindrical bore in the tested material and heated by electron impact. Additionally, a tungsten-based thermocouple was used for a second independent temperature determination.

O 58.11 Wed 18:15 Poster B

Removal of carbon impurities in tungsten by extended annealing — •Sven Kalka — Heinrich Heine Universität, Düsseldorf

In order to carry out experiments in the field of surface science, atomically clean surfaces have to be prepared. A clean surface on the atomic scale is also important when used as a substrate for further experiments, like deposition of thin films. In the case of W(110) surfaces, most of the adsorbates can easily be removed by heating the crystal to about 2000K. Tungsten carbides however are stable even at high temperature and need to be removed separately. Carbon is an impurity within the bulk and diffuses to the surface again, so the cleaning procedure needs to be repeated. Thus, the removal of the carbon impurities within the bulk or at least the near surface region is desirable. We exposed the crystal to an oxygen atmosphere of 10^{-6}mbar, while heating it for several days. With this approach, we reduce the carbon content within the crystal and the subsequent diffusion of carbon to the surface. By STM imaging and LEED, we can evaluate the remaining impurities on the surface directly. Comparison of STM images at different stages of the annealing process indicates a reduction of carbon within the bulk.

O 58.12 Wed 18:15 Poster B

Investigation of the laser-cleaning process on Lead photocathodes — •Susanne Schubert[1], Roman Barday[1], Thorsten Kamps[1], John Smedley[2], Robert Nietubyc[3], Andrei Varykhalov[1], and Giesela Weinberg[4] — [1]HZB, Berlin, Germany — [2]BNL, Upton, USA — [3]NCBJ, Swierk, Poland — [4]FHI, Berlin, Germany

Metal photocathodes are widely used in electron injectors due to their stability and long life time. Due to adsorption of contaminants the work function increases and thus the quantum efficiency is reduced. In order to increase the quantum efficiency of our Pb cathode we performed a cleaning procedure by means of a high power excimer laser as suggested by Smedley [1]. We present the results of a combined photo emission, SEM and quantum efficiency measurement study on witness samples. Thin Lead films were arc-deposited on optical polished Mo-substrates [2]. Before and after irradiation the sample was analyzed at 140 eV photon energy at a XPS/ARPES end station at the synchrotron radiation source Bessy II. Since the surface roughness is of concern for the injector performance it was examined before and after the irradiation procedure with white-light-interferometry and the surface morphology by means of SEM.

[1]J. Smedley et al, PRST-AB 11, 013502 (2008) [2]Rao, T. et al., IPAC 2010, THPEC020 (2010)

O 58.13 Wed 18:15 Poster B

Anisotropic Change in Surface Resistance upon Adsorption of Oxygen on Cu(110) as observed by IRRAS — •Jan Pischel, Olaf Skibbe, and Annemarie Pucci — Kirchhoff-Institut für Physik, Im Neuenheimer Feld 227, D-69120 Heidelberg

Adsorbate induced changes in the electrical conductivity of thin metal films are of great interest because of their importance in technological applications, e.g. microelectronic devices. By developping the concept of surface friction between conduction electrons and adsorbate, Persson showed that changes in surface resistance will result in a broadband infrared absorption feature in the case of reflection experiments with p-polarized radiation [1]. Taking advantage of that fact, Otto et al. showed that on the highly anisotropic Cu(110) surface, interaction between conduction electrons and adsorbates settling on top of the close-packed rows of the surface is restricted to the case where the plane of incidence is parallel to these rows [2].

Tying in with these findings, we investigated the anisotropic change in surface resistance induced by formation of the (2×1)O-Cu(110) *Added-Row* reconstruction, where involvement of the second layer lead to a non-vanishing change in surface resistance also in the case of perpendicular orientation of the plane of incidence with respect to the rows.

[1] B. N. J. Persson. Phys. Rev. B, **44**:3277-3296, 1991.

[2] A. Otto et al. New J. Phys., **9**:288, 2007.

O 58.14 Wed 18:15 Poster B

Adsorption geometry and phase diagram of Br/Pd(110)

— •Alexander Menzel, Peter Amann, Michael Cordin, and Erminald Bertel — Institute for Physical Chemistry, University of Innsbruck, Austria

As the adsorbate system Br/Pt(110)-c(2x2) at 0.5ML Bromine coverage can be used as a low-dimensional model system [1], we were interested in the phase diagram of Br and Cl on the isoelectronic Pd(110) surface.

The electronic surface resonances, which are responsible for the low-dimensional behavior in the case of Pt(110), can be found in ARPES spectra at Pd(110), too. The phase diagram of Br- and Cl-covered Pd(110) was studied for coverages below 1ML. Using LEED, well ordered c(2x4) and c(4x2) Br/Pd(110) phases were found for a coverage of 0.25ML and 0.75ML, respectively. A continuous spot splitting of fractional order spots is observed for coverages in between. As shown by STM, the spot splitting below 0.5ML is due to anti-phase domains in [001]-direction, whereas above 0.5ML, the splitting is caused by continuous compression along [110]-direction. Interestingly, the c(2x2) phase expected for 0.5ML cannot be observed in the temperature range of the experiments (above 100K). A diagram of the observed phases is presented.

[1] P. Amann et al., Eur. Phys. J B 10, 15 (2010).

O 58.15 Wed 18:15 Poster B

DFT Studies on the Adsorption of *R,R*-Tartaric Acid at Copper Surfaces

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The adsorption of organic molecules at metal surfaces has a wide range of applications, e.g. in corrosion protection, surface functionalization and heterogeneous catalysis. Typically, the products in heterogeneous catalysis are a mixture of enantiomers, but there are some systems yielding an excess of one species. Such enantioselective processes at surfaces have received a lot of attention in recent years. An important aspect of these systems is the modification of the bare metal surface by chiral modifier molecules. An important model system for the formation of globally chiral phases at surfaces is the adsorption of *R,R*-tartaric acid at the Cu(110) surface. Using density-functional theory, we investigate the structural and energetic properties of a variety of phases. Further, the influence of surface defects on the adsorption energy is studied.

O 58.16 Wed 18:15 Poster B

Co-Phtalocyanine on Au(100) Surfaces

— •Eva Rauls and Wolf Gero Schmidt — Theoretische Physik, Universität Paderborn, Warburger Str. 100, 33100 Paderborn

For several reasons, phtalocyanines (Pc) with or without metal center are currently under intense investigation in surface physics. The biocompatibility of these molecules together with their electronic structure makes them highly interesting for energy transfer processes in medical applications. In nanotechnology, they are especially useful due to their flexibility, since the basis of these molecules can easily be varied with different functional groups substituting parts of the molecule or simply attached to the core of the molecule. But already upon exclusively exchanging the center atom, the binding energy to a substrate, the molecular deformation or the spin state can be tailored.

In this work, we present our first principles investigations of Co-Pc on Au(100)-surfaces. In contrast to our previous studies of similar porphyrins on Au(111) [1] or Au(110), the flat surface geometry does not induce the strong deformation observed in these cases. A comparatively strong interaction of the complete molecule with the substrate is observed.

[1] S. Müllegger, E. Rauls, et al. ACS Nano 5, 6480 (2011).

O 58.17 Wed 18:15 Poster B

Adsorption dependent charge state of self-assembled donor-acceptor complexes on Au(111)

— •Tobias R. Umbach, Isabel Fernández-Torrente, Jose I. Pascual, and Katharina J. Franke — Institut für Experimentalphysik, Freie Universität Berlin, Arnimallee 14, 14195 Berlin, Germany

The redistribution of charge between organic species and surfaces plays a key role for tuning the electronic functionality of molecular organic compounds on metal surfaces. We investigate self-assembled monolayers of 11,11,12,12-tetracyanonaphtho-2, 6-quinodimethane (TNAP) mixed with sodium (Na) on a Au(111) surface by low temperature scanning tunneling microscopy and spectroscopy (LT-STM, LT-STS). Successive deposition of TNAP and Na leads to the formation of an ordered windmill structure of TNAP and Na. The molecules close to the soliton lines are single charged accompanied by a Kondo resonance observed in STS transport experiments. In contrast, all other TNAP molecules show no Kondo resonance. The adsorption site dependent charge state of the TNAP molecules in the Na-TCNQ layer is an indication for different alignments of the molecular orbitals and therefore variations of the charge transfer process.

O 58.18 Wed 18:15 Poster B

Adsorption of Diindenoperylene on Cu(111) Surfaces

— •Hazem Aldahhak, Eva Rauls, and Wolf Gero Schmidt — Theoretische Physik, Universität Paderborn, Warburger Str. 100, 33100 Paderborn

Thin films of organic molecules like diindenoperylene (DIP) on metal substrates are of great interest for the further miniaturization of organic optoelectronic devices. As recently reported, films of DIP molecules on Cu(111) surfaces behave ambipolarly. In contrast to deposition on largely extended terraces, deposition of DIP molecules on narrow terraces (<15 nm) of Cu(111) leads to an interesting structure with co-directionally oriented molecules, the symmetry of which is not dictated by the hexagonal substrate symmetry [1].

In order to clarify this behavior, we investigated the balance between intermolecular and molecule-substrate interactions in this system. We performed first principles density functional theory calculations for various adsorbate structures. For isolated DIP molecules, the calculation of the potential energy surface (PES) allows us to determine the activation energy for the mobility of the molecules as a prerequisite for self organisation. At higher coverages, the molecules are found to organise in adsorbate structures which agree well with the experimental findings in [1].

[1] De Oteyza et al., Phys. Chem. Chem. Phys. 11, 8741 (2009).

O 58.19 Wed 18:15 Poster B

Observing Structural Phase Dynamics and Molecular Aggregation in Real Time: Dispersive NEXAFS Applied to Organic Films

— •Markus Scholz[1,2], Christoph Sauer[1,2], Michael Wiessner[1,2], Holger Wetzstein[1,2], Achim Schöll[1,2], and Friedrich Reinert[1,2] — [1]Physikalisches Institut, Experimentelle Physik VII und Wilhelm Conrad Röntgen Research Center for Complex Material Systems (RCCM), Universität Würzburg, D-97074 Würzburg — [2]Gemeinschaftslabor für Nanoanalytik, Karlsruher Institut für Technologie KIT, D-76021 Karlsruhe

We present a novel experimental approach which allows following structural and electronic changes in organic films by quick near edge X-ray absorption fine-structure spectroscopy (QNEXAFS). This technique utilizes the energy-dispersive mode of the BESSY UE52-PGM beamline[1] and allows NEXAFS with about one second time resolution. We show the potential of the method on the example of thin films of the organic molecule 1,4,5,8-naphthalene-tetracarboxylicacid-dianhydride (NTCDA). The time-evolution of the NEXAFS signal recorded at different temperatures allows distinguishing between different processes that are involved in the reorganization of the film. Moreover, since the technique also monitors spectroscopic details we are able to observe changes within the signature of the NEXAFS spectra during the phase transition.

[1] Batchelor, Schmidt, Follath, Jung, Fink, Knupfer, Schöll, Noll, Siewert, Büchner, Umbach, Nuclear Inst. And Methods in Physics

Research Section A, Volume 575, Issue 3 (2007), 470

O 58.20 Wed 18:15 Poster B

Chemisorptive bonding of Pyrenetetraone on Cu(111) and Ag(111) measured with XSW — •Christoph Bürker[1], Jens Niederhausen[2], Steffen Duhm[3], Takuya Hosokai[4], Jörg Zegenhagen[5], Ralph Rieger[6], Joachim Räder[6], Klaus Müllen[6], Alexander Gerlach[1], Norbert Koch[2], and Frank Schreiber[1] — [1]Universität Tübingen, Germany — [2]Humboldt-Universität zu Berlin, Germany — [3]Chiba University, Japan — [4]Iwate University, Japan — [5]ESRF, France — [6]Max-Planck-Institut für Polymerforschung Mainz, Germany

The X-ray Standing Wave (XSW) technique [1] is a high precision method to obtain the vertical bonding distance for each chemical element of the molecule. In recent years it was shown that the bonding distance may be dependent on the substrate and correlated with the interaction strength [2].

We present the adsorption geometry of PYTON (4,5,9,10-Pyrenetetraone, $C_{16}H_6O_4$) on Cu(111) and Ag(111). Our results show a significant bending of the oxygen atoms towards the substrate, both for Cu(111) and for Ag(111). Furthermore, for both metals the bonding distance of PYTON is relatively small, indicating a strongly interacting, chemisorbed system with a possible charge transfer between PYTON and substrate. Comparing these results with PTCDA ($C_{24}H_8O_6$) adsorbed on the same metals [2,3] we see a stronger and almost substrate independent interaction of PYTON with Cu(111) and Ag(111). [1] J. Zegenhagen, Surf. Sci. Rep. **18** (1993),199 [2] S. Duhm et al., Org. Electr. **9** (2008),111 [3] A. Gerlach et al., Phys. Rev. B **75** (2007)

O 58.21 Wed 18:15 Poster B

Pentacene/Ag(110): A comparison of DFT and GW results with photoemmision data — •Daniel Lüftner[1], Thomas Ules[2], Georg Koller[2], Michael G. Ramsey[2], and Peter Puschnig[1] — [1]Lehrstuhl für Atomistic Modelling and Design of Materials, Montanuniversität Leoben, Franz-Josef-straße 18, A-8700 Leoben, Austria — [2]Institut für Physik, Karl-Franzens-Universität Graz, Universitätsplatz 5, A-8010 Graz, Austria

We have prepared a monolayer of pentacene on Ag(110) and studied its valence electronic structure by angle-resolved photoemission spectroscopy. Thereby, an extensive data set of the photocurrent I as a function of parallel momenta (k_x, k_y) and binding energy E_b has been obtained. By comparing this data cube with simulated momentum maps of various pentacene molecular orbitals, we unambiguously identify four molecular states between the Fermi level and the top of the Ag *d*-band. This allows us to investigate in detail their energetic positions, broadenings, and modifications in orbital shapes upon adsorption. Moreover, we have calculated the electronic structure of different geometric arrangements of pentacene molecules within the framework of density functional theory (DFT) and – on top of that – the G_0W_0 approximation. We show that G_0W_0 corrections greatly improve DFT band gaps and demonstrate that the G_0W_0 gaps are strongly dependent on the local environment of the pentacene molecule, an effect which is absent in DFT orbital energies. Finally, we compare the orbital energies from DFT and G_0W_0 calculations to the experimental values obtaiend for the pentacene monolayer on Ag(110).

O 58.22 Wed 18:15 Poster B

Spin crossover effect in single aza-BODIPY molecule — •Jörg Meyer, Anja Nickel, Robin Ohmann, Cormac Toher, Francesca Moresco, and Gianaurelio Cuniberti — Institute for Materials Science and Max Bergmann Center of Biomaterials, TU Dresden, 01062 Dresden, Germany

Aza-BODIPY are a class of organic fluorescent dyes which have recently become interesting for organic photovoltaics because of their strong tuneable infrared absorption and their high stability. We investigated two molecular species consisting of two aza-BODIPY core units bound to one central metal atom by low temperature STM/STS and ab initio DFT calculations. The aim of this study was to find out how the different metal atoms (Co, Zn) influence the properties of the organic molecules. Because of steric hindrance among the aza-BODIPY ligands these molecules have a three dimensional structure. That is why the inner structure of the molecule could not be imaged by STM. We evaporated the aza-BODIPY onto a Ag(110) surface, separately. Both molecular species show two different adsorption geometries and are topographically identical. In the STS measurements of the Co-aza-BODIPY different spectra were obtained for the same position on the same molecule. One part of the spectra was very similar to those measured on Zn-aza-Bodipy, while the other spectra showed additional states near the Fermi level. DFT calculations indicate that the changes in these spectra are related to the spin crossover effect.

[1]J. Meyer et. al, Phys. Chem. Chem. Phys. 13, 14421 (2011).

O 58.23 Wed 18:15 Poster B

Self-assembled monolayers of phthalocyanines on gold substrates — •Nadezda Lilicenko[1], Florian Vogel[1], Ulrich Glebe[2], Ulrich Siemeling[2], and Frank Träger[1] — [1]Institur für Physik and Center for Interdisciplinary Nanostructure Scienece and Technology - CINSaT, Universität Kassel, Germany — [2]Institur für Chemie and Center for Interdisciplinary Nanostructure Scienece and Technology - CINSaT, Universität Kassel, Germany

Stable self assembled monolayers (SAMs) of advanced molecules on metal surfaces have attracted considerable attention over the last years. SAMs have found many applications, for example in nanotechnology, as biosensors, for chemical vapour sensing or molecular electronics. In this context, phthalocyanines (PCs) are of great interest, because they exhibit fascinating physical properties, which arise from their delocalized pi-electrons. In our experiments we have used two thioether substituted (sub-)phthalocyanine derivatives for SAM formation, one subphthtalocyanine with boron as central atom and one bis(phthalocyaninato)terbium - single molecular magnet. To study the adsorption of the molecules, we applied optical second harmonic generation (SHG). SHG permits to monitor adsorption process as well as the ordering within the film. The information about monolayer formation kinetics was obtained by fitting the measured SHG data with three kinetic models: first-order, second-order and diffusion limited Langmuir kinetic. As a complementary technique to proof that only monolayer formation takes place, ellipsometric measurements have been performed.

O 58.24 Wed 18:15 Poster B

Plasmonic light emission boosted by the charging of a molecule — Alexander Kabakchiev[1], Theresa Lutz[1], •Christian Dette[1], Christoph Grosse[1], Klaus Kuhnke[1], Uta Schlickum[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

The efficiency of light generation in a scanning tunneling microscope (STM) can depend on the accumulated charge on an individual organic molecule. We employ STM in ultra-high vacuum at liquid helium temperature to study tunnel-current-induced luminescence on the single molecule level. *fac*-Ir(ppy)$_3$ molecules deposited on a C_{60} double layer on Au(111) are investigated by spatially resolved differential conductance spectroscopy and luminescence spectroscopy. We observe that individual Ir(ppy)$_3$ molecules are surrounded by an extended area in which the light emission is boosted by up to two orders of magnitude above the emission on the C_{60} layer. This area increases with the applied bias voltage. Optical spectroscopy reveals that the luminescence is not intrinsic to Ir(ppy)$_3$ but is due to locally excited tip-induced plasmons. Differential conductance maps exhibit a strong ring-like feature which coincides with the margins of the area of enhanced luminescence. We demonstrate that the efficiency of plasmon generation can thus be controlled by a reversible electric-field-induced elementary charge transfer.

O 58.25 Wed 18:15 Poster B

Deposition and investigation of Mn_{12} single molecule magnets on surfaces — •Philipp Erler[1], Stefan Ambrus[2], Sebastian Höll[1], Samuel Bouvron[1], Sönke Voss[1], Michael Burgert[2], 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) represent a class of metalorganic compounds which show magnetic bistability of purely molecular origin and a rich quantum spin behavior below a certain blocking temperature. Because of their superparamagnetic properties and the additional benefits of a monodisperse size distribution, an inexpensive fabrication through self-assembly and the chemical tunability of their molecular ligand shell, SMMs are particularly interesting for applications in spin-based data storage and quantum-computing technologies.

Here we present a detailed study of several Mn_{12} derivatives chemically bound to a gold surface. We investigated the structural and electronic properties of the Mn_{12} molecules in a self-assembled monolayer by means of scanning tunneling microscopy (STM) and spectroscopy (STS) and X-ray photoelectron and absorption spectroscopy (XPS, XAS). Low temperature STM images are shown, revealing a submolecular resolution. Furthermore, we implemented electrospray ionization (ESI) for the deposition of Mn_{12} molecules in ultra high vacuum. In contrast to a wet chemical preparation procedure, this method offers the advantages of a control over the surface coverage and a free choice of the substrate and the molecular ligand.

O 58.26 Wed 18:15 Poster B

Characterizing a Charge Transfer Complex by nc-AFM/STM — •Fabian Schulz, Isabel Fernandez-Torrente, Adrian Olivera, Christian Lotze, Martina Corso, Katharina Franke, and Jose Ignacio Pascual — Freie Universität Berlin, Institut für Experimentalphysik, Arnimallee 14, 14195 Berlin, Germany.

The F4-TCNQ/Au(111) metal-organic interface is a promising candidate for the design of molecular organic electronics, due to its potential regarding Fermi level alignment and facilitation of charge-carrier injection. Therefore, much experimental and theoretical effort has been made to understand the charge transfer process taking place upon adsorption of F4-TCNQ on Au(111). Still, the results remain controversial [1], making more in-depth investigations necessary [2].

By combined qPlus noncontact-AFM/STM measurements - in both imaging and spectroscopy mode - we find the co-existence of two different ordered submonolayer F4-TCNQ/Au(111) phases, yielding also two different charge states. One of them shows a Kondo resonance in conductance experiments, indicating the existence of a single occupied molecular orbital and thus, charge transfer of one electron from the substrate to the molecule. Measurements of the local contact potential difference (LCPD) on different molecular sites reveal that the different charge states can be correlated with different LCPD values [3].

[1] Z.G. Soos *et al.*, Organic Electronics **12**, 39 (2011).
[2] G.M. Rangger *et al.*, Physical Review B **79**, 165306 (2009).
[3] L. Gross *et al.*, Science **324**, 1428 (2009).

O 58.27 Wed 18:15 Poster B

Triazatriangulenium on Ag(111) investigated with scanning tunneling and atomic force microscopy — •Katharina Scheil[1], Nadine Hauptmann[1], Christian Hamann[1], Thiruv. Gopakumar[1], Franziska Otte[2], Rainer Herges[2], and Richard Berndt[1] — [1]Institut für Experimentelle und Angewandte Physik, Christian-Albrechts-Universität zu Kiel, 24098 Kiel, Germany — [2]Otto-Diels-Institut für Organische Chemie, Christian-Albrechts-Universität zu Kiel, 24098 Kiel, Germany

Triazatriangulenium (TATA) has been proposed as a platform to controllably attach functional molecules to metallic surfaces. We used a combined low-temperature scanning tunneling and atomic force microscope in ultra high vacuum to investigate this platform on Ag(111) surfaces. The molecule TATA was deposited using electrospray ionization. TATA molecules arrange in a complex pattern comprising ring-like subunits. The underlying intermolecular interactions will be discussed. Financial support by the Deutsche Forschungsgemeinschaft via the SFB 677 is gratefully acknowledged.

O 58.28 Wed 18:15 Poster B

Mixing Chromophores in SAMs of Azobenzene Derivatives — •Daniel Brete[1,2], Daniel Przyrembel[2], Wolfgang Freyer[1], Robert Carley[1,2], Cornelius Gahl[1,2], and Martin Weinelt[1,2] — [1]Max-Born-Institut Berlin — [2]Freie Universität Berlin

Since photoisomerisation of azobenzene-functionalised alkanethiols in self-assembled monolayers (SAMs) on gold is generally suppressed, controlled dilution of the switching moieties is desirable.

In a solution of dissimilar thiols in general one component is preferentially adsorbed leading to a single component SAM. From a solution of two similar azobenzene-functionalised alkanethiols differing only by their tail group, 6-(4-trifluoromethyl-4'-azobenzeneoxy)-hexane-1-thiol and 6-(4-cyano-4'-azobenzeneoxy)-hexane-1-thiol, we obtained mixed SAMs. HR-XPS measurements show that the composition of the SAM reflects the concentrations of the two components in solution. Shifts in the XPS peak positions indicate that real mixing and not the formation of uniform islands occurs at the surface while NEXAFS data demonstrate that the orientation of the molecules in the mixed SAM is identical to that of the single component SAMs. This is a first step towards decoupling of the chromophores.

O 58.29 Wed 18:15 Poster B

Adsorption of fluorinated and non-fluorinated CuPc on Ag(111) — •Christoph Kleimann, Sonja Schröder, Benjamin Stadtmüller, Ingo Kröger, Christa Elsaesser, and Christian Kumpf — Peter Grünberg Institut (PGI-3), Forschungszentrum Jülich, 52425 Jülich, Germany and Jülich-Aachen Research Alliance (JARA) - Fundamentals of Future Information Technology

Organic thin films usually exhibit a variety of different structures when they adsorb on metal surfaces, depending on the particular interface properties. It is our goal to obtain a fundamental understanding of molecular assembly and the interaction characteristics for both, organic-metal contacts and hetero-organic interfaces.

Here we present results on the adsorption of copper(II)-hexadecafluoro-phthalocyanine (F16CuPc) on Ag(111). We have used spot-profile-analysis LEED (SPA-LEED) for identifying different phases, and scanning tunneling microscopy (STM) as well as x-ray standing waves (XSW) for further characterization.

At low coverages and room temperature a disordered phase is observed. When the first monolayer is closed, the molecules arrange themselves in long rows. Along the rows the molecules are very well ordered, but neighboring rows are often slightly shifted with respect to each other, which is reflected by well defined streaks in the SPA-LEED images.

We also present first results obtained for mixed layers of fluorinated and non-fluorinated molecules (F16CuPc and CuPc).

O 58.30 Wed 18:15 Poster B

Revealing molecular dynamics through Scanning Noise Microscopy and Spectroscopy — •Johannes Schaffert[1], Maren C. Cottin[1], Andreas Sonntag[1], Hatice Karacuban[1], Christian A. Bobisch[1], Nicolás Lorente[2], Jean-Pierre Gauyacq[3], and Rolf Möller[1] — [1]Faculty of Physics, Center for Nanointegration Duisburg- Essen, University of Duisburg-Essen, 47048 Duisburg, Germany — [2]Centre d'Investigació en Nanociència i Nanotecnologia (CSIC-ICN), Campus UAB, E-08193 Bellaterra, Spain — [3]Institut des Sciences Moléculaires d'Orsay, CNRS-Université Paris-Sud 11, UMR 8214, Bâtiment. 351, Université Paris-Sud, F-91405 ORSAY Cedex, France

We show how by adding the real-time characterization of the tunnelling current noise to the standard operation of Scanning Tunneling Microscopy (STM), switching processes on surfaces can be analyzed. This kind of Scanning Noise Microscopy (SNM) was applied for individually adsorbed organic CuPc molecules on Cu(111). It reveals excitation spectra as well as excitation maps with Angstrom spatial resolution. The Noise Spectroscopy clearly exhibits the molecular orbitals LUMO, HOMO and HOMO-1, which could be observed by conventional Scanning Tunneling Spectroscopy only faintly. The mechanism of the molecular switch could be identified as an in-plane libration between the ground state and two transiently occupied states. The findings are confirmed by Density Functional Theory calculations.

O 58.31 Wed 18:15 Poster B

Binary donor acceptor films of TTT and TNAP on Au(111) investigated by LEED and STM — •Benjamin Fiedler[1], Elena Rojo-Wiechel[1], Julia Simon[2], Johannes Beck[2], and Moritz Sokolowski[1] — [1]Institut für Physikalische und Theoretische Chemie der Universität Bonn — [2]Institut für Anorganische Chemie der Universität Bonn

We prepared pure and mixed monolayers of electron accepting and electron donating molecules, namely Tetrathiotetracene (TTT) and Tetracyanonaphthoquinodimethane (TNAP), on Au (111) under ultrahigh vacuum conditions. The films were studied by LEED and STM. Pure TTT shows a complex film growth with a disordered phase at low coverage and an ordered phase at high coverage. In addition, the deposition of TTT leads to a lifting of the Au (111) surface reconstruction. For TNAP the Au(111) surface reconstruction is preserved after deposition. The unit cells of the ordered monolayers of TTT and TNAP are orientated differently with respect to Au(111) surface, but exhibit similar size and shape. Both molecules arrange in brick wall type structures. Quite differently, in the mixed film the molecules are arranged in alternating parallel rows of one type of molecule. Interestingly, the two dimensional arrangement of TTT and TNAP is rather similar to that in alternating stacks of TTF/TCNQ bulk charge transfer crystals.

This work was supported by the DFG through SFB 813.

O 58.32 Wed 18:15 Poster B

HREELS Investigation of Ethene Chemisorption on Cu(110)

— •Emanuel Welsch, Olaf Skibbe, Jan Pischel, and Annemarie Pucci — Kirchhoff-Institut für Physik, Im Neuenheimer Feld 227, D-69120 Heidelberg

Nowadays, the adsorption of ethene has been studied extensively and is well understood on a large number of the many possible single crystal metal subtrates. However, the properties of the chemisorption systems C_2H_4 on Cu(110) and on roughened copper substrates have always been discussed controversially [1-3], comprising the questions of adsorption geometry and of the anomalous IRRAS intensity of the observed gas phase Raman active vibrational modes. Whilst the former has implications on the issue whether a certain mode is dipole allowed or not, the explanation of the latter demanded a new excitation mechanism. Such a mechanism, based on the creation of electron hole pairs, has been established for the case of roughened copper substrates [4].

In this work we present the results of recent HREELS measurements which clearly demonstrate that the abovementioned model cannot explain the activation of the Raman active modes in the case of C_2H_4/Cu(110). Furthermore the selection rules of impact scattering are applied in order to discuss the compatibility of the spectra with several of the possible adsorption geometries.

[1] C. J. Jenks et al. Surf. Sci. Lett., **277**:L89-L94, 1992.
[2] J. Kubota et al. Phys. Chem., **98**:7653-7656, 1994.
[3] R. Raval. Surf. Sci., **331-333**:1-10, 1995.
[4] A. Priebe et al. J. Phys. Chem. B, **110**:1673-1679, 2006.

O 58.33 Wed 18:15 Poster B

Chemical transformations drive complex self-assembly of uracil on close packed coinage metal surfaces

— •Anthoula C. Papageorgiou, Sybille Fischer, Joachim Reichert, Katharina Diller, Florian Blobner, Florian Klappenberger, Francesco Allegretti, and Johannes V. Barth — Physik Department E20, Technische Universität München, 85748 Garching, Germany

We address the interplay between adsorption, chemical nature and self-assembly of uracil on Ag(111) and Cu(111) surfaces as a function of molecular coverage and temperature. We find that the metal surface acts both as a template and a catalyst for the resulting self-assembled structures. With a combination of STM, synchrotron XPS and NEXAFS studies, we unravel a molecular phase map on Cu(111) consisting of three phases, in stark contrast to what is observed for the case of uracil on the more inert Ag(111) surface. On Ag(111) uracil adsorbs flat, intact and forms close packed two-dimensional islands. The self-assembly is driven by stable hydrogen bonded dimers with poor two-dimensional order. On Cu(111) complex structures are observed and we determine these phase transformations to be driven by gradual deprotonation of the uracil molecules. Our XPS study reveals the tautomeric signature of uracil in the contact layer and its deprotonation site. Our data show a dependence between molecular coverage and molecule-metal interaction, as the molecules tilt at higher coverages in order to accommodate for a higher packing density. After deprotonation of both uracil N atoms, the observed adsorption geometry can be understood only with significant charge redistribution in the molecule.

O 58.34 Wed 18:15 Poster B

Evolution of metallophthalocyanine multilayers on Cu(111) during thermal treatment depends on the type of metal center

— •Jie Xiao[1], Min Chen[1], Hans-Peter Steinrück[1], and J. Michael Gottfried[2] — [1]Lehrstuhl für Physikalische Chemie II, Universität Erlangen-Nürnberg, 91058 Erlangen, Egerlandstrasse 3, Germany — [2]Fachbereich Chemie, Universität Marburg, 35032 Marburg, Hans-Meerwein-Strasse, Germany

Vapor deposited multilayer (> 20 ML) Co-phthalocyanine (CoPc) on Cu(111) behaves differently than other transition metal phthalocyanines (MPcs) with the same coverage, such as ZnPc, CuPc and NiPc, when the respective multilayers are heated to a temperature well above their multilayer desorption temperature. For CoPc, the residual coverage is about 6 monolayers after annealing to 650 K, compared to 1-2 monolayers for the other MPcs. This has been found by X-ray and ultraviolet photoemission measurements. Transition metal phthalocyanines, including CoPc, have been demonstrated to adopt a flat-lying orientation on metal substrates, at least at submonolayer and monolayer coverages. However, the residual layer after CoPc desorption shows a different UP spectrum than a directly deposited film of the same coverage, suggesting that the post-heating step causes a different molecular orientation. Possible origins of this effect, including partial reaction of the peripheral C-H bonds with the Cu substrate, will be discussed. Support by the DFG through SFB 583 and the Alexander-von-Humboldt Foundation is gratefully acknowledged.

O 58.35 Wed 18:15 Poster B

STM Signatures of C60 and C58 on Au(111) Surfaces: a DFT Study

— •Melanie Stendel[1,2], Alexej Bagrets[2], Christian Seiler[1,2], and Ferdinand Evers[1,2] — [1]Institut für Theorie der Kondensierten Materie, Karlsruhe Institute of Technology (KIT), 76131 Karlsruhe, Germany — [2]Institut für Nanotechnologie, Karlsruhe Institute of Technology (KIT), 76344 Karlsruhe, Germany

Recent STM-experiments [1] have measured the surface topography of C60 molecules and two isomers of C58 adsorbed on a Au(111) surface. This topography exhibits a pronounced variation for the C60-fullerene and the C58 derivates, which highlights the significantly different electronic structure of the underlying species. Hence, the functionality of a putative fullerene-based thin film technology would be very sensitive to the use of the constituting molecule, C60, C58 and others.

Here, we present a systematic study of the possible adsorption geometries of C60 and C58 on Au(111) within the density functional theory (DFT). Further, we calculate a map of the local density of states in the tip-plane above the molecule for each geometry. Based on this map a qualitative comparison with experimentally determined topographies will be given.

[1] AG Kappes and AG Wulfhekel, Karlsruhe Institute of Technology (KIT), 76131 Karlsruhe, Germany, measurements to be published.

O 58.36 Wed 18:15 Poster B

Scanning tunneling microscopy and spectroscopy of TMP-TCNQ

— •Sandra Perkert[1], Katerina Medjanik[1], Shahab Naghavi[2], Milan Rudloff[3], Vita Solovyeva[3], Dennis Chercka[4], Torsten Methfessel[1], Sergej Nepijko[1], Michael Huth[3], Claudia Felser[2], Martin Baumgarten[4], Klaus Müllen[4], Gerd Schönhense[1], and Hans-Joachim Elmers[1] — [1]Institut für Physik, Johannes Gutenberg-Universität, 55099 Mainz, Germany — [2]Institut für Analytische und Anorganische Chemie, Johannes Gutenberg-Universität, 55099 Mainz, Germany — [3]Physikalisches Institut, Goethe-Universität, 60438 Frankfurt am Main, Germany — [4]Max-Planck-Institut für Polymerforschung, 55128 Mainz, Germany

Organic charge transfer (CT) salts are promising new materials for electronic devices. For a better understanding of their interaction with metal substrates we investigate thin films of the well-known acceptor 7,7,8,8-Tetracyanoquinodimethane (TCNQ) and the new synthesized donor Tetramethoxypyrene (TMP) on a W(110) and an Au(111) surface with scanning tunneling microscopy (STM) and spectroscopy (STS). The topographic images show a self-organized structure of TMP and TCNQ on both substrates. On the Au(111) surface TCNQ assembles in an oblique Bravais lattice with different orientational domains. STS measurements reveal the electronic structure of the molecules and the energetic position of HOMO and LUMO. The measured energy gap between HOMO and LUMO is much smaller for the CT-salt TMP-TCNQ than for the pure donor TMP and the pure acceptor TCNQ. These results fit well to theoretical calculations.

O 58.37 Wed 18:15 Poster B

Planar gold nano crystals as photonic substrate for single-molecule mechano-optical investigations

— •Sören Grannemann, Tamara Münnich, Volker Walhorn, and Dario Anselmetti — Biophysics and Applied Nanoscience, Faculty of Physics, Bielefeld University, Germany

The combination of scanning probe microscopy and optical microscopy techniques is a valuable tool for biological and biomedical investigations at the single molecule level. For these investigations transparent substrates are needed that allow easy sample immobilization. Thin (approx. 20nm) gold films are (quasi) transparent materials whose surface modification by thiol-chemistry is easy and well established. Planar gold nano crystals (PGNC) grown via the thermal aqueous solution method [1] exhibit sizes ranging from some 100 nm to several microns while their thickness lies in the range of roughly 20 nm. Furthermore, the Gold (111) surface is atomically smooth and ideally allows for the immobilization of self-assembled monolayers. We synthesized PGNC and immobilized them on indium tin oxide (ITO) coated glass cover slips. The nano-crystals were investigated by atomic force microscopy (AFM) to characterize their size, thickness and surface roughness. Furthermore, the excitation and detection of single molecule fluorescence through the PGNC by total internal reflection fluorescence (TIRF) microscopy is demonstrated. Therefore, we modified the immobilized PGNC with a mercapto-alkyl self-assembled monolayer exhibiting sparsely distributed amino moieties for dye attachment. [1] H.-C. Chu, C.-H. Kuo and M. H. Huang, Inorg. Chem., 808, 2006.

O 58.38 Wed 18:15 Poster B

UV-Vis spectroscopy studies of photoswitching of azobenzene-containing molecular platform adlayers on Au — •Nicolai Krekiehn[1], Ulrich Jung[1], Mathias Müller[1], Jens Kubitschke[2], Sandra Ulrich[2], Rainer Herges[2], and Olaf Magnussen[1] — [1]Institut für Experimentelle und Angewandte Physik der Christian-Albrechts-Universität, Kiel, Deutschland — [2]Otto-Diels-Institut für Organische Chemie Christian-Albrechts-Universität, Kiel, Deutschland

Photofunctional self-assembled monolayers (SAMs) on solid substrates are of current interest for the preparation of functional nanosystems. These SAMs, however, often exhibit inherent disadvantages as reduced structural order or strong electronic coupling with the substrate (in particular pronounced for metals), which may cause an efficient quenching of the desired functions. We recently introduced a novel aproach for formation of such SAMs basing on molecular platforms, whose structural properties (orientation of the function, lateral and vertical distances of the platforms) can be precisely controlled and verified this concept by STM[1] and various spectroscopies[2].

Here, we present preliminary spectroscopic studies of photoswitching in platform SAMs containing azobenzene, a prototypical molecular switch. Measurements were performed in either transmission or reflection geometry. The photoswitching reactions were found to obey 1st order kinetics and exhibit high quantum efficiencies.

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O 58.39 Wed 18:15 Poster B

Ultrathin films of NTCDA on Ag(111): Growth and thermal evolution beyond the monolayer — •Carolin R. Braatz, Gregor Öhl, and Peter Jakob — Fachbereich Physik, Philipps-Universität Marburg

The growth of well defined thin films of large organic molecules using molecular deposition techniques depends critically on the structural properties of the substrate and/or the contact layer between organic film and the substrate. A comprehensive characterization of these is therefore vital to arrive at an improved understanding of the growth mechanisms of organic layers with destined properties. In this contribution the growth and the thermal evolution of NTCDA layers on Ag(111) have been studied in the temperature range 80 – 550 K using FT-IRAS, SPA-LEED, and TPD. Particular attention is devoted to phase transformations of monolayer and bilayer NTCDA/Ag(111) under different growth conditions and their effect on the initial growth of multilayer films. The potential of IRAS as an in-situ analytical technique to characterize organic film growth is discussed.

O 58.40 Wed 18:15 Poster B

STM investigation on the adlayer structures of the ionic liquids EMIM-TFSA and BMP-TFSA on Au(111) in the submonolayer regime — •Benedikt Uhl, Michael Roos, and Rolf Jürgen Behm — Ulm University, Institute of Surface Chemistry and Catalysis, D-89069 Ulm, Germany

The adlayer structures of the ionic liquids (IL) 1-butyl-1-methylpyrrolidinium-bis(trifluoromethylsulfonyl)imide (BMP-TFSA) and 1-ethyl-3-methylimidazolium-bis(trifluoromethylsulfonyl)imide (EMIM-TFSA) on Au(111) have been investigated by scanning tunneling microscopy (STM). Especially the structure of the first layer of adsorbates on the metal surface is under investigation. The measurements were performed in ultra high vacuum (UHV) at temperatures between 100 K and 298 K, with coverages in the submonolayer and the monolayer regime. At temperatures around 100 K the BMP-TFSA as well as the EMIM-TFSA adsorbates appear as round shaped protrusions in the STM pictures. The nature of these protrusions, which may represent cations, anions or both of them, is discussed. Depending on the preparation process, the adsorbates form different structures, a 2D glass-like phase as well as 2D crystalline structures with long-range order. The different structures are presented in detail (2D density, unit cell) and their dependence on surface coverage is elucidated. The 2D crystalline structures show strong dependence on the Au(111) reconstruction pattern. In this context the influence of the substrate on the structure formation is discussed.

O 58.41 Wed 18:15 Poster B

STM investigation of PbPc adsorbed on Ag(111) — •jiang peng and hietschold michael — Chemnitz University of Technology, Institute of Physics, Solid Surfaces Analysis Group, D-09107 Chemnitz, Germany

We have investigated the adsorption of PbPc on Ag(111). Using OMBE, an ultrathin film of PbPc (a little more than one monolayer) has been deposited on Ag(111) and annealed for 20min to 250°C. Two different adsorption structures have been found. The molecular unit cells characterise A=1.59nm, B=1.84nm with a angle of 87°, and A=1.75nm, B=1.626nm with a angle of 79°, respectively. On the Ag(111) surface we found all of the shuttle-cock shaped molecules in the Pb-down adsorption configuration, no molecules have been adsorbed with the Pb atom up. PbPc molecules on the second layer lie directly on top of the first layer making a direct stack. The molecular adsorption structures found suggest at relatively strong interaction between Pb and Ag substrate, which forces central Pb atom in the down position.

O 58.42 Wed 18:15 Poster B

Ultraviolet photoemission from ionic liquids — •Rebecca Pöschel and Thomas Fauster — Friedrich-Alexander Universität Erlangen, Lehrstuhl für Festkörperphysik, Staudtstr. 7, 91058 Erlangen, Germany

Room-temperature ionic liquids entirely consist of molecular ions. Due to their very low vapor pressure they can be used and studied under ultrahigh vacuum conditions on single-crystal surfaces.

In this study we used two ionic liquids containing the same cation 1-ethyl-3-methylimidazolium $[\mathrm{EMIM}]^+$ and two different anions bis(triflouromethylsulfonyl)amide $[\mathrm{Tf_2N}]^-$ and tetracyanoborate $[\mathrm{TCB}]^-$. Films of different thicknesses between 0.3 and 20 monolayers were deposited on a well-defined Cu (100) single-crystal surface via evaporation. The samples were measured by vacuum ultraviolet (VUV) photoelectron spectroscopy (21.2 eV) under normal emission. The molecular orbitals were studied as a function of layer thickness and a strong radiation damage was observed.

O 58.43 Wed 18:15 Poster B

Ultrathin samaria films on Pt(111) studied by PES and LEED — •J.H. Jhang[1], A. Schaefer[1], D. Ragazzon[2], L.E. Walle[3], M.H. Farstad[3], A. Borg[3], A. Sandell[2], and M. Bäumer[1] — [1]Institute for Applied and Physical Chemistry, Universität Bremen, Germany — [2]Department of Physics and Astronomy, Uppsala University, Sweden — [3]Department of Physics, NTNU, Trondheim, Norway

Rare earth oxides (REOs) exhibit high potential as catalysts due to the ability to easily switch between oxidation states. Their catalytic capability depends strongly on the storage and release of oxygen. The tendency to promote partial or total oxidation reactions is influenced by the existing oxidation states and oxygen mobility: While ceria (3+ and 4+ as stable oxidation states) is a good catalyst for total oxidation, samaria (only 3+ as stable oxidation state) seems to be the most effective REO for partial oxidation of methane, to just name one example. Therefore, in order to look into the atomic details of oxygen transport and transfer a simplified two dimensional model system may be prepared and studied under controlled conditions in ltra-high vacuum (UHV). Studies of REO films other than ceria are however very limited. This makes the exploration of other REOs highly motivated. We present first results on samaria growth on Pt(111) by using physical vapour deposition (PVD) in UHV. Two methods will be presented for samaria growth: oxidation of a surface alloy and deposition in elevated oxygen background pressure. The generated oxide layers are investigated by synchrotron radiation based photoelectron spectroscopy (PES) and low energy electron diffraction (LEED).

O 58.44 Wed 18:15 Poster B

STM investigation of ultra thin silver films on Nb(110) — •Matthias Stocker, Holger Pfeifer, Berndt Koslowski, and Paul Ziemann — Institut für Festkörperphysik, Universität Ulm, D-89081 Ulm

Thin silver films (in the monolayer range) were thermally evaporated onto Nb(110) at approximately 100 °C and analyzed by scanning tunneling microscopy (STM) and spectroscopy (STS) at 5.3 K. The Ag/Nb(110) forms islands of 2ML height which coalesce to form a contiguous layer at a nominal coverage of 2ML. On the islands we find quasi-periodic depressions of depth ~0.1 nm and period ~2 nm pointing to a significant stress within the Ag layer. Spectroscopy reveals a marked difference between the DOS off and on the island with strong resonances at (-1.4, -1.0, 0.0, 0.7) eV which cannot be attributed to quantum well states in the silver. The origin could be hybridization of Ag with Nb states at the interface. On the island, the DOS is strongly reduced above the Fermi energy indicating the development of the L gap in the Ag layer. The stress in the Ag layer with the locally varying strain leads to prominent changes in the DOS as revealed by dI/dV maps.

O 58.45 Wed 18:15 Poster B

Adsorption of CO on Rh_N/Ru(0001) Films — •Sebastian Thussing, Pawel Gazdzicki, and Peter Jakob — Fachbereich Physik, Philipps-Universität Marburg, 35032 Marburg, Germany

The growth of thin ($\leq$ 3 ML) Rh/Ru(0001) films and the adsorption of CO on these films have been investigated in the temperature range 85 – 1350 K using IRAS, TPD, and LEED. Specifically, the shifts of the CO stretching vibration due to lateral interactions, lattice strain and influence by the substrate were investigated. Furthermore, the dependence of CO adsorption energies and coverages on the Rh-film thickness were explored. A minimum in CO desorption energy was thereby found for the first Rh monolayer. For these layers four distinct long-range ordered phases of CO, with characteristic occupation of the various CO adsorption sites, have been observed. Based on our ability to discriminate the various CO species according to their local binding geometry, morphological changes in the island size distribution (ranging from single Rh atoms to extended Rh islands and Rh/Ru surface alloys) have been analyzed. The findings are discussed in the context of recent work on Pt_N/Ru(0001) layers [1, 2].

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[2] Jakob, P. and Schlapka, A., Surf. Sci. 601, 3556 (2007).

O 58.46 Wed 18:15 Poster B

Preparation and in-situ analysis of MOVPE-prepared Si(111) surfaces — •Thomas Haensel[1], Weihong Zhao[1], Henning Döscher[1,2], Sebastian Brückner[1], Peter Kleinschmidt[3], Oliver Supplie[2], Matthias M. May[2], and Thomas Hannappel[1,3] — [1]Technische Universität Ilmenau, Institut für Physik, Fachgebiet Photovoltaik, Gustav-Kirchhoff-Straße 5, D-98684 Ilmenau — [2]Helmholtz-Zentrum Berlin für Materialien und Energie, Hahn-Meitner-Platz 1, D-14109 Berlin — [3]CiS Forschungsinstitut für Mikrosensorik und Photovoltaik GmbH, Konrad-Zuse-Straße 14, D-99099 Erfurt

III-V nanowires are one example for new solar cell concepts aiming at high efficiency. Compared to III-V wafers, silicon substrates benefit from low cost and mature high quality manufacturing. Generally, III-V nanowires are prepared on {111} surfaces. While the preparation of pristine Si(111) is well-established in ultra-high vacuum (UHV), little is known about the preparation of Si(111) surfaces grown in metal organic vapor phase epitaxy (MOVPE) ambient. A contamination-free transfer system enables us to relate in situ reflection anisotropy spectroscopy (RAS) and UHV based techniques such as scanning tunneling microscopy (STM), low energy electron diffraction (LEED) and X-ray photoelectron spectroscopy (XPS). Similarly, we analyzed the nucleation of GaP on Si(111).

O 58.47 Wed 18:15 Poster B

Double layer steps on Silicon(100) prepared in H_2 ambient — •Wei Hong Zhao[2], Johannes Luczak[1], Peter Kleinschmidt[1,3], Sebastian Brückner[1,2], Henning Döscher[1,2], Oliver Supplie[1], and Thomas Hannappel[1,2,3] — [1]Helmholtz-Zentrum Berlin, Institut Solare Brennstoffe und Energiespeichermaterialien, D-14109 Berlin — [2]TU Ilmenau, Institut für Physik, Fachgebiet Photovoltaik, D-98693 Ilmenau — [3]CiS Forschungsinstitut für Mikrosensorik und Photovoltaik, D-99099 Erfurt

Preparation of double-layer steps is important for heteroepitaxial growth of III-V semiconductors on Si(100). Single-layer steps on Si(100) are associated with the presence of two domains with different dimer orientations on the reconstructed surface, leading to the initiation of anti-phase domains (APDs) in the epitaxial III-V layer. Our process consists of deoxidation, homoepitaxial growth employing silane, annealing and cooling in hydrogen ambient. We studied the surface structure using Fourier-transform infrared spectroscopy, low-energy electron diffraction and scanning tunneling microscopy (STM). STM measurements on Si(100) show the formation of D_A and D_B -double-steps on a surface with an intermediate offcut of 2° in [011] direction dependent on cooling procedere. The STM images on 6° misoriented samples revealed a preference for D_B double layer steps.

O 58.48 Wed 18:15 Poster B

Adsorption of Organic Molecules on Potassium Chloride — •Hazem Aldahhak, Eva Rauls, and Wolf Gero Schmidt — Theoretische Physik, Universität Paderborn, Warburger Str. 100, 33100 Paderborn

The ability to grow self-assembled supramolecular nanostructures on solid surfaces has important implications in both basic science and nanotechnology. The constraint to two dimensions enables us to reduce the molecular mobility and study the various interactions between the adsorbed molecules on the one hand and between molecule and surface on the other hand, separately. In recent years, metal surfaces were used as the most common substrate. However, the surfaces of alkali salts like sodium or potassium chloride, open up new possibilities. Surface symmetry and ionicity as well as technological reasons, like e.g. simple mechanisms for the desorption of grown supramolecular assemblies, make these surfaces a worthwile alternative to metal substrates.

We present our investigations of the adsorption of organic molecules like PTCDA on KCl and NaCl surfaces. To this aim, we have performed first principles density functional theory calculations and focussed on both the geometric and electronic structure of single molecules as well as molecular layers at higher coverages.

O 58.49 Wed 18:15 Poster B

Charge Localization Dynamics Induced by Oxygen Vacancies on the TiO2(110) Surface and Titania and Gold-promoted Titania Surfaces Interaction with small molecules — •Matteo Farnesi Camellone — Ruhr-Universität Bochum D-44780 Bochum

We use ab initio molecular dynamics to investigate the dynamics of an F–center created by an oxygen vacancy on the TiO2(110) rutile surface. The simulations uncover a truly complex, time-dependent behavior of fluctuating electron localization topologies in the vicinity of the oxygen vacancy. Although the two excess electrons are found to populate preferentially the second subsurface la<x>yer, they occasionally visit surface sites and also the third subsurface layer [1]. We then study the interaction of CO with the (110) Au supported (110) TiO2 surface catalysts. The structural, electronic, dynamical and thermodynamic properties of the gold promoted titania surfaces are investigated by means of density functional theory calculations that account for the on site Coulomb interaction via the inclu sion of a Hubbard term (GGA+U). The interaction between gold and substrate is accompained by an extensive charge reorganization at the metal-oxide contact wich leads to Au oxidation and the reduction of the titanum dioxide substrate. It is shown that the catalytic activity of the (110) TiO2 substrate is efficiently improved by supported and dispersed Au adatoms on the same substrate. [2]

[1] P. M. Kowalski, M. Farnesi Camellone, N. N. Nair, B. Meyer, and D. Marx, Phys. Rev. Lett. , 146405 (2010). [2] M. Farnesi Camellone, P. M. Kowalski, and D. Marx, Phys. Rev. B 84, 035413 (2011)

O 58.50 Wed 18:15 Poster B

Density functional calculation of interface structure of Fe/ZnO — •Sougata Pal and Eckhard Pehlke — Institut für Theoretische Physik und Astrophysik, Universität Kiel, Germany

Interfaces between magnetic and piezoelectric materials bear the possibility of magnetoelectric coupling phenomena which occur at the interface, in addition to coupling via long range strain fields [1]. As a model system, we have started to investigate the adsorption of 1/4 – 1 ML Fe on both the unreconstructed and the (2×2) vacancy-reconstructed ZnO($000\bar{1}$) surfaces by means of density functional calculations. First, the lowest-energy structures have to be identified. Among the calculated adsorption sites, the *fcc* hollow position is energetically favorable. At sufficiently large oxygen chemical potential, the energy can be further lowered by substituting the top layer Zn-atoms with Fe atoms. In this case the Zn-atoms created by the Zn-Fe exchange are assumed to become oxidized and included into the ZnO bulk. It has turned out be energetically unfavorable, however, to exchange Zn-atoms in deeper layers with Fe-atoms. The interface between ZnO and the locally formed Fe-oxide is thus expected to be sharp. The findings are consistent with Fe-oxidation observed experimentally [2,3].

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[3] Guo-Dong Wang *et al.*, Surf. Review and Lett. **15**, 295 (2008).

O 58.51 Wed 18:15 Poster B

III-V on Si(100) for photoelectrocatalysis — •Matthias M. May[1,2], Oliver Supplie[1,2], Henning Döscher[1], Sebastian Fiechter[1], Hans-J. Lewerenz[1,3], Klaus Schwarzburg[1], and Thomas Hannappel[1,4,5] — [1]Helmholtz-Zentrum Berlin, Institut Solare Brennstoffe und Energiespeichermaterialien, D-14109 Berlin — [2]Humboldt-Universität zu Berlin, Institut für Physik, D-12489 Berlin — [3]California Institute of Technology, Pasadena, USA — [4]TU Ilmenau, Institut für Physik, Fachgebiet Photovoltaik, D-98693 Ilmenau — [5]CiS Forschungsinstitut für Mikrosensorik und Photovoltaik, D-99099 Erfurt

III-V semiconductors on Si(100) represent possible candidates for photoelectrochemical splitting of H_2O. InP grown by MOVPE has proven to be a promising photocathode for H_2 evolution [1]. GaP is closely related to InP and can be grown on Si(100) [2] combining a III-V semiconductor with the inexpensive Si substrate. Lattice match and band gap engineering can be achieved via incorporation of e.g. N [3]. This heteroepitaxial system also opens the possibility of a monolithically integrated photoelectrochemical tandem device addressing both hydrogen and oxygen evolution. First experiments investigating the fundamental properties regarding surface chemistry and topography of these III-V systems on Si are presented.

[1] Lewerenz et al., *Energy Environ. Sci.* **3** (2010)
[2] Döscher et al., *J. Appl. Phys.* **107**, 123523 (2010)
[3] Shan et al., *Phys. Status Solidi B* **223**, (2001)

O 58.52 Wed 18:15 Poster B

Laser interferometric observations of capillary rise in arrays of silicon nanochannels — •Mark Busch[1] and Patrick Huber[1,2] — [1]Experimental Physics, Saarland University, Saarbrücken, Germany — [2]Faculty of Physics and Astronomy, Pontifical Catholic University, Santiago, Chile

We present measurements on the capillary rise of liquids in mesoporous silicon films. The time-dependent rise level of the liquid within the pores has been determined with laser interferometry [1]. The measurements are based on the change of refractive index during the filling of the pores. Such measurements allow one to explore the initial stages of nanochannel filling.

In particular we focus on the orientation and temperature dependence of the filling process. The presented measurements were taken with 2-Propanol and 1-Decanol.

[1] Acquaroli, L. N. *et al.* Capillary Filling in Nanostructured Porous Silicon, *Langmuir* **2011**, *27(5)*, 2067-2072

O 58.53 Wed 18:15 Poster B

On the GaN crystal growth in the MOCVD method: a DFT study — Maria Ptasińska[1], •Jacek Piechota[1], Jakub Sołtys[1], and Stanisław Krukowski[1,2] — [1]Interdisciplinary Centre for Materials Modelling, University of Warsaw, Pawińskiego 5a, 02-106 Warsaw, Poland — [2]Institute of High Pressure Physics (UNIPRESS), Polish Academy of Sciences, Sokołowska 29/37, 01-142 Warsaw, Poland

The purpose of this study is to construct the GaN (gallium nitride) crystal growth model of MOVPE (Metal Organic Vapor Phase Epitaxy) method employing TMG (trimetylogallium) and NH3 (ammonia) as reaction precursors. Two possible reaction paths are taken into consideration. The first one is the decomposition of TMG in the gas phase under high temperature and pressure in the MOVPE chamber and the atomic Ga adsorption on the GaN crystal surface. The second one is TMG decomposition at GaN crystal surface. Calculations indicate that there is charge transfer from the TMG molecules to the GaN surface during approach of TMG molecules to the GaN surface. This may result in bonds breaking in the TMG molecule and Ga adsorption at the surface. Two cases were examined: First the adsorption on the GaN(000-1) surface with broken bonds and second the adsorption on the GaN(0001) surface covered with NH2. Under some special conditions the TMG decomposition was observed close to the GaN surface which is preliminary step to construct general theory of decomposition of various molecules during the GaN crystal growth in the MOCVD method.

O 58.54 Wed 18:15 Poster B

Theoretical investigation of the Zn, O, O2, and H2O adsorption on the polar ZnO(0001) and ZnO(000-1) surfaces — Jakub Sołtys[1], •Jacek Piechota[1], and Stanisław Krukowski[1,2] — [1]Interdisciplinary Centre for Materials Modelling, University of Warsaw, Pawińskiego 5a, 02-106 Warsaw, Poland — [2]Institute of High Pressure Physics (UNIPRESS), Polish Academy of Sciences, Sokołowska 29/37, 01-142 Warsaw, Poland

Performed density functional theory simulations of adsorption of the Zn and O atoms, as well as O2 and H2O molecules on the polar ZnO(0001) and ZnO(000-1) surfaces clarify the principal processes, important for growth of ZnO from the vapor. Demonstrated results indicate that Zn atom is adsorbed at both ZnO surfaces without any energy barrier, but with ultimately different adsorption energies: 0.34 eV for the metallic, and 3.37 for the nonmetallic surface, respectively. In contrast, O atoms are attached very strongly at both polar surfaces, with energies equal to 5.47 eV for the metallic and 2.47 eV for the nonmetallic surface, respectively. The difference between both polar surfaces is the highest for adsorption of molecular oxygen, the O2 molecule is adsorbed on the Zn-face with the energy of 2.45 eV, while in contrast is not adsorbed at the oxygen face of ZnO at all. Some results of adsorption of H2O at both ZnO surfaces are also presented.

O 58.55 Wed 18:15 Poster B

Scanning Tunneling Microscopy study of single-crystalline $Sr_3Ru_2O_7$ — •Bernhard Stöger[1], Zhiming Wang[1], Michael Schmid[1], Ulrike Diebold[1], David Fibes[2], and Zhiqiang Mao[2] — [1]Institute of Applied Physics, Vienna University of Technology, Vienna, Austria — [2]Department of Physics and Engineering Physics, Tulane University, New Orleans, LA, USA

Perovskite oxides play an important role as cathodes in solid oxide fuel cells (SOFC) and in catalysis. Investigating surface defects such as oxygen vacancies and the adsorption of relevant molecules helps gaining more insight into the physics behind SOFCs and catalytic processes.

High quality $Sr_3Ru_2O_7$ (SRO) single crystals were grown using the floating zone technique. $Sr_3Ru_2O_7$ is part of the ruthenate Ruddlesden-Popper series $Sr_{n+1}Ru_nO_{3n+1}$, which have a layered structure. We investigated the surface of SRO, by means of Scanning Tunneling Microscopy (STM) at 78 K. The single crystals were cleaved in ultra-high vacuum at 150 K, which results in rather large terraces. We have characterized the defects that are present at as-cleaved surfaces, and how their appearance changes with applied STM tunneling parameters. Adsorption of carbon monoxide dosed at 105 K, results in asymmetric cross-like features that span several surface unit cells.

This work was supported by the Austrian Science Fund (FWF project F45)

O 58.56 Wed 18:15 Poster B

Vibronic states of Br_4TPP porphyrines on a Cu_3N insulating film — •Martina Corso[1], Jingcheng Li[1], Zechao Yang[1], Christian Lotze[1], Anna Strozecka[1], Lena Kaufmann[2], Max Kerbs[2], Arno Wiehe[2], Christoph A. Schalley[2], Katharina Franke[1], and Jose Ignacio Pascual[1] — [1]Institut für Experimentalphysik, Freie Universität Berlin, Arnimallee 14, 14195 Berlin, Germany — [2]Institut für Chemie und Biochemie, Freie Universität Berlin, Takustr. 3, 14195 Berlin, Germany

Insulating thin films grown on metal surfaces decouple adsorbates from the electron density of the underlaying substrate. In this work we use low temperature STM to study the vibronic states of tetra(4-bromophenyl)porphyrin (Br_4TPP) molecules decoupled from a Cu(110) surface by a single copper nitride layer (Cu_3N). Differential conductance spectra (dI/dV) taken on isolated Br_4TPP show that two types of molecules coexist on the surface, probably due to a different local adsorption environment. They preserve the same electronic structure but shifted of 350 meV. A series of equally spaced peaks ($\sim$ 170 meV) corresponding to vibronic states appears in the LUMO of Br_4TPP measured in dI/dV spectra. The detection of this vibronic progression, not observed on Cu(110), is enabled by the extended lifetime of the transient charged states of individual Br_4TPP which is seven times larger on copper nitride than on the bare metal.

O 58.57 Wed 18:15 Poster B

LEED and PIRS study of SF_6 physisorption on NaCl(100) — •Mirko Langer, Stephan Härtel, Jochen Vogt, and Helmut Weiss — Chemisches Institut der Universität Magdeburg, Universitätsplatz 2, 39106 Magdeburg, Germany

The interaction of the antropogenic greenhouse gas SF_6 with the NaCl(100) surface was investigated using low-energy electron diffraction (LEED) and polarization infrared spectroscopy (PIRS) under ultrahigh vacuum conditions and cryogenic temperatures. Consistent with the results of a previous study of SF_6 adsorption on NaCl thin films [1], SF_6 exhibits a complicated Stranski-Krastanov film growth behavior on NaCl(100): pronounced 3D nano crystal formation occurs at a substrate temperature of 64 K, indicated by strong absorptions in the region of the asymmetric S-F stretch mode. The observed characteristic Davydov splitting of about 100 cm^{-1} is consistent with the large vibrational polarizability of SF_6 and its bcc bulk structure. In contrast to many other physisorption systems, a 2D adsorbate of SF_6 is formed only at lower temperatures below 45 K, indicated by the appearance of superstructure spots in the LEED patterns. The unusual

growth behavior is attributed to the strong lattice mismatch between adsorbate and substrate.
[1] A. Klekamp, E. Umbach, Surf. Sci. Lett. 284 (1993), 291

O 58.58 Wed 18:15 Poster B

Growth and characterisation of Fe thin films on MgO(100) — •Hendrik Bettermann, Wolfgang Rosellen, Torsten Veltum, and Mathias Getzlaff — Institute of Applied Physics, University Duesseldorf

This investigation focuses on Fe films on commercially available MgO substrates. MgO as an insulating material is an interesting substrate for the deposition of thin films. It can provide a cost-efficient one-time alternative to W(110)-substrates.

One possible application for Fe films is the use of it as a supporting and magnetically conducting material for the deposition of magnetic nanoparticles consisting of Ni, Co, or alloys thereof. These are interesting from a technological point regarding data storage due to their size dependent electronic and magnetic properties.

The Fe thin films are investigated and characterised in-situ by LEED (low energy electron diffraction), AES (Auger electron spectroscopy), and STM (scanning tunneling microscopy). XRF (X-ray fluorescence spectroscopy) is also available to perform ex-situ investigations.

We focus on optimized parameters during deposition to produce flat films and wide terraces by variation of both film thickness and annealing temperature.

O 58.59 Wed 18:15 Poster B

Ferrocene ultrathin films on NaCl(100) – a high resolution FTIR study — Birgit Vogt and •Jochen Vogt — Chemisches Institut der Universität Magdeburg, Universitätsplatz 2, 39106 Magdeburg, Germany

Ferrocene $(C_5H_5)^-Fe^{2+}(C_5H_5)^-$ is a prototype of an organometallic sandwich complex. The thin film properties of ferrocene are of interest in many respects, e. g. due to its potential use as a precursor for the deposition of iron or iron oxide films on surfaces [1]. We report on the preparation of ultrathin films of ferrocene on the NaCl(100) surface below 30 K and ultrahigh vacuum conditions. The films were characterized using polarization fourier transform infrared spectroscopy (PIRS). Upon cooling the films from 180 K to 25 K, pronounced reversible frequency shifts and splittings of the distortion modes of the cyclopentadienyl rings are observed. The bending mode at 818 cm^{-1} splits into at least six narrow components between 810 and 830 cm^{-1} with different fractions of absorption in s- and p-polarization, respectively. These are consistent with different orientations of the associated dipole moments with respect to the substrate surface, and a high degree of film crystallinity. Coadsorption experiments with CO_2 reveal that the applied method of preparation results in ferrocene films which cover 60 to 80 percent of the substrate surface.
[1] A. B. F. Martinson et al., J. Phys. Chem. C 115 (2011), 4333

O 58.60 Wed 18:15 Poster B

Morphology and structure of epitaxial films of TiO_x, BaO_x, and $BaTiO_3$ on Pt(100) — •Klaus Meinel[1], Stefan Förster[1], Henning Neddermeyer[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

Interesting applications are expected for films of ternary oxides with perovskite structure such as $BaTiO_3$ which display ferroelectric behavior. In previous work of epitaxial $BaTiO_3$ films on Pt, magnetron sputtering from a $BaTiO_3$ target has been used for film deposition [1]. In the present work, the more gentile reactive vapor deposition of Ti and BaO in an O_2 atmosphere is used for film preparation. STM, SPA-LEED, AES, and XPS have been applied for investigating morphology, structure, thickness, and composition of the binary oxide (TiO_x and BaO_x) films on Pt(100). After carefully adjusting the deposition rates, the simultaneous growth of both materials yields high quality $BaTiO_3$(100) films. With respect to Pt(100), their unit mesh is rotated by 45° yielding a misfit of only 2%. Several superstructures develop which are induced by O vacancies. With the calibrated deposition of the oxides of Ti and Ba, in principle, also a layer by layer construction of $BaTiO_3$ films is possible which allows a deliberate assessment of the interface and surface terminations.

[1] S. Förster, W. Widdra, Surf. Sci. 604, 21631 (2010).

O 59: Invited talk (Mads Brandbyge)

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

Invited Talk O 59.1 Thu 9:30 HE 101

Electronic transport, Joule-heating, and current-driven dynamics in molecular contacts - theory and simulations — •Mads Brandbyge[1], Jing-Tao Lü[1], Tue Gunst[1], and Per Hedegård[2] — [1]Dept. of Micro and Nanotechnology (DTU-Nanotech), Technical Univ. of Denmark build. 345 east, DK-2800 Kongens Lyngby, Denmark — [2]Niels Bohr Inst., Univ. of Copenhagen, Universitetsparken 5, DK-2100, Denmark

Computer simulation and theoretical modelling play an vital role in the emerging field of nanoelectronics with device dimensions down to the molecular scale. Interpretation of experimental results and prediction of novel mechanisms for device operation poses many challenges especially for first principles theory, that is, calculations without fitting parameters. We have developed methods to address aspects of electron transport though nanoconductors from first principles based on density functional theory.

The influence of an electronic current on atomic dynamics is an important and intriguing problem in nanoelectronics. We have recently proposed an approach to molecular dynamics simulations which encompass Joule heating as well as current-induced forces not conserving the energy. We will discuss mechanisms where the current can lead to instabilities in the dynamics e.g. resulting in contact fluctuations or disruption at certain critial voltages. These mechanisms include "runaway" vibrational modes resulting from non-conservative forces, and a laser-type instability in certain types of molecular conductors (donor-acceptor-type systems).

O 60: [MA] Joint Session "Surface Magnetism II" (jointly with O)

Time: Thursday 9:30–13:00 Location: EB 301

O 60.1 Thu 9:30 EB 301

Magnetism of Cobalt Nanoclusters on Graphene on Ir(111) — •Stefan Schumacher[1], Chi Vo-Van[2], Johann Coraux[2], Violetta Sessi[3], Olivier Fruchart[2], Nick B. Brookes[3], Philippe Ohresser[4], and Thomas Michely[1] — [1]II. Physikalisches Institut, Universität zu Köln, D-50937 Köln — [2]Institut Néel, CNRS et Université Joseph Fourier, F-38042 Grenoble — [3]European Synchrotron Radiation Facility, F-38043 Grenoble — [4]Synchrotron SOLEIL, F-91192 Gif-sur-Yvette

On the moiré pattern of graphene on Ir(111) a variety of highly perfect cluster superlattices with narrow size distribution can be grown. The magnetic properties of Co clusters comprising from 26 to 2700 atoms, densely self-organized on the graphene/Ir(111) moiré as well as in more sparse arrangements, were studied *in situ* by means of scanning tunneling microscopy (STM) and X-ray magnetic circular dichroism (XMCD). Surprisingly the small clusters show almost no magnetic anisotropy. We find indication for a magnetic coupling between the clusters. Experiments have to be performed carefully as the clusters get readily damaged by soft X-rays.

O 60.2 Thu 9:45 EB 301

The role of the chemical and van der Waals interactions in defining the spin-polarization at the hybrid graphene-metal interfaces — •Nicolae Atodiresei[1], Vasile Caciuc[1], Predrag

Lazić[2], Martin Callsen[1], and Stefan Blügel[1] — [1]Peter Grünberg Institut & Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, 52425 Jülich, Germany — [2]Massachusetts Institute of Technology, Cambridge, 02139 Massachusetts, USA

By performing density functional theory calculations we reveal the bonding mechanism and the adsorption geometry of graphene on Ir(111) and Co/Ir(111) surfaces. Our simulations included the van der Waals interactions by employing a semi-empirical [1] and an *ab initio* [2] approach, as implemented in the JuNoLo code [3]. The binding of the graphene to the metal is dominated by van der Waals interactions although, locally, a polar covalent-like chemical interaction takes place. In turn, this leads to strong variation of the local spin-polarization at the hybrid graphene-Co/Ir(111) interface. [1] S. Grimme, J. Comput. Chem. **27** 1787 (2006); [2] M. Dion *et al.*, Phys. Rev. Lett. **92**, 246401 (2004); [3] P. Lazić *et al.*, Comp. Phys. Commun. **181**, 371 (2010).

O 60.3 Thu 10:00 EB 301

Magnetic coupling in metal organic networks on surfaces — •Tobias R. Umbach, Christian Felix Hermanns, Matthias Bernien, Alex Krüger, Isabel Ferández-Torrente, Paul Stoll, Katharina J. Franke, Jose I. Pascual, and Wolfgang Kuch — Institut für Experimentalphysik, Freie Universität Berlin, Arnimallee 14, 14195 Berlin, Germany

Metal organic networks offer the possibility to alter the electronic and magnetic functionality of surfaces on a nanometer scale. Here we report on the bilayer metal organic network of Fe atoms and 2,4,6-Tris(4-pyridyl)-1,3,5-triazine (T4PT) on a Au(111) surface. The network is investigated in terms of scanning tunneling microscopy (STM) and X-ray circular dichroism (XMCD). Fe atoms and T4PT molecules form a mixed ordered phase consisting of two distinct layers. The first layer has a triangular structure and every Fe atom is surrounded by three pyridyl groups of three different T4PT molecules. The second layer is exclusively built of T4PT molecules, centered with the triazine ring on top of the Fe atoms of the first layer. XMCD measurements reveal sizable magnetic moments of the Fe sites and an out of plane magnetic anisotropy. The field dependence of the XMCD signal reveals a finite ferromagnetic coupling of the Fe atoms in the Fe-T4PT network.

O 60.4 Thu 10:15 EB 301

Electronic and magnetic properties of free and supported transition metal phthalocyanines — •Roberto Robles, Richard Korytar, and Nicolás Lorente — Centre d'Investigacions en Nanociència i Nanotecnologia, CIN2 (CSIC-ICN), Barcelona, Spain

By performing density functional theory calculations we have studied the electronic and magnetic properties of transition metal phthalocyanines (MPc, with M=Fe,Co,Ni,Cu), both in the gas phase and supported on Ag (100) surfaces. First we investigate the properties of the gas-phase MPc's as we change the transition metal and ionize the system. Then we deposit the molecules on the Ag (100) surface, showing how charge transfer and spin moment change by the hybridization with the surface states. We discuss the utility of the anion as a model of the supported situation. We also explore the effect of different exchange-correlation potentials, as well as the influence of van-der-Waals interactions and electronic correlation beyond DFT (GGA+U). Finally, we analyse our results in view of recent STM experiments on the same systems, specially regarding the Kondo effect observed in some of the systems.

- Mugarza, A. et al. Spin coupling and relaxation inside molecule-metal contacts. Nat. Commun. 2:490 doi: 10.1038/ncomms1497 (2011).

O 60.5 Thu 10:30 EB 301

Spin resolved measurements of magnetic molecules on surfaces — •Jens Brede[1], Régis Decker[1], Jörg Schwöbel[1], Svetlana Klyatskaya[2], Mario Ruben[2,3], and Roland Wiesendanger[1] — [1]Institute of Applied Physics, University of Hamburg, 20355 Hamburg, Germany — [2]Institute of Nanotechnology, Karlsruhe Institute of Technology, 76344 Eggenstein-Leopoldshafen, Germany — [3]IPCMS, Université de Strasbourg, 67034 Strasbourg, France

The use of magnetic molecules opens a gateway to a flexible design of novel spintronic devices to store, manipulate, and read spin information at 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. Here, we applied spin-polarized scanning tunneling microscopy to resolve the physics of the molecule-ferromagnet interface. The analysis focuses on different phthalocyanine molecules. 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.

O 60.6 Thu 10:45 EB 301

Controlling the spin and the magnetic coupling of adsorbed molecules by on-surface coordination chemistry — •Christian Wäckerlin[1], Kartick Tarafdar[3], Dorota Chylarecka[1], Jan Girovsky[1], Tatjana Hählen[1], Cristian Iacovita[4], Armin Kleibert[2], Frithjof Nolting[2], Thomas A. Jung[1], Peter M. Oppeneer[3], and Nirmalya Ballav[5] — [1]Laboratory for Micro- and Nanotechnology and — [2]Swiss Light Source, Paul Scherrer Institute, Switzerland — [3]Department of Physics and Astronomy, Uppsala University, Sweden — [4]Department of Physics, University of Basel, Switzerland — [5]Department of Chemistry, Indian Institute of Science Education and Research, India

The chemical and magneto-electronic interaction of metalloporphyrins with axial ligands has been investigated for the specific case where the paramagnetic molecules [1] are supported on ferromagnetic substrates. Specifically, nitric oxide (NO) can coordinate to the porphyrin center and compete with the surface ligand in its influence of the structural and electronic integrity of the porphyrin [2]. The coordination of NO (S=1/2) with Co(II) (S=1/2) [3], Fe(II) (S=1) and Mn(II) (S=5/2) tetraphenyl porphyrins on ferromagnetic Ni or Co thin film substrates is analyzed by combining X-ray magnetic circular dichroism (XMCD), scanning tunneling microscopy (STM) and density functional theory + additional Hubbard U interaction (DFT+U) calculations.

[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).

O 60.7 Thu 11:00 EB 301

Probing individual spin states of Fe-Porphyrins on a superconductor — •Benjamin W. Heinrich, Lukas Z. Braun, José I. Pascual, and Katharina J. Franke — Institut für Experimentalphysik, Freie Universität Berlin, Germany

Scanning Tunneling Microscopy/Spectroscopy (STM/STS) allows for studying the competition between magnetism and superconductivity at a single-impurity level. Commonly, the adsorption of a magnetic atom [1,2], or molecule [3], on a superconductor locally breaks the time-reversal symmetry and gives rise to bound states in the superconducting (SC) gap [4], and/or Kondo quasi-particle states [3]. However, here we can show that decoupling the impurity spin from the SC substrate preserves both the local spin and the SC state.

We use inelastic electron tunneling spectroscopy (IETS) to probe the spin state of single Fe(III)-Octaethylporphyrin-Cloride (FeOEP-Cl) molecules adsorbed on Pb(111). Due to the bulky ligand, the interaction between the central Fe ion, holding the molecular spin, and the substrate is strongly reduced. At 4.5 K, we can observe spin flips on the molecule, while the SC quasi-particle resonances remain unchanged. Reducing the tip-sample distance allows for altering the local anisotropy, while desorbing the chlorine ligand via controlled voltage pulses results in a change of the spin state as revealed by energy shifts of the IETS signal.

[1] A. Yazdani et al., Science 275, 1767 (1997) [2] S.-H. Ji et al., Phys. Rev. Lett. 100, 226801 (2008) [3] K.J. Franke et al., Science 332, 940 (2011) [4] H. Shiba, Prog. Theor. Phys. 40, 435 (1968)

15 min. break

O 60.8 Thu 11:30 EB 301

Spatially modulated tunnel magnetoresistance on the nanoscale — •Hirofumi Oka, Kun Tao, Sebastian Wedekind, Guillemin Rodary, Valeri Stepanyuk, Dirk Sander, and Jürgen Kirschner — Max-Planck-Institut für Mikrostrukturphysik, Weinberg 2, D-06120 Halle, Germany

We investigate the tunnel magnetoresistance (TMR) effect within a single Co nano-island by low-temperature spin-polarized scanning tunneling microscopy in magnetic fields. We measure the tunnel current as a function of the bias voltage and extract the TMR. We find a TMR of 290 MΩ for the anti-parallel and 190 MΩ for the parallel state at −0.27 V at the center of a Co island. This gives a TMR ratio of ∼50%. The TMR ratio depends on energy and position within the nano-island. We observe a clear spatial modulation of the TMR ratio with an amplitude of ∼20% and a spacing of ∼1.3 nm between maxima and minima around the Fermi level. This result can be ascribed to a spatially modulated spin-polarization within the Co island due to spin-dependent quantum interference [1]. Our combined experimental and theoretical study reveals that spin-dependent electron confinement affects all transport properties such as differential conductance, conductance and TMR. We demonstrate that the TMR within a nanostructured magnetic tunnel junction can be controlled on a length scale of 1 nm through spin-dependent quantum interference [2].

[1] H. Oka et al., Science 327, 843 (2010).
[2] H. Oka et al., PRL 107, 187201 (2011).

O 60.9 Thu 11:45 EB 301

First-principles investigation of g-shifts and damping of dynamical magnetic excitations in adatoms on surfaces

— •Samir Lounis[1], Antonio T. Costa[2], Bruno Chilian[3], Alexander A. Khajetoorians[3], Jens Wiebe[3], Roland Wiesendanger[3], and Douglas L. Mills[4] — [1]Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, D-52425 Jülich, Germany — [2]Instituto de Fisica, Universidade Federal Fluminense, 24210-340 Niteroi, Rio de Janeiro, Brazil — [3]Institute of Applied Physics, Hamburg University, Jungiusstrasse 11, D-20355 Hamburg, Germany — [4]Department of Physics and Astronomy, University of California Irvine, California, 92697 USA

Recently, spin excitations in Fe adatoms on Cu(111) and Ag(111) surfaces are probed with magnetic field dependent inelastic scanning tunneling spectroscopy[1]. The calculation of the transverse dynamical magnetic susceptibility allows to analyse the electronic signature of these excitations[2]. We show that an Fe adatom on Ag(111) surface, contrary to other atoms embedded in various lattice configurations, has a surprisingly large g-value of 3 instead of the regular value of 2.

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

[1] A. A. Khajetoorians *et al.*, Phys. Rev. Lett. 106, 037205 (2011); B. Chilian *et al.*, Arxiv:1108.2443
[2] S. Lounis *et al.*, Phys, Rev, Lett. 105, 187205 (2010); S. Lounis *et al.*, Phys. Rev. B 83, 035109 (2011)

O 60.10 Thu 12:00 EB 301

Anomalously large *g*-factor of single atoms adsorbed on a metal substrate

— •Jens Wiebe[1], Alexander A. Khajetoorians[1], Samir Lounis[2], Antonio T. Costa[3], Bruno Chilian[1], Douglas L. Mills[4], and Roland Wiesendanger[1] — [1]Institute of Applied Physics, Hamburg University, Germany — [2]Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich, Germany — [3]Instituto de Física, Universidade Federal Fluminense, Rio de Janeiro, Brazil — [4]Department of Physics and Astronomy, University of California Irvine, USA

We performed magnetic field dependent inelastic scanning tunneling spectroscopy (ISTS) on individual Fe atoms adsorbed on different metal surfaces. ISTS reveals a spin excitation which is shifting linearly to higher energies in the magnetic field. The magnetic anisotropies and the *g*-factors of the Fe atoms, as well as the lifetimes of the excitations, are extracted. We find lifetimes of hundreds of fs limited by coupling to electron-hole pairs in the substrate and decreasing linearly in the magnetic field. As expected, the magnetic anisotropy strongly depends on the substrate. Astoundingly, the *g*-factor is $g \approx 3.1$ for Ag(111) [1] instead of the regular value of 2 which is observed for the Cu(111) substrate [2]. This very large *g*-shift can be understood when considering the complete electronic structure of both the Ag(111) surface state and the Fe atom, as shown by *ab initio* calculations of the magnetic susceptibility.

[1] B. Chilian et al., Phys. Rev. B, accepted (2011).
[2] A. A. Khajetoorians et al., Phys. Rev. Lett. **106**, 037205 (2011).

O 60.11 Thu 12:15 EB 301

Detecting spin excitation of rare-earth atoms and clusters on metallic surfaces

— •Toshio Miyamachi[1], Tobias Schuh[1], Stefan Gerstl[1], Arthur Ernst[2], and Wulf Wulfhekel[1] — [1]Physikalisches Institut, Karlsruher Institut für Technologie, Germany — [2]Max-Planck-Institut für Mikrostrukturphysik, Halle, Germany

At the heart of the stability of magnetic bits in information storage is a magnetic anisotropy energy (MAE) and magnetization dynamics. Recent inelastic tunneling spectroscopy (ITS) studies have revealed that the spin states of 3d transition metal atoms and clusters on metallic substrates have extremely short lifetimes of the order of femtosecond due to strong hybridization of 3d states and substrates [1]. To reduce the influence of substrates from atoms and clusters, 4f rare-earth Gd atoms and clusters on Pt(111) and Cu(111) were studied with ITS. Since the 4f states are inner orbitals, the hybridization with substrates could be decreased. In addition, as the relativistic spin orbit interaction plays a crucial role for the MAE, 4f atoms with larger spin and orbital momenta could show larger MAEs than 3d atoms [2]. Obtained results show that the spin excitation of 4f states can be accessed with ITS, and that giant magnetic anisotropies and lifetimes of the excited states of Gd are nearly independent of supporting substrate or size of the cluster, reflecting the strongly localized character of 4f electrons in Gd atoms and clusters.

[1] T. Balashov et al., Phys. Rev. Lett. 102, 257203 (2009)
[2] T. Schuh et al., Phys. Rev. B. 84, 104401 (2011)

O 60.12 Thu 12:30 EB 301

Spin-transfer torque switching efficiency in SP-STM experiments

— •Andreas Sonntag, Stefan Krause, Gabriela Herzog, Anika Schlenhoff, and Roland Wiesendanger — Institute of Applied Physics, University of Hamburg, Germany

The tunnel current generated in spin-polarized scanning tunneling microscopy (SP-STM) experiments can be used to manipulate the switching behavior of superparamagnets [1] or even to reverse the quasistable magnetization of nano-islands [2]. Two main contributions involved in magnetization switching could be identified: Joule heating and the spin-transfer torque.

In our study we investigate the influence of a spin-polarized tunneling current on the switching behavior of superparamagnetic Fe nanoislands on the W(110) surface. Analyzing the lifetimes of the two magnetic states in dependence of the current, Joule heating and spin-torque effects are separated and quantified [3]. While the Joule heating decreases both lifetimes equally, the spin-torque lifts their degeneracy. Both effects are found to scale linearly with the tunneling current. By introducing the so-called spin-transfer torque viscosity and normalizing the torkance with respect to the magnetic moment of the free layer, we compare our findings to experiments performed on lithographically fabricated magneto-tunnel junctions. The results show a comparatively high spin-transfer torque efficiency in our experiments.

[1] S. Krause et al., Science **317**, 1537 (2007).
[2] G. Herzog et al., Appl. Phys. Lett. **96**, 102505 (2010).
[3] S. Krause et al., Phys. Rev. Lett. **107**, 186601 (2011).

O 60.13 Thu 12:45 EB 301

Spin transfer torque and Joule heating of field-emitted electrons

— •Anika Schlenhoff, Andreas Sonntag, Stefan Krause, and Roland Wiesendanger — Institute of Applied Physics, University of Hamburg

Since the detection of the spin polarization of field-emitted electrons in the 1970's [1], it is an open question which type of effects a high spin-polarized current of field-emitted electrons has onto a magnetic sample. Though spin-polarized two-photon photoemission has gained first insight into the interaction of hot electrons with an underlying spin system [2], the microscopic details still remain to be discovered.

In our studies, we utilize spin-polarized scanning tunneling microscopy (SP-STM) in the field emission mode [3] for the direct observation of the influence of field-emitted electrons onto atomic-scale superparamagnets [4]. The experiments reveal that the injection of high spin-polarized currents via the first field emission resonance (FER) significantly changes the superparamagnet's switching behavior. Telegraphic noise experiments allow for a detailed current-dependent lifetime analysis, thereby quantifying the spin-transfer torque and Joule heating of the field-emitted electrons. The results are compared to low energy electrons tunneling directly into the nanoisland.

[1] N. Müller *et al.*, Phys. Rev. Lett. **29**, 1651 (1972).
[2] A. B. Schmidt *et al.*, Phys. Rev. Lett **105**, 197401(2010).
[3] A. Kubetzka *et al.*, Appl. Phys: Lett. **91**, 012508 (2007).
[4] S. Krause *et al.*, Phys. Rev. Lett. **103**, 127202 (2009).

O 61: [TT] Focused Session: Charge and Spin Transport through Junctions at the Nanometre Scale

Time: Thursday 9:30–13:00 Location: H 0104

Invited Talk O 61.1 Thu 9:30 H 0104
The information is the noise: shot noise a tool for investigating atomic and molecular nanowires — •Jan van Ruitenbeek — Kamerlingh Onnes Laboratory, Leiden University, Netherlands

Shot noise is the intrinsic noise in an electron current arising from the discrete character of the electron charge. It carries information on the quantum mechanical electronic structure of nanoscale conductors. In atomic wires shot noise can be exploited for obtaining information on the number of conductance channels and their transmission probability. We have applied shot noise analysis to single-molecule junctions. The outstanding property that distinguishes a molecule from a quantum dot is its floppy character. This leads to the observation of electron scattering on vibration modes of the molecule, known as Inelastic Electron Tunneling Spectroscopy (IETS). While IETS is now being exploited by many groups for the study and characterization of metal-molecule junctions, the influence of inelastic scattering is expected to affect electron transport more deeply. The conductance can be viewed as the first moment in the probability distribution of a charge q being transmitted through the junction during a given period of time. The second moment is the shot noise in the current. For bias voltages above the vibration mode energy corrections to shot noise have recently been predicted by several groups. As a first test of these predictions measurements will be discussed in terms of two-electron effects.

Invited Talk O 61.2 Thu 10:10 H 0104
Electronic transport and magnetism in one-atom contacts — •Carlos Untiedt — Dep. Fisica Aplicada. Facultad de Ciencias (Fase II). Universidad de Alicante. Alicante. Spain

The smallest object that we could connect to an electronic circuit will be formed by just a single atom. With the use of the Scanning Tunneling Microscope (STM) we can fabricate and modify such bridges. There has been a great advance in the understanding of the electronic properties of these [1]. However it has been very difficult to extract consequences of the magnetism on their transport properties.

Recently we reported the observation of an effective Kondo screening of the magnetic moment of one-atom contacts between pure ferromagnetic metals by the conduction electrons [2]. Using a STM or Electromigrated Break Junctions we fabricated atomic contacts on these ferromagnetic materials and Fano-Kondo resonances where found in the conductance with the characteristic behavior of a Kondo system.

One of the advantages of our set-up configuration is the capability of the STM to study and analyze hundreds of atomic contacts. This has given us the unique opportunity of performing statistics on the Fano parameters of our conductance curves. A statistical analysis allow us to discuss on the dependence of the Kondo system with the different degrees of couplings to the environment. Finally we will show some of our latest results including Pt chains suggesting a magnetic moment being developed.
[1] Agraït,Yeyati, Ruitenbeek, Phys. Rep. 377 (2003)
[2] Nature 458, 1150(2009)

Topical Talk O 61.3 Thu 10:50 H 0104
Metallic atomic-size contacts: The role of absorbed noble gas atoms and anisotropic magnetoresistance — •Juan Carlos Cuevas — Departamento de Física Teórica de la Materia Condensada, Universidad Autónoma de Madrid, E-28049 Madrid, Spain

In this talk I will review our efforts to resolve two basic puzzles in the context of metallic atomic-size contacts. First, I will discuss how the presence of noble gas atoms affects the electronic transport through atomic contacts. In particular, I will present ab initio results for the conductance of atomic junctions comprising single noble gas atoms (He, Ne, Ar, Kr, and Xe) coupled to gold electrodes. These results show that for the lightest elements (He and Ne) no significant current flows through the noble gas atoms and their effect is to reduce the conductance of the junctions by screening the interaction between the gold electrodes. This explains the observations reported in atomic contacts with adsorbed He atoms. Conversely, the heaviest atoms (Kr and Xe) increase the conductance because of the additional current path provided by their valence p states.

On the other hand, I will address the origin of the anomalous anisotropic magnetoresistance (AMR) observed in different experiments in ferromagnetic atomic-size contacts, which is still under debate. I will present theoretical results that strongly suggest that the anomalous AMR stems from the reduced symmetry of the atomic contact geometries. This reduced symmetry leads to both a great enhancement of the AMR magnitude and an anomalous angular dependence, as compared to bulk devices.

10 min. break.

Topical Talk O 61.4 Thu 11:40 H 0104
Spin transport through organic molecules — •Wulf Wulfhekel — Physikalisches Institut, Karlsruhe Institute of Technology, Germany

We demonstrate that with the help of spin-polarized Scanning Tunneling Microscopy the spin transport across single organic molecules can be investigated and a molecular GMR junction can be realized. For this, single hydrogen phthalocyanine molecules were contacted by two ferromagnetic electrodes, i.e. a magnetic substrate and a magnetic STM tip. As substrate, ferromagnetic Co nano-islands grown Cu(111) were used, onto which the molecules were deposited. The magnetic state of the islands was determined by spin-polarized Scanning Tunneling Spectroscopy (STS) with Co tips. Then, the tip of the STM was approached in a controlled way towards a single molecule to contact the molecule. Below 0.4 nm distance, an attractive interaction between the tip and the molecule leads to a jump to contact of one of the side groups of the molecule, leading to a well defined molecular junction. Through the contacted molecule a GMR of 60% was observed which is one order of magnitude larger than the magnetoresistance without the molecule. This is explained on basis of ab initio calculations showing a selective hybridization of the molecular states with minority states of the electrodes. Finally, one of the electrodes has been replaced by an antiferromagnet forming an ideally hard magnetic layer. Due to the local character of the hybridization with the molecular states, a significant magnetoresistance can also be observed.

Topical Talk O 61.5 Thu 12:20 H 0104
Spin-current manipulation of atomic-scale magnets using SP-STM — •Stefan Krause — Institute of Applied Physics, University of Hamburg, Germany

A prerequisite on the way to advanced applications in spintronics is the detailed understanding of current-induced magnetization switching (CIMS). Here, the spin-transfer torque generated by a spin current forces a magnet to reverse its magnetization. Spin-polarized scanning tunneling microscopy (SP-STM) provides an ideal representation of a tunneling magneto-resistance device, with vacuum serving as the tunnel barrier between a biased magnetic tip and a magnetic sample.

In our experiments the ultimate lateral resolution of SP-STM is used for a very local observation and manipulation of individual Fe/W(110) nanoislands in the superparamagnetic regime. Performing a current-dependent lifetime analysis of the magnetic states, three fundamental contributions to CIMS are clearly separated and quantified: spin-transfer torque, Joule heating and Oersted field [1,2].

Lowering the temperature leads to a stabilization of the nanomagnets. In this regime the high spin-polarized tunnel current solely triggers magnetization reversal, and the threshold is determined by ramping the tunnel current. For fast reversal, short high-current pulses are applied, thereby demonstrating the capability of SP-STM for the reliable manipulation of magnetism on the atomic scale[3].
[1] S. Krause *et al.*, Science **317**, 1537 (2007).
[2] S. Krause *et al.*, Phys. Rev. Lett. **107**, 186601 (2011).
[3] G. Herzog *et al.*, Appl. Phys. Lett. **96**, 102505 (2010).

O 62: [TT] Transport: Graphene 1 (jointly with MA, HL, DY, DS, O)

Time: Thursday 9:30–13:00 Location: BH 334

O 62.1 Thu 9:30 BH 334

Spin relaxation in graphene induced by adatoms — •Jan Bundesmann and Klaus Richter — Institut für Theoretische Physik, Universität Regensburg, 93040 Regensburg, Germany

By means of a recursive Green's function method we study diffusive spin-dependent transport through graphene and graphene nanostructures. Diffusion in graphene mainly originates from charges trapped in the substrate. In addition we assume the presence of adsorbed atoms or molecules. These are the origin of a locally fluctuating spin-orbit coupling. While both intrinsic spin-orbit interaction and spin-orbit coupling induced by electric fields or curvature are rather weak (typically $\mathcal{O}(\mu eV)$), underneath adatoms these values can reach the height of meV. Our results show that adatoms clearly reduce the spin relaxation time in graphene. The ones we obtain are on the order of magnitude as the ones found in experiments ($\mathcal{O}(ns)$).

Depending on the type of adatom, the effect on intrinsic and extrinsic spin-orbit interaction is of different strength. We study how this influences the relaxation of in-plane or out-of-plane polarized spins.

Lastly we plan to address the questions if adatoms tend to relax spins via the Elliot-Yafet or rather via the Dyakonov-Perel mechanism.

O 62.2 Thu 9:45 BH 334

Emergent Gauge Fields in Bilayer Graphene — •Roland Winkler[1,2,3] and Ulrich Zülicke[4] — [1]University of Basque Country and IKERBASQUE Foundation, Bilbao, Spain — [2]Northern Illinois University, DeKalb, Illinois 60115, USA — [3]Argonne National Laboratory, Argonne, Illinois 60439, USA — [4]School of Chemical and Physical Sciences and MacDiarmid Institute for Advanced Materials and Nanotechnology, Victoria University of Wellington, Wellington 6140, New Zealand

We present a detailed study of the electronic properties of bilayer graphene. Group theory is used to derive an invariant expansion of the Hamiltonian for electron states near the **K** point taking into account the effect of electric and magnetic fields, strain and spin-orbit coupling. We obtain several new gauge fields for band electrons in bilayer graphene, resulting in novel orbital and spin-related effects.

RW is supported by IKERBASQUE Foundation, Bilbao, Spain. Work at Argonne was supported by DOE BES under Contract No. DE-AC02-06CH11357. UZ is supported by MacDiarmid Institute for Advanced Materials and Nanotechnology.

O 62.3 Thu 10:00 BH 334

Single-parameter pumping in graphene — •Sigmund Kohler[1], Pablo San-Jose[2], Elsa Prada[1], and Henning Schomerus[3] — [1]Instituto de Ciencia de Materiales de Madrid, CSIC, 28049 Madrid, Spain — [2]Instituto de la Estructura de la Materia, CSIC, 28006 Madrid, Spain — [3]Department of Physics, Lancaster University, Lancaster, LA1 4YB, United Kingdom

The ratchet or pump effect, which is the induction of a dc current by an ac force in the absence of any net bias, represents one of the most intriguing phenomena in non-equilibrium transport. For graphene, one expects that its gapless and chiral nature negatively affects pumping, because it hinders the confinement of electrons. Despite this expectation, a pump mechanism that is particularly efficient in graphene exists [1]: It is based on barriers in which the, say, left half is modulated by an ac gate voltage. Then electrons entering the barrier in evanescent modes from that side may be excited to propagating modes. Evanescent mode entering from the right, by contrast, decay before reaching the driving region. This mechanism is rather efficient in graphene, because all evanescent modes within a certain energy range contribute. The corresponding mechanism in a two-dimensional electron gas works only with modes that fulfill certain resonance conditions, which leads to a much smaller pump current.

[1] P. San-Jose, E. Prada, S. Kohler, and H. Schomerus, Phys. Rev. B **80**, 155408 (2011)

O 62.4 Thu 10:15 BH 334

Self-consistent theory of the second-harmonic generation in graphene — •Sergey Mikhailov — Institute of Physics, University of Augsburg, 86135 Augsburg, Germany

A self-consistent-field theory of the second-order nonlinear electromagnetic response of graphene is developed. The second-order polarizability and the corresponding second-order self-consistent dielectric response function of graphene are calculated for the first time. The second harmonic generation in graphene is shown to be about two orders of magnitude stronger than in typical semiconductor structures. Under the conditions of 2D plasmon resonances the second harmonic radiation intensity is further increased by several orders of magnitude.

O 62.5 Thu 10:30 BH 334

The Hubbard model on the bilayer honeycomb lattice with Bernal stacking — •Thomas C. Lang[1], Stefan Übelacker[1], Zi Yang Meng[2], Michael Scherer[1], Carsten Honerkamp[1], Alejandro Muramatsu[3], Fakher F. Assaad[4], and Stefan Wessel[1] — [1]RWTH Aachen, Aachen, Germany — [2]Louisiana State University, Baton Rouge, USA — [3]Universität Stuttgart, Stuttgart, Germany — [4]Universität Würzburg, Würzburg, Germany

Using a combination of quantum Monte Carlo, the functional renormalization group and mean-field theory we study the Hubbard model on the bilayer honeycomb as a model for interacting electrons on bilayer graphene. The free bands consisting of two Fermi points with quadratic dispersions lead to a finite density of states, which triggers the antiferromagnetic instability and spontaneously breaks sublattice and spin rotational symmetry once a local Coulomb repulsion is introduced. We show that the antiferromagnetic instability is insensitive to the inclusion of extended Coulomb interactions and discuss effects on the sublattice magnetization and of finite size systems in numerical approaches.

O 62.6 Thu 10:45 BH 334

Coulomb drag in graphene via kinetic equation approach — •Michael Schuett[1], Pavel M. Ostrovsky[1,2], Igor V. Gornyi[1,3], Mikhail Titov[4], Boris N. Narozhny[5], and Alexander D. Mirlin[1,5,6] — [1]Institut für Nanotechnologie, Karlsruhe Institute of Technology, 76021 Karlsruhe, Germany — [2]L. D. Landau Institute for Theoretical Physics RAS, 119334 Moscow, Russia — [3]A.F. Ioffe Physico-Technical Institute, 194021 St. Petersburg, Russia. — [4]School of Engineering & Physical Sciences, Heriot-Watt University, Edinburgh EH14 4AS, UK — [5]Institut für Theorie der kondensierten Materie, Karlsruhe Institute of Technology, 76128 Karlsruhe, Germany — [6]Petersburg Nuclear Physics Institute, 188350 St. Petersburg, Russia.

We calculate the Coulomb drag resistivity at finite temperature for two graphene monolayers within the kinetic equation approach. The emphasis is put on the case of fast electron-electron collisions compared to disorder induced scattering. We obtain the asymptotic behavior of the Coulomb drag resistivity ρ_D both for small chemical potentials (μ_1, μ_2) in the two layers as well as chemical potentials larger than temperature. When only one layer is at the Dirac point the Coulomb drag resistivity is zero. However when approaching the Dirac point of both layers simultaneously, the Coulomb drag resistivity does not vanish as long as $\mu_1 \propto \mu_2 \to 0$. For any finite disorder strength or alternating current Coulomb drag resistivity obeys again $\rho_D(\mu_1 = 0, \mu_2 = 0) = 0$, as expected from the particle hole symmetry argument. When both layers have large chemical potentials we recover the Fermi liquid behavior.

O 62.7 Thu 11:00 BH 334

Manifestation of electron-electron interaction in the magnetoresistance of graphene — •Johannes Jobst[1], Daniel Waldmann[1], Igor V. Gornyi[2,3], Alexander D. Mirlin[2,4,5], and Heiko B. Weber[1] — [1]Lehrstuhl für Angewandte Physik, Universität Erlangen-Nürnberg, Erlangen, Germany — [2]Institut für Nanotechnologie, Karlsruhe Institute of Technology, Karlsruhe, Germany — [3]A.F. Ioffe Physico-Technical Institute, St. Petersburg, Russia — [4]Inst. für Theorie der kondensierten Materie, Karlsruhe Institute of Technology, Karlsruhe, Germany — [5]Petersburg Nuclear Physics Institute, St. Petersburg, Russia

We investigate the magnetotransport in large area graphene Hall bars epitaxially grown on silicon carbide. In the intermediate field regime between weak localization and Landau quantization the observed temperature-dependent parabolic magnetoresistivity is a manifestation of electron-electron interaction. We can consistently describe the data with a model for diffusive (magneto)transport that covers the crossover to the ballistic regime. We find a temperature-driven crossover related to the reduction of the multiplet modes contributing to electron-electron interaction from 7 to 3 due to intervalley scattering. In addition we find a field-driven crossover from purely diffusive to partially ballistic behavior.

15 min. break.

O 62.8 Thu 11:30 BH 334

Orbital Magnetism in graphene bulk and nanostructures — •Lisa Hesse, Jürgen Wurm, and Klaus Richter — Institut für Theoretische Physik, Universität Regensburg, Germany

We study the magnetic response of finite and bulk graphene structures due to orbital motion of the charge carriers. Besides a semiclassical approach we use exact quantum mechanical calculus within the Dirac formalism to derive different analytic expressions for the magnetic susceptibility of extended systems at various field regimes. This allows us to study on the one hand edge effects which are accessible through our semiclassical treatment but also to gain profound knowledge of the importance of bulk effects in finite systems. In order to provide an independent confirmation of the theory we also perform numerical calculations on graphene nanostructures based on a tight-binding approximation.

O 62.9 Thu 11:45 BH 334

Klein paradox for arbitrary spatio-temporal scalar potential barrier and Josephson-like current in graphene — Sergey E. Savel'ev[1], •Wolfgang Häusler[2], and Peter Hänggi[2] — [1]Department of Physics, Loughborough University, Loughborough LE11 3TU, United Kingdom — [2]Institut für Physik Universität Augsburg, D-86135 Augsburg, Germany

We derive the exact time evolution according to the Dirac-Weyl equation, describing a mono-layer of graphene, in the presence of a scalar potential $U(x,t)$ of arbitrary spatial and temporal dependence at normal incidence, $p_y = 0$. This solution shows that the Klein paradox (the absence of backscattering) persists even for arbitrary temporal modulations of the barrier. Moreover, we identify an unusual oscillating current j_y running along the barrier, despite of the vanishing momentum in y-direction. This current exhibits resemblence to the Josephson current in superconductors, including the occurance of Shapiro steps and its sine-like dependence on the phase difference of wave functions.

O 62.10 Thu 12:00 BH 334

Relaxation in graphene quantum dots — •Christoph Neumann[1], Christian Volk[1,2], Sebastian Kazarski[1], Stefan Fringes[1], Stephan Engels[1,2], Bernat Terres[1,2], Jan Dauber[1,2], Stefan Trellenkamp[2], and Christoph Stampfer[1,2] — [1]JARA-FIT and II. Institute of Physics B, RWTH Aachen, 52074 Aachen, Germany — [2]Peter Grünberg Institut (PGI-8/9), Forschungszentrum Jülich, 52425 Jülich, Germany

Graphene quantum dots (QDs) have received increasing attention over the last years as interesting candidates for the future implementation of spin qbits. Compared to GaAs-based QDs, their smaller hyperfine and spin-orbit coupling promises more favorable spin coherence times. However, while the preparation, manipulation, and read-out of single spins has been demonstrated in GaAs structures, research on graphene QDs is still at an early stage. Although Coulomb blockade phenomena and excited state spectroscopy is already well established, experimental signatures allowing the identification of relaxation times have been hard to trace. Here we report on pulse gating experiments on graphene quantum devices. We will present measurements of the relaxation rates in single-layer graphene QDs. The investigated devices consist of an island with a diameter of 120 nm, 4 lateral graphene gates and 2 charge detectors. From so-called diamond measurements we extract a charging energy of 11 meV and excited state level spacings of 2-4 meV. The gates enable us to tune the tunnelling rates from the GHz down to the low MHz regime. Finally low-bias pulse gate measurements allow us to extract relaxation rates on the order of 50 ns.

O 62.11 Thu 12:15 BH 334

Minimal tight-binding model for transport in graphene heterojunctions — •Ming-Hao Liu, Jan Bundesmann, and Klaus Richter — Institut für Theoretische Physik, Universität Regensburg, 93040 Regensburg, Germany

A real-space Green's function formalism based on a minimal tight-binding model is adopted to efficiently simulate ballistic transport in graphene heterojunctions. The basic idea is to make use of the Bloch theorem along the transverse dimension of the bulk graphene, which greatly reduces the computation load and hence allows experimental sizes in the longitudinal dimension. Numerically, we will show (i) consistency with the existing results based on the effective Dirac theory for chiral tunneling through *pnp* junctions in monolayer graphene (MLG) and bilayer graphene, (ii) good agreement with recent ballistic experiments on *pnp* junctions in MLG, and (iii) new predictions for spin-dependent tunneling through *pn* junctions in MLG in the presence of the Rashba spin-orbit coupling.

O 62.12 Thu 12:30 BH 334

Quantum Hall effect in graphene with superconducting electrodes — •Markus Weiss, Peter Rickhaus, and Christian Schönenberger — Departement Physik, Universität Basel, Klingelbergstrasse 82, CH-4056 Basel

We report on the realization of an integer quantum Hall system with superconducting electrodes. Graphene was contacted to niobium electrodes that show a critical field of about 4 tesla, where electronic transport passes mainly through quantum Hall edge-states and bulk transport is largely suppressed. We find a magnetic field range of more than one tesla where well developed quantum Hall plateaus coexist with superconductivity in the leads. In high magnetic fields with the electrodes in the normal state we observe plateaus at $G=\nu e^2/h$ for $\nu=2$, 4, and 10. Reducing the magnetic field to below the upper critical field of the electrodes, the conductance on the plateaus shows a sudden increase. Whereas the conductance on the $\nu=2$ plateau increases only by 10%, the increase on the $\nu=6$ and $\nu=10$ plateau is considerably larger with 60% and 80%, respectively. We attribute this conductance enhancement to multiple Andreev reflection processes along the graphene-superconductor interface, that lead to the formation of Andreev edge-states. The observed conductance enhancement of the $\nu=6$ and 10 plateaus is consistent with a doubling of the conductance contribution of the second and third edge-states. We attribute the small conductance increase on the $\nu=2$ plateau to the special nature of the zero energy Landau level, that makes the corresponding edge-state sensitive to the structure of the graphene edge.

O 62.13 Thu 12:45 BH 334

Klein paradox for arbitrary spatio-temporal scalar potential barrier and Josephson-like current in graphene — Sergey E. Savel'ev[1], •Wolfgang Häusler[2], and Peter Hänggi[2] — [1]Department of Physics, Loughborough University, Loughborough LE11 3TU, United Kingdom — [2]Institut für Physik Universität Augsburg, D-86135 Augsburg, Germany

We derive the exact time evolution according to the Dirac-Weyl equation, describing a mono-layer of graphene, in the presence of a scalar potential $U(x,t)$ of arbitrary spatial and temporal dependence at normal incidence, $p_y = 0$. This solution shows that the Klein paradox (the absence of backscattering) persists even for arbitrary temporal modulations of the barrier. Moreover, we identify an unusual oscillating current j_y running along the barrier, despite of the vanishing momentum in y-direction. This current exhibits resemblence to the Josephson current in superconductors, including the occurance of Shapiro steps and its sine-like dependence on the phase difference of wave functions. [1] S.E. Savel'ev, W. Häusler, and P. Hänggi, ArXiv: 1107.4983 .

O 63: Focussed session: Frontiers of electronic structure theory: Strong correlations from first principles IV (jointly with TT)

Time: Thursday 10:30–13:15 Location: HE 101

Topical Talk O 63.1 Thu 10:30 HE 101

Random phase approximation and *GW* for correlated systems — •Patrick Rinke — Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, Germany

In the quest for finding an “optimal" first principles electronic structure method, that combines accuracy and tractability with transferability across different chemical environments and dimensionalities (e.g. molecules, wires/tubes, surfaces, solids), the treatment of exchange and correlation in terms of “exact-exchange plus correlation in the random-phase approximation (EX+cRPA)” offers a promising avenue. Likewise one can express the same level of theory in the Green’s function context through the *GW* approximation, which has the additional advantage that quasiparticle spectra as measured by direct and inverse photoemission become accessible. For lanthanide and actinide oxides as prototypical f-electron solids, I will demonstrate that *GW* calculations yield spectral properties in good agreement with experiment, provided a suitable starting point like density-functional theory in the local-density approximation augmented by Hubbard U corrections (LDA+U) is used [1]. For the f-electron metal Cerium, for which (semi)local DFT functionals fail to reproduce the isostructural α-γ phase transition, EX+cRPA calculations based on hybrid functionals yield a double minimum in the total energy versus volume curve, indicative of the phase transition. For correlations in molecular systems, I will contrast EX+cRPA with *GW* and discuss recent schemes that go beyond cRPA [2]. [1] H. Jiang, *et al.*, Phys. Rev. Lett. **102**, 126403 (2009), [2] J. Paier *et al.*, arXiv:cond-mat/1111.0173

O 63.2 Thu 11:00 HE 101

Renormalized second-oder perturbation theory for the electron correlation energy: concepts and benchmarks — •Xinguo Ren[1], Patrick Rinke[1], Gustavo E. Scuseria[2] und Matthias Scheffler[1] — [1]Fritz-Haber-Institut der MPG, Berlin, Germany — [2]Rice University, Houston, USA

We present a renormalized second-oder perturbation theory (R2PT) for the electron correlation energy that combines the random-phase approximation (RPA), second-order screened exchange (SOSEX) [1], and renormalized single excitations (rSE) [2]. These three terms all involve a summation of certain types of diagrams to infinite order, and can be viewed as a “renormalizationöf the direct, the exchange and the single excitation (SE) term of 2nd-order Rayleigh-Schrördinger perturbation theory based on an (approximate) Kohn-Sham reference state. A preliminary version of R2PT has been benchmarked for covalently-bonded molecular systems and chemical reaction barrier heights [3] and shows an overall well balanced performance. We have extended this, by including “off-diagonal” diagrams into the rSE term and expect this refined version of R2PT to be more generally applicable to electronic systems of different bonding characteristics. Extended benchmarks of van-der-Waals-bonded molecules and crystalline solids will be presented. [1] A. Grüneis *et al.*, J. Chem. Phys. **131**, 154115 (2009). [2] X. Ren *et al.*, Phys. Rev. Lett. **106**, 153003 (2011). [3] J. Paier *et al.*, arXiv:cond-mat/1111.0173.

O 63.3 Thu 11:15 HE 101

Energetics of LDA+DMFT(CTQMC) in a fully charge self-consistent pseudopotential formulation — •Daniel Grieger, Christoph Piefke, Oleg E. Peil, and Frank Lechermann — 1. Institut für Theoretische Physik, Universität Hamburg, Germany

In recent years, the combination of the local-density approximation (LDA) to density functional theory with the dynamical mean-field theory (DMFT) has proven to be a powerful and reliable tool to describe explicit strong electronic correlations in realistic materials. In order to obtain information about observables like equilibrium lattice constants, bulk moduli, phase stability and many more, it is essential to calculate total energies in this formalism in a consistent and physically sound way. A key step is to converge the correlated charge density within a comprehensive LDA+DMFT interface (charge self-consistency). We use a mixed-basis pseudopotential implementation of DFT and a numerically exact hybridisation-expansion continuous-time QMC solver for DMFT, so that we can combine the highest possible accuracy with a minimum of further approximations. Besides illuminating the crucial parts of the theoretical total-energy formalism, we will present the application of the method to calculate details of the phase diagram of several realistic materials in the realm of intermediate to strong electronic correlations.

O 63.4 Thu 11:30 HE 101

Unraveling the α-γ phase transition in Ce from first principles — •Marco Casadei[1], Xinguo Ren[1], Patrick Rinke[1], Angel Rubio[1,2], and Matthias Scheffler[1] — [1]Fritz-Haber-Institut der MPG (TH), Berlin, Germany — [2]UPV/EHV, San Sebastian (Fisica Materiales), Spain

The presence of localized, partially occupied f-electron states dictates many of the peculiar physical properties of rare-earth materials. In particular, the description of the isostructural α-γ phase transition in Cerium poses a great challenge to density-functional theory (DFT) based approaches since local/semilocal functionals (LDA/GGA) fail to produce the phase transition. We approach this problem by treating all electrons (including the f-electrons) at the same quantum mechanical level. The calculations are performed using both hybrid functionals (e.g. PBE0), that incorporate a portion of exact-exchange, and full exact-exchange plus correlation at the level of the random phase approximation (EX+cRPA). The PBE0 hybrid functional predicts the correct magnetic properties of both phases and yields a double minimum in the total energy versus volume curve, indicative of the phase transition, although with the wrong energetic order. EX+cRPA is then essential to capture the right energetic ordering of the minima. Our results suggest a hypothetical persistence of the phase transition to zero temperature, the driving mechanism being the change of the hopping amplitude between f-type orbitals.

O 63.5 Thu 11:45 HE 101

Electron correlation effects in americium metal under pressure — •Alexander Shick[1,2], Jindrich Kolorenc[2], and Roberto Caciuffo[1] — [1]European Commission, Joint Research Centre, Institute for Transuranium Elements, Karlsruhe — [2]Institute of Physics ASCR, Prague

Evolution of the electronic structure of elemental americium due to the lattice compression is investigated. We make use of a version of the LDA+DMFT method based on the "exact diagonalization" of the multi-orbital Anderson impurity Hamiltonian with the full Coulomb interaction matrix and the spin-orbit coupling [1]. Also, we include the charge density self-consistency [2]. We observe only a relatively minor modifications of the electronic structure with compression, which appears to be in accord with the RXES and XANES spectra at the L_3 edge that were recently determined experimentally [3]. Neither these experiments nor our calculations support the earlier theoretical proposal that the f-electron occupation should increase with compression, leading eventually to a mixed-valence ($5f^6$ + $5f^7$) behavior [4].

[1] A. B. Shick, J. Kolorenc, V. Janis, A. I. Lichtenstein, Phys. Rev. **B 84**, 113112 (2011). [2] A. B. Shick, J. Kolorenc, L. Havela, A. I. Lichtenstein, Phys. Rev. **B 80**, 085106 (2009). [3] S. Heathman, J.-P. Rueff, L. Simonelli, M. A. Denecke, J.-C. Griveau, R. Caciuffo, G. H. Lander, Phys. Rev. **B 82**, 201103 (2010). [4] S. Y. Savrasov, K. Haule, G. Kotliar, Phys. Rev. Lett. **96**, 036404 (2006).

O 63.6 Thu 12:00 HE 101

DFT and beyond-DFT derived tight-binding parameters for RMnO$_3$ using the VASP2WANNIER90 interface — •Sowmya Sathyanarayana Murthy[1], Roman Kovacik[2], Martijn Marsman[1], Cesare Ederer[2], Georg Kresse[1], and Cesare Franchini[1] — [1]Faculty of Physics, University of Vienna and Center for Computational Materials Science, A-1090 Wien, Austria — [2]School of Physics, Trinity College Dublin, Dublin 2, Ireland

By combining the Vienna ab initio simulation package with the wannier90 code we have constructed maximally localized Wannier functions (MLWFs) for the Jahn-Teller/GdFeO$_3$ distorted insulating perovskites RMnO$_3$ (R=La, Pr, Nd, Sm and Eu) at different levels of approximation for the exchange-correlation kernel (PBE, HSE and GW)[1]. By suitably mapping the MLWFs onto an effective e_g tight-binding (TB) Hamiltonian[1,2] we have computed a complete set of TB parameters using two alternative model parameterizations, with and without an explicit treatment of the electron-electron interaction. The so obtained set of tabulated TB parameters provide band dispersion in excellent agreement with the underlying *ab initio* and MLWF bands. The evolution of the structural and electronic properties of RMnO$_3$ as a function of the atomic radius of R[3] is discussed in terms of the corresponding changes in the TB parameters and MLWFs properties.

References:

[1] C. Franchini *at. al* arXiv:1111.1528 (2011).
[2] R. Kovacik & C. Ederer Phys. Rev. B **81** 245108 (2010).
[3] T.Kimura *et al.* Phys. Rev. B **68** 060403(R) (2003).

O 63.7 Thu 12:15 HE 101

A periodic implementation of hybrid functionals for numeric atom-centered orbitals

— Sergey Levchenko, Rainer Johanni, Xinguo Ren, Jürgen Wieferink, Patrick Rinke, •Volker Blum und Matthias Scheffler — Fritz-Haber-Institut der Max-Planck-Gesellschaft, D-14195 Berlin

Traditional density functional theory based on the electron density and its gradients has a successful track record in condensed matter theory, but is also subject to some well known limitations: For instance, the residual self-interaction of the electrons; or, failure to cover the fundamental band gap of solids. Hybrid density functionals that add some non-local exchange are becoming a *de facto* strategy to remedy such issues; however, evaluating the non-local exchange operator in periodic systems efficiently can be nontrivial. We here describe an implementation of periodic non-local exchange using numeric atom-centered basis functions within the FHI-aims [1] all-electron code. The implementation is based on a localized “resolution of identity” strategy for the Coulomb operator, coupled with efficient integral and density matrix screening operations (in real space) that allow to cover periodic systems up to (currently) $O(100)$ atoms at essentially converged basis set accuracy, and seamlessly in parallel (memory and CPU time, tested up to hundreds of CPUs). We prove the accuracy of our approach for bulk semiconductors and their surfaces, using the PBE0 and HSE density functionals. [1] V. Blum *et al.*, Comp. Phys. Comm. **180**, 2175 (2009).

O 63.8 Thu 12:30 HE 101

Precise all-electron response functions from a combined spectral sum and Sternheimer approach: application 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

The optimized-effective-potential (OEP) method is used to construct local potentials from non-local, orbital-dependent exchange-correlation functionals, e.g., exact exchange (EXX). The method involves two response functions, which have to be converged to very high precision to obtain smooth and stable local potentials. Usually, this requires an exceptionally large orbital basis, leading to very costly calculations, especially for all-electron methods such as FLAPW [1,2]. In this work, we propose a scheme that combines the usual spectral sum from standard perturbation theory with a radial Sternheimer approach. It also comprises a, albeit small, Pulay-type correction, which refines the results especially for small basis sets. We demonstrate that with this new approach already the conventional minimal LAPW basis set is sufficient to yield precise response functions. Furthermore, very few unoccupied states are required, which reduces the computational cost considerably. The numerically important Sternheimer contribution arises from the potential dependence of the LAPW basis functions and is constructed by solving inexpensive radial differential equations. We show results for complex transition-metal oxides.

[1] M. Betzinger *et al.*, Phys. Rev. B **83**, 045105 (2011)
[2] Fleur code: http://www.flapw.de

O 63.9 Thu 12:45 HE 101

Accurate electronic structure calculation on transition metal defects in SiC by HSE06+U functional

— •Viktor Ivády[1] and Ádám Gali[1,2] — [1]Research Institute for Solid State Physics and Optics, Hungarian Academy of Sciences, PO Box 49, H-1525 Budapest, Hungary — [2]Department of Atomic Physics, Budapest University of Technology and Economics, Budafoki út 8, H-1111 Budapest, Hungary

Relatively little is known about transition metal impurities in semiconductors. The accurate treatment of these systems require the exact description of strongly correlated partially occupied d and f shells of the impurities in host materials of sp^3 bonds. In our study we investigate the electronic structure of transitional metals (Ti, V and Cr) in 4H-SiC by means of PBE (semi)local functional and HSE06 range separated hybrid functional calculations in 576-atom supercell where experimental data are available for these impurities. While HSE06 functional yielded superior results over (semi)local functionals regarding the Mott-insulators with correlated states our results show that HSE06 are not sufficiently accurate for the chosen isolated transition metal defects. The application of HSE06+U functional allow us to apply orbital dependent corrections on the correlated orbitals in the experimental band gap of SiC. We chose the U to fulfill the generalized Koopmann's and Janak's theorems that is presumably an "exact" functional of the system. Our investigations show that U should be energy dependent and its acutal value depends also on the given defect configuration even for the same type of the impurity. We compare the experimental and calculated transition levels obtained by the "exact" functional.

O 63.10 Thu 13:00 HE 101

Origin of magnetism and qausiparticle properties of Cr-doped rutile and anatase TiO2

— •Fabiana Da Pieve[1,2,3], Sergio Di Matteo[4], Tonatiuh Rangel[2,3], Matteo Giantomassi[2,3], Gian-Marco Rignanese[2,3], and Xavier Gonze[2,3] — [1]EMAT, University of Antwerp, Groenenborgerlaan 171, B-2020 Antwerp, Belgium — [2]Unité NAPS, Université Catholique de Louvain,Place Croix du Sud 1, 1348 Louvain-la-Neuve, Belgium — [3]ETSF, European Theoretical Spectroscopy Facility — [4]Groupe theorique Departement Materiaux et Nanoscience Institut de Physique de Rennes,UMR UR1-CNRS 6251, Université de Rennes 1, F-35042 Rennes Cedex, France

We studied magnetic ground-state properties, band gaps and quasiparticle excitations in the rutile and anatase phases of Cr-doped TiO2, by combining LSDA+U ab-initio calculations and many-body GW perturbative corrections to LSDA+U results. The position of Cr-impurity states and band gaps found by GW on top of LSDA+U is in good agreement with available experimental data. The magnetic ground-state is characterized by a different geometrical coordination of Cr-ions in rutile and in anatase: interestingly, these constraints, due to correlated hopping (superexchange, direct exchange or F-center exchange) lead to ferromagnetic or antiferromagnetic couplings of Cr-ions depending on the number of O vacancies. We suggest two key experiments that could confirm our calculations by measuring directly Cr-t2g states, which play a central role in our model and in optical properties.

O 64: Plasmonics and nanooptics III

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

O 64.1 Thu 10:30 MA 005

Antenna-enhanced Photocurrent Microscopy on Single-Walled Carbon Nanotubes

— •Nina Rauhut[1], Nitin Saxena[1], Michael Engel[2], Ralph Krupke[2], Mathias Steiner[3], and Achim Hartschuh[1] — [1]Department Chemie und CeNS, LMU, München, Germany — [2]Karlsruher Institut für Technologie, Karlsruhe, Germany — [3]T. J. Watson Research Center, IBM, Yorktown Heights, NY,USA

The unique optical and electronic properties of single-walled carbon nanotubes (SWCNTs) make these quasi 1D structures promising building blocks for nanoscale electronic and optoelectronic devices [1]. A powerful method to characterize SWCNT based field-effect transistors is scanning photocurrent microscopy (SPCM), where a focused laser spot is raster scanned across a device, recording the photocurrent signal at the same time. Due to diffraction SPCM measurements have been restricted so far to a spatial resolution of few hundred of nanometers.

We report on the first photocurrent measurements along single SWCNTs with sub 30 nm spatial resolution. Our approach extends conventional tip-enhanced near-field optical microscopy (TENOM) in which the diffraction limit is overcome by exploiting antenna-enhanced localized fields [2]. Combining SPCM and TENOM, we succeeded in simultaneously recording enhanced optical and photocurrent images with nanoscale resolution providing new insight into the optoelectronic properties of nanostructures.

[1] Avouris, P.; Chen, Z.; Perebeinos, V. Nat. Nanotechnol. 2007, 2,

605 [2] Hartschuh, A. Angew. Chemie (Int. Edition) 2008, 47, 8178

O 64.2 Thu 10:45 MA 005

Near-Field Investigation of Nanostructures with Normal Incidence Photoemission Electron Microscopy

— •Pascal Melchior[1], Ernst Jan Vesseur[2], Alexander Fischer[1], Markus Rollinger[1], Daniela Bayer[1], Christian Schneider[1], Albert Polman[2], and Martin Aeschlimann[1] — [1]Fachbereich Physik and Research Center OPTIMAS, Technische Universität Kaiserslautern, Germany — [2]FOM Institute AMOLF, Amsterdam, The Netherlands

Photoemission electron microscopy (PEEM) enables the mapping of the near-field distribution of nanostructures under broadband laser excitation with a subwavelength spatial resolution. The combination with ultrafast laser pulses makes PEEM to an excellent technique to address the electron dynamics of nanoantennas by means of nonlinear photoemission. In standard PEEM systems, a grazing angle of incidence is used for illumination. However, the asymmetric illumination causes phase retardation effects and complex intensity distributions because of the superposition of higher order plasmonic modes. The complexity of the observed photoemission behavior under grazing angle makes the interpretation of static near-field distributions as well as time-resolved measurements challenging. With a new PEEM configuration we now excite the sample under normal-incidence and are thus able to eliminate these effects. We show first results of phase-resolved normal-incidence (NI) measurements on gold ring resonators that enable us to distinguish the resonance behavior of individual nanostructures with a subwavelength spatial resolution. The results are corroborated with FDTD calculations of the near-field properties of the structures.

O 64.3 Thu 11:00 MA 005

Time resolved near-field microscopy of metal nanoparticles

— •Matthias Brandstetter[1,2], Ralf Vogelgesang[1], and Markus Lippitz[1,2] — [1]Max-Planck Institut für Festkörperforschung, Stuttgart — [2]4. Physikalisches Institut, Universität Stuttgart

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 periodically modulates the geometry of a nanoparticle. The mechanical oscillations launched by the laser pulse lead to a variation in the local electron density of the nanoparticle and therefore a local variation in the dielectric properties. Using an AFM tip as near-field scatterer, we locally detect these changes of the dielectric properties of a nanoparticle on the nanoscale. The confinement of the near-fields will allow us to explore the elastomechanical properties of nanoparticles with a spatial resolution of 20nm. We present our combination of an apertureless scanning near-field microscope and a pump probe setup as well as first experimental results.

O 64.4 Thu 11:15 MA 005

Light Emission Mediated By A Lifted Conjugated Polymer

— •Jingcheng Li[1], Gunnar Schulze[1], Luz M. Ballesteros[2], Anna Strozecka[1], Robin Schürmann[1], Katharina J. Franke[1], and Jose I. Pascual[1] — [1]Institut für Experimentalphysik, Freie Universität Berlin, Arnimallee 14, D-14195 Berlin, Germany — [2]Departamento de Química Física, Facultad de Ciencias, Universidad de Zaragoza, 50009 Spain

In molecular junctions, the coupling between transporting electrons and molecular vibrations can lead to molecular heating. Understanding and controlling the heat generation and dissipation are essential for future molecular electronics. In this project, combined with scanning tunneling microscope (STM) light emission, we explored the mechanism of molecular heating in the junction. The STM tip was used to contact a single conjugated polymer and lift it from surface to form molecular junction. Light emission induced by tunneling electrons through the molecular junction was collected. After removing the plasmon background, the strong coupling between electrons and molecular vibrations is uncovered. Black body radiation theory is used to determine the temperature of polymer chains.

O 64.5 Thu 11:30 MA 005

Magic Angles in Metamaterials

— •Sven M. Hein[1], Lutz Langguth[1,2], and Harald Giessen[1] — [1]4th Physics Institute and Research Center SCOPE, University of Stuttgart, D-70569 Stuttgart, Germany — [2]Center for Nanophotonics, FOM Institute for Atomic and Molecular Physics (AMOLF), Science Park 104, 1098 XG Amsterdam, The Netherlands

When coupling two dipoles to each other in three dimensions, there are certain conditions under which the interaction vanishes. This effect is known for example in Nuclear Magnetic Resonance as "Magic Angles". It arises from the fact that at certain geometric arrangements the dipole coupling changes from attractive to repulsive. In 3D metamaterials [1], we have to consider the electric as well as the magnetic dipoles, and beyond spatial variation also twisting is possible, e.g. in stereometamaterials [2]. We investigate this intriguing effect in detail and show that it could be useful to elucidate quadrupole- and higher-order interactions. Allowing for retardation leads to a plethora of fascinating new effects.

[1] N. Liu et al., Nature Materials 7, 31 (2008).
[2] N. Liu and H. Giessen, Nature Photonics 3, 157-162 (2009).

O 64.6 Thu 11:45 MA 005

Near-field infrared microscopy with a broadband light source

— •Stefanie Bensmann[1], Christoph Janzen[1], Reinhard Noll[1], and Thomas Taubner[1,2] — [1]Fraunhofer-Institut für Lasertechnik (ILT), Aachen — [2]1. Physikalisches Institut 1A, RWTH Aachen

Scattering-type near-field infrared microscopy (s-SNOM) allows to record IR spectra at a wavelength-independent spatial resolution of approx. 30 nm. In general these spectra are taken sequentially by repeating a measurement at different wavelengths which can be time-consuming. Furthermore, conventional MIR laser sources have a limited spectral range excluding the possibility to examine samples like e.g. certain semiconductors, polar crystals and different polymers.

These problems can be circumvented by using broadband IR light sources covering an extended frequency range. They allow to record a full spectrum within a single measurement (interferogram with Fourier transformation) [1-3]. However, thermal sources or a laser power of less than 1 mW only permit the study of samples with a strong resonance. We present first spectra recorded with a broadband IR laser with a power of several milliwatt at 8.9-13.7 μm that is currently developed at the ILT with the NeaSNOM (near-field optical microscope from Neaspec, www2.neaspec.com). This new system will extend the spectral range covered and allow to examine samples with weaker resonances.

[1] M. Brehm et al., Optics Express 15, p. 11222, 2006.
[2] S. Amarie et al., Optics Express 17, p. 21794, 2009.
[3] F. Huth et al., Nature Materials 10, p. 352, 2011.

O 64.7 Thu 12:00 MA 005

Quantitative analysis and modeling of the near-field optical signals on vertically layered samples

— •Benedikt Hauer, Andreas Engelhardt, and Thomas Taubner — I. Institute of Physics (IA), RWTH Aachen University, Sommerfeldstraße 14, 52074 Aachen, Germany

In scattering-type scanning near-field optical microscopy (s-SNOM) the evanescent electric fields at the apex of a sharp illuminated tip can be used to probe the dielectric properties of a sample with a subwavelength resolution given by the tip radius. The near-field coupling depends on both the three-dimensional composition of the sample and the tip's material and geometry.

We present a quantitative and fully analytical theory to predict the s-SNOM signal strength of layered sample systems depending on the vertical tip–sample separation. The calculation is based on the well-established contrast model by Cvitković et al. [1] and coincides much better with experimental approach curves than a multilayer model in which the tip is approximated as a point dipole [2]. By varying the layer thickness and the imaging parameters we demonstrate the validity of our theory in the infrared spectral range. The findings are used to determine the optimum microscope settings in order to distinguish small differences in layer thickness or dielectric properties. Our work demonstrates the capability of s-SNOM to extract quantitative information on the vertical structure of a sample up to a depth of 100 nm.

[1] A. Cvitković et al., Optics Express 15, 8550 (2007)
[2] J. Aizpurua et al., Optics Express 16, 1529 (2008)

O 64.8 Thu 12:15 MA 005

Near-field Spectroscopic Imaging with Parabolic Mirror Assisted Gap-Mode Optical Microscopy

— •Kai Braun, Dai Zhang, Xiao Wang, and Alfred J. Meixner — Institut für Physikalische und Theoretische Chemie, Universität Tuebingen, Germany

The recognition and identification of individual components is essential in many scientific issues. Raman microscopy is well established to detect chemical contrasts, however with a diffraction limited resolution. In this work we will present our recent work of high-resolution spectroscopic imaging using parabolic mirror assited gap-mode optical microscopy. A high NA parabolic mirror has been adopted in this new type of microscope as focusing and collecting element [1] which enables to investigate opaque samples with the highest NA achievable in air. Optical field enhancement is achieved in the gap between a sharp Au-tip and the substrate. The tip is excited efficiently by a radially polarized laser beam [2]. The optical signal emerging from the gap is simultaneously collected by an avalanche photo diode and a spectrometer. In addition the simultaneously obtained topographic information can be used for analysing the morphology correlated local material distribution We will show topographic and spectroscopic imaging of different components in a modified Diamond like Carbon (DLC) film etc. We demonstrate the prospective application of this microscope in a variety of important fields.

[1] M. A. Lieb, A. J. Meixner, Opt. Exp. 2001, 8, 456. [2] D. Zhang et all. PRL, 2010, 104, 5.

O 64.9 Thu 12:30 MA 005

Phase-sensitive near-field mapping

— •Stefan Griesing, Andreas Englisch, and Uwe Hartmann — Institute of Experimental Physics, Universität des Saarlandes, P.O. Box 15 11 50, D-66041 Saarbrücken

The combination of a standard SNOM set-up with an interferometer give an access to the phase information of the optical near-field. Fiber-based aperture SNOMs connected to a pseudoheterodyne set-up are sensitive to low-frequency phase variations which are caused by environmental effects. In order to stabilize the reference phase, we introduced an active phase stabilization system in our setup. The detected near-field signal is demodulated by a lock-in amplifier. The real part of the second harmonic of the fiberstretchers drive frequency is detected and used as input signal for a PID feedback loop. The stretcher is then driven by a signal composed of the modulation part and the feedback part. In the case of a slow PID loop which solely follows the environmentally caused phase fluctuations, amplitude and phase information of the sample are obtained by demodulation of the first harmonic. The most interesting application is the investigation of highly dispersive media. In this case, a second wavelength is injected in the system. The PID feedback loop is fed with the real part of the second harmonic of one wavelength as described above. If a short time constant of the feedback-loop is chosen it becomes fast and compensates completely for phase variations of the input wavelength. Solely the difference phase of both wavelengths, caused by the dispersion of the sample, remains in the interference signal and can be measured.

O 64.10 Thu 12:45 MA 005

Investigation of mid-infrared s-SNOM subsurface imaging on topography-free samples

— •Andreas Engelhardt, Benedikt Hauer, and Thomas Taubner — I. Institute of Physics (IA), RWTH Aachen University, Sommerfeldstraße 14, 52074 Aachen, Germany

Scattering-type scanning near-field optical microscopy (s-SNOM) provides optical information of a sample with a nanoscale-resolution in the order of the probing tip radius ($\sim 30\,\mathrm{nm}$) which allows for material-specific imaging and even spectroscopy on the nanoscale. Optical coupling of the probe with nanoscale objects also occurs through thin cover layers of low refracting materials enabling the detection of objects underneath the surface [1].

We demonstrate subsurface s-SNOM imaging of metallic nanostructures with mid-infrared light through thin ($30 - 100\,\mathrm{nm}$) and flat dielectric layers. The latter do not reveal the geometry of the structures in their surface topography, thus topography artifacts are avoided. We observe that the visibility of the buried objects improves with increasing oscillation amplitude of the probe due to a better signal-to-noise ratio, however at the cost of contrast loss. The study provides basic experimental data for the theoretical development of a powerful s-SNOM based nondestructive nano-tomography characterization method [2].

[1] T. Taubner *et al.*, Optics Express, **13**, 8893 (2005)
[2] J. Sun *et al*, APL, **95**, 121108 (2009)

O 65: Graphene V

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

O 65.1 Thu 10:30 MA 041

The Suitability of Single Crystal Metal Films as Substrates for Graphene Growth

— •Patrick Zeller[1], Michael Weinl[2], Matthias Schreck[2], and Joost Wintterlin[1] — [1]LMU München, Department Chemie — [2]Universität Augsburg, Institut für Physik

We report about a project in which thin, single crystal films of various metals are investigated as substrates for the epitaxial growth of graphene. The films consist of 100 to 150 nm thick, epitaxially oriented metal layers grown on Si(111) wafers. 40 to 100 nm thick yttria-stabilized zirconia (YSZ) buffer layers separate the metal from the Si substrate [1]. As metals we have investigated Ir(111), Ru(0001), and Ni(111). All metal films display high crystalline quality with a typical mosaic spread in the range of 0.2 to 0.9°. Ir films have the lowest values down to 0.1°. Graphene was grown on the films by chemical vapor deposition (CVD) of ethylene at elevated temperatures. Methods used were scanning tunneling microscopy (STM), low-energy electron diffraction (LEED), Auger electron spectroscopy (AES), atomic force microscopy (AFM) and scanning electron microscopy (SEM). The topography of the as-grown metal films can be improved by annealing in UHV. Investigations of the thermal stability and dewetting of the films were done. AFM and SEM show the size of the graphene domains. We show that the quality of the graphene layers achieved on these metal films is comparable to epitaxial graphene grown on bulk metal single crystals. [1] Gsell, S., et al., Journal of Crystal Growth 2009, 311, 3731.

O 65.2 Thu 10:45 MA 041

Epitaxial growth of graphene on Ir(111) by liquid precursor deposition

— •Samuel Grandthyll[1], Frank Müller[1], Christian Zeitz[1], Karin Jacobs[1], Stefan Hüfner[1], Stefan Gsell[2], and Matthias Schreck[2] — [1]Saarland University, Experimental Physics, D-66041 Saarbrücken, Germany — [2]University Augsburg, Institut Phys. D-86135 Augsburg, Germany

The epitaxial growth of graphene on the surface of an Ir/YSZ/Si(111) multilayer substrate via the deposition of a liquid carbon precursor (acetone) was investigated by x-ray photoelectron spectroscopy, x-ray photoelectron diffraction, low-energy electron diffraction (LEED), and Fermi surface mapping. It is shown that the onset of graphene formation starts in a low temperature range around 600 K and that subsequent annealing up to 1000 K finally results in well-ordered graphene monolayers. Comparison of temperature-dependent LEED data with model calculations suggests that the growth of graphene takes place via a backbonelike growth by the formation of a hexagonal network connecting the hcp and fcc configuration sites within the similar to 10x10/9x9 supercell. In LEED, the low intensities of the superstructure related satellite spots give evidence for only small corrugations of the graphene layer due to weak interaction with the Ir(111) surface, making graphene on Ir(111) similar to free-standing graphene with the Fermi surface providing distinct spots at the K points.

O 65.3 Thu 11:00 MA 041

Local tunneling spectroscopy of the Hydrogen-induced impurity state in quasi-freestanding graphene

— •Ronny Schlegel[1], Martha Scheffler[1], Danny Haberer[1], Rico Pohle[1], Torben Hänke[1], Alexander Grüneis[1,2], Christian Hess[1], and Bernd Büchner[1] — [1]Leibniz Institute for Solid State and Materials Research Dresden — [2]University of Vienna, Austria

Graphene has a unique electronic structure, which is expected to exhibit a linear dispersion near the Fermi edge. Usually this peculiar feature is difficult to observe due to proximity effect from the substrate. However, the fabrication of quasi-freestanding graphene on specific multi-layer metal surfaces has recently been demonstrated.

Manipulation of such graphene through selective insertion of impurities may allow to tune the electronic structure and thus to open up new routes towards graphene based device functionalities. Hydrogenation leads to a reversible gap opening at the Fermi edge. Also a dispersionless, hydrogen-induced state appears in the center of this gap.

Here we use scanning tunneling microscopy and spectroscopy (STM/STS) to study graphene samples with an outstanding cleanness obtained by in-situ preparation under UHV conditions. The surfaces are investigated by STM and atomically resolved images of the pristine graphene as well as the hydrogen adsorbate sites were achieved. STS measurements reveal an enhanced DOS near the Fermi edge after hydrogenation, consistent with theoretical predictions and ARPES experiments.

O 65.4 Thu 11:15 MA 041

Investigation of the electronic structure of bilayer graphene on Ni(111) — •Martin Weser[1], Roland Koch[2], Elena Voloshina[3], Alex Generalov[1,4], Hendrik Vita[1], Thomas Seyller[2], Karsten Horn[1], and Yuriy S. Dedkov[5] — [1]Fritz-Haber Institut, Berlin, Germany — [2]Universität Erlangen-Nürnberg, Erlangen, Germany — [3]Freie Universität, Berlin, Germany — [4]Technische Universität Dresden, Germany — [5]SPECS Surface Nano Analysis GmbH, Germany

Among the many proposed applications of graphene in electronic devices, its use as a spin-filter has received attention, because the electronic structure of graphene and that of close-packed surfaces of ferromagnetic metals such as Ni and Co overlap only for the minority spin bands at the Fermi level. The effect was predicted to strongly increase with increasing of the number of graphene layers. We have developed a method for multilayer preparation using pyridine cracking on Ni(111) in ultrahigh vacuum. We characterize our multilayer films using low energy electron diffraction, core and angle-resolved valence level photoelectron spectroscopy. Multilayers are found to grow in a manner where consecutive layers are rotated against each other by well-defined angles, a fact that may lead to a decoupling of layers as found in multilayer growth on the carbon face of SiC(000-1). It was found that twisted stacking occurs for the overlayer, with two favorable rotation angles. In spite of this arrangement, spin filtering may still be possible because of the specific shape of the majority spin states in Ni(111) at EF.

O 65.5 Thu 11:30 MA 041

DFT studies of Graphene on Ni(111) and Surface Nickel Carbide Ni_2C — •Andreas Garhofer[1], Peter Jacobsen[1,2], Bernhard Stoeger[1], Gareth S. Parkinson[1], Michael Schmid[1], Roman Caudillo[3], Florian Mittendorfer[1], Josef Redinger[1], and Ulrike Diebold[1,2] — [1]Institute of Applied Physics, TU Wien, Austria — [2]Tulane University, USA — [3]Intel Corporation

Graphene with its unique transport properties supported on ferromagnetic materials is a promising candidate for the fabrication of spin-filtering devices. In order to study the growth of graphene on metal surfaces, graphene on Ni(111) is a perfect system from a structural point of view.

We studied the systems using the DFT program package VASP with the vdW-DF method in the flavor of optB88 to include van der Waals interactions. In our theoretical discussion we analyzed the growth of graphene and Ni_2C on Ni(111). We calculated the stability of the surface carbide phase and the binding energies of rotated and unrotated graphene on Ni(111) as well as on Ni_2C. Graphene and Ni_2C have no epitaxial relationship due to their incommensurate lattices, leading to a spread in grain rotations. The CVD growth of graphene on Ni(111) was also studied with STM. The experiments showed not only perfect aligned (1x1) structures, but also several moiré patterns. They are due to grain rotations of graphene on both Ni(111) and also surface nickel carbide Ni_2C. During CVD growth, carbon atoms segregate into the Ni bulk. With an increasing carbon concentration first the surface carbide and then a graphene layer on top is built.

O 65.6 Thu 11:45 MA 041

Freely spanned graphene membranes from epitaxal graphene — •Daniel Waldmann[1], Johannes Jobst[1], Konrad Ullmann[1], Felix Fromm[2], Sebastian Bauer[3], Benjamin Butz[4], Jan Englert[5], Thomas Seyller[2], Patirk Schmuki[3], Erdman Spieker[4], and Heiko Weber[1] — [1]Lehrstuhl für Angewandte Physik, Universität Erlangen-Nürnberg — [2]Lehrstuhl für Technische Physik, Universität Erlangen-Nürnberg — [3]Lehrstuhl für Korrosion und Oberflächentechnik, Universität Erlangen-Nürnberg — [4]Center for Nanoanalysis and Electron Microscopy, Universität Erlangen-Nürnberg — [5]Zentralinstitut für Neue Materialien und Prozesstechnik, Universität Erlangen-Nürnberg, Germany

We developed a fabrication process for freestanding graphene membranes from high-quality epitaxial graphene on silicon carbide (SiC) by electrochemical removal of the SiC. The membranes with areas up to 700 μm^2 are freely spanned over holes in the substrate. Thus we can perform measurements on epitaxial graphene without the disturbing influence of the substrate. The homogeneity is controlled by scanning electron microscopy and scanning transmission electron microscopy. Raman measurements display a strongly enhanced signal of the membranes compared to epitaxial graphene on substrate. Using high resolution transmission electron microscopy we imaged the graphene membranes with atomic resolution.

O 65.7 Thu 12:00 MA 041

Transfer methods of large-scale graphene — •Marco Kraft[1,2], Marc A. Gluba[2], Gerald Troppenz[2], and Norbert H. Nickel[2] — [1]Institut für Physik, Humboldt Universität zu Berlin — [2]Helmholtz Zentrum Berlin für Materialien und Energie GmbH

Graphene has attracted significant attention due to its unusual high carrier mobility and low sheet resistivity. It would be diserable to combine these outstanding properties with the already established technology of silicon. Unfortunately, it is not possible to grow large-scale graphene on silicon. Hence, graphene has to be grown on foreign substrates and subsequently transferred to the silicon based device. Different approaches for this transfer process (e.g. by adhesive foils, protective resist, etc.) are compared by means of their transfer efficiency. For this purpose large scale graphene was grown by low-pressure chemical vapor deposition (CVD) on copper using methane as a precursor. Raman spectroscopy on the as-grown graphene revealed characteristic defect modes, which might be due to the non planar surface of the copper foil. Afterwards the graphene layer was transferred on a Si/SiO2 substrate by using different methods. The transfer process is monitored by raman spectroscopy, atomic force microscopy (AFM) and scanning electron microscopy (SEM) and the resulting graphene layers are compared with samples from mechanical exfoliation on mica muscovite as de facto standard for high quality graphene.

O 65.8 Thu 12:15 MA 041

Conversion of aromatic self-assembled monolayers on Cu substrates into graphene sheets — •Nils-Eike Weber[1], Dan Matei[1], Rainer Stosch[2], Armin Gölzhäuser[1], and Andrey Turchanin[1] — [1]Physik supramolekularer Systeme und Oberflächen, Universität Bielefeld — [2]Physikalisch-Technische Bundesanstalt, Braunschweig

Aromatic thiol-based self-assembled monolayers (SAMs) on gold can be converted into nanocrystalline graphene sheets via electron irradiation induced cross-linking and thermal annealing [1, 2]. To realize the role of substrate in this process, we study the conversion of biphenylthiol SAMs into graphene on copper substrates. To this end, Low Energy Electron Diffraction, Scanning Tunneling Microscopy, X-ray Photoelectron Spectroscopy and Raman Spectroscopy were employed. The use of copper substrates leads to an increase of the crystallinity of graphene sheets in comparison to those obtained on gold substrates. This result makes it promising to attempt the synthesis of high quality graphene for electronic applications using the suggested molecular approach.

[1] A. Turchanin et al., Adv. Mater. 21, 1233 (2009)
[2] A. Turchanin et al., ACS Nano 5, 3896 (2011)

O 65.9 Thu 12:30 MA 041

Extreme UV interference lithography of carbon nanomembranes and graphene — •Andreas Winter[1], Annika Willunat[1], Michaela Vockenhuber[2], Yasin Ekinci[2], Andre Beyer[1], Armin Gölzhäuser[1], and Andrey Turchanin[1] — [1]Physics of Supramolecular Systems and Surfaces, University of Bielefeld, D-33615 Bielefeld — [2]Laboratory for Micro and Nanotechnology, Paul Scherrer Institute, 5132 Villigen, Switzerland

Two-dimensional (2D) carbon materials like graphene, graphene oxide, carbon nanomembranes (CNMs) or ultrathin polymeric films have recently attracted enormous interest due to their potential for use in electronics, chemical and biological sensors, nanofilters, hybrid materials, etc. Most of these applications require lithographic patterning of these 2D carbon materials with the nanoscale resolution. In this respect, Extreme UV Interference Lithography (EUV-IL) provides both large-scale patterning and high resolution with an ultimate limit in the sub-10 nm range. We employ EUV-IL to generate two-dimensional nanopatterns of ca. 1 nm thick CNMs as well as of graphene. We characterize these structures with a Helium Ion Microscope (HIM), which allows imaging of topographic and chemical features of both supported CNMs on insulating substrates, freely suspended CNMs and graphene sheets.

O 65.10 Thu 12:45 MA 041

Layer-by-layer engineering of novel 2D carbon materials with tunable optical, chemical and electrical properties — •Andrey Turchanin[1], Christoph Nottbohm[1], André Beyer[1], Rainer Stosch[2], and Armin Gölzhäuser[1] — [1]Physik supramolekularer Systeme und Oberflächen, Universität Bielefeld — [2]Physikalisch-Technische Bundesanstalt, Braunschweig

We present a route to the fabrication of novel layered 2D carbon materials with tunable electrical, optical and chemical properties on various substrates and as suspended membranes [1]. These materials are engineered via simple layer-by-layer mechanical stacking of carbon (organic) nanomembranes with a thickness of about 1 nm. We characterize physical and chemical properties of these materials via optical microscopy, UV/Vis reflection spectroscopy, X-ray photoelectron spectroscopy, Raman spectroscopy and electrical measurements. Vacuum annealing of the multilayer stacks results in their conversion into graphene at temperatures above 800 K. The degree of this conversion and the thickness of the resulting layers can be precisely controlled. The suggested route opens broad avenues to the engineering of novel 2D carbon hybrid materials for applications ranging from electronics to biophysics.

[1] C.T. Nottbohm et al., Small 7, 874 (2011)

O 66: Nanostructures at surfaces III

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

O 66.1 Thu 10:30 MA 042

Conductance measurements of single graphene nanoribbons with scanning tunnelling microscopy — •Matthias Koch[1], Francisco Ample[2], Christian Joachim[2,3], and Leonhard Grill[1] — [1]Dept. of Physical Chemistry, Fritz-Haber-Institute of the Max-Planck-Society, Berlin, Germany — [2]Institute of Materials Research and Engineering (IMRE), Singapore — [3]Nanosciences Group, CEMES-CNRS, Toulouse, France

Graphene nanoribbons (GNR) are promising candidates for molecular wires in future nanotechnology. Their planar atomic structure leads to electronic properties that strongly depend on their edge-structure and width. We have assembled such GNRs in a bottom-up approach directly on a metal surface and characterized them by low temperature scanning tunneling microscopy (LT-STM). Such a process leads to atomically defined edges, which are required for charge transport studies as structural defects have been predicted to modify the electronic structure and to reduce the conductance. After their characterization by STM, we have performed conductance measurements of single GNRs by pulling them off the surface with the STM tip. In this way, single molecules are contacted to two electrodes in a controlled way and can at the same be characterized before and after such a procedure at the atomic level. Importantly, the electrode-electrode distance is varied during the measurements, thus allowing length-dependent conductance measurements, which are necessary for a fundamental understanding of charge transport. We find that the conductance exponentially decreases with the molecular length in the junction.

O 66.2 Thu 10:45 MA 042

Measuring the one-dimensional band structure of an armchair graphene nanoribbon — •Christopher Bronner[1], Felix Leyssner[1], Stephan Meyer[1], Manuel Utecht[2], Peter Saalfrank[2], Tillmann Klamroth[2], and Petra Tegeder[1] — [1]Freie Universität Berlin, Fachbereich Physik, Arnimallee 14, 14195 Berlin, Germany — [2]Universität Potsdam, Institut für Chemie, Karl-Liebknecht-Straße 24-25, 14476 Potsdam, Germany

Besides other low-dimensional carbon materials, graphene nanoribbons (GNRs) have attracted great interest in the past years. These flat, quasi-one-dimensional structures which can be thought of as stripes cut out of graphene, offer a wide range of band structures depending e.g. on their width, edge shape and applied electric fields, which makes them interesting for nanotechnology applications. Despite the intriguing properties predicted by theory, relatively few experiments have been conducted on GNRs because the fabrication of well-defined, narrow ribbons is challenging. Recently, surface-assisted bottom-up fabrication has been employed on the Au(111) surface to produce a defect-free GNR [1]. We employed complementary surface-sensitive spectroscopies and supporting DFT calculations to determine the electronic structure of those particular GNRs, especially the band gap and dispersion. [1] J. Cai et al., Nature 466, 470-473 (2010)

O 66.3 Thu 11:00 MA 042

Characterization of nano-scale electrical contacts using dynamical Coulomb blockade — Christophe Brun[1], •Konrad H. Müller[2], I-Po Hong[1], François Patthey[1], Christian Flindt[2], and Wolf-Dieter Schneider[1] — [1]Institut de Physique de la Matière Condensée, Ecole Polytechnique Fédérale de Lausanne, CH-1015 Lausanne, Switzerland — [2]Département de Physique Théorique, Université de Genève, CH-1211 Genève, Switzerland

The theory of dynamical Coulomb blockade (DCB) has in the past been successful in describing transport measurements in carefully engineered tunnel junctions by explicitly taking into account the electrical circuits in which they are embedded [1,2]. Here we use the theory of DCB to explain recent scanning tunneling spectroscopy measurements on flat metallic nano-scale islands electrically coupled to their supporting substrates [3]. The observed suppression of the differential tunnel conductance at small bias voltages is due to DCB and can be understood by considering the island–substrate contact as an Ohmic resistor in parallel with a plate capacitor. Our theoretical calculations are in good agreement with the measurements and allow us to investigate the systematic dependence of the resistances and capacitances on the island–substrate contact area.

[1] M. H. Devoret *et al.*, Phys. Rev. Lett. 64, 1824 (1990).

[2] G.-L. Ingold and Yu. V. Nazarov, in *Single Charge Tunneling* (Plenum, New York, 1992).

[3] C. Brun, K. H. Müller, I-P. Hong, F. Patthey, C. Flindt, and W.-D. Schneider, in preparation (2011).

O 66.4 Thu 11:15 MA 042

Characterization of Different Growth Regimes on Prepatterned Surfaces — Fabian Lied[1], •Tanja Mues[1], Wenchong Wang[2], Lifeng Chi[2], and Andreas Heuer[1] — [1]Institut für Physikalische Chemie, Westfälische Wilhelms-Universität Münster — [2]Physikalisches Institut, Westfälische Wilhelms-Universität Münster

Molecule deposition on a prepatterned substrate is a recently developed technique to generate structures of organic molecules on surfaces via self-organization. For the case of prepatterned stripes the time-resolved process of structure formation is studied via Lattice Monte Carlo simulations. By systematic variation of the interaction strength three distinct growth regimes can be identified: localized growth, bulge formation and cluster formation. All three growth regimes can be recovered in the experiment when choosing appropriate organic molecules. Some key microscopic observables, reflecting the properties of the structure formation, display a non-monotonous dependence on the interaction strength.

O 66.5 Thu 11:30 MA 042

Pt(111) supported monolayer graphene as template for Pt nanoparticle formation. — Nadja E. Wagner, •Albert K. Engstfeld, and R. Jürgen Behm — Ulm University, Institute of Surface Chemistry and Catalysis, D-89069 Ulm, Germany

Recent investigations have shown that graphene monolayer films deposited on metal single crystal surfaces can be used as templates for the nucleation of periodic arrays of metal nanoparticles. These surfaces are promising model systems to study the electrocatalytic properties of very small metal nanoparticles. For the electrochemical measurements it is crucial that the graphene layer is perfectly closed to prevent electrooxidation and exposition of the substrate. It has been shown that graphene on Pt(111) can be grown,[1] the requirement of a closed layer, however, could not yet be fulfilled.

In this work the graphene layer was prepared by ethene exposure at elevated temperatures and different pressures in UHV. The properties of graphene monolayers on Pt(111) were studied by high resolution STM. We will show that it is possible to form a compact graphene layer on Pt(111) under these conditions. The ethylene pressure was found to play an important role on the homogeneity of the graphene layer. With increasing ethylene pressure the amount of domain boundaries rises due to an increasing number of smaller rotational domains. The homogeneity of the surface is checked by electrochemical measurments. Evaporation of Pt on gr/Pt(111) was investigated, and results will be presented.

[1] T. A. Land et al., Surface Science. 264, 1992, 261-270

O 66.6 Thu 11:45 MA 042

Anisotropic behavior of organic molecules on prepatterned surfaces — •Stefan Frieder Hopp and Andreas Heuer — Institut für Physikalische Chemie, Universität Münster, 48149 Münster, Germany

The nucleation of organic molecules on surfaces, prepatterned with gold stripes, is investigated with emphasis on anisotropy effects. Representing the molecules as ellipsoids, the related particle-particle interaction is modeled by means of a generalized Gay-Berne potential for similar biaxial particles [1]. The orientational behavior of these ellipsoidal molecules with respect to the stripe pattern is studied for the first monolayer by performing kinetic Monte Carlo simulations. It is shown how the properties of the particle alignment depend on energy scales, temperature and flux. Based on the fact the particles strictly arrange in rows, it is furthermore instructive to analyze the orientation behavior within the different rows. Finally, the transfer of orientation from a preset row of molecules with fixed orientation to other nucleating particles is examined.

[1] R. Berardi, C. Fava and C. Zannoni, Chem. Phys. Lett. 236, 462 (1995).

O 66.7 Thu 12:00 MA 042

Scanning tunneling microscopy study of antimony clusters on Si(111)7x7 — •Stephan Appelfeller, Martin Franz, and Mario Dähne — Institut für Festkörperphysik, Technische Universität Berlin, Hardenbergstr. 36, D-10623 Berlin

The growth regime of surface clusters is located between single atom adsorption processes and long range surface reconstructions. These surface clusters are interesting structures to analyze not only because of their possible use in nanocatalysis and the miniaturization of nanodevices but also for their unique physical properties. Here, clusters were grown on heated, 7x7 reconstructed Si(111) substrates by molecular beam epitaxy with submonolayer antimony coverages. Several different cluster appearances were found depending on the exact preparation conditions using a scanning tunneling microscope. The structural and electronic properties of the dominant cluster types were studied with a focus on antimony clusters which appear ring like in empty state images. These ring clusters form preferentially at an edge of a faulted half unit cell and represent up to 75% of all clusters observed in the measurements. A structure model that explains the experimental results well was developed for these ring clusters. This work was supported by the DFG through FOR 1282 project D.

O 66.8 Thu 12:15 MA 042

Separation of length scales to estimate the elastic energy of a heteroepitaxially deposited crystal — •guillaume boussinot — MPIE, Duesseldorf, Germany — PGI, Forschungszentrum Juelich, Germany

In heteroepitaxy problems, the elastic energy of the system is in general a very non-trivial function of the shape of the deposited crystal. We use the separation of length scales describing this shape to estimate the elastic energy of a cylindrical crystal and find its equilibrium dimensions for a given volume.

O 66.9 Thu 12:30 MA 042

Diamond-Like Carbon Coatings on Selected Plastic Materials — •Christian B. Fischer[1], Magdalena Rohrbeck[1], Stefan Wehner[1], Matthias Richter[2], and Dieter Schmeisser[2] — [1]Universität Koblenz-Landau, IfIN - Physik, 56070 Koblenz, Germany — [2]BTU Cottbus, Angewandte Physik II / Sensorik, 03046 Cottbus, Germany

The manufacturing of synthetic materials and their wide range of use for daily life is accompanied by essential requirements. Besides the basic performance of materials such as flexibility, elasticity, fracture strength and chemical resistance, further determinants are long term stability or biocompatibility. To overcome mismatches in surface characteristics of optimal parent material they can be customized for their intended use resulting in suitable coatings for profitable applications. The determining factor for such modifications is the preservation of basic material performance in addition to the benefit of further advantages like changed adhesive, improved repellent or antibacterial behavior. Protective coatings of selected plastic materials have been realized by depositing a few layers of diamond-like carbon (DLC). The assembly of soft plastic material and robust DLC coating is important for the resulting material characteristics. The detailed understanding of materials interphasing between these unequal materials and the conjunction of carbon centers in chemically different neighborhood is part of the presented work. Results will be transferable to other plastic materials with diverse needs, e.g. energy storage devices, water treatments and coatings for everyday commodities or industrial parts.

O 66.10 Thu 12:45 MA 042

Continuum modeling of particle redeposition during ion-beam erosion — •Christian Diddens and Stefan J. Linz — Institut für Theoretische Physik, Universität Münster, Wilhelm-Klemm-Straße 9, 48149 Münster, Germany

We have studied the redeposition mechanism during ion-beam erosion and its impact on the formation of nanopatterns within a suitable continuum model [1]. Since particle redeposition is a complex and highly non-local process, one is interested in an approximation which holds for generic surface morphologies. The detailed analysis of this model reveals, that the redeposition yield can be approximated by a Taylor expansion around the surface mean height, as it has already been shown in a discrete solid-on-solid model [2]. In addition, by combining a common erosion model (Kuramoto-Sivashinsky equation) with the presented redeposition model, we show, that redeposition of eroded particles is able to trigger the emergence of long-range ordered nanopatterns.

[1] C. Diddens, S. J. Linz, unpublished

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

O 67: Metal surfaces: Adsorption of H/O and inorganic molecules

Time: Thursday 10:30–12:45 Location: MA 043

O 67.1 Thu 10:30 MA 043

Two-Level Conductance Fluctuations of a Single-Molecule Junction — •Nicolas Néel[1,2], Jörg Kröger[2], and Richard Berndt[1] — [1]Christian Albrechts Universität zu Kiel — [2]Technische Universität Ilmenau

The conductance of a single-molecule junction in a low temperature scanning tunneling microscope has been measured at nanosecond time resolution. In a transition region between tunneling and contact the conductance exhibits rapid two-level fluctuations which are attributed to different geometries of the junction. The voltage dependence of the fluctuations indicates that electrons injected into the lowest unoccupied molecular orbital may efficiently couple to molecular vibrations. Financial support through SFB 677 is acknowledged.

N. Néel, J. Kröger, and R. Berndt, Nano Lett. 11, 3593 (2011)

O 67.2 Thu 10:45 MA 043

Tilting, bending and nonterminal sites in CO on Cu(001) — •Holger L. Meyerheim[1], Ramesh Thamankar[1], Arthur Ernst[1], Sergei Ostanin[1], Igor V. Maznichenko[2], Elena Soyka[1], Ingrid Mertig[2], and Jürgen Kirschner[1] — [1]Max-Planck-Institut f. Mikrostrukturphysik, D-06120 Halle — [2]Institut f. Physik, Martin-Luther-Universität Halle-Wittenberg, D-06099 Halle

Carbon monoxide (CO) adsorbed on metals represents an archetype system in surface science. In the case of CO on Cu(001) it is undisputed that the ($\sqrt{2}\times\sqrt{2}$) structure is characterized by θ=0.5 monolayers (MLs) of CO molecules located on top of every other Cu atom with carbon bonded to the metal.

We have studied the geometric structure of the compressed c($7\sqrt{2}\times\sqrt{2}$) anti-phase domain structure of CO on Cu(001) by using scanning tunnelling microscopy experiments in combination with first principles calculations. We find direct evidence for structural relaxations involving an inhomogeneous CO-environment characterized by molecular tilting, bending and non-terminal sites [1]. Our study resolves the so far unresolved problem to explain coverage dependent changes in RAIRS spectra reported previously [2,3].

[1] R. Thamankar, H. L. Meyerheim, A. Ernst, S. Ostanin, I.V. Maznichenko, E. Soyka, I. Mertig, and J. Kirschner, Phys. Rev. Lett. 106, 106101 (2011); [2] C.J. Hirschmugl et al., Phys. Rev. Lett. 65, 480 (1990); [3] J.C. Cook at al., J. Chem. Soc. Faraday Trans. 93, 2315 (1997)

O 67.3 Thu 11:00 MA 043

Ab-initio study of the stability of Fe_3Al surfaces in contact with an oxygen atmosphere — •Afshin Izanlou, Mira Todorova, Martin Friak, and Jörg Neugebauer — Department for Computational Materials Design, Max-Planck-Institut für Eisenforschung GmbH, Düsseldorf

Iron-aluminides are potential candidates for high temperature applications, but their deformability, which is necessary for manufacturing processes, is reduced by hydrogen diffusion at room temperature. The presence of passive surface films has been reported to reduce H embrittelment [1] by lowering the H liberation rate at the surface. It has been further suggested that addition of passivity inducing alloying elements would have a beneficial effect on their thermo-mechanical and electro-chemical behaviour, as well [2].

In a first step towards the identification of suitable alloying elements that reduce H liberation over a wide range of environmental conditions, we study by density functional theory both clean and oxygen covered low index Fe_3Al surfaces. We find the mixed FeAl termination to be most stable on the [001] and [110] clean surfaces, while an Fe-termination is most favourable on the [111] surface. Having identified the likely clean surface terminations, we study low coverage oxygen structures and assess the impact the environment has on surface structure and stability by employing thermodynamic concepts.

[1] C.T. Liu *et al.*, Scr. Metall. Mater. **24** (1990) 385.

[2] R. Balasubramaniam, Bull. Mater. Sci. **3** (1999) 571; D.G. Morris and M. A. Muñoz-Morris, Adv. Eng.Mater., **13** (2011) 43.

O 67.4 Thu 11:15 MA 043

Iodine on Pt(110) - competing phases — •Nadja Oberkalmsteiner, Michael Cordin, and Erminald Bertel — Institute of Physical Chemistry, University of Innsbruck, Innsbruck, Austria

The adsorption of halogens on Pt(110) leads to an exceedingly rich phase diagram. This is due in part to the competition between different ordered phases at the same coverage of Θ=0.5 ML. In previous experiments with Br/Pt(110) a c(2x2) structure was observed at room temperature, while a small excess coverage led to the appearance of a threefold periodicity. The latter structure however, was strongly fluctuating, thus neither the exact coverage nor the structure could be determined unambiguously. Here we present STM data on the Θ=0.5 ML room temperature phase of Iodine on Pt(110). Similarly to Bromine, a long-range ordered c(2x2) structure is observed. A minute excess coverage leads to nucleation of a (3x1) structure with local coverage of Θ=0.66 ML. The presence of such a few highly dispersed (3x1) nuclei, however, switches the rest of the surface with Θ=0.5 ML local coverage into a global (3x2) structure. Since the Iodine adlayer does not fluctuate at room temperature, one can determine precisely the excess coverage required to switch the whole surface to the threefold periodicity. The observed transition clearly demonstrates the long-range nature of the interaction in real space, thus arguing for an electronically driven phase transition. Remarkably, the (3x2) structure involves a considerably buckling of the substrate pointing towards an inherent instability of the Pt(110) surface. Apparently both halogens promote a charge density wave/periodic lattice distortion transition of Pt(110).

O 67.5 Thu 11:30 MA 043

Structure and characterization of the hydrogen-bonded NH_3-NO coadsorption on Pt(111): an ab-initio study. — •Andrea Cepellotti[1], Angelo Peronio[2], and Maria Peressi[3] — [1]Theory and Simulation of Materials, École Polytechnique Fédérale de Lausanne — [2]IOM-CNR Laboratorio TASC, Trieste — [3]Dipartimento di Fisica, Università di Trieste

The study of coadsorption states is an important subject in heterogeneous catalysis, since interactions between adsorbates can inhibit or allow specific reaction pathways. As such the coadsorption of NH_3 and NO on Pt(111) is an interesting system that still lacks a satisfactory characterization both on theoretical and experimental grounds. Early EELS and TDS experiments [1] and recent STM measurements have suggested the formation of complexed structures composed by the two molecules.

Available observations are not able to unambiguously characterize the observed structures, therefore we employ density functional theory to demonstrate the existence of two stable structures, determining the geometrical structure by means of total energy minimization and reproducing the available experimental data. The electronic structure has been characterized, proving that the interaction between adsorbates arises from a hydrogen bond between each H and O. Such interaction suggests an explanation for the high selectivity of NH_3 in the reduction with NO on platinum-based catalysts, which makes this class of systems suitable for combustion-gas treatment.

[1] J. L. Gland and B. A. Sexton, J. Catal. 68, 286 (1981)

O 67.6 Thu 11:45 MA 043

Ordered domain-wall structure of Ir(100)-(2×1)-O — •Pascal Ferstl, Tobias Schmitt, Lutz Hammer, and M. Alexander Schneider — LS f. Festkörperphysik, Universität Erlangen-Nürnberg, Germany

Oxygen adsorption on Ir(100) leads to the formation of a (2×1) superstructure, whereby 0.5 ML of oxygen atoms are adsorbed in bridge positions [1,2]. A recent SXRD study [2] found an additional partial occupation of the hollow sites in the centres of the (2×1) cell by oxygen atoms. This finding is now validated by our STM measurements where we could directly image these extra atoms, which, however, are still very mobile at room temperature.

A slight reduction of the amount of oxygen adsorbed by heating the sample to the onset of oxygen desorption does not depopulate the hollow sites but creates light domain walls perpendicular to the oxygen rows instead. The mutual spacing of the domain walls is rather regular and decreases with coverage eventually leading to a (2×n) superstructure. The occurrence of such a superstructure has been inferred from very early LEED work [3], but its origin remained unclear. We argue that the domain walls already exhibit the hexagonal reconstruction of the clean surface.

[1] K. Johnson *et al.*, J. Chem Phys. **112** (2000) 10460;
[2] D. Sander *et al.*, Phys. Rev. B **81** (2010) 153403;
[3] J. Küppers & H. Michel; Appl. Surf. Sci. **3** (1979) 179

O 67.7 Thu 12:00 MA 043

Interactions of 2nd row high electron affinity elements with Mg(0001) — •Su-Ting Cheng, Mira Todorova, and Jörg Neugebauer — Max-Planck-Insitut für Eisenforschung GmbH, Düsseldorf, Germany

The high corrosion susceptibility of magnesium can be either beneficial or detrimental, depending on the application. For use in biodegradable implants fast, but controllable, degradation behavior is desirable. However, in engineering applications the low corrosion resistance of magnesium and its alloys is a considerable drawback.

Aiming to gain a better understanding of the corrosion behavior of Mg and its alloys we investigate the interaction of oxidizing species such as O, F, N and Cl with the Mg (0001) surface using density functional theory calculations. Accounting for the effect of the environmental conditions within a thermodynamic picture we find that adsorbate phases can only be stable kinetically and are always thermodynamically unstable with respect to the corresponding bulk compounds.

O 67.8 Thu 12:15 MA 043

Coadsorption of deuterium and CO on PtRu/Ru(0001) model surfaces - The influence of surface structure — •Thomas Diemant, Heinrich Hartmann, Joachim Bansmann, and Rolf Jürgen Behm — Institute of Surface Chemistry and Catalysis, Ulm University, D-89069 Ulm, Germany

The study of the interaction of hydrogen (deuterium) and/or CO with bimetallic PtRu surfaces is of high interest for an improved understanding of the chemistry of low temperature Polymer Electrolyte (PE) fuel cells. Studies with structurally well-defined model surfaces can contribute significantly in this respect. In our study, we used PtRu/Ru(0001) model surfaces of two distinct structural configurations: (i) monolayer Pt islands on a Ru(0001) substrate and (ii) PtRu/Ru(0001) surface alloys with almost random distribution of the two metal components in the surface layer. We studied the coadsorption of deuterium and CO on these bimetallic model surfaces using temperature-programmed desorption (TPD) and infrared reflection absorption spectroscopy (IRAS). We will show how the adsorption properties of both species are affected by the deposition of Pt, the metal distribution in the surface and the presence of the co-adsorbed species.

O 67.9 Thu 12:30 MA 043

Exceptionally low friction of CrN/TiN multilayer coatings – a combined experimental and theoretical study — •David Holec, Jörg Paulitsch, and Paul H. Mayrhofer — Department of Physical Metallurgy and Materials Testing, University of Leoben, Leoben, Austria

Recently we have have demonstrated that CrN/TiN multilayer coatings, deposited using the hybrid high power impulse magnetron sputtering (HIPIMS)/direct current magnetron sputtering (DCMS), exhibit extremely low friction coefficients below 0.1 when tested at room temperature and ambient air conditions. By performing dry-sliding tests in an atmosphere with reduced humidity we identified relative humidity of approximately 13% as the necessary condition for the friction to drop to values below 0.1. Density functional theory was used to study the properties of the CrN/TiN system. While the surface energy of the (100) surface is lower than that of (111) in TiN, the situation reverses in CrN. Subsequently we studied the binding energies of H and O atoms on the (100) surfaces. It has turned out that both atoms are weaker bonded on TiN than on CrN. Moreover, the barrier for surface diffusion of H on TiN is significantly lower (~0.5eV) than on CrN (~0.8eV), thus suggesting that H atoms are more mobile on TiN surfaces while stronger bonded on CrN surfaces. Based on both evidences we therefore speculate that the extraordinary low friction coefficient of the CrN/TiN multilayer may be related to accumulation of water molecules from humid air (creation of water droplets) on the CrN on the expense of the TiN surfaces, thus providing a bearing-like effect.

O 68: Focussed session: Functional molecules at surfaces III

Time: Thursday 10:30–13:00 Location: A 053

Topical Talk O 68.1 Thu 10:30 A 053

Frontier Nanoscience: Molecular Superconductors to Molecular Machines — •SAW WAI Hla — Center for Nanoscale Materials, Argonne National Laboratory, IL 60439, and Department of Physics and Astronomy, Ohio University, Athens, OH 45701, USA.

We combine a variety of scanning tunneling microscope (STM) manipulation schemes with tunneling spectroscopy techniques to image and manipulate properties of molecules on surfaces. This talk will include our recent results and achievements: In molecular spintronics area, orbital Kondo effect of single molecules generated by an interfacial charge transfer process will be discussed. In nanoscale superconductivity area, we will present the smallest molecular superconductor ever studied to date. Here, the finding of superconductivity in just four pairs of (BETS)2-GaCl4 molecules opens the possibility of investigating superconducting phenomena locally. Finally, in molecular nanomachine area, complex rotation mechanisms of Ru based multicomponent molecular rotors operated by injecting tunneling electrons from an STM tip will be presented. These experiments are innovative, and are tailored to address several critical issues covering both for fundamental understanding, and for demonstration of novel molecule based nanodevices on materials surfaces.

Topical Talk O 68.2 Thu 11:00 A 053

Directional motion of a four-wheeled molecule on a metal surface — •Manfred Parschau — Empa - Swiss Federal Laboratories for Materials Science and Technology , Nanoscale Materials Science Laboratory, Ueberlandstrasse 129, CH-8600 Dübendorf, Switzerland

Propelling single molecules in a controlled manner along an unmodified surface remains extremely challenging because it requires molecules that can use light, chemical or electrical energy to modulate their interaction with the surface in a way that generates motion. Although controlled movement of molecules along a surface has been reported, the molecules in these examples act as passive elements that either diffuse along a preferential direction with equal probability for forward and backward movement or are dragged by a tip of a scanning tunneling microscope. Here I present a molecule with four functional units that undergo continuous and defined conformational changes upon sequential electronic and vibrational excitation. Scanning tunneling microscopy confirms that activation of the conformational changes of the rotators through inelastic electron tunneling propels the molecule unidirectionally across a Cu(111) surface. The system can be adapted to follow either linear or random surface trajectories or to remain stationary, by tuning the chirality of the individual motor units.

Topical Talk O 68.3 Thu 11:30 A 053

Charge transfer dynamics in assemblies of functional molecules — •Michael Zharnikov — Angewandte Physikalische Chemie, Universität Heidelberg, 69120 Heidelberg, Germany

Development of future technologies such as molecular electronics and sustained progress in organic electronics and photovoltaics rely on reliable information about the charge transport (CT) through individual molecular units (or loosely ”molecular wires”) which serve as important building blocks of a variety of potential devices. In this context, femtosecond CT dynamics in a series of self-assembled monolayers with different backbones, which are prototypes of potential molecule wires, was addressed by resonant Auger electron spectroscopy using the core hole clock approach. The CT pathway was unambiguously defined by resonant excitation of a special marker group attached to the backbone. The length of the backbone was varied to monitor the respective dependence of the CT time. Similar to the static conductance, this dependence can be coarsely described by an exponential function. The respective attenuation factors and CT time associated with the anchoring to the substrate were determined. These factors and characteristic CT times through molecular frameworks are found to depend strongly on the character of the molecular orbital which mediates the CT process. Thus, the efficiency of tunnelling in molecular wires can be significantly affected by controlling the specific orbitals into which charge carriers are injected. This can be a valuable input for theory and an important consideration for molecular electronics devices where improvements in conductance can have significant technological impact.

O 68.4 Thu 12:00 A 053

Electronic and structural properties of azobenzene adsorbed on layered materials — •Eric Ludwig[1], Torben Johannsen[1], Michael Naboka[2], Thomas Strunskus[3], Alexei Nefedov[2], Christof Wöll[2], Lutz Kipp[1], and Kai Rossnagel[1] — [1]Institut für Experimentelle und Angewandte Physik, Universität Kiel, D-24098 Kiel — [2]Institut für Funktionelle Grenzflächen, Karlsruher Institut für Technologie, D-76344 Eggenstein-Leopoldshafen — [3]Institut für Materialwissenschaft, Universität Kiel, D-24098 Kiel

Molecular switches with optically tunable properties are often ascribed a high potential in the field of molecular electronics. However, one of the main challenges has not yet been solved, namely to attach a large number of molecules to a solid surface in a way that efficient switching remains possible.

Here, we present a combined direct and inverse photoelectron spectroscopy and NEXAFS study of azobenzene adsorbed on layered transition metal dichalcogenides. Specifically, we have used a metallic and a semiconducting substrate to determine the influence of the substrate electronic structure and a novel sublimation setup to deposit azobenzene non-destructively from sub-monolayer to multilayer coverages.

Our results indicate generally weak substrate-adsorbate interactions, which is reflected, for instance, in Vomer-Weber growth on the semiconducting substrate and almost flat-lying molecules for monolayer coverage. The photoemission and NEXAFS data also show evidence for photoswitching of multilayers on both substrates. This work was supported by the DFG through SFB 677.

O 68.5 Thu 12:15 A 053

First-principles calculations on dependence of electron transport through molecular junctions on the anchoring groups — •Shigeru Tsukamoto, Vasile Caciuc, Nicolae Atodiresei, and Stefan Blügel — Peter Grünberg Institut & Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, D-52425 Jülich

Molecular electronics is exciting by the perspective that various types of electric properties are potentially realized only by single molecules with unique electronic structures. In particular, the anchoring groups in a molecular junction, which link a molecule to an electrode, are recognized as an important part to control the electron conductivity.

Here, by means of first-principles calculations we report how the anchoring groups of molecular junctions affect the electron transmissions. The systems used here are M–R–C_6H_4–R–M, where M is a Cu or Au electrode, and R is an anchoring group as R=S, COO, BOO, NOO.

The transport calculations have revealed significant differences in the electron transmissions of the four molecular junctions: The molecular junctions with S and BOO anchoring groups have finite electron transmissions at the Fermi level, and the transmission of the system with the BOO group changes rapidly at the energies above and below the Fermi level. For the molecular junctions with COO and NOO anchoring groups, the electron transmissions at the Fermi level are small but they increase at the energies above and below the Fermi level, respectively. The difference in the electron transmissions obviously originates from the difference in the anchoring groups, and the variation in electric functionality of single molecular junctions is suggested.

O 68.6 Thu 12:30 A 053

Electron Dynamics in Azobenzene SAMs on Gold — •Stefanie Paarmann, Cornelius Gahl, and Weinelt Martin — Fachbereich Physik, Arnimallee 14, 14195 Berlin

Electronic structure and femtosecond electron dynamics of self-assembled monolayers of azobenzene functionalized alkanethiols on gold have been investigated with time-resolved two-photon photoemission spectroscopy (2PPE). Two excited electronic states at 2.4 and 3.6 eV above E_F are attributed to unoccupied states in the chromophores, which are populated via charge transfer from the metal substrate and exhibit lifetimes in the order of 100 fs. Additional to the ultrafast dynamics we observe a continuous change of the monochromatic 2PPE spectra on the time scale of hours. While at a photon energy of $h\nu$=4.2 eV the SAM is irreversibly modified by the UV illumination, reversible changes attributed to photoisomerization occur at $h\nu$=3.6 eV. The low cross-section of $< 10^{-22}$ cm^2 is in accordance with earlier experiments where within the experimental error no photoresponse to UV light was observed.

O 68.7 Thu 12:45 A 053

Orbital tomography: Deconvoluting photoemission spectra of organic molecules — •F. S. Tautz[1], P. Puschnig[2,3], E.-M. Reinisch[2], T. Ules[2], G. Koller[2], S. Soubatch[1], M. Ostler[4], L. Romaner[3], C. Ambrosch-Draxl[3], and M. G. Ramsey[2] — [1]Peter Grünberg Institut, Forschungszentrum Jülich — [2]Institut für Physik, Karl-Franzens Universität Graz — [3]Chair of Atomistic Modeling and Design of Materials, Montanuniversität Leoben — [4]Lehrstuhl für Technische Physik, Universität Erlangen-Nürnberg

We propose a tomographic method which uses the energy and momentum dependence of photoemission from adsorbed molecules to deconvolute valence band spectra spectra into individual orbitals beyond the limits of energy resolution.

The method allows the purely experimental determination of molecule-projected densities of state (PDOS), to be compared to theoretically calculated PDOS. The method further allows the direct observation of the effects of bonding on individual orbitals, and in so doing, provides stringent tests for the development of ab-initio electronic structure theory.

Photoemission experiments on PTCDA/Ag(110) were performed at BESSYII using a toroidal electron energy analyzer. The valence band of PTCDA was unambiguously disentangled into contributions from six molecular orbitals with a binding energy below 4 eV, four of them within an energy range of only 0.4 eV.

O 69: Competition for Gerhard Ertl Young Investigator Award

Time: Thursday 10:30–13:00 Location: A 060

O 69.1 Thu 10:30 A 060

Selective Growth of Nanostructured Oxides on Au(111) as Model Catalysts — •Xingyi Deng — National Energy Technology Laboratory (NETL), United States Department of Energy, P.O. Box 10940, Pittsburgh, Pennsylvania 15236, United States — URS, P.O. Box 618, South Park, Pennsylvania 15129, United States

Metal oxides are widely used in heterogeneous catalysis as supports, promoters, additives, and catalysts, but often appear in variable phases possessing complex structural characteristics, presenting many unique challenges to elucidate mechanistic information of these catalysts. In this work, we demonstrate and highlight the use of surface-grown nanostructured oxides as model catalysts to gain fundamental insight into the reactivity of these complex systems. The key is to grow nanostructured oxides with precisely controlled composition, phase and morphology. We find that a variety of nanostructured iron-oxides (including FeO, Fe_3O_4 and α-Fe_2O_3) with well-defined morphology can be selectively grown Au(111) by carefully controlling of deposition/oxidation conditions. In addition, the polar ZnO nanostructures with a bulk-type O-ZnO(000-1) phase have been grown and discovered on the Au(111) surface which are likely stabilized via a support effect from the growth substrate. Coupling of traditional surface science techniques (STM, XPS and LEIS) with in situ capabilities at elevated pressures (AP-XPS), we have characterized these model catalysts at an atomistic detail and investigated their activity toward water and CO simultaneously. The studies of the nanostructured FeO and α-Fe_2O_3 using in situ techniques unequivocally illustrate the enhanced activities associated with the presence structural features such as edges and interfacial sites, which tend to dominate reactivity of materials in the nanocrystalline size regions.

O 69.2 Thu 11:00 A 060

Thin Film and Crystal growth on Semiconductor Surfaces — •Soon Jung Jung — CRANN, TCD, Dublin 2, Ireland

The challenges to use the unique properties of surface onto the fascinating technologies are quite exiting. As a chemist, the research interest is to develop new ways to modify the surface properties by attaching organic molecules on the semiconductor surfaces and to understand their interfacial architecture at the atomic level. Various adsorption structure and mechanism of simple *gas phase molecules*: H_2, *liquid phase molecules*: pyrimidine ($C_4H_4N_2$), water (H_2O), thiophene (C_4H_4S) and the complex *solid phase molecules*: purine ($C_5H_4N_4$), histidine ($C_6H_9N_3O_2$) will be introduced. In the second part, by using the unique surface properties, I will introduce a novel method to synthesize single crystal NWs by using the surface energy difference between several materials. By simply heating a multilayer film, the energy stored up in the film is released by heating to promote NW formation. This low temperature homogenous growth process does not require added growth precursors and produces high quality single crystalline materials. This method is general so that I could demonstrate Au NW, Cu NW, Fe Nano block and carbon nano tube growth. I will introduce these results and discuss about the future application of this method.

O 69.3 Thu 11:30 A 060

Exploring quantum magnetism at the single atom level — •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. In this talk, I will review the recent developments in this field, ranging from newly studied material systems like semiconductors [3], and demonstrate how single atom magnetometry (SAM) can be combined with an atom-by-atom bottom-up fabrication to realize complex atomic-scale magnets with tailored properties as well as all-spin based atomic-scale technology. I will also discuss the application of these techniques to explore the impact of itinerant electrons on the magnetization dynamics of single atoms as well as the magnetization dynamics of strongly exchanged coupled systems.

[1] R. Wiesendanger, *RMP*, **81**, 1495 (2009); [2] A. J. Heinrich, *et al.* , *Science*, **306**, 466 (2004); [3] A.A. Khajetoorians, *et al.* , *Nature*, **467**, 1084 (2010); [4] A.A. Khajetoorians, *et al.* , *PRL*, **106**, 037205 (2011); [5] A.A. Khajetoorians, *et al.* , *Science*, **332**, 1062 (2011)

O 69.4 Thu 12:00 A 060

Disentangling the Degrees of Freedom of a Charge Density Wave in Momentum, Temperature and Time — •Robert Moore — Stanford Institute for Materials and Energy Sciences, SLAC

National Accelerator Laboratory, Menlo Park CA, USA

Understanding the emergence of collective behavior in correlated electron systems remains at the forefront of modern condensed matter physics. The key to such an understanding is disentangling the contributions from the coupling of degrees of freedom in exotic many body states. Density waves, both of charge and spin, have been studied for decades, however, there are still open questions that need to be resolved for a complete description of the phenomena. As an example, the family of the rare earth tri-tellurides (RTe3) exhibits prototypical charge density wave behavior while dramatically violating traditional theory. Its simplicity in atomic and electronic structure provides unique opportunities to gain further insight in such discrepancies between theoretical descriptions and experimental realizations of electron-phonon coupling. Our recent results will be reviewed from angle resolved photoemission spectroscopy (ARPES), time-resolved ARPES and time-resolved resonant soft x-ray diffraction techniques focusing on both electronic and lattice response to the density wave instability in momentum, temperature and time. New insights into electron-phonon coupling and the density wave phenomena are revealed and will be discussed.

O 69.5 Thu 12:30 A 060

Surface Science Studies of the Catalytic Solid-Liquid Interface Utilizing Single Molecule Spectroscopy and Calorimetry — •Robert M Rioux — Department of Chemical Engineering, The Pennsylvania State University, University Park, PA 16801

The study of the gas-solid interface has been the hallmark of surface science. In his Nobel talk, Professor Ertl highlighted the surface thermodynamics, kinetics and dynamics of catalytic reactions on well-defined single crystal surfaces. Research efforts in gas-solid surface science are highly relevant in a number of technological areas; however, a detailed molecular understanding of the catalytic solid-liquid interface is still lacking. Fundamental properties critically important to catalysis, such as the heat of adsorption of a reactant have not been measured in the solution phase and there are very few structure-activity/selectivity studies of catalytic reactions occurring at this interface. A quantitative picture of the effect of solvent at this interface on catalysis is lacking. The study of this interface requires a new approach since many of the techniques of surface science will not work in this situation. We will demonstrate with a combination of non-linear optical spectroscopy, solution-phase calorimetry, and single molecule approaches adapted from biophysics to measure reactivity and selectivity, we are beginning to elucidate a molecular-level understanding of the catalytic solid-liquid interface on extended and nanoscale surfaces. In this talk, we will review recent efforts to quantify this technologically important interface.

O 70: Invited talk (Nobuo Ueno)

Time: Thursday 15:00–15:45 Location: HE 101

Invited Talk O 70.1 Thu 15:00 HE 101

First-principles experiment on electrical conductivity of organic devices with UPS: Charge delocalization, vibration coupling and band-gap states — •Nobuo Ueno — Graduate School of Advanced Integration Science, Chiba University, Chiba, Japan

We will discuss following two topics, which are related to quantum mechanical/chemical studies of electrical conductivity in organic devices, by using UV photoelectron spectroscopy (UPS):

(i) Energy band dispersion, electron-phonon coupling and polaron.

(ii) Direct detection of very low density of electronic states in organic HOMO-LUMO gap.

As the electrical conductivity (σ) is given by $\sigma = ne\mu$, where n is the carrier concentration and e the charge and μ the charge mobility, the topic (i) is a direct experimental study of μ in molecular aggregates and in a molecule based on energy and momentum conservation rules, and the topic (ii) is related to study n, since n is related to the energy level alignment/the Fermi level position that must be controlled by unknown and undetectable electronic states in organic HOMO-LUMO gaps. The topic (ii) is thus related to elucidation of a well-known mystery; why do the transport types appear depending on molecules without impurity doping? In other words why does the Fermi level move in HOMO-LUMO gap? The mystery might be originated from a primary deference between organic semiconductors and their inorganic counter parts.

O 71: [MA] Joint Session "Graphen: Spin Transport" (jointly with DS, DY, HL, O, TT)

Time: Thursday 15:00–16:45 Location: H 1012

Topical Talk O 71.1 Thu 15:00 H 1012

Spin transport in graphene — •Bernd Beschoten — II. Institute of Physics, RWTH Aachen University and JARA: Fundamentals of Future Information Technology, 52074 Aachen

Graphene is considered as promising candidate for spintronics applications. The reason is the weak spin-orbit coupling, the absent hyperfine interaction and the observation of micrometer long spin relaxation lengths [1]. So far most spin transport studies have focused on single layer graphene (SLG). However, bilayer graphene (BLG) has unique electronic properties, which differ greatly from those of SLG by its effective mass of carriers, interlayer hopping and electric-field induced band gap. Our studies of spin transport in BLG as a function of mobility μ, minimum conductivity, charge carrier density and temperature reveal the importance of the D'yakonov - Perel' (DP)-type spin scattering mechanism [2]. In BLG samples, the spin relaxation time τ_s scales inversely with μ both at room temperature and at low temperatures. τ_s times of up to 2 ns are observed in samples with the lowest mobility. We discuss the role of intrinsic and extrinsic factors that could lead to the dominance of the DP-type spin scattering mechanism in BLG. Remarkably, similar spin transport properties are also observed in large area graphene grown by the CVD method on copper foils demonstrating the potential of CVD graphene in spintronics devices [3].

Work supported by DFG/FOR 912.

[1] N. Tombros *et al.*, Nature 448, 571 (2007).

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

[3] A. Avsar *et al.*, Nano Letters 11, 2363 (2011).

Invited Talk O 71.2 Thu 15:30 H 1012

Long spin relaxation times in epitaxial graphene on SiC(0001) — •Thomas Maassen[1], Jan Jasper van den Berg[1], Natasja IJbema[1], Felix Fromm[2], Thomas Seyller[2], Rositsa Yakimova[3], and Bart Jan van Wees[1] — [1]Zernike Institute for Advanced Materials, University of Groningen, The Netherlands — [2]Lehrstuhl für Technische Physik, Universität Erlangen-Nürnberg, Germany — [3]Department of Physics, Chemistry and Biology (IFM), Linköping University, Sweden

Spin transport in graphene draws great interest because of recent promising measurements at room temperature (RT). At the same time the limiting factor for spin relaxation seems to be the substrate. By replacing the commonly used SiO_2 substrate we aim to observe improved spin transport. We developed an easy process to prepare lateral spin-valve devices on epitaxial grown monolayer graphene on SiC(0001), that enables us to upscale the production to wafer size. We examine the spin transport properties of this material by performing nonlocal spin-valve and Hanle spin precession measurements. We observe the longest spin relaxation time τ_S in single layer graphene at RT (1.5 ns) and $T = 4.2$ K (2.3 ns), while the spin diffusion coefficient is strongly reduced by nearly 2 orders of magnitude. The increase in τ_S is probably related to the changed substrate, while the small value for D_S is until now unexplained. Nevertheless, the high values for τ_S, combined with the easy production method on a large scale, clear the way for graphene based spintronic devices and applications in the future.

O 71.3 Thu 16:00 H 1012

Manipulation of spin transport properties in graphene — •Frank Volmer^{1,2}, Tsung-Yeh Yang^{1,2}, Eva Maynicke^{1,2}, Marc Drögeler^{1,2}, Sebastian Bläser^{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

It has been shown that the dominant spin relaxation mechanism in bilayer graphene is of the D'yakonov-Perel' type [1]. In this case the spin dephasing time increases with decreasing momentum scattering time or, respectively, with decreasing charge carrier mobility.

Therefore, it is desirable to control and to manipulate the mobility of a single device in order to get a further insight into the dephasing mechanisms. As the charge transport through the two-dimensional graphene is known to be strongly affected by adatoms, it is furthermore interesting to explore their influence on the spin transport. Hence we use current annealing, chemical solvents and electron beam induced deposition to add or to remove impurities on the graphene surface and study their influence on the spin transport properties.

First results indicate that even in single-layer graphene devices (nonlocal spin valves with Co/MgO injectors) a D'yakonov-Perel'-type dephasing mechanism is dominating.

This work has been supported by DFG through FOR 912.

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

O 71.4 Thu 16:15 H 1012

Anisotropic super-spin at the end of a carbon nanotube — •Manuel J. Schmidt — RWTH-Aachen, Deutschland

The interplay of edge magnetism and spin-orbit interactions is studied theoretically on the basis of zigzag ends of carbon nanotubes. Spin-orbit coupling, generally weak in ordinary graphene, is strongly enhanced in nanotubes and thus cannot be neglected at low energies. In the present case it leads to a magnetic anisotropy on the order of 10 mK. Also the relation to correlated topological edge states is shortly discussed.

Carbon nanotubes with zigzag ends have localized electronic states at those ends. These localized states correspond to the edge states in graphene and are equally susceptible to Coulomb interactions. The latter drive a transition, known as edge magnetism in graphene. However, due to the very limited spatial size of this magnetic state, it should not be considered as a symmetry broken state but rather as a super-spin, composed of a few individual electron spins. Without spin-orbit interaction, the ground state of this super-spin would be 2S+1 fold degenerate. Finite spin-orbit coupling, however, breaks this degeneracy in such a way that the true ground state is unique and time-reversal invariant. Furthermore, it turns out that the magnitude of this effect may be tuned by a partial suppression of the magnetism (tunable edge magnetism).

15 min. break

O 72: [MA] Joint Session "Surface Magnetism III" (jointly with O)

Time: Thursday 15:15–19:15 Location: BH 243

O 72.1 Thu 15:15 BH 243

Ultimate limit of electron-spin precession upon reflection in ferromagnetic films — A. Hallal^{1}, T. Berdot^{1}, P. Dey^{1}, L. Tati Bismaths^{1}, L. Joly^{1}, A. Bourzami^{2}, F. Scheurer^{1}, H. Bulou^{1}, •J. Henk^{3}, M. Alouani^{1}, and W. Weber^{1} — ^{1}Institut de Physique et Chimie des Matériaux de Strasbourg, France — ^{2}Université Ferhat-Abbas, Sétif, Algeria — ^{3}Max-Planck-Institut für Mikrostrukturphysik, Halle, Germany

We report the discovery of 180° electron-spin precession in spin-polarized electron-reflection experiments on Fe films on Ag(001) [1], the largest possible precession angle in a single electron reflection. Both experiments as a function of Fe film thickness and *ab initio* calculations show that the appearance of this ultimate spin precession depends with utmost sensitivity on the relaxation of the Fe surface layers during growth. Similar spin precession is also predicted for other ferromagnetic films.

[1] A.Hallal *et al.*, Phys. Rev. Lett. **107** (2011) 087203.

O 72.2 Thu 15:30 BH 243

High resolution electron energy loss spectroscopic studies of surface spin waves in ultrathin Co films on Cu(001) — •Rajeswari Jayaraman^{1}, Harald Ibach^{1}, Antonio Toninho Costa^{2}, and Claus Michael Schneider^{1} — ^{1}Peter Grünberg Institut, Forschungszentrum Jülich, 52425 Jülich, Germany — ^{2}Departamento de Ciências Exatas, Universidade Federal de Lavras, 37200-000 Lavras, Minas Gerais, Brazil

Electron energy loss spectroscopy has become a valuable tool for studies of the dispersion of spin waves at ferromagnetic surfaces. Using our recently developed high resolution spectrometer [1] we have extended a previous study [2] of the surface spin waves of fcc cobalt films deposited on Cu(001) along the [011] direction to lower wave vectors $k_{\parallel}$ and lower spin wave energies. Spin waves are resolved down to $k_{\parallel} = 0.2\text{Å}^{-1}$ and spin wave energies of 15meV. For $k_{\parallel} = 0.2 - 0.35\text{Å}^{-1}$ spectra with resolution of 7meV exhibit a noticeable contribution of bulk spin waves, in agreement with theoretical calculations. We have furthermore studied the dispersion along the [001] direction. In agreement with theory [3] we find that the spin wave dispersion is nearly isotropic in this system even at higher wave vectors.

[1] H. Ibach et al., to be published.

[2] R. Vollmer et al., Phys. Rev. Lett. 91, 147201 (2003).

[3] A.T. Costa et al., Phys. Rev. B 69, 64413 (2004); A.T. Costa et al., Phys. Rev. B 70, 054406 (2004).

O 72.3 Thu 15:45 BH 243

Ultrafast Magnetization Dynamics of Gadolinium and Terbium Studied by XUV Photoelectron Spectroscopy — •Martin Teichmann^{1,2}, Kristian Döbrich^{1,2}, Björn Frietsch^{1,2}, Cornelius Gahl^{1,2}, Robert Carley^{1,2}, Olaf Schwarzkopf^{3}, Philippe Wernet^{3}, and Martin Weinelt^{1,2} — ^{1}Max-Born-Institut, Max-Born-Straße 2a, 12489 Berlin — ^{2}Freie Universität Berlin, Fachbereich Physik, Arnimallee 14, 14195 Berlin — ^{3}Helmholtz-Zentrum für Materialien und Energie GmbH, Albert-Einstein-Straße 15, 12489 Berlin

Recent results from IR-pump-XUV-probe angle-resolved photoelectron spectroscopy (ARPES) experiments on the ultrafast demagnetization of thin films of Gd(0001) and Tb(0001) on W(110) will be presented. Following excitation by an intense IR pulse, ARPES with 35 eV photons allows us to directly probe the response of the exchange-split valance band. As a signature of ultrafast demagnetization by the IR pulse, we see a rapid reduction of the exchange-splitting in the valence band of both metals. However, due to its larger spin-lattice coupling, the response of terbium to laser excitation is far stronger than gadolinium. We also observe significant differences between the responses of the minority and majority bands in the first picosecond, both within and between the two metals. This ultrafast response is in contrast to quasi-equilibrium thermal demagnetization, and reveals a spin dependence to the exchange coupling between the valence and 4f states responsible for magnetic ordering. Laser excitation drives the system out of magnetic equilibrium on the picosecond timescale.

O 72.4 Thu 16:00 BH 243

Structural aspects of magnetic coupling in a bilayer CoO(111) on Ir(100) — Florian Mittendorfer^{1}, Raimund Podloucky^{2}, and •Josef Redinger^{1} — ^{1}Inst. of Applied Physics, Vienna University of Technology, Vienna, Austria — ^{2}Inst. of Physical Chemistry, University of Vienna, Vienna, Austria

Experimentally, stoichiometric CoO is found to form a (111)-like hexagonal c(10x2) bilayer on the square fcc Ir(100) surface [1]. Besides lateral displacements and vertical bucklings two distinct local building blocks can be detected: hexagonal BN-like almost co-planar Co-O fragments and NaCl-type O atoms above Co triangles. Consequently, different magnetic couplings for the different arrangements should be expected, which will be further modified by the coupling to the non-magnetic substrate. We have performed DFT and DFT+U calculations for the proposed c(10x2) CoO(111)/Ir(100) structure and structural variants and also for the NaCl (RS) and Wurtzite (WZ) type bulk phases. Quite interestingly for the bulk phases PBE and even HSE predict the WZ to be the stable one, a trend which could only be reversed in PBE+U calculations for high values of U. Furthermore

ferromagnetic coupling for bulk WZ CoO is found to be energetically much closer to the antiferromagnetic groundstate as compared to RS CoO. For the bilayer CoO(111)/Ir(100) systems this translates into a rather complex magnetic arrangement of ferro and antiferromagnetc couplings, which could be easily modified by small changes to the geometrical structures as determined by the CoO/Ir interface.
[1] C. Ebensperger et al., Phys Rev. B81, 235405 (2010).

O 72.5 Thu 16:15 BH 243

Interfacial uniaxial anisotropy and magnetization reversal of $Fe/BaTiO_3(001)$ layers — •Vasili Hari Babu[1], Remya Kunjuveettil Govind[2], Joachim Gräfe[1], Martin Welke[1], Karl-Michael Schindler[2], and Reinhard Denecke[1] — [1]Wilhelm-Ostwald-Institut für Physikalische und Theoretische Chemie, Universität Leipzig, Germany — [2]Institut für Physik, Martin-Luther-Universität Halle-Wittenberg, Germany

Multiferroics, consisting of both ferroelectric and ferromagnetic phases, have attracted scientific and technological interest due to the magnetoelectric coupling between the phases. In these heterostructures, the growth and magnetic anisotropy of the ferromagnetic phase are to be known to exploit the sizeable magnetoelectric effects. In the present work, Fe films were grown up to 24 *ML* thickness on a ferroelectric $BaTiO_3(001)$ substrate by electron beam evaporation in an ultra high vacuum chamber and the determination of the magnetic properties was carried out by using *in-situ* magneto-optic Kerr effect. The layers were seen to have onset of ferromagnetic ordering at 6 *ML* thickness and the layers up to 12 *ML* thick were seen to exhibit uniaxial magnetic anisotropy (UMA) in the Fe[110] direction. However, the magnetization reversal of layers above 16 *ML* thick was seen to exhibit a growing cubic anisotropy along with the UMA from the fact that the growth of Fe(10) unit cell is 45° rotated to the $BaTiO_3(10)$ direction in order to reduce the lattice mismatch. The competition between the uniaxial (aided by the interface) and cubic anisotropies of these layers is explained by accounting the quadratic magneto-optic Kerr effects.

O 72.6 Thu 16:30 BH 243

Electric-field induced phase transition in Fe/Ni(111) — •Lukas Gerhard, Moritz Peter, and Wulf Wulfhekel — Physikalisches Institut, Karlsruher Institut für Technologie (KIT), Germany

It is known that both the crystallographic and the magnetic structure of Fe thin films exhibit a rich phase diagram. As has been found recently, this can be exploited to trigger a phase transition in 2 ML thick Fe films by magento electric coupling (MEC) [1]. In order to show that the phenomenon is not limited to this particular system, we studied 1 ML Fe films on a Ni(111) substrate. In atomically resolved scanning tunneling microscopy (STM) images two different crystallographic structures were revealed: Fcc and hcp domains coexist and show slightly different local densities of states. Indeed these domains can be switched by the application of very high electric fields. The induced crystallographic phase transition is studied with atomic resolution showing the lateral displacement of every Fe atom. The dynamic behaviour of the observed transition shows the same characteristics as the MEC in Fe/Cu(111) and can be explained by electric field induced lattice relaxations. A full understanding of the magnetism in this system requires additional theoretical efforts. [1] L. Gerhard et al. Magnetoelectric coupling at metal surfaces. Nat. Nano 5, 792-797 (2010)

O 72.7 Thu 16:45 BH 243

Enhanced magnetoelastic coupling of Fe layers on the NiO/Ag(001) — •Anita Dhaka, Dirk Sander, and Jürgen Kirschner — Max-Planck-Institut für Mikrostrukturphysik, 06120 Halle, Germany

Magnetoelastic (ME) coupling is the driving force for magnetostriction of bulk samples. The ME coupling coefficients B_1 and B_2 determine the magnetostriction λ_{100} and λ_{111}, respectively, of cubic systems. They also determine the impact of lattice strain on the magnetic anisotropy. Therefore their experimental determination is of utmost importance for the understanding of magnetic anisotropy of epitaxially strained monolayers [1]. We have performed *in-situ* ME stress measurements on Fe monolayers on epitaxially grown NiO/Ag(001) to investigate the effect of an antiferromagnetic (AFM) buffer layer on the magnetoelasticity of ferromagnetic (FM) monolayers. Here, we measured the ME coupling coefficient B_2 of 6 monolayer (ML) Fe, which is unexpectedly large. We find $B_2 = -19.6 \pm 1.6$ MJ/m^3, which differs in both magnitude and sign from the bulk value of $+7.83$ MJ/m^3 [1]. For the deposition of 6 ML Fe on Ag(001) we measure $B_2 = +2 \pm 0.6$ MJ/m^3, which is almost a factor of four smaller than the bulk value. Notably, the induced strain in the Fe film on both substrates is comparable. This suggests that the FM-AFM interface plays an important role for the enhanced B_2 of Fe on NiO.

[1] D. Sander, Rep. Prog. Phys. 62, 809 (1999).

O 72.8 Thu 17:00 BH 243

Growth mode and atomic structure of MnSi thin films on the Si(111) surface — •Benjamin Geisler[1], Peter Kratzer[1], Takayuki Suzuki[2,3], Theresa Lutz[2], Giovanni Costantini[2,4], and Klaus Kern[2,5] — [1]Fakultät für Physik and Center for Nanointegration, Universität Duisburg-Essen, 47048 Duisburg, Germany — [2]Max-Planck-Institut für Festkörperforschung, D-70569 Stuttgart, Germany — [3]Department of Electronics Engineering and Computer Science, Fukuoka University, Fukuoka 814-0180, Japan — [4]Department of Chemistry, University of Warwick, Coventry, CV4 7AL, United Kingdom — [5]Institut de Physique de la Matière Condensée, Ecole Polytechnique Fédérale de Lausanne, CH-1015 Lausanne, Switzerland

Thin films of MnSi, epitaxially grown on Si(111), are interesting in the field of spin injection into semiconductors. However, due to the complexity of the material, little is known about the film atomic structure and its dependence on the growth conditions. We performed DFT calculations for thin films of MnSi on Si(111) in their ground state crystal structure (B20) to analyze experimental STM images which recently revealed the coexistence of different surface terminations. We give an explanation for the atomic structure behind this observation and present evidence that the film structure depends on the growth protocol (codeposition vs. reactive epitaxy). Furthermore, our calculations indicate an increased magnetic moment of the films due to the biaxial strain induced by the substrate and a preference of ferromagnetic alignment over antiferromagnetic orderings. This makes the material promising for applications in Si-based spintronics.

15 min. break

O 72.9 Thu 17:30 BH 243

Surface morphology and atomic structure of Fe_3Si on GaAs(001) and GaAs(110) and magnetic correlations — •Sani Noor[1], Igor Barsukov[2], M. Samet Özkan[1], Lina Elbers[1], Nikita Melnichak[2], Benjamin Geisler[3], Jürgen Lindner[2], Peter Kratzer[3], and Ulrich Köhler[1] — [1]Experimentalphysik IV, AG Oberflächen, Ruhr-Universität Bochum — [2]Experimentalphysik - AG Farle, Universität Duisburg-Essen — [3]Fakultät für Physik and Center for Nanointegration (CeNIDE), Universität Duisburg-Essen

The system Fe_3Si/GaAs is a FM/SC combination that possesses properties such as a low lattice mismatch, high thermal stability and half-metallic behaviour that make it an interesting candidate for spintronic devices.

In this contribution we present STM studies of stoichiometric Fe_3Si layers grown epitaxially on GaAs(001) and GaAs(110) and compare the structural findings with the magnetic behaviour. From MOKE, SQUID and FMR measurements the magnetic moments as well as the magnetic anisotropies could be determined as a function of the layer thicknesses. Furthermore, we find a transition from superparamagnetic behaviour to ferromagnetic behaviour at a thickness of 3 ML. In accordance with theoretical calculations an enhanced magnetic moment can be observed for thicknesses below 20 ML. We also compare STM simulations of the Fe_3Si surface with the experimental filled and empty state images.

O 72.10 Thu 17:45 BH 243

Interplay between magnetic anisotropy and quantum-well states in thin magnetic films — •Tamene Dasa, Pavel Ignatiev, and Valeriy Stepanyuk — Max-Planck-Institut für Mikrostrukturphysik Weinberg 2, D-06120 Halle, Germany

In this work the magnetic properties of thin magnetic films on non magnetic substrate have been investigated. The main focus is on the interplay between the magnetic anisotropy (MA) and the spin-polarized qauntum-well states arising in such films. The study is performed in the framework of the Density Functional Theory (DFT) by means of the VASP code and the LSDA for the exchange-correlation. We consider Co and Fe films, with vertical size varying from 1 to 6 monolayers, on Pt(001) surface. The Pt substrate is expected to provide high MA.[1] Our results demonstrate that the magnetic anisotropy energy (MAE) and the easy axis direction can be altered by changing the thickness of the film. This effect is explained in terms of the spin-polarized quantum-well states within the film. We also show the possibility to tune the MAE by means of capping the magnetic film by non-magnetic material.

[1] P. Gambardella, S. Rusponi, M. Veronese, S. S Dhesi, C. Grazioli, A. Dallmeyer, I. Cabiria, R. Zeller, P. H. Dederichs, K. Kern, C. Carbone, and H. Brune, Science **300**, 1130 (2003).

[2] M. Tsujikawa, A. Hosokaw and Tatsuki Oda, Phys. Rev. B **77**, 054413 (2008).

O 72.11 Thu 18:00 BH 243

Effect of the external electric field on surface states — •Pavel Ignatiev, Oleg Brovko, and Valeri Stepanyuk — Max-Planck-Institut für Mikrostrukturphysik, Weinberg 2, D-06120 Halle, Germany

We present an *ab initio* study of surface states exposed to the external electric field (EEF). We consider two examples: the Shockley-type surface state on Cu(111) and spin-polarized surface states arising on Co nanoislands. Using the KKR method supplemented with a possibility to account for the EEF, we demonstrate that the EEF affects both energetics and intensities of surface states. Our results on Cu(111) are compared with recent STS studies on the Stark shift of the Cu(111) Shockley surface state.[1] For spin-polarized surface states on a Co bilayer on Cu(111), we show that the spin-selective screening of the EEF by evanescent vacuum surface states tails leads to a possibility of reversing the sign of the surface states spin polarization.[2] Field-induced variations of the majority and the minority surface states band structures change significantly standing-wave patterns [3] of the spin-polarized electrons opening, thus, another way to locally switch spin-polarization of confined surface states. The effect of the electric field on magnetism of the Co bilayer is characterized also in terms of the effective magnetoelectric coefficient.[4]

[1] L. Limot *et al.*, Phys. Rev. Lett. **91**, 196801 (2003); J. Kröger *et al.*, Phys. Rev. B **70**, 033401 (2004).

[2] P. A. Ignatiev, V. S. Stepanyuk, Phys. Rev. B **84**, 075421 (2011).

[3] H. Oka *et al*, Science **327**, 843 (2010).

[4] C.-G. Duan *et al.*, Phys. Rev. Lett. **101**, 137201 (2008).

O 72.12 Thu 18:15 BH 243

Quantum Spin Holography with Surface State Electrons — •Oleg O. Brovko[1,2] and Valeri S. Stepanyuk[1] — [1]Max-Planck-Institut für Mikrostrukturphysik, Halle, Germany — [2]Martin-Luther-Universität Halle-Wittenberg, Halle, Germany

Recently Moon and coworkers have shown that information can be stored in a fermionic state of a two-dimensional electron gas and have dubbed the proposed concept quantum holographic encoding [1]. They have constructed molecular holograms of CO molecules on a Cu(111) surface, hosting a Shockley-type surface state (SS) [2]. Interference of electron waves scattered at the molecules led to the formation of an electron density pattern representing an information page [1]. This page has then been read out with an STM. It has been also shown that using the innate energy dispersion of SS electrons one can not only project the hologram in two spatial degrees of freedom but also stack them one on top the other in the energy dimension.

In our contribution we expand the concept and show that the spin of the electron can also act as a new dimension for information storage. If the molecules or atoms used in creation of a hologram are magnetic, then the scattering of surface state electrons becomes spin-dependent, allowing one to store different information pages in different spin channels. As an example we demonstrate the possibility of simultaneous encoding of two different information pages with electrons of the same energy but opposite spins.

[1] C.R. Moon et al., Nature Nano. 4, 167 (2009)

[2] W. Shockley, Phys. Rev. 56, 317 (1939)

O 72.13 Thu 18:30 BH 243

First-principles investigation of energy– and impurity–dependent electron focusing effect — •Mohammed Bouhassoune, 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 the electronic signature of subsurface impurities can be revealed using Scanning Tunneling Spectroscopy (STS) [1,2]. A single impurity buried below the surface induces anisotropic spatial oscillations of the charge density due to a focused coherent interference of scattered electrons. These oscillations whose strength is determined by the shape of the host Fermi surface can be observed at the surface even if the impurity is far below the substrate. Using the full-potential Korringa-Kohn-Rostoker Green-function (KKR-GF) method, we investigate the energy dependent scattering of electrons at several magnetic and non-magnetic buried impurities below the Cu(100) surface. This allows a real-space mapping of the constant energy surfaces of the host material and a possible characterization of the impurity through the analysis of the induced phase shifts of the electron-density oscillations.

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

[1] A. Weismann et al., Science **323**, 1190 (2009).

[2] S. Lounis *et al.*, Phys. Rev. B **83**, 035427 (2011) and references therein.

O 72.14 Thu 18:45 BH 243

Spin-dependent two-electron emission from ferromagnetic Fe(001) — •Jürgen Kirschner[1], Frank O. Schumann[1], Carsten Winkler[1], Franz Giebels[2], Herbert Gollisch[2], and Roland Feder[2] — [1]Max-Planck-Institut für Mikrostrukturphysik, Weinberg 2, 06120 Halle — [2]Theoretische Festkörperphysik, Universität Duisburg-Essen, 47048 Duisburg

We present a joint experimental and theoretical study of correlated electron pair emission from a ferromagnetic Fe(001) surface induced by spin-polarized low-energy electrons [1]. Spin-dependent angular and energy distributions of the emitted pairs have been measured and calculated. They are analyzed with the aid of the spin-, momentum-, symmetry-, and layer-resolved valence electron density of states, which we obtained by an ab-initio density functional theory calculation. The observed spectra are found to arise almost completely from only three surface parallel atomic layers. Momentum distributions for parallel spins of the emitted electrons exhibit an exchange-correlation hole, which is larger than the correlation hole in the antiparallel spin case. By comparing experimental antiparallel-spin pair spectra with their theoretical counterparts we determine an effective screening strength of the Coulomb interaction in the surface region.

[1] F. Giebels, H. Gollisch, R. Feder, F.O. Schumann, C. Winkler, and J. Kirschner, Phys. Rev. B 84, 165421 (2011).

O 72.15 Thu 19:00 BH 243

Extending the two-dimensional electron spin-filter to a larger range of scattering energies and angles — •D. Kutnyakhov[1], K. Medjanik[1], S.A. Nepijko[1], H.J. Elmers[1], G. Schönhense[1], C. Tusche[2], J. Kirschner[2], F. Giebels[3], H. Gollisch[3], and R. Feder[3] — [1]Inst. f. Physik, Univ. Mainz — [2]MPI f. Mikrostrukturphysik, Halle — [3]Theor. Festkörperphysik, Univ. Duisburg-Essen

In continuation of recent work on the novel imaging spin-filter technique based on electron diffraction from W(001) in the specular (00)-LEED spot [1,2], we studied the scattering energy (E) and angle of incidence (theta)-landscape of the spin sensitivity S, and reflectivity I/I_0. The setup includes a spin-polarized GaAs electron source and a delayline detector for spatially-resolving detection. Intensities, spin-orbit-induced asymmetries and figures of merit have been calculated by means of a relativistic layer KKR SPLEED code [3]. We assumed a 6 % inward relaxation of the topmost layer. The quasi-particle potential input for the SPLEED calculations was obtained by computing the ab-initio ground state electronic structure (FLAPW) and secondly augmenting the resulting potential by a complex self-energy correction. E-theta-behaviour studies open a path to an increased angular acceptance and energy range of the approach, thus increasing the performance of the multichannel spin-filter for electron spectroscopy [2].

Funded by DFG (Scho341/9 and TR 49), graduate school MAINZ.

[1] C. Tusche et al., APL 99 (2011) 032505; [2] M. Kolbe et al., PRL 107 (2011) 207601; [3] R. Feder in Polarized Electrons in Surface Physics, ed. by R. Feder (World Scientific, Singapore, 1985).

O 73: Focussed session: Frontiers of electronic structure theory: Strong correlations from first principles V (jointly with TT)

Time: Thursday 16:00–19:00 Location: HE 101

Topical Talk O 73.1 Thu 16:00 HE 101

Symmetry Breaking and Restoration in Electronic Structure Theory — •Gustavo Scuseria — Rice University, Houston, Texas, USA

We have derived and implemented symmetry-projected Hartree-Fock-Bogoliubov (HFB) equations and apply them to the molecular electronic structure problem. All symmetries (particle number, spin, spatial, and complex conjugation) are deliberately broken and restored in a self-consistent variation-after-projection approach. We show that the resulting method yields a comprehensive black-box treatment of static correlation with effective one-electron (mean-field) computational cost. The ensuing wave function is of multireference character and permeates the entire Hilbert space of the problem. The energy expression is an independent quasiparticle density matrix functional. All reduced density matrices are expressible as an integration of transition one-particle density matrices over a gauge grid. I will present several proof-of-principle examples demonstrating the compelling power of this new method for electronic structure theory [1].

[1] Projected Quasiparticle Theory for Molecular Electronic Structure, G. E. Scuseria, C. A. Jimenez-Hoyos, T. M. Henderson, J. K. Ellis, and K. Samanta, J. Chem. Phys. 135, 124108 (2011).

O 73.2 Thu 16:30 HE 101

generator coordinate method to recover residual correlation energy — •Daniel Rohr and Gustavo Scuseria — Rice University, Houston, Texas, USA

Building on previous work in our group [1] we explore the possibilities to recover the residual correlation energy with the generator coordinate method (GCM). GCM allows for the expansion of the wave function in a set of non-orthogonal functions. In addition, the expansion functions may not be single slater determinants but rather multi-determinantal wave functions.

As input for the GCM we use wave functions generated by Projected Quasiparticle Theory (PQT) presented in the talk "Symmetry Breaking and Restoration in Electronic Structure Theory". The wave functions generated by PQT are multi-determinantal and non-orthogonal.

We explore the prospects of GCM to recover the residual correlation energy, not captured by PQT. Different generator coordinates are investigated for model hamiltonians and small test systems.

[1] Projected Quasiparticle Theory for Molecular Electronic Structure, G. E. Scuseria, C. A. Jimenez-Hoyos, T. M. Henderson, J.K. Ellis, and K. Samanta, *J. Chem. Phys.* **135, 124108 (2011).**

O 73.3 Thu 16:45 HE 101

reatment of strongly correlated systems within the framework of reduced density matrix functional theory — Sangeeta Sharma, •J. K. Dewhurst, and E. K. U. Gross — Max-Planck-Institut fur Mikrostrukturphysik, Weinberg 2, D-06120 Halle, Germany

One of the most dramatic failures of the usual local density approximation or generalized gradient type approximations to the exchange-correlation functional of density functional theory is the incorrect prediction of a metallic ground state for the strongly correlated Mott insulators, of which transition metal oxides (TMOs) may be considered as prototypical. In the present work we extend reduced density matrix functional theory (RDMFT) to the case of solid-state systems and introduce a new functional for their accurate treatment [1]. Furthermore, a method for calculating the spectrum of extended solids within RDMFT is presented and an application of this method to the strongly correlated TMOs demonstrates: (i) an insulating state is found in the absence of magnetic order and, in addition, (ii) the interplay between the charge transfer and Mott-Hubbard correlation is correctly described. In this respect we find 1. S. Sharma, J. K. Dewhurst, N. N. Lathiotakis and E. K. U. Gross Phys. Rev. B 78, 201103 Rapid Comm. (2008) 2. S. Sharma, S. Shallcross, J. K. Dewhurst and E. K. U. Gross cond-mat/0912.1118

O 73.4 Thu 17:00 HE 101

Treatment of spin in reduced density-matrix functional theory — •Nicole Helbig[1,2], Nektarios Lathiotakis[3], Stefan Kurth[2,4], and Angel Rubio[2] — [1]Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, 52425 Jülich, Germany — [2]NanoBio Spectroscopy group and ETSF Scientific Development Centre, Dpto. Física de Materiales, Universidad del País Vasco, Centro de Física de Materiales CSIC-UPV/EHU-MPC and DIPC, 20018 San Sebastián, Spain — [3]Theoretical and Physical Chemistry Institute, NHRF, Vass. Constantinou 48, 11635 Athens, Greece — [4]IKERBASQUE, Basque Foundation for Science, 48011 Bilbao, Spain

Many currently used approximations to the exchange-correlation energy in reduced density-matrix functional theory do not satisfy the spin constancy condition. Hence, these approximations yield different energies for ensembles of degenerate spin configurations both in an ensemble approach and a direct minimization of the energy. These findings are hardly surprising since the approximations were originally derived and optimized for closed shell systems. We discuss possible extensions to open-shell and spinor functionals.

O 73.5 Thu 17:15 HE 101

Kinetic-energy Functional of Interacting Electrons: Numerical Procedure and Its Statistical Interpretation — •Luca M. Ghiringhelli[1] and Luigi Delle Site[2] — [1]Fritz Haber Institute, D-14195, Berlin — [2]Institute for Mathematics, Freie Universität, Berlin

We introduce a numerical procedure, based on the extension of the Levy-Lieb constrained search principle and Monte Carlo sampling of electron configurations in space, for the derivation of the kinetic-energy functional for interacting particles. We consider a quasi-uniform gas of interacting electrons, for which spin statistics play a crucial role, and we show that when the fermionic character of the electrons is included via a statistical–spin approach, our procedure leads to correlation terms, that have the form of the Shannon entropy and the resulting kinetic-energy functional does satisfy the Lieb-Thirring inequality. By mapping the quantum problem onto a classical one, a statistical interpretation of the results is obtained that clarifies the possible physical meaning of the calculated quantity.

O 73.6 Thu 17:30 HE 101

Electron Tunneling - The Influence of Interaction — •Jessica Walkenhorst[1], Nicole Helbig[2,1], Heiko Appel[3], Angel Rubio[1], and E.K.U. Gross[4] — [1]NanoBio Spectroscopy group and ETSF, Universidad del País Vasco, San Sebastián, Spain — [2]Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, Jülich, Germany — [3]NanoBio Spectroscopy group and ETSF, Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, Germany — [4]MPI of Microstructure Physics, Halle, Germany

Electron tunneling plays a fundamental role in many chemical and physical processes and provides evidence of quantum mechanics at the macroscopic level. Whilst much effort has been devoted to modelling electron tunneling, doing so in a non-perturbative way remains a major challenge. Even though time-dependent density functional theory (TDDFT) has become a popular tool to describe and predict many electronic properties, it still fails to describe the tunneling process correctly. This failure of TDDFT is due to the electron-electron interaction being described only approximately through the exchange-correlation potential. To elucidate this further, we investigate the fingerprints of electron-electron interaction in few electron systems during the tunneling process. This is done by exact time propagation of electronic wave functions in different external potentials. For computational feasibility, we consider one-dimensional model Hamiltonians with variable electron-electron interaction.

O 73.7 Thu 17:45 HE 101

Dynamical Vertex Approximation for Nanoscopic Systems — •Giorgio Sangiovanni, Angelo Valli, Georg Rohringer, Alessandro Toschi, and Karsten Held — TU Wien

With the aim of calculating strongly correlated materials more and more reliably, different novel approaches have been proposed in recent years. Quantum Cluster Theories turned out to be very successful for 2- and 3- dimensional Hubbard and related models. Complementary approaches, like Dual Fermion and Dynamical Vertex Approximation, classifiable as diagrammatic extensions of single-site Dynamical Mean Field Theory, become superior when long-range spatial correlations need to be accurately described. An interesting application of Dynamical Vertex Approximation is the one for nanoscopic systems [Phys. Rev. Lett. 104, 246402 (2010)]. The increasing complexity of nanoscopic systems and the possibility of tuning their physical properties through nano-engineering constitute a new challenge for theories, in particular when strong electronic correlations are involved. I will discuss how Dynamical Vertex Approximation can be applied to such problems. I will show how to model a quantum point contact with 110 atoms and present our finding that the contact becomes insulating already before entering the tunneling regime due to a local Mott-Hubbard transition occurring on the atoms which form the point contact. I will also present results for the realistic case of a manganite nano-cluster where we combined our algorithm with a one- electron Hamiltonian calculated within Density Functional Theory [Phys. Rev. Lett. 107, 197202 (2011)].

O 73.8 Thu 18:00 HE 101

Full ab initio theory of the Kondo effect in molecular devices — •David Jacob — MPI für Mikrostrukturphysik Halle

When a magnetic molecule is deposited on a metallic substrate or attached to metallic contacts its magnetic moment can actually be screened by the conduction electrons due to the Kondo effect. In view of possible applications of magnetic molecules for nanoscale spintronics and magnetic storage devices, it is important to reliably predict whether the Kondo effect will take place or not in a given system, and how it can be controlled by various parameters. From a more fundamental point of view, magnetic molecules in contrast to bulk systems offer the possibility to study exotic variants of the Kondo effect such as the orbital Kondo effect [1] or the underscreened Kondo effect [2]. Here we present a *full ab initio* method for molecular devices that combines the COHSEX approximation with more sophisticated many-body techniques like the One-Crossing-Approximation for treating the strong correlations of localized electrons that give rise to the Kondo effect. This method is a further development of our previous method [3,4] that was not yet fully ab initio due its dependence on the interaction between the localized electrons as a parameter. The application of our method to various magnetic molecules attached to metallic leads or deposited on surfaces sheds light on the complex nature of the Kondo effect in molecular-scale devices. [1] M. Karolak *et al.*, PRL **107**, 146604 (2011); [2] J. J. Parks *et al.*, Science **328**, 1370 (2010); [3] D. Jacob *et al.*, PRL **103**, 016803 (2009); [4] D. Jacob *et al.*, PRB **82**, 195115 (2010)

O 73.9 Thu 18:15 HE 101

Charge Kondo effect in PbTe doped with Tl impurities — •Theo Costi[1] and Veljko Zlatic[2] — [1]Peter Grünberg Institut (PGI-2) and Institut for Advanced Simulation (IAS-3), Forschungszentrum Jülich, 52425 Jülich, Germany — [2]Institute of Physics, 10001 Zagreb, Croatia

Semiconducting PbTe is one of the most interesting materials for thermoelectric applications. When doped with a small concentration of Tl impurities, acting as acceptors, a number of anomalous properties are found: e.g.,beyond a critical concentration of about 0.3% Tl, the system exhibits superconductivity with remarkably high critical temperatures for such a low carrier system. This and other anomalous phenomena prompted the idea that Tl impurities act as negative U centres leading to a charge Kondo effect and to superconductivity. Here, we combine ab-initio information and numerical renormalization group methods to explore the consequences of this model for the normal state properties, showing that it can explain a number of features in the temperature and doping dependence of the resistivity, and carrier density. Predictions for the photoemission spectrum are also discussed [1].

[1] T. A. Costi and V. Zlatić, Phys. Rev. Lett. (arXiv:1109.1824).

O 73.10 Thu 18:30 HE 101

Critical properties of the half-filled Hubbard model in three dimensions — •Georg Rohringer[1], Alessandro Toschi[1], Andrey Katanin[2], and Karsten Held[1] — [1]Institute for Solid State Physics, Vienna University of Technology 1040 Vienna, Austria — [2]Institute of Metal Physics, Ekaterinburg, Russia

By means of the dynamical vertex approximation(DΓA) [1] we include spatial correlations on all length scales beyond the dynamical mean field theory (DMFT) for the half-filled Hubbard model in three dimensions. The most relevant changes due to non-local fluctuations are [2]: (i) a deviation from the mean-field critical behavior with the same critical exponents as for the three dimensional Heisenberg (anti)-ferromagnet and (ii) a sizable reduction of the Néel temperature (T_N) by $\sim 30\%$ for the onset of antiferromagnetic order. Finally, we give a quantitative estimate of the deviation of the spectra between DΓA and DMFT in different regions of the phase-diagram.

[1] A. Toschi, A. Katanin, and K. Held, PRB 75, 045118 (2007).

[2] G. Rohringer, A. Toschi, A. Katanin, and K. Held, PRL in press [arXiv:1104.1919].

O 73.11 Thu 18:45 HE 101

Study of strontium vanadate using a dynamical cluster approximation in the linear augmented plane-wave basis — •Hunpyo Lee[1], Kateryna Foyevtsova[1], Johannes Ferber[1], Markus Aichhorn[2], Harald O. Jeschke[1], and Roser Valentí[1] — [1]Institute of Theoretical Physics, University of Frankfurt, Frankfurt, Germany — [2]Institute of Theoretical and Computational Physics, TU Graz, Graz, Austria

Even though the local density approximation in combination with a single-site dynamical mean field theory (LDA+DMFT) explains the Mott transition and the enhancement of the effective mass in real compounds, a numerical approach taking spatial correlations into account would be desirable. In this talk, we introduce a combination of LDA with dynamical cluster approximation (LDA+DCA) in the framework of the full-potential linear augmented plane-wave basis in WIEN2k and apply it to $SrVO_3$. We compare our LDA+DCA results with LDA+DMFT as well as with angle-resolved photoemission spectra (ARPES). We find that LDA+DCA results compare better with ARPES than the LDA+DMFT results due to the inclusion of short-range spatial correlations.

O 74: Plasmonics and nanooptics IV

Time: Thursday 16:00–18:30 Location: MA 005

O 74.1 Thu 16:00 MA 005

The chirp of a surface plasmon polariton probed via plasmon-plasmon interference — •Christoph Lemke[1], Till Leissner[1], Stephan Jauernik[1], Alwin Klick[1], Jacek Fiutowski[2], Jakob Kjelstrup-Hansen[2], Horst-Günter Ruhbahn[2], and Michael Bauer[1] — [1]IEAP, Christian- Albrechts-Universität zu Kiel, 24098 Kiel, Germany — [2]2Mads Clausen Institute, NanoSYD, University of Southern Denmark, Alsion 2, DK-6400 Sønderborg, Denmark

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 sub 20 fs ultrashort laser pulses [1].

Here, 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 SPP wavepacket dynamics. We exemplify the potential of the scheme by probing the chirp of phase modulated SPPs in a time resolved plasmon-plasmon-interference experiment. Wavepacket simulations quantitatively reproduce the experimental data and allow for a characterization of the phase modulated ultrashort plasmon pulses.

[1] A. Kubo et al., Nano Lett. 7, 470 (2007)

O 74.2 Thu 16:15 MA 005

Light trapping in thin-film solar cells characterized by fs-laser pulse backscattering — •Michael Birlo[1], Dominik Differt[1], Florian Lükermann[1], Christian Strüber[1], Helmut Stiebig[2], and Walter Pfeiffer[1] — [1]Universität Bielefeld, Universitätsstrasse. 25, 33615 Bielefeld, Germany — [2]Malibu GmbH & Co.KG, 33609 Bielefeld, Germany

Multiple light scattering at randomly nanostructured interfaces leads to light trapping and enhances the light absorption and efficiency of thin-film silicon solar cells. To increase the trapping efficiency the scattering mechanism has to be understood and selective characterization tools are needed. In this study we use dual-channel spectral interferometry in order to fully characterize the temporal properties of backscattered radiation from thin-film solar cells illuminated by ultra short laser pulses. The so obtained spectral phase, amplitude and polarization state of the scattered light reveals light localization in the few-micron thick randomly nanostructured thin-film solar cell. In comparison a reference cell with flat interfaces exhibits no light trapping. Spectral interference measurements of broadband coherent radiation represents a suitable tool for light trapping characterization.

O 74.3 Thu 16:30 MA 005

Normal Incidence Photoemission Electron Microscopy for the Observation of Surface Plasmon Polaritons — •P. Kahl[1], S. Wall[1], C. Witt[1], C. Schneider[2], D. Bayer[2], A. Fischer[2], P. Melchior[2], M. Horn-von Hoegen[1], M. Aeschlimann[2], and F.-J. Meyer zu Heringdorf[1] — [1]Faculty of Physics and CeNIDE, University of Duisburg-Essen — [2]Department of Physics and OPTIMAS, University of Kaiserslautern

Up to now the imaging of surface plasmon polaritons (SPPs) has been achieved in photoemission electron microscopy (PEEM) in a 2PPE process by illuminating a sample with fs laser pulses under grazing incidence. Under such conditions the experimentally observed Moiré-patterns can be explained by a time-integrated superposition of the light pulse and the SPP, resulting from the simultaneous propagation of the two pulses with different velocities, wavelengths and directions. This prevents a direct observation of SPPs, for example is the wavelength of the Moiré-pattern one order of magnitude larger than the SPP wavelength.

In normal incidence PEEM (NI-PEEM) the contrast mechanism is easier to interpret, because the propagation directions of the light and SPP pulse are perpendicular to each other. Experimentally, however, normal incidence is difficult to obtain. We will discuss two approaches to achieve NI-PEEM, based on different instrument designs. We demonstrate that the observed wavelength corresponds to the real SPP wavelength and that the location of excitation of the SPP on a silver island is adjustable by turning the polarization of the laser pulse.

O 74.4 Thu 16:45 MA 005

Coupling of Excitons in Carbon Nanotubes to Propagating Surface Plasmons — •Nicolai Hartmann[1], Johann Berthelot[2], Padmnabh Rai[2], Francesco Tantussi[3], Francesco Fuso[3], Maria Allegrini[3], Alexandre Bouhelier[2], and Achim Hartschuh[1] — [1]Department Chemie and CeNS, Ludwig-Maximilians-Universität, München, Germany — [2]Département Nanosciences, Université de Bourgogne, Dijon, France — [3]Dipartimento di Fisica E. Fermi, Università di Pisa, Italy

We report on the coupling between excitonic states in semiconducting single-walled carbon nanotubes and propagating surface plasmons in thin metal films.

First we show that upon optical excitation in the visible regime a single carbon nanotube acts as a directive near-infrared dipolar source for surface plasmons propagating mainly along the direction of the nanotube axis. Plasmon excitation and propagation is monitored in Fourier and real space by leakage radiation microscopy [1, 2] and is modelled by rigorous theoretical calculations. Coupling to plasmons almost completely reshapes the emission of nanotubes both spatially and with respect to polarization as compared to photoluminescence on a dielectric substrate. Second we visualize the remote excitation of single nanotubes via propagating surface plasmons.

Our results demonstrate the potential of carbon nanotubes as active elements in plasmonic circuits.

[1] B. Hecht, et.al., Phys. rev. Lett. 77, 1889 (1996) [2] M. Böhmler, et.al., Opt. Express 18, 16443 (2010)

O 74.5 Thu 17:00 MA 005

Organic nanofibers as waveguides and emitters of surface plasmon polaritons — •Till Leissner[1], Jacek Fiutowski[2], Christoph Lemke[1], Kasper Thilsing-Hansen[2], Stephan Jauernik[1], Alwin Klick[1], Jakob Kjelstrup-Hansen[2], Michael Bauer[1], and Horst-Günter Rubahn[2] — [1]IEAP, Christian-Albrechts-Universität zu Kiel, 24098 Kiel, Germany — [2]Mads Clausen Institute, NanoSYD, University of Southern Denmark, Alsion 2, DK-6400 Sønderborg, Denmark

Surface plasmon polariton (SPP) excitation and propagation at gold films as governed by the presence of organic nanofibers composed of self-assembled para-Hexaphenylene (p6P) molecules is studied using interferometric time-resolved photoemission electron microscopy (ITR-PEEM). Two different SPP modes are identified in the experiment: a) the nanofibers act as superior sources for the emission of SPPs at the gold-vacuum interface [1]; b) along the interface between nanofiber and goldfilm we observe 1-d SPP waveguiding as recently also reported by Radko et al. [2]. A quantitative analysis of the data enables us to determine critical SPP propagation parameters such as damping length and group velocity. The results are compared with model simulations based on Hugyens principle and the effective index method [3].

[1] T. Leißner et al., Plasmonics, accepted, [2] Radko et al., Opt. Ex. 19, 16 (2011), [3] Holmgaard and Bozhevolnyi, Phys. Rev. B 75, 245405 (2007)

O 74.6 Thu 17:15 MA 005

Surface plasmon near-field intensity switching using spectral intensity variation combined with photoemission electron microscopy — •Christian Schneider[1], Martin Piecuch[1], Daniela Bayer[1], Alexander Fischer[1], Pascal Melchior[1], Christoph Lemke[2], Michael Bauer[2], and Martin Aeschlimann[1] — [1]Department of Physics and Research Center OPTIMAS, University of Kaiserslautern, 67663 Kaiserslautern — [2]Institut für Experimentelle und Angewandte Physik, Universität Kiel, 24118 Kiel

The physical effects at interfaces between metallic and dielectric media attract more and more attention due to the possibility to generate collective electron density oscillations. These propagating surface plasmon polaritons (SPPs) open the opportunity to guide the electrical field energy. By tailoring a gold microstructure in an appropriate manner, we are able to focus the electrical field energy at a given point of the structure. In addition, based on the coherence between the SPP and the light pulse the field concentration can be switched on and off by alternating the laser pulse spectrum. Applying photoemission electron microscopy (PEEM) as a near field probe and our fast and effective algorithm based on Huygens principle, we can experimentally and theoretially show that by altering the spectral intensity of a 30 fs laser pulse at 800 nm using a Mach-Zehnder-interferometer, we are able to shift the electrical field energy in a controlled manner. First consistent results comparing simulated and measured data of a Fresnel type focusing device show a very good agreement.

O 74.7 Thu 17:30 MA 005

Transmission of Light through Magnetic Nanocavities — •Piotr Patoka, Michael Hilgendorff, and Michael Giersig — Institut für Experimentalphysik, Freie Universität Berlin, Arnimallee 14, 14195 Berlin

The transmission of light through a metallic film stack on a transparent substrate, perforated with a periodic array of cylindrical holes/nanocavities, is studied. The structure is fabricated by using self-assembled nanosphere lithography. Since one layer in the film stack is made of a ferromagnetic metal (iron), exposure of the structure to a solution containing iron oxide nanoparticles causes nanoparticle accumulation inside the nanocavities. This changes the dielectric constant inside the nanocavities and thus affects the light transmission. Simulations are in good agreement with experiment, and show large sensitivity of the response to the amount of iron oxide nanoparticles deposited. This could be used in various sensor applications.

O 74.8 Thu 17:45 MA 005

Time-Resolved PEEM Investigation of the Interaction of Surface Plasmons with Hot Spots — •Martin Wiesenmayer, Alexander Fischer, Pascal Melchior, Christian Schneider, Daniela Bayer, and Martin Aeschlimann — University of Kaiserslautern, Department of Physics, 67663 Kaiserslautern, Germany

In our talk we present a spatially and time-resolved investigation of a rough, polycrystalline silver surface. The acquisition of phase resolved autocorrelation traces ($h\nu = 1.55$ eV and 3.1 eV, p- and s-polarized) enables a detailed analysis of such data, especially with respect to the interference fringes. The interaction of the laser induced surface plasmons with local hot spots on the silver surface is the focus of our work. We observe a significant broadening of the autocorrelations which exceeds the dephasing times of a smooth metal surface. Using photoemission electron microscopy (PEEM) allows for a parallel detection in the micron regime (field of view below 20 μm) which is crucial for the interpretation of the observed broadening effects. Our investigations contribute to a deeper understanding of the time dependent evolution of the local near field enhancement on rough silver surfaces, as used in surface enhanced Raman scattering (SERS).

O 74.9 Thu 18:00 MA 005

Dispersion control of propagating surface plasmons on nanoporous gold — •Neha Sardana[1,2] and Jörg Schilling[1] — [1]Centre for Innovation Competence SiLi-nano, Martin Luther University of Halle-Wittenberg, Karl-Freiherr-von-Fritsch-Str. 3, 06120 Halle (Saale), Germany — [2]International Max Planck Research School for Science and Technology of Nanostructures, Weinberg 2, 06120 Halle (Saale), Germany

Surface Plasmons (SPs) have wavelengths shorter than light and allow its strong confinement hence forming the backbone of current subwavelength optics. Their dispersion relation on plane metal/dielectric surfaces follows directly from Maxwell equations and is given as $k_x{=}(\omega/c) * \sqrt[2]{[\varepsilon_m * \varepsilon_d/(\varepsilon_m + \varepsilon_d)]}$, 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 respectively. To control the dispersion of the SPs, normally ε_d is varied. An increase in ε_d causes a red shift of the SP at constant k_x or an increase of k_x for constant SP frequency ω. However in our experiments we explore the same possibility by changing the value of ε_m by introducing nanoporosity by dealloying method into the metal. Reflection measurements in the Kretchmann configuration are used to determine the dispersion relation of the SP on nanoporous gold/air interface. A characteristic dip in reflectivity, which shifted to shorter wavelength with increasing angle of incidence, was identified. This shift is compared with the Bruggeman effective medium theory. The experimental analysis proves that SP dispersion relation can be controlled by porosity of metal leading to larger flexibility in SP devices.

O 74.10 Thu 18:15 MA 005

Excitation of radial and other complex polarization states in special optical fibers by long period fiber gratings — •Christoph Zeh[1], Rico Illing[1], Bernd Köhler[1], Jörg Opitz[1], and Lukas M. Eng[2] — [1]Fraunhofer Institut für Zerstörungsfreie Prüfverfahren, Institutsteil Dresden, Maria-Reiche-Str. 2, 01109 Dresden — [2]Institut für Angewandte Photophysik, TU Dresden, 01069 Dresen

Radial polarization has drawn much attention in recent years, especially in the nano-optics and plasmonics community, because of its enhanced focusing properties as well as its ability to efficiently excite plasmons in radially symmetric structures.

Here, we present polarization mode excitation by long period fiber gratings (LPGs) in a special optical fiber. LPGs are able to efficiently transfer energy between co-propagating modes of the fiber. Since the field of a waveguide can always be represented as a set of mode fields with respective amplitudes and phases, polarization control is achieved by controlling the relative amplitudes and phases of the guided modes. We will demonstrate the use of a tunable acoustic LPG for this task and compare the results to other mechanical and UV-induced gratings.

The special fiber used in the above experiments is simulated by the multiple multipole technique (MMP) for a better understanding of the mode fields. This results in the transverse vector fields and propagation constants of the modes. The latter are necessary for designing the LPGs and for understanding the measurement results.

O 75: Particles and clusters

Time: Thursday 16:00–17:45 Location: MA 041

O 75.1 Thu 16:00 MA 041

Towards Catalysis by Gold Clusters: reaction cycles and poisons — Elizabeth C. Beret, •Luca M. Ghiringhelli, and Matthias Scheffler — Fritz Haber Institute, D-14195, Berlin

Nanosized gold particles are good catalysts in a variety of oxidation reactions. These reactions, for which oxidation of CO to CO_2 serves as a paradigm, imply a transition in the total spin and therefore do not occur spontaneously in the gas phase. In the catalytic process, the catalyst clusters are exposed to an atmosphere of gas-phase O_2 and CO reactants at finite temperature and pressure. We have thus modeled free gold clusters in contact with an atmosphere composed of O_2 and CO by means of DFT calculations (PBE functional), and accounted for both temperature and pressure effects employing *ab initio* atomistic thermodynamics. On the basis of this analysis, we could recognize the thermodynamic driving force of the catalytic CO oxidation process and single out the possible (p,T)-dependent reaction cycles and those paths leading to stable structures that poison the catalytic process. This as a useful (exploratory) theoretical step, before taking chemical reaction kinetics into consideration. In the proposed reaction paths, the total spin is conserved in each elementary step, and it is the adsorption of an incoming O_2 molecule that drives the catalyst cluster from the singlet to the triplet spin state, and *vice versa*

O 75.2 Thu 16:15 MA 041

Endohedral doping of hydrogenated Si fullerenes: A route to magnetic Si building blocks? — •Dennis Palagin and Karsten Reuter — TU München

Metal encapsulation was found to produce fullerene and other polyhedral cage structures of silicon and therewith provides an intriguing novel nanoform of Si for device applications. In these structures the cage geometry is stabilized through a strong interaction with the endohedral dopant atom. The recent suggestion that also hydrogen termination of Si_{16} could yield an empty fullerene configuration has raised hopes that metal-doping corresponding $Si_{16}H_{16}$ fullerenes would yield cage structures with minimized M-Si interaction [1]. With the atomic character of e.g. magnetic dopants then likely conserved, this would offer a route to develop Si fullerene species with large magnetic moments. We scrutinize this proposition through density-functional theory based global geometry optimization. While we can confirm that the fullerene is indeed the ground-state structure of $Si_{16}H_{16}$, this is unfortunately not the case for Ti or Cr dopant atoms. Strongly distorted or even broken cages are instead significantly more stable. We therefore screen a larger range of dopant atoms and critically discuss the resulting M-Si interaction in all of these cases.

[1] V. Kumar and Y. Kawazoe, Phys. Rev. Lett. 90, 055502 (2003).

O 75.3 Thu 16:30 MA 041

The size-dependent agglomeration of nanoparticles in solvents — Gediminas Galinis, Gauthier Torricelli, Hanieh Yazdanfar, Atea Akraiam, Mark Watkins, and •Klaus von Haeften — Department of Physics and Astronomy, University of Leicester, Leicester, LE1 7RH, United Kingdom

Nanoparticles suspended in solvents usually tend to agglomerate by mutual physisorption. We have investigated this phenomenon by depositing silicon clusters with a broad size distribution (peak size 40 to 60 nm) into water. Drops of the cluster-water suspension were then placed on highly oriented pyrolitic graphite (HOPG) and dried in vacuum. AFM measurements in UHV revealed a height distribution peaking at 1 to 2 nanometers, which was much smaller than the original size distribution. We explain this observation as being due to size-dependent agglomeration in water caused by the balance of thermal energy and van der Waals attraction. The maximum height of 3 nm diameter was consistent with the prediction of the Hamaker theory [1]. While single clusters where identified most clusters were laterally agglomerated and for high densities a distinct second layer was identified. In addition, the clusters showed various forms of self-organisation such as rings or gratings depending on the wetting behaviour of the solvents.

[1] G. Torricelli, A. Akraiam, K. von Haeften, Nanotechnology 22, 315711 (2011).

O 75.4 Thu 16:45 MA 041

Traceable size determination of spherical nanoparticles via Small Angle X-ray Scattering (SAXS) — •Gudrun Gleber[1], Michael Krumrey[1], Armin Hoell[2], Levent Cibik[1], Stefanie Marggraf[1], and Peter Müller[1] — [1]Physikalisch-Technische Bundesanstalt, Abbestr. 2-12, 10587 Berlin — [2]Helmholtz-Zentrum Berlin, Albert-Einstein-Str. 15, 12489 Berlin

Although various methods to measure the size of nanoparticles are available, the results of different methods often do not agree. In the framework of an European metrology project, several methods were used for traceable size determination and their results were compared.

As samples, spherical particles made of gold, PMMA, Silica, and Latex of nominal sizes between 10 nm and 200 nm in aqueous solution were used. The Small Angle X-ray Scattering (SAXS) experiments were performed at the Four-Crystal Monochromator (FCM) beamline in the laboratory of Physikalisch-Technische Bundesanstalt (PTB) at BESSY II using the SAXS setup of the Helmholtz-Zentrum Berlin (HZB). Besides the setup based uncertainties such as the uncertainties of photon energy, of detector pixel size, and of the distance between sample and detector, those based on the analysis process as e. g. assumption of particle shape, size distribution function, and background contribution were investigated.

O 75.5 Thu 17:00 MA 041

Ultraviolet photoelectron spectroscopy of mass selected metal clusters on graphite (HOPG) — •Natalie Miroslawski[1], David Engemann[1], Niklas Grönhagen[1], Bernd von Issendorff[2], and Heinz Hövel[1] — [1]Experimentelle Physik I, Technische Universität Dortmund, Germany — [2]Fakultät für Physik, Universität Freiburg, Germany

Mass selected silver and copper clusters between 34 and 923 atoms were deposited with less then 0.1eV/atom kinetic energy on graphite (HOPG) and investigated with ultraviolet photoelectron spectroscopy (UPS) with a photon energy of 21.2eV. The clusters were deposited with different coverage for each cluster size and measured at 125K. For a better interpretation we subtracted normalized HOPG spectra from the measured cluster spectra to extract the d-band structure of the clusters. To investigate the cluster mobility and coalescence we varied the deposition temperature and the cluster coverage. Additionally we annealed the sample after deposition at different temperatures and observed changes in the UPS spectra depending on the cluster coverage.

O 75.6 Thu 17:15 MA 041

Ag clusters on SiO_2 and in matrices: UV-VIS absorption and XANES — •Stefanie Duffe[1], Sabrina Hoffmann[1], Kamil Latussek[1], David Engemann[1], Christian Sternemann[1], Christoph J. Sahle[1], Heinz Hövel[1], Ralph Wagner[2], and Pieter Glatzel[3] — [1]TU Dortmund, Experiment. Physik I/DELTA, Dortmund, Germany — [2]BU Wuppertal, Fachgruppe Physik-Materialwiss., 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 (SiO_2) [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. We investigate the plasmon resonance of Ag clusters on SiO_2, in PDMS (polydimethylsiloxane) or aerogel before and after exposure to air by optical spectroscopy [3]. XANES measurements at the Ag $L_{1,2,3}$-edges [4] were carried out at the synchrotron radiation sources DELTA and ESRF. Embedding the clusters into PDMS [5] or aerogel enables the investigation of a much higher amount of separated clusters which is otherwise limited by coalescense and electromagnetic coupling.

[1] O. F. Hagena, Z. Phys. D 20, 425 (1991). [2] H. Hövel et al., Phys. Rev. B 48, 18178 (1993). [3] U. Kreibig et al. In: Advances in Metal and Semiconductor Clusters Vol. 4, (ed. M.A. Duncan), JAI press Inc., 345 (1998). [4] P. Behrens et al., Z. anorg. allg. Chem. 625, 111 (1999). [5] L. Ravagnan et al., J. Phys. D 42, 082005 (2009).

O 75.7 Thu 17:30 MA 041

How do metal clusters split water?
Towards a theoretical understanding of co-catalysts for water oxidation — •Harald Oberhofer and Karsten Reuter — TU Munich, Garching, Germany

Efficient, sustainable production of molecular hydrogen—a promising alternative to batteries in terms of energy storage—is still an unsolved problem. Implementation of direct water splitting using only sunlight and suitable photo-catalysts so far has been hampered by poor photon absorption properties of the materials and low reaction efficiencies. One ansatz of overcoming the latter obstacle is the use of small metal clusters as co-catalysts, a method that yielded promising results in experiments. Yet, the actual effect of co-catalysts on the reaction is poorly understood. In our contribution we discuss our DFT-based efforts towards a microscopic understanding of small metal clusters as co-catalysts. We present our studies, based on a thermodynamic approach pioneered by Nørskov and Rossmeisl [J. Phys. Chem. B **108**, 17886 (2004)], of the water oxidation reaction on various metal clusters in the non-scalable size regime (less than 20 atoms) and compare with the extended surface. On top of these results we discuss the influence of solvent on the reaction as well as the stabilisation of electron holes necessary for the reaction. Conclusions of the presented work will in the future be used to postulate micro-kinetic reaction pathways and determine reaction rates comparable with experiment.

O 76: Nanostructures at surfaces IV

Time: Thursday 16:00–17:30 Location: MA 042

O 76.1 Thu 16:00 MA 042

Silicon micro-tip arrays for fast-switchable cold electron sources — •Pavel Serbun[1], Aliaksandr Navitski[1], Benjamin Bornmann[1], Stephan Mingels[1], Günter Müller[1], Florian Dams[2], Christian Prommesberger[2], and Rupert Schreiner[2] — [1]FB C Physics Department, University of Wuppertal, 42119, Wuppertal, Germany — [2]Faculty of Microsystems Technology, University of Applied Sciences Regensburg, Germany

Silicon-based cathodes with precisely aligned field emitter arrays applicable for miniaturized electron sources were successfully fabricated. The cathode chips contain about 3x10^5 Si tips/cm^2 in a triangular array with a tip height of 1 or 2.5 um, tip radius of about 20 nm, and 20 um pitch. Amazingly homogeneous and well-aligned field emission (FE) from all tips (100% efficiency) and maximum stable currents of about 0.1 uA for p- and 0.6 uA for n-type Si were reproducibly achieved. Additional coating with a bimetallic layer (5 nm Cr and 10 nm Au) resulted in at least 5 times higher average FE current i.e. typically 3 uA but lead, however, to a 30% increase of the onset voltage. I-V characteristics of p-type Si tips exhibit the expected I-V characteristics consisting of a linear FN-like part at low field/current, a current saturation region, and finally a rapid current rise at high field due to secondary charge effects. Moreover, a high photosensitivity of the saturation current was observed which provides a unique possibility to modulate the electron current by ultra-short light pulses. Detailed FE and light-modulation results of p-type arrays of varying size and tip-number will be presented and discussed at the conference.

O 76.2 Thu 16:15 MA 042

Photo sensitivity and field emission properties of B-doped Si-tip arrays — •Benjamin Bornmann[1], Stephan Mingels[1], Aliaksandr Navitski[1], Pavel Serbun[1], Florian Dams[2], Christian Prommesberger[2], Rupert Schreiner[2], Dirk Lützenkirchen-Hecht[1], and Günter Müller[1] — [1]FB C Physics Department, University of Wuppertal, 42119, Wuppertal, Germany — [2]Faculty of Microsystems Technology, University of Applied Sciences Regensburg, 93053, Regensburg, Germany

Field emission (FE) cathodes have shown significant advantages over thermionic electron sources. For sensor applications Si tips are favored because they can be easily integrated with other Si based components. p-semiconductors have a limited number of free electrons thus being highly sensitive to photonic excitation. This allows the realization of compact fast switchable e^--sources. We report on FE-spectroscopy on B-doped Si-tip arrays with optional tunable laser illumination (0.5-5.9 eV). The current-voltage curve exhibits three emission regimes: a Fowler-Nordheim regime at low currents, a saturation region due to electron depletion and secondary carrier generation at high currents. The corresponding spectra show an increased charging in saturation by a shift and splitting of the peaks. A high conductivity is observed under secondary carrier generation. The FE is most stable in saturation as the emission strongly depends on the supply function here rather than on the surface sensitive tunneling probability. Accordingly, the highest photosensitivity is observed in saturation. Optimization of the quantum efficiency with tunable laser illumination is ongoing.

O 76.3 Thu 16:30 MA 042

Template-based surface nano-patterning to realize high performance devices — •Liaoyong Wen, Huaping Zhao, Fabian Grote, Yan Mi, Ranjith Vellacheri, Zhibin Zhan, Ahmed Al-

Haddad, Yaoguo Fang, Kin Mun Wong, and Yong Lei — Fachgebiet 3D-Nanostrukturierung, Institut für Physik & ZIK MacroNano, Technische Universität Ilmenau, 98693 Ilmenau, Germany

Surface patterning using nano-templates are highly efficient in preparing large-scale ordered arrays of surface nanostructures. Here we introduce surface patterning processes using two templates that are prepared using self-assembly processes: ultra-thin alumina membranes (UTAMs) and monolayer polystyrene (PS) sphere arrays. The surface patterns have promising device applications due to the low-cost and time-saving fabrication processes of surface structures. The feature size of the building blocks of the surface patterns prepared using UTAM and PS templates can be adjusted from the quantum size to the nanometer size and to the micrometer size range. Different functional surface nano-patterns have been developed using the UTAM and PS templates, including 1D nanostructure arrays, quantum-sized nanodot arrays, and metallic hollow sphere arrays. The device applications in photocatalytic devices, supercapacitors, solar cells, SERS sensors, and field emission device will be demonstrated.

1.Lei, Y.; Yang, S. K.; Wu, M. H.; Wilde, G., Chem. Soc. Rev. 2011, 40, 1247. 2.Yang, S. K.; Xu, F.; Ostendorp, S.; Wilde, G.; Zhao, H.; Lei, Y., Adv. Funct. Mater. 2011, 21, 2446. 3.Wu, M. H.; Wen, L. Y.; Lei, Y.; Ostendorp, S.; Chen, K.; Wilde, G., Small 2010, 6, 695.

O 76.4 Thu 16:45 MA 042

Magnetic nanowire arrays prepared by electrodeposition using AAO templates — •Nina Winkler, Jörn Leuthold, Martin Peterlechner, Yong Lei, and Gerhard Wilde — Institute of Materials Physics and Center for Nanotechnology, University of Münster, 48149 Münster, Germany

Regular magnetic nanowire arrays with large wire aspect ratios have possible applications, amongst others, in high density magnetic recording media and biological sensing of carbohydrates. Porous Anodic Alumina Oxide (AAO) is a versatile template for surface nanostructuring and in this talk, the fabrication of nanowire arrays by electrodeposition using AAO will be addressed. The AAO template enables control of regularity and shape of nanostructures by its pores which are hexagonally arranged and stand perpendicularly on an Aluminum substrate. Two different pretreatments of the AAO template will be presented to either remove or perforate the insulating alumina barrier layer between Al substrate and pores of the AAO template. Electrodeposition is applied using a potential pulse sequence to obtain nickel, iron, cobalt or FeNiP nanowire arrays. The structure of the nanowire arrays has been observed by SEM and TEM. The magnetic properties of the nanowire arrays have been characterized by Vibrating Sample Magnetometer (VSM) measurements and Magnetic Force Microscopy (MFM). The high regularity of a nanowire array is demonstrated using an image-based analysis tool which compares the arrangement of the wires to a mathematically perfect hexagonal pattern and therefore allows a quantitative analysis of the hexagonal regularity of the nanowire array.

O 76.5 Thu 17:00 MA 042

Highly sensitive gas sensors based on three-dimensional surface nano-patterns realized by UTAM nano-structuring technique — •Yan Mi[1,2], Zhibin Zhan[1,2], Hui Sun[1,2], Fabian Grote[1,2], Huaping Zhao[1,2], and Yong Lei[1,2] — [1]Fachgebiet 3D-Nanostrukturierung, Institut für Physik & Zentrum für Mikro- und Nanotechnologien (ZIK MacroNano), Technische Universität Ilmenau, 98693 Ilmenau, Germany — [2]Institut für MaterialPhysik, Westfälische Wilhelms-Universität Münster, 48149 Münster, Germany

Using an innovative three-dimensional (3D) surface nano-structuring technique, highly ordered functional surface nano-patterns can be synthesized with high application potentials. In this talk, we demonstrate an excellent device application of the 3D surface nano-patterns - gas sensors with extremely high sensitivity. The basic structures of the high sensitive gas sensors are template-prepared ZnO nanotube arrays via atomic layer deposition process. The sensitivity of the gas sensor to NO2 gases could reach 25 ppb level, which has not been reported before for commercial gas sensors. Such kind of high sensitivity to NO2 is quite attractive to environmental protection and atmospheric quality monitoring. The high regularity and controllability to the structural parameters of the 3D nano-patterns make it possible to investigate the surface chemistry and physics of the gas sensors and hence to optimize the device performance.

O 76.6 Thu 17:15 MA 042

High performance super-capacitors based on template-prepared one-dimensional MnO_2 nanostructures — •Fabian Grote[1,2], Yan Mi[1,2], Huaping Zhao[1,2], and Yong Lei[1,2] — [1]Institut für Physik & Zentrum für Mikro- und Nanotechnologien, Technische Universität Ilmenau, Germany — [2]Institut für Material Physik, Westfälische Wilhelms-Universität Münster, Germany

MnO_2 is a promising candidate for future applications in high performance super-capacitors, since it possesses a high specific capacitance. A way of selectively control the growth of highly ordered MnO_2 nanowire and nanotube arrays for fabricating a super-capacitor electrode will be demonstrated using an electrochemical deposition technique in combination with porous aluminium oxide as a template. The morphology is investigated by field emission scanning electron microscopy and transmission electron microscopy. Electrochemical properties of different structures will be shown and compared.

O 77: Electronic structure I

Time: Thursday 16:00–17:30 Location: MA 043

O 77.1 Thu 16:00 MA 043

Electron-phonon coupling investigated by laser-photoemission spectroscopy in Pb/Si(111) — •Mathias Sandhofer, Dimitrios Papoutzis, Laurenz Rettig, Simon Freutel, Ltaief Ben Ltaief, Isabella Avigo, Manuel Ligges, and Uwe Bovensiepen — Fakultät für Physik, Universität Duisburg-Essen, 47048 Duisburg

We investigate different contributions to electron scattering rates in epitaxial Pb/Si(111) thin films by a linewidth analysis in photoemission spectroscopy, using frequency-quadrupled Ti:Sa laser pulses (6 eV). We consider contributions from electron-electron (e-e), electron-phonon (e-ph) and electron defect (e-df) scattering. For the investigated electronic quantum well states at five and seven monolayer film thickness the e-e contribution is 4 meV[1]. This simplifies the observation of the e-ph coupling through a temperature dependent linewidth analysis which is expected to yield a contribution one or two orders of magnitude higher[2]. A linear temperature-dependence of the linewidth is found for 40 K<T<120 K, indicating the increase of e-ph scattering rate due to an increase of the number of phonons. The obtained e-ph coupling constant is λ=0.7+-0.1. For higher temperatures (T>120 K) the linewidth remains constant. Supported by a lower linewidth for T=40 K after heating to 180 K, we explain this by a decrease in e-df scattering through a reduction of defects.

[1] Kirchmann et al., Nature Physics 6, 782 (2010)

[2] Hong I-Po et al., Phys Rev B 80, 081409 (2009)

O 77.2 Thu 16:15 MA 043

Investigation of the hybridization between the unoccupied Shockley surface state and bulk electronic states on Cu(111) — •Aimo Winkelmann, A. Akin Ünal, Christian Tusche, Cheng-Tien Chiang, Safia Ouazi, Sebastian Wedekind, Masaki Takada, Dirk Sander, Jürgen Henk, and Jürgen Kirschner — Max-Planck-Institut für Mikrostrukturphysik, Halle

Shockley surface states and image-potential states in the bulk L-gap of the (111) surfaces of Cu, Ag, and Au are well-known models for the study of quasi-two-dimensional electron systems. We have applied k-resolved multiphoton photoemission using a *momentum microscope*, scanning tunneling spectroscopy using Fourier-transformation and Bessel-function fitting, together with first-principles electronic structure calculations to determine the dispersion of the occupied and unoccupied Shockley surface state of Cu(111). We verify that the dispersion of this state deviates significantly from the paradigmatic parabolic behavior of quasi-free electrons with increasing energy above the Fermi level [1]. Based on our calculations, we ascribe this deviation to the shift of the spectral weight of the surface state into the bulk, and of bulk states toward the surface, which leads to an enhanced hybridization between the states with increasing energy.

[1] A.A. Ünal, C. Tusche, S. Ouazi, S. Wedekind, C.-T. Chiang,

A. Winkelmann, D. Sander, J. Henk, J. Kirschner Phys. Rev. B 84, 073107 (2011)

O 77.3 Thu 16:30 MA 043

Spectral and spatial redistribution at the $LaAlO_3/SrTiO_3$ interface — •Tim Günter[1], Andrea Rubano[1,2], Thomas Fink[1], Domenico Paparo[3], Lorenzo Marrucci[3], Fabio Miletto Granozio[3], Umberto Scotti di Uccio[3], Jochen Mannhart[4], and Manfred Fiebig[1,5] — [1]HISKP, University Bonn, Germany — [2]Fritz-Haber-Institut, Berlin, Germany — [3]Dip. di Scienze Fisiche, University Naples, Italy — [4]MPI for Solid State Research, Stuttgart, Germany — [5]Materials Departement, ETH Zürich, Switzerland

A conductive two-dimensional electron liquid (2DEL) appears at the $LaAlO_3/SrTiO_3$ (LAO/STO) interface for a LAO thickness of n≥4 unit cells. Despite the tremendous research interest, many questions regarding the origin and characteristics of the 2DEL have to be addressed yet. In particular, this includes the electronic structure of the 'buried interface'. Optical second harmonic generation (SHG) is an ideal tool for studying interfaces, since it is sensitive to the interfacial symmetry breaking along the stacking direction. Using SHG with frequency-tunable amplified femtosecond laser pulses we obtain information about the structural reorganization of the interfacial STO conduction band for SHG photon energies up to 6.2 eV. A massive spectral weight redistribution is present for n≥3, indicating a global reorganization of the conduction band structure. At low temperatures the spectral resolution is enhanced which alleviates the distinction of interfacial electronic transitions. Our data are supported by a theoretical framework based on symmetry selection rules that allows a specific assignment of interfacial O(2p)-Ti(3d) transitions to the SHG spectrum.

O 77.4 Thu 16:45 MA 043

Energy level alignment and ultrafast electron dynamics at pristine and pyridine-covered ZnO(10$\bar{1}$0) — •Jan-Christoph Deinert, Daniel Wegkamp, Julia Stähler, and Martin Wolf — Fritz-Haber-Institut der MPG, Abt. Physikalische Chemie, Faradayweg 4-6, 14195 Berlin

Organic adlayers on semiconductor surfaces are promising candidates for highly functional molecular electronics devices, e. g. organic LEDs. Such hybrid systems may exhibit electronic and excitonic properties that go beyond the linear combination of the two material classes' stand-alone properties. An example is the formation of new interface states through hybridization of molecular and semiconductor states. Efficient functionalization requires sound knowledge of both occupied and unoccupied electronic structure at the hybrid interface. In our experiment we can directly access these states and examine their ultrafast dynamics upon excitation using femtosecond time-resolved two-photon photoemission (2PPE). Characterization of the pristine ZnO(10$\bar{1}$0) surface yields the valence and conduction band (CB) edge energies. Besides a time-dependent down shift of the sample work function by few 10 meV, our spectra show the hydrogen-induced downward shift of the CB minimum below E_F. Furthermore, we directly monitor the hot electron relaxation in the ZnO CB on femtosecond timescales and subsequent formation of a long-lived state. Adsorption of pyridine leads to a massive reduction of the work function of the sample up to $\Delta\Phi = -2.7\,\mathrm{eV}$, which makes this system a good candidate for further studies of energy level alignment.

O 77.5 Thu 17:00 MA 043

Character of the valence band states in the Kondo surface alloys $CeAg_x$/Ag(111) and $CePt_5$/Pt(111) — •Holger Schwab[1,2], Mattia Mulazzi[1,2], Kenya Shimada[3], and Friedrich Reinert[1,2] — [1]Physikalisches Institut, Experimentelle Physik VII und Wilhelm Conrad Röntgen Research Center for Complex Material Systems (RCCM), Universität Würzburg, D-97074 Würzburg — [2]Gemeinschaftslabor für Nanoanalytik, Karlsruher Institut für Technologie KIT, D-76021 Karlsruhe — [3]Hiroshima Synchrotron Radiation Center, Hiroshima University, Higashi-Hiroshima 739-0046, Japan

Recently we have shown the transition from the single impurity to the Kondo lattice regime in the surface alloy $CePt_5$. [1] Now we have prepared a new Ce based surface alloy: $CeAg_x$. The electronic and crystal structures of both materials have been investigated by means of low-energy electron diffraction and angle-resolved photoelectron spectroscopy (ARPES). With resonant PES near the $4d$-$4f$ absorption edge we were able to infer the weight of the $4f$-electron spectral function with respect to single-particle density of states. While the typical Kondo features at the Fermi energy (Kondo resonance and spin orbit partner) in the $CePt_5$ surface alloy are observed, $CeAg_x$ shows a different behaviour. By comparing our experiments to model calculations [2,3], we were able to estimate the Kondo temperature in the two systems and investigate parameters contributing to the hybridisation.
[1] M. Klein et al.,Phys. Rev. Lett. 106, 186407 (2011).
[2] F. Patthey et al., Phys. Rev. B 42, 8864 (1990).
[3] S. Gardonio et al., Phys. Rev. Lett. 107, 026801 (2011).

O 77.6 Thu 17:15 MA 043

Spectroscopic Characterisation of Insulating and Superconducting Cement *$12CaO{\cdot}7Al_2O_3$ (C12A7)* — •Anna Buling[1], John McLeod[2], Manfred Neumann[1], Ernst Kurmaev[3], Hideo Hosono[4], and Peter Sushko[5] — [1]D-Fachbereich Physik, Universität Osnabrück — [2]CA-Department of Physics and Engineering Physics,University of Saskatchewan — [3]RU-Institute of Metal Physics, Russian Academy of Sciences - Ural Division, Yekaterinburg — [4]JP-Materials and Structurs Laboratory, Tokyo Institute of Technology — [5]UK-University College London

The nanoporous complex oxide $C12A7$, which is a wide bandgap insulator, is produced as a main constituent of commercial alumina cement but has great potential for other applications in electronics and catalysis. By introducing oxygen deficiency, conductivity can be realized in the system up to superconductivity with a T_C ≈0.14 - 0.4 K. Currently, there are two competing models explaning the existence of conductivity in this compound: One involves the electron hopping along framework lattice sites, the other the electron transfer via a cage conduction band.

Here we present the investigation of insulating and superconducting $C12A7$ by means of X-ray photoemission, X-ray absorption and X-ray emission spectroscopy measurements completed with DFT calculations to illuminate the relations in the conduction and the valence bands. Our measurments suggest that free electrons in oxygen-deficient $C12A7$ occupy a narrow band which exists between the main conduction band and the valence bands.

O 78: Metal substrates: Adsorption of organic / bio molecules IV

Time: Thursday 16:00–17:45 Location: A 053

O 78.1 Thu 16:00 A 053

1D growth of α-Sexithiophene on Au(110) — •Rene Hammer[1], Tobias Leopold[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 quality of the interface between a metal electrode and the organic semiconducting device is a central issue in organic electronics. Typically the structures of the first layers are quite different from its bulk single crystal structures. However for the growth of α-Sexithiophene (6T) on Au(110) a rather bulk like interface has been proposed [1].

Here we present a scanning tunneling microscopy study of the 6T adsorption on Au(110) at 300K. At low coverages (0.05 monolayer (ML)) the growth of one-dimensional(1D) chains of molecules in [1-10] direction is observed. The structures are 2 molecules wide and several 100nm in length. This chain formation is independent of step edges. At coverages close to a ML a packing of the 1D structures with distances of 4, 5 and 6 Au lattice constants is observed

Single molecular rows grow by a zipper-like mechanism: A topmost atomic row of the (2x1) Au(110) reconstruction shifts by one lattice constant, which leads to a local (1x1) Au(110) micro-facet. These are the preferred adsorption sites of the 6T molecules, in contrast to the previously proposed model [1].

[1] Prato et al., J. Phys. Chem. B 103 (1999)

O 78.2 Thu 16:15 A 053

Single-molecule spectroscopy of terthiophene adsorbed on

Au(111): electronic and vibronic properties — •Berndt Koslowski, Norbert Maurer, Anna Tschetschetkin, and Paul Ziemann — Institute of Solid State Physics, University of Ulm, D-89069 Ulm, Germany

Because of their expedient properties and their diversity, oligo- and polythiophenes are among the most investigated organic semiconductors. We investigated the adsorption of terthiophene molecules (3T) on Au(111) at low temperature by means of Scanning Tunneling Microscopy and Spectroscopy. 3T adsorbs preferentially in the fcc regions and orients perpendicularly to the soliton walls of the herringbone reconstructed Au(111). Tunneling spectroscopy in the center of the molecule shows the broad LUMO of the molecule at +2.3 eV on a background resembling properties of the gold surface. The HOMO was determined to lie at -1.3 eV leaving the optical gap unchanged as compared to the gas-phase molecule. dI/dV maps reveal a very inhomogeneous distribution of the LUMO/HOMO across the molecule indicating a significant interaction of molecular states with the substrate [1]. By inelastic electron tunneling spectroscopy we find very rich vibrational spectra on the molecules containing more than 30 modes. We analyze the vibronic spectrum and compare it to spectra expected for the free molecules and other experimental results. [1] Koslowski et al., Beilstein J. Nanotechnol. 2, 561-568 (2011).

O 78.3 Thu 16:30 A 053

Using polarized light in photoelectron emission microscopy — •Thorsten Wagner[1], Zdena Druckmüllerova[1,2], Daniel Roman Fritz[1], and Peter Zeppenfeld[1] — [1]Johannes Kepler University Linz, Institute of Experimental Physics, Linz, Austria — [2]Brno University of Technology, Institute of Physical Engineering, Brno, Czech Republic

Photoelectron emission microscopy (PEEM) combines a high lateral resolution with the capability to monitor processes at surfaces in real-time. For experiments in the lab, unpolarized light of a Hg lamp is commonly used to excite the photoelectrons. In this case, valuable information about the optical anisotropy of the surface under investigation is lost. On the other hand, techniques like reflectance difference spectroscopy (RDS) which are focussed on this anisotropy have proven to be useful tools to study thin adsorbate films of organic molecules. So why not combining both in a single experiment? In this presentation we will show, how polarized light can be used to study the growth of α-sexithiophene on silver and nickel oxide surfaces. As the ionization potential of the molecules is higher than the photon energy, the light of the Hg lamp only excites electrons from the metal-organic interface. In this case, no direct response of the molecules to the polarized light can be expected in the PEEM image. Nevertheless, the molecules are optical anisotropic and act as dichroic filters for the incident light. This effect can actually be used, e.g., to probe the orientation of the molecules even during growth.

O 78.4 Thu 16:45 A 053

Theoretical Insight into the Growth Mechanisms of 6P Monolayers on Copper Substrates — •Giulio Biddau[1], Peter Puschnig[1], Margareta Wagner[2], Stephen Berkebile[2], Alexander Fleming[2], Falko Netzer[2], Michael Ramsey[2], and Claudia Ambrosch-Draxl[1] — [1]Chair of Atomistic Modelling and Design of Materials, Montauniversitaet Leoben, Austria — [2]Institute of Physics, Surface and Interface Physics, Karl-Franzens University, Graz, Austria

We present a multi-technique study of the deposition and adsorption of para-sexiphenyl (p-6P) on the Cu(110) substrate and of its first monolayer (1ML) growth at high coverage, while at low coverages the adsorbed molecules repel forming a dense wetting monolayer. The characterization has been carried out by low-temperature STM experiments and Density Functional Theory calculations, performed using the generalized gradient approximation and considering van der Waals interactions with the DFT-D2 approach.Insight in the diffusion barriers is obtained by the Nudged Elastic Band method and the comparison with experimental STM results carried out with the Tersoff-Hamann approximation.We show that island growth occurs through diffusion of admolecules deposited in the second monolayer along [110] directions in a 2D Frank-van-der-Merwe layer by layer behavior.We show that molecules of the 1ML, efficiently screen the interaction of 2ML molecules with the metallic substrate.Thus,the weakly bound 2ML admolecules are allowed to diffuse with low Ehrlich-Schwoebel barrier along [110],favoring the formation a high-density reconstruction.

O 78.5 Thu 17:00 A 053

The role of molecular orbitals in scanning tunneling induced luminescence — •Christoph Grosse[1], Theresa Lutz[1], Christian Dette[1], Alexander Kabakchiev[1], Klaus Kuhnke[1], Uta Schlickum[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

The plasmonic light spectrum of pristine metals excited by scanning tunneling microscopy (STM) can be affected in many different ways by the adsorption of organic molecules. In this study we elucidate the role of molecular orbitals in the light emission process and employ STM to investigate the optical and electronic properties of individual *fac*-Ir(ppy)$_3$ molecules on top of a C_{60} monolayer on Ag(111). In this binary system, the C_{60} monolayer acts as a molecular decoupling layer. Compared to this, the light excitation on the Ir(ppy)$_3$ molecules increases locally by half an order of magnitude due to a more efficient excitation of tip induced plasmons. Mapping the molecular orbitals by differential conductance (dI/dV) images reveals three distinguishable molecular orbitals. A comparison of their shape with sub-molecular resolved light excitation maps shows a clear correlation between the light enhancement and the orbital closest to the Fermi energy of the substrate.

O 78.6 Thu 17:15 A 053

Controlled rotation of single molecules and sub-angstöm determination of intrinsic molecular elasticity — •Rémy Pawlak[1], Sweetlana Fremy[1], Shigeki Kawai[1], Thilo Glatzel[1], Hongjuan Fang[2], Lesli-Anne Fendt[2], François Diederich[2], and Ernst Meyer[1] — [1]DepaDepartement of Physics, University of Basel, Switzerlandrtement of Physics, University of Basel, Switzerland — [2]Laboratorium für Organische Chemie, ETH Zürich, Switzerland

Directed molecular repositioning is a key step towards the built-up of molecular machines. To artificially generate and control motion on a surface, molecules are generally excited by an exchange of light, chemical or electrical energy. Although the elasticity of molecular structures plays a role in all diffusion processes, such intrinsic properties are rather poorly known. Here, we explore by scanning probe microscopy directed manipulations of single porphyrin derivatives equipped with peripheral carbonitrile end groups confined on Cu(111). Using 3D-spectroscopic measurements with sub-angström precision, these chemical end-groups have been accurately identified as four reactive centers. By attaching the tip to one of them, a mechanical stress is applied until a directed motion of the whole molecule is induced. Depending on the selection of one of the CN end-groups, the molecule is either rotated clockwise or anticlockwise in a controlled way. The energy transferred between the molecule and the tip during this mechanically-induced manipulation, which is closely related to its diffusion energy, are directly quantified.

O 78.7 Thu 17:30 A 053

Controlled rotation of single molecules and sub-angstöm determination of intrinsic molecular elasticity — •Rémy Pawlak[1], Sweetlana Fremy[1], Shigeki Kawai[1], Thilo Glatzel[1], Hongjuan Fang[2], Lesli-Anne Fendt[2], François Diederich[2], and Ernst Meyer[1] — [1]Departement of Physics, University of Basel, Switzerland — [2]Laboratorium für Organische Chemie, ETH Zürich, Switzerland

Directed molecular repositioning is a key step towards the built-up of molecular machines. To artificially generate and control motion on a surface, molecules are generally excited by an exchange of light, chemical or electrical energy. Although the elasticity of molecular structures plays a role in all diffusion processes, such intrinsic properties are rather poorly known. Here, we explore by scanning probe microscopy directed manipulations of single porphyrin derivatives equipped with peripheral carbonitrile end groups confined on Cu(111). Using 3D-spectroscopic measurements with sub-angström precision, these chemical end-groups have been accurately identified as four reactive centers. By attaching the tip to one of them, a mechanical stress is applied until a directed motion of the whole molecule is induced. Depending on the selection of one of the CN end-groups, the molecule is either rotated clockwise or anticlockwise in a controlled way. The energy transferred between the molecule and the tip during this mechanically-induced manipulation, which is closely related to its diffusion energy, are directly quantified.

O 79: Experimental methods

Time: Thursday 16:00–17:45 Location: A 060

O 79.1 Thu 16:00 A 060

Scanning tunneling potentiometry on the Au/Ge(001) surface — •Christian A. Bobisch[1], Mark R. Kaspers[1], Alexander M. Bernhart[1], Mateusz Wojtaszek[2], Franciszek Krok[2], Marek Szymonski[2], and Rolf Möller[1] — [1]Faculty of Physics, Center for Nanointegration Duisburg-Essen, University of Duisburg-Essen, 47048 Duisburg, Germany — [2]Department of Physics of Nanostructures and Nanotechnology, Jagiellonian University, 30-059 Krakow, Poland

Recently many studies focus on self organized Au atom wires on the Ge(001) surface. This surface offers the unique opportunity to study a Tomonoga-Luttinger liquid, i.e. a one dimensional electronic system [1,2]. In order to study electron transport through such a surface, the coupling of the metallic leads to the surface is a crucial parameter. We use a multiprobe scanning tunneling microscope (STM) to analyze the lateral variation of the electrochemical potential caused by a current parallel to the surface induced by two tips. In the scheme of scanning tunneling potentiometry a third STM tip measures the topography and the electrochemical potential μ_{ec} of the surface simultaneously [3]. The excess amount of Au deposited onto the Ge(001) surface condenses into crystalline islands. However, our potentiometry data reveal a discontinuity of μ_{ec} at the edges of these islands. This indicates that the islands do not couple to the electronic system of the Au reconstructed Ge(001) surface.

[1] Phys. Rev. Lett. 101, 236802 (2008). [2] Nat. Phys. 7, 776, (2011). [3] Nano Lett. 9, 1588 (2009).

O 79.2 Thu 16:15 A 060

Quantitative investigation and optimization of porous anodic alumina for surface nanostructuring beyond existing limitations — •Stefan Ostendorp[1], Jörn Leuthold[1], Yong Lei[1,2], and Gerhard Wilde[1] — [1]Institut für Materialphysik, WWU Münster — [2]Institut für Physik & IMN (ZIK) MacroNano, TU Ilmenau

Porous anodic alumina (PAA) is a versatile and cost-efficient template material for various applications in surface nano-structuring. As porous anodic alumina membranes (PAAMs), it can be used for arrays of 1-dimensional nano-structures. Arrays of nano particles can be fabricated by ultra-thin alumina membranes (UTAMs). Thereby this PAA based nano-structuring techniques allow to modify structural parameters of fabricated nano-structures such as size, shape and spacing of nano-particles as well as diameter and length of wires or tubes. The outstanding ability of creating large scale arrays of hexagonally arranged nano-structures makes this technique interesting for different fields from fundamental physical studies to applications in optics or electronics. But actually the range of fabrication conditions resulting in regular PAA was rather limited so far. Here we present our recent progress extending these limitations. By detailed studies of the formed porous structures and by applying a newly developed method for quantifying their regularity we were able to tune the fabrication conditions and realize regular PAA with structural parameters beyond the known limitations. Furthermore, we present a novel fabrication technique to realize regular UTAMs for nano-structuring purposes within the newly extended range of accessible structural parameters.

O 79.3 Thu 16:30 A 060

Development of a stress measurement for pulsed laser deposition of BaTiO$_3$ — •Jörg Premper, Dirk Sander, and Jürgen Kirschner — Max-Planck-Institut für Mikrostrukturphysik, Weinberg 2, D-06120 Halle

The structural analysis of BaTiO$_3$ monolayers on Fe(001) reveals unexpected structural relaxations near the interface and a minimum thickness for polarisation was deduced from theory to be 2 unit cells [1]. Structural relaxation and onset of polarization are expected to induce characteristic signatures of both interface and film stress of this system. To measure these stresses, we set up an optical 2-beam crystal curvature measurement, which allows stress measurements during pulsed laser deposition of BaTiO$_3$. We use a scanning mirror for the homogeneous ablation of the BaTiO$_3$ target to avoid a rotary UHV-feedthrough of a rotating target. First results on the stress measurements during PLD of BaTiO$_3$ are presented, which indicate the feasibility of reliable stress measurements. This is a comforting result in view of the plasma bloom of the ablation process hitting the thin crystal, where one might have expected a detrimental disturbance on the optical curvature measurement.

[1] H.L. Meyerheim, F. Klimenta, A. Ernst, K. Mohseni, S. Ostanin, M. Fechner, S. Parihar, I.V. Maznichenko, I. Mertig and J Kirschner: Phys. Rev. Lett. **106** (2011), 087203

O 79.4 Thu 16:45 A 060

Time-resolved Nanojoule Adsorption Calorimetry — •Ole Lytken[1], Hans-Peter Steinrück[1], Hans-Jörg Drescher[2], and J. Michael Gottfried[2] — [1]Universität Erlangen-Nürnberg — [2]Universität Marburg

In a typical nanojoule adsorption calorimeter, the average heat of adsorption of a small pulse of molecules is measured as a temperature change in a thin single-crystal sample. The temperature change is often measured using a pyroelectric polymer pressed gently against the backside of the sample. For calibration of the calorimeter, a laser beam with known intensity is used to deposit a known amount of heat in the sample. This calibration works well when the reaction studied is fast. If, however, the initial fast adsorption is followed by a slower secondary reaction, such as a slow desorption, dissociation or segregation into the sample, the shape of the measured signal and the calibration signal start to deviate. Here we will present a method to analyze calorimeter signals which include such slow reactions and extract information, not only of the total amount of heat deposited in a given pulse, but also kinetic information about the slow reaction.

O 79.5 Thu 17:00 A 060

Characterisation and compression of pJ white-light continuum pulses — •Daniel Wegkamp[1], Simon Wall[1], Daniele Brida[2], Stefano Bonora[2], Giulio Cerullo[2], Julia Stähler[1], and Martin Wolf[1] — [1]Fritz-Haber-Institute of the MPG, Dep. of Physical Chemistry, Berlin, Germany — [2]Politecnico di Milano, Dipartimento di Fisica, Milan, Italy

Pump-probe-spectroscopy using ultrashort laser pulses allows access to the temporal evolution of electron and lattice dynamics. Probing the system in spectral regions that differ from the pump wavelength can give additional insights into those dynamics. White-light continuum pulses enable probing of wide spectral regions without the need of tuning the light source and their bandwidth enables the generation of ultrashort pulses for pump-probe experiments. Compression of the white-light pulses allows us to measure spectrally resolved as well as integrated *without* the loss of temporal resolution and, furthermore, the pulses may be incorporated in *nonlinear* optical probing schemes. White-light pulses are generated by self-phase modulation due to focusing of 40 fs laser pulses (800nm, 300 kHz Ti:Sa amplifier system) into a YAG crystal. To compress the pulses we measure the wavelength-dependent group delay in a simple pump-probe-setup. On this basis, we compensate for the phase of the laser pulse by adapting a deformable mirror, which is placed in the fourier-plane of a 4-f-compressor. Near transform-limited pulses of about 10 fs duration are achieved. These are applied to measure the ultrafast dynamics of VO$_2$ below and above the threshold for the photoinduced phase transition.

O 79.6 Thu 17:15 A 060

Optimizing the sensitivity of energy-selective photon detectors for use in inverse photoemission: VUV-transmission properties of CaF$_2$ windows — •Christian Thiede, Karen Zumbrägel, Matthias Rüter, Anke B. Schmidt, and Markus Donath — Westfälische Wilhelms-Universität, Münster, Nordrhein-Westfalen

Band-pass photon detectors are widely used in inverse-photoemission experiments performed in the isochromat mode. In Geiger-Müller counters, the band-pass behavior is realized by combining the photoionization threshold of a suitable counting gas (high pass) with the transmission characteristics of an alkaline earth fluoride window (low pass). Since inverse photoemission generally suffers from a low photon yield, an optimized detector efficiency is crucial for this technique.

One of the critical parameters is the transmission characteristics of the entrance window. We present transmission measurements for CaF$_2$ windows in the vacuum-ultraviolet spectral range in the vicinity of the transmission cutoff as a function of crystal purity as well as surface finish, adsorbate coverage, thickness, and temperature. Our findings reveal that the sensitivity of the photon counter depends critically on these window parameters.

O 79.7 Thu 17:30 A 060

Nanojoule Adsorption Calorimetry — •Hans-Jörg Drescher[1,2], Han Zhou[1], Ole Lytken[2], Hans-Peter Steinrück[2], and J. Michael Gottfried[1] — [1]Philipps-Universität Marburg — [2]Friedrich-Alexander-Universität Erlangen-Nürnberg

Nanojoule Adsorption Calorimetry (NAC) is a modern technique for measuring adsorption enthalpies of molecules or atoms on well-defined substrates, such as thin metal or oxide single crystals and organic thin films. Similar to previous adsorption calorimeters by Černy, King and Campbell, NAC relies on the direct measurement of tiny temperature changes induced by adsorption utilizing pyroelectric detectors. Thus, its scope extends beyond that of conventional methods such as temperature-programmed desorption (TPD), which require reversible adsorption and cannot be used if thermal decomposition occurs at a lower temperature than desorption. The apparatus is optimized for investigating well-defined metal-organic interfaces, which are models for interfaces in organic electronic devices. Specifically, this contribution covers the design considerations arising from constructing and optimizing a calorimetry apparatus with outstanding sensitivity and accuracy in the nanojoule and picomole regimes as well as first proof of concept measurements. These basic studies aim at interfaces between low-work function metals and π-conjugated semiconducting polymers playing an important role in the above-mentioned devices.
Support by the A. v. Humboldt Foundation, the DAAD, the Graduate School Molecular Science Erlangen-Nürnberg and the Universitätsbund Erlangen-Nürnberg e.V. is gratefully acknowledged.

O 80: General meeting of the Surface Science Division

Time: Thursday 19:30–20:00 Location: HE 101

O 81: Post deadline session

Time: Thursday 20:00–21:00 Location: HE 101

Some contributed talks.

O 82: Invited talk (Willi Auwärter)

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

Invited Talk O 82.1 Fri 9:30 HE 101

Nanochemistry with functional molecules - a 2D perspective — •Willi Auwärter — Physik Department E20, Technische Universität München, James-Franck Str. 1, D-85748 Garching, Germany

The comprehensive characterization and engineering of low-dimensional nanostructures on surfaces is of significant current interest, both from a scientific and technological point of view. Specifically, the fabrication of molecular nano-architectures on metal surfaces, applying self-assembly protocols inspired from supramolecular chemistry, is a maturing and rapidly advancing field of research. We will put particular emphasis on recent results elaborated with porphyrins. Given their intriguing variety of functional properties, which are exploited in both biological and artificial systems, porphyrins are ideally suited as building blocks for surface-confined nanostructures. Moreover, they represent model systems to explore surface coordination chemistry. Scanning tunneling microscopy (STM) and spectroscopy (STS) allows the inspection of the interior of these molecules and their electronic characteristics. Supported with complementary theoretical modeling and space-averaging techniques we address key questions related to their functionality: How does the molecular conformation respond to surface anchoring and how do specific groups guide the self-assembly? What determines the response of adsorbed metalloporphyrins towards small gas molecules? Can we achieve and control conductance switches or molecular rotors?

O 83: [TT] Transport: Graphene 2 (jointly with MA, HL, DY, DS, O)

Time: Friday 9:30–12:45 Location: BH 334

O 83.1 Fri 9:30 BH 334

Transport study of graphene with artificially induced defects — •Verena Martin, Johannes Jobst, Michael Krieger, and Heiko B. Weber — Lehrstuhl für Angewandte Physik, Universität Erlangen-Nürnberg, Staudtstr. 7, 91058 Erlangen

We report on transport properties of ion irradiated graphene which is grown epitaxially on 6H semi-insulating silicon carbide (SiC) substrate. We investigate both monolayer graphene [1] and quasi-free standing epitaxial graphene [2]. Subsequent irradiation steps of argon and carbon ions with different ion energies into the graphene/SiC stack are performed at low temperature (4K) and room temperature. The resistivity of the graphene layer is monitored in situ. After each irradiation step temperature dependent measurements and magnetoresistance measurements are performed to study the effect of the damage. An increase of resistivity with decreasing temperature as well as a broadening of the weak localization peak could be correlated to an increase of the defect amount.
[1] K. Emtsev et al., Nat. Mater. **8**, 203 (2009)
[2] C. Riedl et al., Phys. Rev. Lett. **103**, 246804 (2009)

O 83.2 Fri 9:45 BH 334

Inelastic Raman scattering on electronic excitations in graphene and carbon nanotubes — •Oleksiy Kashuba[1] and Vladimir Fal'ko[2] — [1]Institut für Theorie der statistischen Physik, RWTH Aachen, 52056 Aachen, Deutschland — [2]Department of Physics, Lancaster University, Lancaster, LA1 4YB, UK

Raman measurements in carbon allotropes are generally associated with the exploration of the vibrational modes. We present a theory of the non-resonant inelastic light scattering accompanied by the excitations of electron-hole pairs and predict the selection rules and polarization properties of the dominant Raman active modes. The prediction of the Raman plot profile for graphene at high magnetic field with pronounced peaks corresponding to the inter-Landau-level transitions [1,2] was confirmed by subsequent experiment [3]. We also provide a theory of Raman scattering on intersubband electron-hole pairs in large diameter carbon nanotubes predicting dominant polarisations and Raman spectra featuring a pattern of van Hove singularities [4].
[1] O. Kashuba and V. I. Fal'ko, Phys. Rev. B 80, 241404(R) (2009).
[2] M. Mucha-Kruczyński, O. Kashuba, and V. I. Fal'ko, Phys. Rev. B 82, 045405 (2010).
[3] C. Faugeras et. al., Phys. Rev. Lett. 107, 036807 (2011).
[4] O. Kashuba and V. I. Fal'ko, submitted to PRL (2011), arXiv:1111.1413

O 83.3 Fri 10:00 BH 334

Transport in clean side-gated graphene nanoribbons —

•Bernat Terrés[1,2], Jan Dauber[1,2], Uwe Wichmann[1], Stefan Trellenkamp[2], and Christoph Stampfer[1,2] — [1]JARA-FIT and II. Institute of Physics B, RWTH Aachen, 52074 Aachen, Germany — [2]Peter Grünberg Institut (PGI-8/9), Forschungszentrum Jülich, 52425 Jülich, Germany

Graphene is a two dimensional form of crystalline carbon with unique electrical properties. However, due to its gap-less nature it is hardly possible to implement concepts of state-of-the-art electronic devices. Recently, it has been shown that by tailoring graphene into narrow ribbons an effective band gap can be induced. Extensive studies have been reported on the transport mechanism in graphene nanoribbons and although being successfully demonstrated as tunneling barriers in quantum dots, graphene nanoribbons show a Coulomb blockade dominated transport behavior. In this work we report on the effects of a symmetrically applied side gate voltage on clean (hydrofluoric acid treated) graphene nanoribbons. In particular we show low-temperature experiments where the overall conductance can be tuned up to a level of about $8e^2/h$. Measurements show evidence that the local resonances in the transport gap can be strongly suppressed by adjusting the side-gate voltages. In summary, the high conductance values together with the observation of onsets of quantized conductance plateaus at integer multiples of $2e^2/h$ indicates that the disorder potential can be dramatically reduced, even though the transport mechanism is still mainly dominated by substrate and rough-edge induced disorder.

O 83.4 Fri 10:15 BH 334

Coulomb drag in graphene: perturbation theory — •Boris Narozhny[1], Michael Titov[2,3], Igor Gornyi[3,4], and Pavel Ostrovsky[3,5] — [1]Institut für Theorie der Kondensierten Materie, Karlsruher Institut für Technologie, 76128 Karlsruhe, Germany — [2]School of Engineering and Physical Sciences, Heriot-Watt University, Edinburgh EH14 4AS, UK — [3]Institut für Nanotechnologie, Karlsruher Institut für Technologie, 76021 Karlsruhe, Germany — [4]A.F. Ioffe Physico-Technical Institute, 194021 St. Petersburg, Russia — [5]L.D. Landau Institute for Theoretical Physics RAS, 119334 Moscow, Russia

We study the effect of Coulomb drag between two closely positioned graphene monolayers. In the limit of weak electron-electron interaction and small inter-layer spacing d ($\mu_{1(2)}, T \ll v/d$) the drag is described by a universal function of the chemical potentials of the layers $\mu_{1(2)}$ measured in the units of temperature T. When both layers are tuned close to the Dirac point, then the drag coefficient is proportional to the product of the chemical potentials $\rho_D \propto \mu_1\mu_2$ (when any of the layers is precisely at the Dirac point, then the drag vanishes due to electron-hole symmetry). In the opposite limit of low temperature the drag is inversely proportional to both chemical potentials $\rho_D \propto T^2/(\mu_1\mu_2)$. In the mixed case where the chemical potentials of the two layers belong to the opposite limits $\mu_1 \ll T \ll \mu_2$ we find $\rho_D \propto \mu_1/\mu_2$. In the case of strongly doped graphene $\mu_{1(2)} \gg v/d \gg T$ the drag coefficient acquires additional dependence on d and we recover the usual Fermi-liquid result if the screening length is smaller than d.

O 83.5 Fri 10:30 BH 334

Dirac boundary condition at the reconstructed zigzag edge of graphene — Jan van Ostaa, Anton Akhmerov, Carlo Beenakker, and •Michael Wimmer — Instituut-Lorentz, Universiteit Leiden, The Netherlands

Edge reconstruction modifies the electronic properties of finite graphene samples. We formulate a low-energy theory of the reconstructed zigzag edge by deriving the modified boundary condition to the Dirac equation. If the unit cell size of the reconstructed edge is not a multiple of three with respect to the zigzag unit cell, valleys remain uncoupled and the edge reconstruction is accounted for by a single angular parameter ϑ. Dispersive edge states exist generically, unless $|\vartheta| = \pi/2$. We compute ϑ from a microscopic model for the "reczag" reconstruction (conversion of two hexagons into a pentagon-heptagon pair) and show that it can be measured via the local density of states. In a magnetic field there appear three distinct edge modes in the lowest Landau level, two of which are counterpropagating.

O 83.6 Fri 10:45 BH 334

Dielectric properties of graphene in the presence of spin-orbit interactions — •Andreas Scholz[1], John Schliemann[1], and Tobias Stauber[2] — [1]Institute for Theoretical Physics, University of Regensburg, 93040 Regensburg, Germany — [2]Departamento de Fisica de la Materia Condensada and Instituto Nicolas Cabrera, Universidad Autonoma de Madrid. E-28049 Madrid. Spain

We study the dielectric function of graphene in the presence of pseudo-Rashba and intrinsic spin-orbit interactions (SOI) for arbitrary frequency, wave vector, doping, and spin-orbit coupling (SOC) parameters. In the static limit, the asymptotic behavior of the screened potential due to charged and magnetic impurities is derived. Due to the existence of a sharp Fermi surface in doped graphene, the screened potential exhibits characteristic (Friedel) oscillations. These oscillations are absent in the undoped case. An analytical expression for the plasmon dispersion is derived from the long-wavelength limit of the dielectric function and afterwards compared to the numerical result. For finite SOC parameters we find the existence of several new plasmon modes. Several limiting cases, namely the case of pure Rashba or pure intrinsic SOC, the case of equally large Rasbha and intrinsic coupling and of zero SOC are opposed.

15 min. break.

O 83.7 Fri 11:15 BH 334

Monolithic Epitaxial Graphene Electronics — •Stefan Hertel[1], Daniel Waldmann[1], Johannes Jobst[1], Sergey Reshanov[2], Adolf Schöner[2], Michael Krieger[1], and Heiko B. Weber[1] — [1]Chair of Applied Physics, Erlangen, Germany — [2]ACREO AB, Kista, Sweden

We developed a scheme to fabricate transistors with high switching performance by employing the whole system epitaxial graphene consisting of the graphene itself, but also include the semiconducting silicon carbide substrate and their common interface.

We used n-type SiC as conducting channel and tailored two different interfaces to the graphene: (a) monolayer epitaxial graphene [1] to provide ohmic contacts and (b) quasi-freestanding bilayer graphene [2](as achieved by hydrogen intercalation of MLG) to get Schottky-like contacts. We developed a method to produce both species side-by-side on the same chip. The resulting transistor works similar to a MeSFET with graphene as source and drain material but also as gate metal. In principal one single lithography step is sufficient to fabricate a transistor.

We demonstrate an epitaxial graphene transistor with on/off ratios exceeding 4 orders of magnitude at room temperature which can operate in both normally-on and normally-off operation mode, adjustable using a parametric backgate voltage. No damping was observed up to MHz frequencies.

[1] Emtsev et al., Nature Material **8**, 203-207 (2009).
[2] Speck et al., Applied Physics Letters **99**, 122106 (2011).

O 83.8 Fri 11:30 BH 334

Field Effect Superconductivity in Multigraphene — •Ana Ballestar[1], Srujana Dusari[1], Jose Barzola-Quiquia[1], Pablo Esquinazi[1], Robson da Silva[2], and Yakov Kopelevich[2] — [1]Division of Superconductivity and Magnetism, Institut für Experimentelle Physik II, Universität Leipzig, Linnéstraße 5, D-04103 Leipzig, Germany — [2]Instituto de Fisica, Unicamp, 13083-970 Campinas, Sao Paulo, Brasil

We have studied the temperature and magnetic field dependence of the electrical resistivity of mesoscopic tens of nanometers thick multigraphene samples as a function of bias voltage applied perpendicular to the graphene planes. We found that the resistivity changes asymmetrically with the bias voltage. For large and negative bias voltages the resistivity shows non-percolative superconducting-like transitions at $T \sim 15 \ldots 20$ K . The transition can be suppressed at high enough magnetic fields applied normal or parallel to the main plain of the samples. We discuss the obtained results in terms of electric field induced superconductivity at localized near surface regions of the graphite sample.

O 83.9 Fri 11:45 BH 334

Graph theory meets ab-initio molecular dynamics: atomic structures and transformations at the nanoscale — •Fabio Pietrucci[1] and Wanda Andreoni[1,2] — [1]CECAM - EPFL Lausanne, Switzerland — [2]Institute of Theoretical Physics - EPFL Lausanne, Switzerland

We introduce a set of Social PeRmutation INvarianT (SPRINT) coordinates which describe the topology of the network of bonds among atoms [1]. These coordinates are obtained from the contact matrix, they are invariant under permutation of identical atoms, and provide a clear signature of the transition between ordered and disordered structures. In combination with first-principles molecular dynamics and metadynamics, the topological coordinates are employed to explore low-energy structures of silicon clusters and organic molecules, demonstrating the possibility of automatically simulating isomerization, association, and decomposition reactions without prior knowledge of the products or mechanisms involved.

Finally we discuss the application of this new approach to the simulation of carbon nanostructures: we obtain transformation pathways for the reconstruction of zig-zag edges of graphene ribbons to 5-7 rings, as well as the folding of graphene into fullerene-like cages. Our results show that it is now feasible the blind exploration of complex structural rearrangements of nanostructures at finite temperature and at density-functional theory level of accuracy.

[1] F. Pietrucci and W. Andreoni, Phys. Rev. Lett. 107 (2011) 085504.

O 83.10 Fri 12:00 BH 334

Localization behavior of Dirac particles in disordered graphene superlattices — Qifang Zhao[1], Jiangbin Gong[1], and •Cord Müller[2] — [1]Department of Physics and Centre for Computational Science and Engineering, National University of Singapore — [2]Centre for Quantum Technologies, National University of Singapore

Graphene superlattices (GSLs) can be used to engineer band structures and, from there, charge transport properties, but these are sensitive to the presence of disorder. We study the localization behavior of massless 2D Dirac particles induced by weak disorder for both scalar-potential and vector-potential GSLs. By an analytical weak-disorder expansion, we investigate how the localization length depends on the incidence angle to a 1D GSL. Delocalization resonances are found for both scalar and vector GSLs. The sharp angular dependence of the Lyapunov exponent may be exploited to realize disorder-induced filtering devices [1].

[1] Q. Zhao, J. Gong, and C. A. Müller, `arXiv:1111.3436`

O 83.11 Fri 12:15 BH 334

Thermal Transport in Graphene: a Large-scale Molecular Dynamics Study — •Luiz Felipe C Pereira and Davide Donadio — Max Planck Insitute for Polymer Research, Mainz, Germany.

Carbon-based materials show exceptional thermal properties. The thermal conductivity of carbon allotropes can range five orders of magnitude. In the bulk, amorphous carbon is a very poor heat conductor, with $\kappa \approx 0.01$ W/m/K, whereas diamond has the highest thermal conductivity among elemental solids, $\kappa \approx 2000$ W/m/K at room temperature. Carbon nanostructures extend the range even further. Thermal conductivities as large as 5000 W/m/K have been measured for suspended graphene and carbon nanotubes. Nonetheless, there is still much controversy over the thermal transport properties of graphene, both experimentally and theoretically. We have performed extensive equilibrium and non-equilibrium molecular dynamics simulations aimed at understanding the mechanism of heat transport in graphene. In order to address the influence of system size on the simulation results, an aspect frequently overlooked in similar computational studies, we perform large scale molecular dynamics simulations of micrometer-size models containing more than 10^6 atoms. Furthermore, we investigate the influence of uniaxial strain on the thermal conductivity of graphene, and show that the resulting strain-induced anysotropy has a profound influence on its thermal conductivity.

O 83.12 Fri 12:30 BH 334

Effect of short-range interactions on the phase diagram of graphene — •David Mesterhazy[1], Jürgen Berges[1], and Lorenz von Smekal[2] — [1]Institut für Theoretische Physik, Universität Heidelberg — [2]Institut für Kernphysik, Technische Universität Darmstadt

We study low-energy theories of suspended monolayer graphene at the charge neutral point by means of functional renormalization group methods. In particular, the role of residual short-range interactions for the expected chiral phase transition is investigated. The resulting effective low-energy description can provide a firm basis for a study of the universal properties of the quantum phase transition. Furthermore, first results for the phase diagram at finite temperature are presented.

O 84: Focussed session: Frontiers of electronic structure theory: Strong correlations from first principles VI (jointly with TT)

Time: Friday 10:30–13:00 Location: HE 101

Topical Talk O 84.1 Fri 10:30 HE 101

Dynamically screened Coulomb interaction and GW self-energy in transition metal compounds — •Takashi Miyake — AIST, Tsukuba, Japan

We present a procedure for constructing low-energy models from first-principles using the GW-RPA and Wannier function technique. The procedure starts with dividing the Hilbert space into two subspaces: the low-energy part (d space) and the rest of the space (r space). The low-energy model is constructed for the d space by eliminating the degrees of freedom of the r space. The effective electron interaction of the model is expressed by a partially screened Coulomb interaction which is calculated in the constrained random-phase-approximation (cRPA), where screening channels within the d space are subtracted. As an illustration, the procedure is applied to 3d transition metals, 3d perovskite oxides, and iron-based superconductors. It is found that strength of electron correlation is strongly material dependent. Self-energy effects in quasiparticle bandstructure are analyzed using the GW approximation, which is the lowest-order expansion in the screened Coulomb interaction. Effects of dynamic screening and non-local self-energy (in the Wannier basis) are discussed.

O 84.2 Fri 11:00 HE 101

The Electronic Structure of CuO: Quasiparticles and Satellites — •Claudia Rödl, Francesco Sottile, and Lucia Reining — Laboratoire des Solides Irradiés, Ecole Polytechnique, CNRS, CEA-DSM, 91128 Palaiseau, France and European Theoretical Spectroscopy Facility (ETSF)

The insulating transition-metal oxide CuO is considered a key to understanding the electronic structure of high-temperature superconducting cuprates, since it features similar bonding geometries. The photoemission spectra of this oxide, which is usually termed to be strongly correlated, have not been explained satisfactorily by first-principles calculations up to now. Special difficulties arise from the close entanglement of the structural and electronic degrees of freedom in this compound, which is due to the unoccupied Cu $3d$ orbitals.

In contrast to the local-density approximation of density-functional theory (DFT), which predicts CuO to be a metal, we obtain finite band gaps by means of hybrid functionals containing screened exchange and the DFT+U method. Starting from these qualitatively correct band structures, we perform many-body calculations in the GW approximation. The various approaches to the one-particle excitation spectra are compared to experimental results. We discuss whether or not the peaks occurring in the photoemission data are quasiparticle excitations or satellite structures, respectively.

O 84.3 Fri 11:15 HE 101

Ab-initio description of satellites in graphite — •Matteo Guzzo[1], Lorenzo Sponza[1], Christine Giorgetti[1], Francesco Sottile[1], Debora Pierucci[2], Mathieu G. Silly[2], Fausto Sirotti[2], Joshua J. Kas[3], John J. Rehr[3], and Lucia Reining[1] — [1]Ecole Polytechnique, Palaiseau, FR — [2]Synchrotron SOLEIL, Gif-sur-Yvette, FR — [3]U. Washington, Seattle, USA

The GW method 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. We have recently shown that including additional diagrams in the Green's function (similarly to what has been done with the cumulant expansion) we obtain an excellent description of satellites series in the test case of bulk silicon [1], where GW is unable to cope. We now focus on a more complex system, i.e. graphite, with this same approach. 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 a single graphene layer. **Refs:** [1] M. Guzzo *et al.*, Phys. Rev. Lett. 107, 166401 (2011)

O 84.4 Fri 11:30 HE 101

Internal elasticity of graphene-based systems — •Pasquale Pavone[1,2], Rostam Golesorkhtabar[1,2], Jürgen Spitaler[1,2], and Claudia Ambrosch-Draxl[1] — [1]Chair of Atomistic Modelling and Design of Materials, University of Leoben, Austria — [2]Materials Center Leoben Forschung Gmbh, Leoben, Austria

When a crystal undergoes a strain deformation, the lower symmetry of the deformed structure may allow for internal relaxations of atomic positions which do not follow the macroscopic applied strain. These relaxations can be described introducing the concept of internal-strain tensor [1], which relates the local deformation to the macroscopic strain. In this work, we present a first-principles calculation of the linear and non linear internal-strain tensors for a monolayer graphene as well as for hexagonal graphite. In order to analyze the relevance of the internal relaxation for hexagonal structures, results are also compared with *ab-initio* data for the cubic diamond phase. Calculations are performed using the pseudo-potential density-functional-theory code Quantum ESPRESSO [2] and both the local-density and generalized-gradient approximations for the exchange-correlation energy. The accuracy of the result of this investigation allows to solve some open issues arising in the literature from previous model [3] as well as *ab-initio* [4] calculations.

[1] C.S.G. Cousins, J. Phys.: Condens. Matter **14**, 5091 (2002)
[2] P. Giannozzi *et al.*, J. Phys. Condens. Matter **21**, 395502 (2009)
[3] C.S.G. Cousins and M.I. Heggie, Phys. Rev. B **67**, 024109 (2003)
[4] R. Wang *et al.*, Physica B: Condens. Matter **405**, 3501 (2010)

O 84.5 Fri 11:45 HE 101

Accounting for dynamical screening in optical absorption spectra — •Lorenzo Sponza[1,2], Matteo Guzzo[1,2], Christine Giorgetti[1,2], and Lucia Reining[1,2] — [1]LSI-Ecole Polytechnique, Palaiseau, France — [2]ETSF : European Theoretical Spectroscopy Facility

In optics, absorption spectra are computed via the evaluation of the two particle correlation function L of the material which is given by the differentiation of the single particle Green-s function G_1 with respect to an external (perturbing) potential U. State of the art calculations of optical absorption spectra rely on the Bethe-Salpeter Equation (BSE) and they make use of static screening W. Though, the inclusion of dynamical effects at a BSE level is a subject of both theoretical and technological interest. As an example, in some photovoltaic cells multiple-exciton generation (MEG)[2] has been proposed to improve drastically the efficiency of the device but to describe absorption in the presence of MEG one has to account for the dynamical screening.

Recently G_1 has been derived as exact solution of a differential functional equation which allows the excplicit treatment of $W(\omega)$ [1]. Inspired by this work, we extended its strategy to the case of absorption, that is to the computation of L. We found a non-linear integro-differential equation that can be solved through some careful approximation. In this work we present an analysis of the solution of the problem and a comparison with standard Bethe-Salpeter approach.

[1] M.Guzzo *et al.*, Phys. Rev. Lett. **107**, 166401 (2011) [2] for MEG see for example Kheifets *et al.*, Phys. Rev. B **68**, 233205 (2003)

O 84.6 Fri 12:00 HE 101

Quasiparticle Spectra from Self-Consistent GW Calculations for Transition-Metal Monoxides — •Merzuk Kaltak and Georg Kresse — Computational Materials Physics University of 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 scGW 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 $\epsilon(\omega)$ is calculated.

O 84.7 Fri 12:15 HE 101

Unified description of ground and excited states of finite systems: the self-consistent *GW* approach — •Fabio Caruso[1], Patrick Rinke[1], Xinguo Ren[1], Angel Rubio[1,2], and Matthias Scheffler[1] — [1]Fritz-Haber-Institut, Berlin, Germany — [2]Universidad del Pais Vasco, San Sebastian, Spain

Fully self-consistent *GW* calculations – based on the iterative solution of the Dyson equation – provide an approach for consistently describing ground and excited states on the same quantum mechanical level. Based on our implementation in the all-electron localized basis code FHI-aims [1], we show that for finite systems self-consistent *GW* reaches the same final Green function regardless of the starting point. The results show that self-consistency systematically improves ionization energies and total energies of closed shell systems compared to perturbative *GW* calculations (G_0W_0) based on Hartree-Fock or (semi)local density-functional theory. These improvements also translate to the electron density as demonstrated by a better description of the dipole moments of hetero-atomic dimers and the similarity with the coupled cluster singles doubles (CCSD) density. The starting-point independence of the self-consistent Green function facilitates a systematic and unbiased assessment of the performance of the *GW* approximation for finite systems. It therefore constitutes an unambiguous reference for the future development of vertex corrections and beyond *GW* schemes.

[1] V. Blum *et al.*, Comp. Phys. Comm. **180**, 2175 (2009).

Topical Talk O 84.8 Fri 12:30 HE 101

Density-functional theory - time to move on? — •Nicola Marzari — Theory and Simulations of Materials, École Polytechnique Fédérale de Lausanne

Density-functional theory can be a very powerful tool for scientific discovery and technological advancement. Still, it remains an imperfect tool, with open and urgent challenges in our quest towards qualitative and quantitative accuracy, and in our ability to perform quantum simulations under realistic conditions.

Several of these challenges stem from the remnants of self-interaction in our electronic-structure framework, leading to qualitative failures in describing some of the fundamental processes involved in energy applications - from charge-transfer excitations to photoemission spectra, to the structure and reactivity of transition-metal complexes.

I'll discuss these challenges in realistic case studies, and our suggestions for possible solutions - including constrained DFT, DFT + onsite and intersite Hubbard terms, and Koopmans' compliant energy functionals. In particular, I'll discuss how self-interaction corrected functionals lead naturally to a beyond-DFT formulation where both total energies and spectroscopic properties can be accounted for.

O 85: Plasmonics and nanooptics V

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

O 85.1 Fri 10:30 MA 005

Spectral near and far field characteristics of single plasmonic nanoantennas in the infrared — •F. Neubrech[1], P. Alonso Gonzalez[2], P. Albella[3], C. Huck[1], F. Casanova[2], L. E. Hueso[2], J. Chen[2], F. Golmar[2], A. Pucci[1], J. Aizpurua[3], and R. Hillenbrand[2] — [1]Kirchhoff-Institut für Physik, Heidelberg, Germany — [2]CIC nanoGUNE Consolider, San Sebastian, Spain — [3]Center for Materials Physics, San Sebastian, Spain

The optical properties of metal nanoparticles are dominated by plasmonic resonances, which cause a huge field enhancement in the vicinity of the nanoparticles. Such huge near-field enhancements can be exploited for SEIRA or SERS. In both techniques one pre-condition is a good match between the vibrational excitation and the plasmonic one. Instead of near-field characteristics, far-field quantities are used to characterize the tuning, since they are easier to obtain experimentally. However, the use of far-field quantities will present several problems, since there is a shift between the near and far-field peak energies. In order to demonstrate this effect experimentally we carried out microscopic infrared spectroscopy fot the far-field optical, which enables us to record far-field spectra of single antennas. Using IR scattering near-field optical microscopy near-field intensities of the same antennas were recorded at a wavelength of 9.3 microns. Comparing the near and far-field response at the given wavelength for antennas with different lengths, we observed a significant shift of the near field peak intensity to lower energies, which is in perfect agreement with FDTD simulations.

O 85.2 Fri 10:45 MA 005

Local Enhancement of Optical Chirality in Planar and 3D Plasmonic Nanostructures — •Martin Schäferling, Mario Hentschel, Daniel Dregely, and Harald Giessen — 4th Physics Institute, Research Center SCoPE and Research Center SimTech, University of Stuttgart, Pfaffenwaldring 57, 70550 Stuttgart, Germany

Chirality – the absence of mirror symmetry – is an integral component of our world. The chirality of electromagnetic fields can be quantified by the so-called optical chirality [1]. Fields with high optical chirality can be utilized to enhance the sensitivity of enantiomer sensors [2]. Such fields can be generated by plasmonic nanostructures.

We numerically calculate and visualize the enhancement of optical chirality in the near-field of different planar and three-dimensional nanostructures. For practical applications not only the absolute values of the enhancement but also the shapes of the regions with enhanced optical chirality are important. Therefore, we present three-dimensional maps of the enhancement which allows a straightforward comparison of the different structures.

We show that planar structures can provide easy access to these chiral fields. As also the fabrication process is simple compared to three-dimensional structures, they are very well-suited for applications such as enantiomer sensing. Three-dimensional structures, on the other hand, allow higher enhancement of optical chirality.

[1] Y. Tang and A.E. Cohen, Phys. Rev. Lett. 104, 163901 (2010).
[2] E. Hendry et al., Nat. Nanotechnol. 5, 783 (2010).

O 85.3 Fri 11:00 MA 005

Three-dimensional chiral plasmonic oligomers — •Mario Hentschel[1,2], Martin Schäferling[1], Thomas Weiss[1], Hans-Georg Kuball[3], Na Liu[4], and Harald Giessen[1] — [1]4. Physikalisches Institut und Research Center SCoPE, Universität Stuttgart — [2]Max-Planck-Institut für Festkörperforschung, Stuttgart — [3]Fachbereich Chemie, Lehrstuhl für Physikalische Chemie, Universität Kaiserslautern — [4]Department of Electrical and Computer Engineering, Rice University

We demonstrate a chiral optical response in stacked arrangements of plasmonic nanostructures. They exhibit resonant plasmonic coupling between particles of similar size and dipole moment. Moreover, we demonstrate that such particle ensembles possess the capability to encode their three-dimensional arrangement in unique and well modulated spectra, making then ideal candidates for a three-dimensional chiral plasmonic ruler [1]. Our results are crucial for the future design and improvement of plasmonic chiral optical systems, e.g., for ultrasensitive enatiomer sensing on the single molecule level [2], for the design of chiral optical modulators and devices [3] as well as applications in medicine and drug development.

[1] Liu, N. et al., Science 332, 1407-1410 (2011).
[2] Hendry, E. et al., Nat. Nanotech. 5, 783-787 (2010).
[3] Gansel, J. K. et al., Science 325, 1513-1515 (2009).

O 85.4 Fri 11:15 MA 005

Simulation of Plasmonic Nanostructures using the Discontinuous Galerkin Time-Domain Method on Graphics Processing Units — •Richard Diehl[1], Jens Niegemann[2], and Kurt Busch[3] — [1]Institut für Theoretische Festkörperphysik and DFG-Center for Functional Nanostructures (CFN), Karlsruhe Institute of Technology (KIT), Wolfgang-Gaede-Straße 1, 76131 Karlsruhe, Germany — [2]IFH - Lab for Electromagnetic Fields and Microwave Electronics ETH Zürich, Gloriastrasse 35, 8092 Zürich, Switzerland — [3]Humboldt-Universität zu Berlin, Institut für Physik, AG Theoretische Optik, Newtonstr. 15, 12489 Berlin, and Max-Born-Institut, Max–Born–Str. 2A, 12489 Berlin, Germany

The discontinuous Galerkin time-domain (DGTD) method is a powerful method to explore the electromagnetic properties of nano-scale plasmonic and dielectric systems. Here, we present the method's advantages and disadvantages when implemented to run on graphic processing units (GPUs). The GPU's superior performance is demonstrated for a realistic split-ring resonator on membrane setup which is characterized by both, optical spectroscopy and electron energy loss spectroscopy. Compared to modern CPU hardware, GPU-based DGTD yields up to two orders of magnitude decreased computational time.

O 85.5 Fri 11:30 MA 005

Plasmon resonances in atomic-scale gaps — •Johannes Kern[1], Swen Grossmann[1], Tim Häckel[1], Nadezda Tarakina[2,3], Monika Emmerling[3], Martin Kamp[3], Jer-Shing Huang[4], Paolo Biagioni[5], Jord C. Prangsma[1], and Bert Hecht[1] — [1]Experimental Physics 5, University of Würzburg, Germany — [2]Experimental Physics 3, University of Würzburg, Germany — [3]Technical Physics, University of Würzburg, Germany — [4]Department of Chemistry, National Tsing Hua University, Taiwan — [5]Dipartimento di Fisica, Politecnico di Milano, Italy

We experimentally investigate the plasmon resonances of side-by-side aligned single-crystalline gold nanorod dimers. Robust gaps between the particles reaching well below 1 nm are obtained by reproducible self-assembly. For such atomic-scale gaps extreme splitting of the symmetric and anti-symmetric dimer eigenmodes is observed in white-light scattering experiments.

Besides providing evidence for atomic-scale gap modes at visible wavelengths with correspondingly small mode volumes, our experimental results can serve as a benchmark for electromagnetic modeling beyond local Maxwell theory.

O 85.6 Fri 11:45 MA 005

Quantum mechanic effects in nanoantenna enhanced infrared spectroscopy — •Jörg Bochterle, Frank Neubrech, and Annemarie Pucci — Kirchhoff-Institute for Phyiscs, Heidelberg, Germany

When light interacts with the conduction electrons of metal nanoparticles, the thereby resonantly excited localized surface plasmon resonance (LSPR) gives rise to a local field enhancement in the vicinity of the particles. Since the resonance frequency is governed by the geometrical shape of the particle, it can be tuned over a large spectral range. The strong fields are of great interest for sensing applications e.g. the detection of molecules by their vibrational fingerprint in the infrared. To measure the signal enhancement as a function of very small distances from the surface, we cooled a gold nanoantenna array on silicon substrate under ultra high vacuum conditions with liquid helium and adsorbed carbon monoxide (CO) gas. The enhanced signal of the CO stretching vibration is shown as a function of the layer thickness. Interestingly, the measurements differ from the classically expected behavior of a monotonically increasing near field towards the surface of the nanoparticle. However, describing the localized plasmon resonance quantum mechanically, the near field exhibits such monotonic increase only down to a certain distance and then decreases for smaller distances to the surface.

O 85.7 Fri 12:00 MA 005

Detecting low concentrations of pollutant chemicals in water by SERS:Combining optimised nanoparticle ensembles and SERDS — •R. Ossig[1], Y.-H. Kwon[2,3], H.D. Kronfeldt[2], and F. Hubenthal[1] — [1]Institut für Physik and CINSaT, Universität Kassel, Germany — [2]Technische Universität Berlin, Institut für Optik und Atomare Physik, Germany — [3]Institute of Lasers, Academy of Sciences, Unjong District, Pyongyang, DPR Korea

We present recently performed surface enhanced Raman spectroscopy (SERS) measurements using the combination of optimised silver nanoparticle (NP) ensembles and shifted excitation Raman difference spectroscopy (SERDS) to perform trace analysis of pollutant chemicals in water. The silver NPs were prepared under ultrahigh vacuum conditions on quartz substrates. The microsystem diode laser used is capable to generate two slightly different emission wavelengths ($\Delta\lambda \approx 0.5$ nm) with a spectral width of ≈ 10 pm, which is ideal for SERDS. To tune the surface plasmon resonance frequency of the NP ensembles in the vicinity of the excitation wavelength of the used diode laser, the morphology of the NPs was varied to obtain the optimal values for the investigated molecule-excitation wavelength combination. In this contribution we demonstrate, that optimising the optical properties of the silver NPs is essential for the detection of low pollutant concentrations. While for plasmon resonances in the vicinity of the excitation wavelength a low limit of detection in the order of 2 μm/l, is obtained, slightly off resonance NP ensembles yield a limit of detection that is at least 10 times higher.

O 85.8 Fri 12:15 MA 005

Plasmonic excitations in quasi 1d structures — •Ulrich Krieg, Christian Brand, Viktoria Meier, Herbert Pfnür, and Christoph Tegenkamp — Institut für Festkörperphysik, Leibniz Universität Hannover, Appelstrasse 2, D-30167 Hannover, Germany

A quasi one dimensional system was prepared by adsorption of 0.5 Ml Ag on vicinal Si (557) via self assembly. The morphology of these single domain wire like structures was characterised by spot profile analysis LEED (SPA-LEED), STM and subsequently studied by electron energy loss spectroscopy. For the latter an instrument with both high energy and momentum resolution was used (ELS-LEED). The measured loss spectra showed a strong anisotropy: In parallel direction the plasmonic loss dispersed linearly while in perpendicular direction the plasmonic loss does not disperse at all. This can be interpreted as an electronic decoupling and subsequently a confinement of the plasmon to the nanowires of finite width.

The quantitative simulation of the plasmonic losses in the low momentum regime is compatible with a wire width of 2.5 nm which agrees well with the width of the (111) terraces of Si (557). Indeed we found with SPA-LEED and STM the overall step-structure unchanged and the step-edges undecorated after the evaporation and annealing process. This confirms the model of a quantum well perpendicular to the nanowires used in our simulations.

O 85.9 Fri 12:30 MA 005

Radiative cooling of nanoparticles close to a surface — •Maria Tschikin and Svend-Age Biehs — Institut für Physik, Carl von Ossietzky Universität Oldenburg, D-26111 Oldenburg

In the present work we investigate the radiative cooling of a heated nanoparticle immersed in a thermal bath close to a partially reflecting surface. In the long-wavelength limit the particle can be considered as a simple dipole that radiates like an antenna. The radiated power of the dipole with a given temperature is then found within the framework of fluctuating electrodynamics. It turns out that the radiated power of the particle is not only proportional to its polarizability but also to the electric and magnetic local density of states. Hence, the radiated power which will determine the thermal relaxation time of the nanoparticle is very sensitive to its environment similar to the lifetime of an excited atom. Now, in our calculations we first introduce a thermal relaxation time τ and compare the results for a metallic and a polar nanoparticle. We demonstrate an oscillating behavior of τ with respect to the separation distance from the surface, an analog of Friedel oscillations in Fermi liquids. In addition it can be shown, that the cooling rate strongly depends not only on the temperature difference between particle and environment, but also on the absolute temperature of the environment.

O 85.10 Fri 12:45 MA 005

Spectral Shifts in Optical Nanoantenna-Enhanced Hydrogen Sensors — •Andreas Tittl[1], Christian Kremers[2], Jens Dorfmüller[1], Dmitry Chigrin[2], and Harald Giessen[1] — [1]4th Physics Institute and Research Center SCoPE, University of Stuttgart — [2]Institute of High-Frequency and Communication Technology, Faculty of Electrical, Information and Media Engineering, University of Wuppertal

We present numerical investigations on the nature of spectral shifts in antenna-enhanced hydrogen sensing geometries consisting of a single gold bowtie antenna situated next to a palladium nanodisk.

We performed extensive numerical FEM calculations and will show how previously published experimental results for this system[1] can be modeled and understood by considering two competing effects: a small spectral blueshift of the resonance caused by the change of the dielectric function from Pd to PdH and a substantial redshift caused by the expansion of the Pd lattice and in turn of the Pd nanodisk.

The insight we gain into the spectral behavior of this system enables us to accurately model antenna-enhanced hydrogen sensors. Furthermore, it allows a numerical characterization and optimization of such structures beyond half bowtie geometries and thus paves the way towards the realization of extremely sensitive plasmonic hydrogen sensors.

[1] Liu et al., Nat. Mater. **10**, 631-636 (2011)

O 86: Graphene VI

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

O 86.1 Fri 10:30 MA 041

Observation of an activation barrier in the interaction between graphene and a metal tip by using atomic force-microscopy and -spectroscopy — •Thomas Hofmann, Alfred J. Weymouth, Joachim Welker, and Franz J. Giessibl — University of Regensburg, Faculty of Experimental and Applied Physics, Universitätsstrasse 31, D-93053 Regensburg

For chemical bonding of adsorbed atoms onto graphene, the participating carbon atom has to change its hybridization state from sp$_2$ to sp$_3$. This rehybridization has been described for bonding of hydrogen on graphite, leading to an activation barrier [1]. We studied the interaction of a tungsten tip with monolayer graphene with a low temperature atomic force microscope. As the tip is approached to the surface, atomic contrast initially is obtained in a repulsive regime, i.e. the carbon atoms appear to repel the tip similar to measurements on pentacene [2]. Upon further reducing the distance, the image contrast flips and the carbon atoms attract the tip, as has been proposed by DFT calculations [3]. Force versus distance spectroscopy shows a pronounced barrier that has to be overcome before the carbon atoms appear attractive.

[1] L. Jeloaica, V. Sidis, Chem. Phys. Lett. 300, 157 (1999)
[2] L. Gross *et al.*, Science 325, 5944 (2009)
[3] M. Ondráĉek *et al.*, Phys. Rev. Lett. 106, 176101 (2011)

O 86.2 Fri 10:45 MA 041

Graphene studied with a multi-tip STM — •Stefan Korte, Vasily Cherepanov, and Bert Voigtländer — Peter Grünberg Institut (PGI-3), Forschungszentrum Jülich, 52425 Jülich, Germany, and JARA-Fundamentals of Future Information Technology

Graphene produced by exfoliation promises clean, defect free two-dimensional sheets. However, for conductance measurements, electrical contacts have to be created. This is usually done by lithography or other processing methods that might contaminate the graphene. With a multi tip STM unprocessed graphene flakes on SiO$_2$ have been contacted for local four point measurements with flexible probe placement and geometry. Four point conductance measurements and potentiometry on graphene will be presented.

O 86.3 Fri 11:00 MA 041

Micro Four-Point Probe Measurements of Graphene on Silicon Carbide — •Edward Perkins[1], Lucas Barreto[1], Felix Fromm[2], Christian Raidel[2], Thomas Seyller[2], and Philip Hofmann[1] — [1]Institut for Fysik og Astronomi, Aarhus Universitet, Ny Munkegade 120, Aarhus 8000C, Denmark — [2]Institut für Physik der Kondensierten Materie, Universität Erlangen-Nürnberg, Erwin-Rommel-Strasse 1, D-91058 Erlangen, Germany

Four-point probe measurements are the classic method for investigating conductivity independent of contact resistances. By implementing this technique at the micron scale, in ultra-high vacuum, clean, local measurement of the conductivity is possible. By varying the effective separation of the contact probes, discrimination between conduction through the bulk and the surface can be achieved.

Data from both monolayer graphene on silicon carbide and hydrogen-intercalated quasi-freestanding graphene will be presented. The transport is shown to be two-dimensional in character, and the measured conductivity is combined with photoemission data to extract the mobility.

O 86.4 Fri 11:15 MA 041

Time-Resolved Two-Photon Photoemission of Unoccupied Electronic States of Periodically Rippled Graphene on Ru(0001) — •Nico Armbrust, Jens Güdde, Peter Jakob, and Ulrich Höfer — Fachbereich Physik und Zentrum für Materialwissenschaften, Philipps-Universität, D-35032 Marburg

The well characterized graphene layers epitaxially grown on Ru(0001) have attracted a lot of interest up to now due to their periodically rippled structure caused by the strong interaction with the metal substrate. Here, the dynamics of unoccupied electronic states of graphene on Ru(0001) have been explored by time- and angle-resolved two-photon photoemission (2PPE). We identify a Ru derived resonance and a Ru/graphene interface state at 0.91 eV and 2.58 eV above the Fermi level, as well as three image-potential derived states close to the vacuum level. The most strongly bound, short lived and least dispersing image-potential state is suggested to have some quantum-well character with a large amplitude below the graphene hills. The two other image-potential states are attributed to a series of slightly decoupled states. Their lifetimes and dispersions are indicative of electrons moving almost freely above the valley areas of the moiré superstructure of graphene.

O 86.5 Fri 11:30 MA 041

Photoluminescence in graphene antidot lattices — Daniel Hutzler, •Stefanie Heydrich, Jonathan Eroms, Dieter Weiss, Tobias Korn, and Christian Schüller — Institut für Experimentelle und Angewandte Physik, Universität Regensburg

We present recent observations of the behavior of photoluminescence in patterned single and bilayer graphene. It was reported previously [1,2], that femtosecond pulsed laser excitation creates an electron-hole plasma in graphene which emits a broadband luminescence. We have observed this luminescence in graphene patterned with antidot lattices as well as in pristine graphene.

We utilize fast, high-resolution scans to map graphene flakes on Si/SiO2-substrates. Thus, a luminescence image of both the flake and its structured areas is created.

In structured areas, the absolute intensity of the photoluminescence is smaller than in pristine flakes due to parts of the graphene having been etched away. However, the observed signal in the patterned flakes is larger than expected from the mere amount of illuminated graphene. This enhancement is roughly 1/15 of the expected signal in single layer and 1/7 in bilayer graphene. It is possible that additional charge carriers at the antidot edges [3] cause this increase in luminescence.

Financial support by the DFG via GRK 1570 is gratefully acknowledged.

[1] R.J. Stöhr et al., Phys. Rev. B 82, 121408(R) (2010)

[2] C.H. Lui et al., Phys. Rev. Lett. 105, 127404 (2010)

[3] S. Heydrich et al., Appl. Phys. Lett. 97, 043113 (2010)

O 86.6 Fri 11:45 MA 041

Angle resolved Coulomb- and phonon-induced carrier dynamics in graphene — •Torben Winzer, Andreas Knorr, and Ermin Malic — Institut für Theoretische Physik, Nichtlineare Optik und Quantenelektronik, Technische Universität Berlin, 10623 Berlin, Germany

We investigate the relaxation dynamics of optically excited charge carriers in graphene within the density matrix formalism resolved in time, momentum, and angle. The focus lies on the interplay between carrier-carrier and carrier-phonon scattering channels immediately after an excitation, when the carrier system is highly anisotropic. We observe that Coulomb-scattering prefers processes of carriers with parallel momentum corresponding to a relaxation dynamics carried out directly toward the Dirac point. In contrast, the emission of phonons leads efficiently and quickly to an isotropic carrier distribution in the states one phonon energy beneath the exciting energy. Accordingly, for large scattering angles Coulomb- and phonon-induced relaxation dynamics complement each other, whereas in the case of narrow scattering angles there is a direct competition [1]. We demonstrate how the combination of all relaxation channels results in an ultrafast thermalization, followed by a slower energy dissipation.

[1] E. Malic, T. Winzer, E. Bobkin, and A. Knorr, Phys. Rev. B 84, 205406, (2011)

O 86.7 Fri 12:00 MA 041

Sheet plasmon dispersion in epitaxial graphene and graphene nanostructures — •Jens Baringhaus, Thomas Langer, Herbert Pfnür, and Christoph Tegenkamp — Institut für Festkörperphysik, Leibniz Universität Hannover, 30167 Hannover, Germany

The dispersion of the two-dimensional sheet plasmon in epitaxial graphene on SiC substrates has been investigated by means of angle resolved high resolution electron energy loss spectroscopy. The dispersion shows a characteristic point of inflection whose position in phase space depends on the interface (Si-face, C- face, H-intercalation). The plasmon dispersions can be quantitatively described by the model of a nearly free electron gas assuming in addition a resonant coupling to long-lived electron-hole pairs. As the characteristic point appears when entering the interband regime, the effect is related to the chemical potential of the graphene film, i.e. the interface structure. This is in agreement with experiments where the chemical potential has been shifted both by adsorption of F4-TCNQ on epitaxial monolayer graphene and heating of quasi freestanding monolayer graphene films. In undoped or barley doped graphene sheets such as graphene on C-face SiC a point of inflection is not visible at all. Furthermore, the uniaxial dispersion on self-assembled multilayer graphene nanoribbons with an average width of 100 nm has been studied as well. In perpendicular direction a strong damping of the plasmon is observed which can be attributed to the roughness of the ribbons whereas in parallel direction the plasmon dispersion is shifted to higher energies. This shift has its origin in the multilayer characteristic of the ribbons.

O 86.8 Fri 12:15 MA 041

Screening of charges by graphene layers — Daniel Niesner[1], Marko Kralj[2], and •Thomas Fauster[1] — [1]Lehrstuhl für Festkörperphysik, Universität Erlangen-Nürnberg, Staudtstr. 7, D-91058 Erlangen, Germany — [2]Institut za fiziku, Bijenička 46, HR-10000 Zagreb, Croatia

The screening of external charges by a two-dimensional electron gas is studied by spectroscopy of loosely bound electrons on graphene grown on various substrates. The charge transfer from the substrate to the graphene layer (doping) is correlated with the work function and the energy of the Dirac point in good agreement with theoretical predictions [1]. The spectroscopy of the unoccupied states by two-photon photoemission reveals that the long-range image potential applies only for energies close to the vacuum level. The lowest state is found at 3.7 eV above the Dirac point independent of the substrate. This indicates that for this state the screening is dominated by the electronic structure of the graphene layer.

[1] P. A. Khomyakov *et al.,* Phys. Rev. B **79**, 195425 (2009).

O 86.9 Fri 12:30 MA 041

Anisotropic quantum Hall effect in graphene on stepped SiC(0001) surfaces — •Timo Schumann, Klaus-Jürgen Friedland, Myriano H. Oliveira Jr., J. Marcelo Lopes, and Henning Riechert — Paul-Drude-Institut für Festkörperelektronik, 10117 Berlin

The synthesis of epitaxial graphene on SiC by surface thermal decomposition is a promising route for future applications, since it produces high-quality and large-area layers directly on an insulating substrate. By this method, a regularly stepped graphene surface is formed with terrace widths in the order of μm and step heights of about 10 nm. Here we report on an anisotropic behavior in the magnetoresistance measured at high magnetic fields for narrow Hall bars patterned on stepped surfaces. The devices morphology and structural quality has been studied by atomic force microscopy and Raman spectroscopy. If the Hall bar is aligned parallel to the terraces, a quantum Hall effect with negative magnetoresistance is observed due to the condensation of the carriers in the Landau levels, away from the Fermi energy. In contrast, a positive magnetoresistance arises if the current crosses many steps (Hall bar perpendicular to the terraces). We tentatively explain this behavior by proposing a model, which is based on the opening of new conducting channels at both edges of the Hall bar in the surface region close to the steps. These additional channels enable the possibility of electron backscattering from one channel to another on the opposite side, since the spatial separation between the additional edge channels is reduced, resulting in a positive magnetoresistance.

O 86.10 Fri 12:45 MA 041

Transmission electron microscopy of biological samples on nanocrystalline graphene support films — •Daniel Rhinow[1], Matthias Büenfeld[2], Nils-Eike Weber[2], André Beyer[2], Armin Gölzhäuser[2], Werner Kühlbrandt[1], and Andrey Turchanin[2] — [1]Max-Planck-Institut für Biophysik, 60438 Frankfurt, Deutschland — [2]Universität Bielefeld, Fakultät für Physik, 33615 Bielefeld, Deutschland

Electron cryo-microscopy (cryoEM) of vitrified biological specimens is a powerful method for the analysis of macromolecular structures. Although theory indicates that atomic resolution should be attainable routinely, resolutions obtained with most ice-embedded specimens are significantly worse. Biomolecules are phase objects and image contrast is degraded by radiation damage, inelastic scattering, electrostatic charging, and specimen movement. Amorphous carbon, used routinely as support film in biological cryoEM, has several disadvantages such as low electrical conductivity at low temperature and mechanical instability below a film thickness of ~ 20 nm. We have tested nanocrystalline graphene as support film for transmission electron microscopy of ice-embedded biological specimens. Nanocrystalline graphene was synthesized by pyrolysis of molecular nanosheets, obtained by cross-linking of self-assembled biphenyl precursors. Due to their transparency, mechanical strength, and conductivity nanocrystalline graphene supports match all requirements for cryoEM of biological specimens.

O 87: Surface chemical reactions

Time: Friday 10:30–12:45 Location: MA 042

O 87.1 Fri 10:30 MA 042

Detection of carbon monoxide in a hydrogen-rich atmosphere with Kelvin Probe measurements. — •Stefan Simon[1], Christoph Senft[1], Roniyus Marjunus[1,2] und Walter Hansch[1] — [1]Universität der Bundeswehr, München, Germany — [2]University of Lampung, Bandar Lampung, Indonesia

For fuel cell applications, it is necessary to have a CO free hydrogen gas, because CO containments lead to a lower efficiency of fuel cells. It is possible to remove this carbon monoxide from the hydrogen gas by mechanisms called water gas shift reaction (WGS) or preferential oxidation catalyst (PROX). For these methods it is important, that the amount of CO has to be known. Therefore, a sensor which can detect CO in hydrogen and regulate these CO adsorption mechanisms would be a great advantage. A problem is that CO and H2 are both reducing gases. So the reaction for the two gases on top of the surface is in principle the same. In this talk a sensitive layer based on modified platinum is presented, which can detect carbon monoxide in a hydrogen-rich atmosphere. The detection mechanism is based on changing the work function by the gases, which is then measured with a kelvin probe system.

O 87.2 Fri 10:45 MA 042

Click-type on-surface formal [2+2] cycloaddition visualized by Scanning Tunneling Microscopy — •Sylwia Nowakowska[1], Petra Fesser[2], Cristian Iacovita[1], Aneliia Shchyrba[1], Christian Wäckerlin[3], Saranyan Vijayaraghavan[1], Nirmalya Ballav[3], Kara Howes[2], Jean-Paul Gisselbrecht[4], Maura Crobu[2], Corinne Boudon[4], Meike Stöhr[5], Thomas A. Jung[3], and François Diederich[2] — [1]University of Basel, Switzerland — [2]ETH Zürich, Switzerland, — [3]Paul Scherrer Institute, Switzerland — [4]C.N.R.S. Université de Strasbourg, France — [5]University of Groningen, The Netherlands

A porphyrin module has been functionalized with one electron-rich alkyne substituent and three di(tert-butyl)phenyl moieties as imaging groups. STM measurements in combination with X-ray photoelectron spectroscopy studies demonstrated the occurrence of a formal [2+2] cycloaddition/cycloreversion between the donor-activated alkyne and the electron-deficient exocyclic double bond of TCNQ on Au(111). At low coverage, monomeric and self-assembled dimeric species of the initial compounds as well as of the reaction product, a TCNQ-conjugated porphyrin, could be visualized and manipulated with the STM tip. [1] These results motivated us to explore the self-assembly and the reactive assembly of difunctionalized porphyrins equipped with two electron-rich alkyne substituents and their reaction with electron-deficient linkers.

[1] P. Fesser et al., Chem. Eur. J., 17 (2011) 5246-5250

O 87.3 Fri 11:00 MA 042

H-atom relay reactions in real space — •takashi kumagai[1], hiroshi okuyama[2], tetsuya aruga[2], ikutaro hamada[3], thomas frederiksen[4], and hiromu ueba[5] — [1]Fritz-Haber Institute of the Max-Planck Society — [2]Kyoto University — [3]Tohoku University — [4]Donostia International Physics Center — [5]Toyama University

The relay mechanism, in which H-atom transfer occurs in a sequential fashion along hydrogen bonds, plays an essential role in many functional compounds. The scanning tunneling microscope (STM) is used to assemble and control a test-bed for real-space observation of H-atom relay reactions at a single-molecule level. We demonstrate that the transfer of H-atoms along hydrogen-bonded chains assembled on a Cu(110) surface is controllable and reversible, and is triggered by excitation of molecular vibrations induced by inelastic tunneling electrons. The one-dimensional chain complexes consisted of water and hydroxyl groups are constructed in a step-by-step manner using a combination of STM manipulation and controlled dissociation of water molecules. Time-resolved measurement of the H-atom relay enables us to determine the rate as a function of tunneling current and bias voltage. The experimental findings are rationalized by ab initio calculations for adsorption geometry, active vibrational modes and reaction pathway, to reach a detailed microscopic picture of the elementary processes.

O 87.4 Fri 11:15 MA 042

Reaction of Monolayer and Multilayer 2H-Phthalocyanine with a Cu(111) Surface — •Min Chen[1], Jie Xiao[1], Hans-Peter Steinrück[1], and J. Michael Gottfried[2] — [1]Friedrich-Alexander-Universität Erlangen-Nürnberg — [2]Philipps-Universität Marburg

The in-situ metalation of adsorbed tetrapyrrole molecules (e.g., porphyrins and phthalocyanines) continues to be a subject of interest. To clarify the mechanism of the initial interaction and subsequent reaction of 2H-phthalocyanine (2HPc) with a Cu(111) surface, various coverages of 2HPc vapor-deposited onto Cu(111) were studied by X-ray photoelectron spectroscopy (XPS) and temperature programmed desorption (TPD). It was found that adsorbed 2HPc is partially or completely metalated by reaction with Cu atoms from the substrate at 300 K, while for other tetrapyrroles such as 2H-tetraphenylporphyrin and 2H-tetrakis(3,5-di-tert-butylphenyl)porphyrin no metalation was observed under these conditions. The differences in reactivity may be related to the specific molecular geometries, which lead to the different distances between the reactive molecular center and the substrate. Furthermore, the metalation mechanism of 2HPc multilayers on Cu(111) will be discussed; in particular the question whether Cu atoms detach from the substrate and diffuse into the 2HPc multilayer or whether the 2HPc molecules in the multilayer migrate to the Cu/organic interface. Our XPS and TPD results suggest that the surface-confined metalation reactions depend critically on the molecular geometry.

O 87.5 Fri 11:30 MA 042

Front dynamics in the O_2 + NH_3 reaction on Rh(110) surfaces investigated with LEEM — •Benjamin Borkenhagen[1], Mathías Rafti[2,3], Gerhard Lilienkamp[1], Winfried Daum[1], and Ronald Imbihl[3] — [1]Institut für Energieforschung und physikalische Technologien, TU-Clausthal, Leibnizstraße 4, D-38678 Clausthal-Zellerfeld — [2]Instituto de Investigaciones Fisicoquímicas Teóricas y Aplicadas (INIFTA), Fac. Cs. Exactas, Universidad Nacional de La Plata. 64 y Diag. 113 (1900) La Plata, Argentina — [3]Institut für Physikalische Chemie und Elektrochemie, Leibniz-Universität Hannover, Callinstraße 3-3a, D-30167 Hannover

Recent research on the O_2 + NH_3 reactions on Rh(110) focused on interface instabilities in this bistable reaction system. Since the surface structures and changes in the surface anisotropy presumably play a central role in the mechanism of the front instabilities we studied this reaction system in the 10^{-6} and 10^{-5} mbar range with LEEM (low energy electron microscopy) and μLEED. We identified the mixed coadsorbate phase c(2 × 4)-O,N and the c(2 × 6)-O phase in the bistable range. At higher temperatures we discovered the formation of μm-sized islands and studied phase transitions on these islands in detail. The phase transition front breaks up into separate fronts on each island. The small fronts are mainly influenced by the microscopic surface structure such as surface steps.

O 87.6 Fri 11:45 MA 042

Surface chemical reactions constrained in one dimension — •Dingyong Zhong[1,2], Gerhard Erker[3], Harald Fuchs[1,2], and Lifeng Chi[1,2] — [1]Physikalisches Institut, Universität Münster, Wilhelm-Klemm-Str. 10, 48149 Münster, Germany — [2]Center for Nanotechnology (CeNTech), Universität Münster, Heisenbergstr. 11, 48149 Münster, Germany — [3]Organisch-Chemisches Institut, Universität Münster, Corrensstr. 40, 48149 Münster, Germany

Although bulk gold has long been considered minimally reactive, exhibiting poor catalytic activity, the Au(110) surface which exhibits a one-dimensional (1D) geometrical constraint, can acts as the platform for carbon-hydrogen bond activation of inert alkanes. The 1.22 nm wide atomic grooves resulting from the missing-row reconstruction of Au(110) surface efficiently confine the diffusion of adsorbed molecules and constrain the molecules into a 1D pathway, their interactions restricted to neighboring molecules in the easy-diffusion direction within the atomic channels. The hydrogen atoms on terminal methyl or penultimate methylene groups can dissociate and desorb from the surface at 420 to 470 K, leading to carbon-carbon bond formation between the residual alkyl chains. The studies imply that the physical and chemical behaviors of molecule-on-surface systems can be dramatically altered by 1D spatial constraint.

O 87.7 Fri 12:00 MA 042

Electrochemically triggered phosphating of Si-Al-coated steel — •Paul Schneider, Andreas Erbe, and Frank Uwe Renner — Max-Planck-Institut für Eisenforschung, Düsseldorf, Germany

Tri-cation phosphating has been investigated on Si-Al-coated steels. Phosphate crystal growth on these surfaces can be initiated by cathodic polarisation, leading to hydrogen evolution and subsequent generation of a pH gradient. The electrochemically generated pH gradient replaces the pH gradient which is obtained by pickling on Fe and Zn-rich surfaces whose oxides are not stable under the technologically relevant pH. The dependence of the crystal morphology and composition on the applied potential has been investigated by scanning electron microscopy (SEM) with energy dispersive X-ray analysis (EDX), X-ray diffraction and X-ray photoelectron spectroscopy (XPS). The obtained phosphate layers mainly consist of hopeite with varying Mn content. In a second step, the time dependence of the crystal nucleation and growth has been studied by switching the passive surface to a potential where crystal growth was observed. First crystals were observed after 2 s of polarisation. Subsequently, both number of crystals as well as crystal size increases. A complete surface coverage is obtained after 2 min of active phosphating.

O 87.8 Fri 12:15 MA 042

Sensor Material for Small Concentration Measurement of Carbon Monoxide in Air at Room Temperature Based on Work Function Properties — •Roniyus Marjunus[1,2], Stefan Simon[1], Josef Biba[1], Michael Görlich[1], Christoph Senft[1], and Walter Hansch[1] — [1]Universität der Bundeswehr München, Neubiberg, Germany — [2]University of Lampung, Bandar Lampung, Indonesia

Carbon monoxide (CO) is a toxic gas and its measurement is very important for safety and fire protection. Until now, many CO sensors can be found in markets but most of them are based on resistance behaviour and the prices are expensive. A different approach in making sensor is using the work function properties of incorporated sensitive layer. We have concerned many materials and their stoichiometry to find a good sensitive layer. Data of work function change/Contact Potential Different (CPD) measurement with Pt-based shows a promising sensitivity. The results exhibit the work function change/CPD is around 10 mV for 30 ppm (MAK-value) of CO in dry/wet air.

O 87.9 Fri 12:30 MA 042

Aggregation and Metal/Surface Reactivity of DPDI on Cu(111) — •Toni Ivas[1], Susanne Martens[1], Manfred Matena[6], Jonas Björk[2], Jorge Lobo-Checa[3], Lutz H. Gade[4], Thomas A. Jung[1], and Meike Stöhr[5] — [1]University of Basel — [2]Linkoping University — [3]CIN2, Barcelona — [4]Universität Heidelberg — [5]University of Groningen — [6]DIPC, San Sebastian

The perylene derivative DPDI (4,9-diaminoperylene-quinone-3,10-diimine) forms a very stable nanoporous network on Cu(111) crystals upon thermal dehydrogenation. This hexagonal network has been intensively investigated and has proven to serve as an ideal structure for the studying of host-guest assemblies, due to the considerably large pore size and the remarkable stability in particular. The pores of the dehydro-DPDI network act as quantum wells confining surface states of copper electrons and thereby producing 2D arrays of quantum dots. The DPDI network was predicted to consists of dehydrogenated DPDI forming hydrogen bonds but the recently obtained data hints at the possibility that DPDI is bound through a complex coordination network which includes copper adatoms after thermal activation/dehyrogenation. A new model has now been developed, where the DPDI is expected to undergo three dehydrogenation steps in total as well as an additional cyclization step. The hereby obtained "dehydro-DPDI" is then thought to form the coordination network. Theoretical studies as well as recent experimental results obtained by Normal Incidence X-ray Standing Wave (NIXSW) technique strongly support this new model.

O 88: Electronic structure II

Time: Friday 10:30–13:00 Location: MA 043

O 88.1 Fri 10:30 MA 043

The XPS-limit in Hard X-ray Angle Resolved Photo emission — •Jürgen Braun, Jan Minar, and Hubert Ebert — Universität München, Department Chemie, Butenandtstr. 5-13, D-81377 München, Germany

A brief introduction to the theory of angle-resolved photo electron spectroscopy (ARPES) of solid materials is given with an emphasis on the so-called one-step-model of photo emission that describes excitation, transport to the surface and the escape into the vacuum in a coherent way. The main aspects of the theory and its implementation within the Munich SPR-KKR program package [1] will be reviewed. As a new feature we present a model that accounts for finite temperatures when calculating photo emission spectra on the basis of the Coherent Potential Approximation (CPA) alloy theory (alloy analogy model). Our method goes well beyond the simple, but standard Debye-Waller approach to photo emission by including in particular the temperature dependence of the effective photo emission matrix elements as well. This allows among others to reproduce the so called XPS- or density of states limit in angle-resolved photo emission which occurs for high photon energies and/or high temperatures due to a full Brillouin zone averaging caused by phonon scattering. To illustrate the applicability of the new formalism examples of soft- and hard X-ray ARPES calculations for W(110), Pt(111) and Au(111) will be presented.

1. H. Ebert et al., The Munich SPR-KKR package, version 5.4, http://olymp.cup.uni-muenchen.de/ak/ebert/SPRKKR (2009)

O 88.2 Fri 10:45 MA 043

Spin- and angle-resolved photoemission spectroscopy on Bi_2Te_3 thin films — •Alexej Herdt[1], Lukasz Plucinski[1], Gustav Bihlmayer[1], Georg Mussler[1,2], Sven Döring[3], Detlev Grützmacher[1,2], Stefan Blügel[1], and Claus Michael Schneider[1,2,3] — [1]Peter Grünberg Institut, Forschungszentrum Jülich — [2]Jülich Aachen Research Alliance - Fundamentals of Future Information Technologies (JARA-FIT), Forschungszentrum Jülich — [3]AG Prof. Dr. C.M. Schneider, University Duisburg-Essen

Recently, topological insulators have attracted wide attention in the field of condensed matter physics. Typical materials showing the topological phase are $Bi_{1-x}Sb_x$, Bi_2Se_3 or Bi_2Te_3, which have been theoretically predicted and experimentally observed in several studies [1]. We investigate the surface state spin texture of an epitaxial MBE-grown Bi_2Te_3/Si(111) thin film using angle- and spin-resolved photoelectron spectroscopy (SP-ARPES). Film growth and characterization are described elsewhere [2,3]. Our study shows, that the linear Dirac cone is accompanied by deeper lying high spin-polarized energy dispersive surface states up to 4 eV binding energy. These states indicate clear reversals of the spin vector components for both chiralities measured on different Fermi surface positions located in the $\boldsymbol{k}$-space. The results are supported by our high-resolved ARPES data as well as theoretical *ab initio* band structure calculations in thin film geometry.

[1] M. Z. Hasan *et al.*, Rev. Mod. Phys. 82, 3045 (2010)
[2] J. Krumrain *et al.*, J. Cryst. Growth 324, 115 (2011)
[3] L. Plucinski *et al.*, Appl. Phys. Lett. 98, 222503 (2011)

O 88.3 Fri 11:00 MA 043

Electronic structure of spatially aligned graphene nanoribbons — •Steffen Linden[1], Dingyong Zhong[1], Alexander

Timmer[1], Haiming Zhang[1], Nabi Aghdassi[1], Xinliang Feng[2], Klaus Müllen[2], Harald Fuchs[1], Helmut Zacharias[1], and Lifeng Chi[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 under UHV conditions is a new concept to create robust, ordered molecular surface structures that may also exhibit novel properties [1]. Starting from specifically designed primer molecules, well-orientated armchair graphene nanoribbons (aGNRs) with well-defined widths have been obtained on a stepped gold surface. To study the structural and electronic properties of these GNRs, scanning tunneling spectroscopy (STM), angle-resolved ultraviolet photoemission spectroscopy (ARUPS) and inverse photoemission (IPE) have been conducted. STM shows the exclusive presence of 7-aGNRs and a few percent of 13-aGNRs on the substrate. The combination of ARUPS and IPE reveals bandgaps of 2.8 eV and 1.6 eV for 7-aGNRs and 13-aGNRs, respectively. These values are in between those obtained from LDA and GW calculations for freestanding aGNRs[2,3]. Thus a weak doping from the underlying gold substrate may occur. These results clearly show the development of a sizable bandgap in narrow aGNRs.

[1] J. Cai et al., Nature 466, 470 (2010), [2] J. W. Son et al., PRL 97, 216803 (2006), [3] Li Yang et al., PRL 99, 186801 (2007)

O 88.4 Fri 11:15 MA 043

Co thin films on Cu(001): dispersion and spin polarisation of the unoccupied quantum well state — •Martin Ellguth, Christian Tusche, Aimo Winkelmann, and Jürgen Kirschner — Max-Planck-Institut für Mikrostrukturphysik, Weinberg 2, 06120 Halle

Co thin films on Cu(001) are a thoroughly investigated material system, where a surface state is present and quantum well states occur in the unoccupied part of the band structure. Using our momentum microscope, we have measured energy-resolved momentum images in two-photon photoemission (2ppe: $h\nu = 3.1$ eV) using 400-nm-photons from a frequency doubled Ti:Sa laser. The momentum imaging principle yields the full $\vec{k}_{||}$-space of photoelectrons in a single measurement. We assemble such images over a range of kinetic energies and select an energy-vs-$k_{||,1}$ cut from the 3-dimensional dataset to visualize the dispersion relation of the unoccupied quantum well states in 2ppe depending on the film thickness (3 to 11 monolayers).

For a selected initial energy of 350 meV below the Fermi level, we obtain a spin-polarised version of such an image by placing a recently developed 2-dimensional imaging spin detector[1] into the electron beam path. We observe a spin polarisation of 0.5 for those $\vec{k}_{||}$, where the resonant excitation via the quantum well state yielded an increased intensity and 0.45 in the remaining $\vec{k}_{||}$-regions.

[1] C. Tusche, M. Ellguth, A.A. Ünal, C.-T. Chiang, A. Winkelmann, A. Krasyuk, M. Hahn, G. Schönhense, J. Kirschner, *Appl. Phys. Lett.* **99**, 032505 (2011)

O 88.5 Fri 11:30 MA 043

Low-Energy Scale Excitations in the Spectral Function of Organic Monolayer Systems — •Achim Schöll[1,2], Johannes Ziroff[1,2], Simon Hame[1,2], Mario Kochler[1,2], Azzedine Bendounan[1,2], and Friedrich Reinert[1,2] — [1]Experimentelle Physik VII und Wilhelm Conrad Röntgen Research Center for Complex Material Systems, Universität Würzburg, 97074 Würzburg, Germany — [2]Gemeinschaftslabor für Nanoanalytik, Karlsruher Institute für Technologie KIT, 76021 Karlsruhe, Germany

Using high-resolution photoemission spectroscopy we demonstrate that the electronic structure of several organic monolayer systems, in particular 1,4,5,8-naphthalene tetracarboxylic dianhydride and Copper-phtalocyanine on Ag(111), is characterized by a peculiar excitation feature right at the Fermi level. This feature displays a strong temperature dependence and is immediately connected to the binding energy of the molecular states, determined by the coupling between the molecule and the substrate. At low temperatures, the line-width of this feature, appearing on top of the partly occupied LUMO (lowest unoccupied molecular orbital of the free molecule), amounts to only ~ 10meV, representing an unusually small energy scale for electronic excitations in these systems. We discuss possible origins, related e.g. to many-body excitations in the organic-metal adsorbate system, in particular a generalized Kondo scenario based on the single impurity Anderson model.

O 88.6 Fri 11:45 MA 043

In situ angle resolved photoelectron spectroscopy (ARPES) during the formation and depth sensitive hard X-ray photoelectronspectroscopy (HAXPES) of a ZnO:Ni nanocomposite — •Arndt Quer, Erik Kröger, Matthias Kalläne, Lutz Kipp, and Kai Rossnagel — Institute of Experimental and Applied Physics, University of Kiel, 24098 Kiel, Germany

Magnetoelectric composits based on piezoelectric and magnetostrictive substances have drawn significant interest in recent years due to their multifunctionality and potential technological aspects, e.g. sensor applications. For the magnetoelectric coupling the interface between the two components and its magnetic and electronic structure is of basic interest. The composite of magnetostrictive Ni thin films on top of pizeoelectric ZnO-substrates was used as a simple basic system. In order to investigate the electronic structure during interface formation, we performed in situ photoelectron spectroscopy (PES), revealing NiO formation at the interface and in addition charge transfer from the Ni adatoms to the ZnO substrate. The resulting enhanced conductivity of the ZnO surface enables high resolution ARPES measurements. These ARPES results of the electronic structure of the composite over the Brillouin zone in ΓMK-plain are shown. Furthermore the "complete" composite of a 5 nm thin film nickel on ZnO substrate was investigated by depth sensitive HAXPES. This work was supported by the DFG via SFB855.

O 88.7 Fri 12:00 MA 043

Extremely short mean free path of electrons in lanthanides — •Karen Zumbrägel, Anke B. Schmidt, and Markus Donath — Physikalisches Institut, WWU Münster

The probing depth of electron spectroscopies is determined by the mean free path of electrons within the investigated material. Schönhense and Siegmann predicted a rule of thumb that for transition metals the electron mean free path for low energies is inversely proportional to the number of d holes [1]. This rule was confirmed for, e.g., Fe with 3 to 5 monolayers [2] and predicts an extremely short mean free path of less than 1 ML for Gd.

We performed overlayer experiments with gadolinium and terbium grown on tungsten. Applying inverse photoemission, we observed the decreasing intensity of tungsten bulk-state transitions as a function of the lanthanide film thickness. Thus we were able to determine the mean free path for low-energy electrons in gadolinium and terbium and confirm therewith the prediction of Schönhense and Siegmann.

[1]Schönhense and Siegmann, Ann. Phys. 2 (1993) 465

[2]Passek et al., J. Magn. Magn. Mat. 159 (1996) 103

O 88.8 Fri 12:15 MA 043

Charge transfer and dipole-dipole repulsion at ultra-thin organic heterojunction on metal — •Patrick Amsalem[1], Jens Nierderhausen[1], Andreas Wilke[1], Raphael Schlesinger[1], Stefanie Winkler[1], Antje Vollmer[2], Jurgen P. Rabe[1], and Norbert Koch[1] — [1]Humboldt-Universität zu Berlin, Institut für Physik, Newtonstrasse 15, Berlin 12489, Germany — [2]Helmholtz-Zentrum Berlin für Materialien und Energie GmbH - BESSY II, Albert-Einstein-Strasse 15, Berlin 12489, Germany

We investigate the electronic properties of a two monolayer thick organic heterojunction grown on a metal surface by photoelectron spectroscopy. The first molecular α-sexithiophene layer is physisorbed on the Ag(111) substrate and the sample work function decreases by 0.7 eV. Upon incremental deposition of an organic C60 overlayer, a charge transfer state, attributed to the partial filling of the C60 LUMO-derived states, is observed. This is accompanied by a work function increase which does not increase linearly as a function of coverage within the sub-monolayer regime. Analysis of the valence band and core level spectra reveals that the overlayer is actually composed of a mixture of charged and neutral species. Noteworthy, the work function behavior is correlated with the ratio of charged and neutral molecules, which depends on coverage. Dipole-dipole repulsion is proposed as the main driving force to explain these charge/neutral molecule ratio variations. The energy level alignment and structural properties are discussed by invoking simple electrostatic considerations.

O 88.9 Fri 12:30 MA 043

Localized Doping on an Atomic Chain System — •I. Barke, S. Polei, V. v. Oeynhausen, and K.-H. Meiwes-Broer — Insuitut für Physik, Universität Rostock, 18051 Rostock, Germany

Adatoms can be used as efficient dopants for band-structure engineering of surfaces. While delocalized electron waves in two or three dimensions are usually affected by an ensemble of impurities, perfect separation of segments between two dopants can be achieved in one dimension. This results in local regions of well-defined charge-carrier concentrations. On the quasi one-dimensional system Si(111)5x2-Au it is shown that quantum wires between two doping adatoms establish a local electronic structure depending on the respective adatom distance. Within a chain segment the effect of a spatially independent charge-carrier concentration is superimposed by a Coulomb-like interaction with the positively charged impurities. This offers a natural explanation for the relatively broad features observed in photoemission [1] and the complex appearance in STM and STS images [2].

[1] J. L. McChesney et al., 70, 195430 (2004).

[2] I. Barke et al., Solid State Commun. 142, 617 (2007).

O 88.10 Fri 12:45 MA 043

Doped silicene: Evidence of a wide stability range — •Udo Schwingenschlögl, Yingchun Cheng, and Zhiyong Zhu — KAUST, PSE Division, Thuwal 23955-6900, Kingdom of Saudi Arabia

The effects of doping on the lattice structure, electronic structure, phonon spectrum, and electron-phonon coupling of low-buckling silicene are studied by first-principles calculations. Although the lattice is found to be very sensitive to the carrier concentration, it is stable in a wide doping range. The frequencies of the G and D Raman modes can be used to probe the carrier concentration. In addition, the phonon dispersion displays Kohn anomalies at the Γ and K points which are reduced by doping. This implies that the electron-phonon coupling cannot be neglected in field-effect transistor applications.

Reference: EPL **95**, 17005 (2011).

O 89: Metal substrates: Adsorption of organic / bio molecules V

Time: Friday 10:30–13:00 Location: A 053

O 89.1 Fri 10:30 A 053

Self-assembly and 2D spontaneous resolution of cyano-functionalized [7] helicenes on Cu(111) — •Tuan Anh Pham[1], Serpil Boz[2], Aneliia Shchyrba[2], Sylwia Nowakowska[2], Michael Schär[3], François Diederich[3], Manh-Thuong Nguyen[4], Daniele Passerone[4], Thomas Jung[5], and Meike Stöhr[1] — [1]University of Groningen, Netherlands — [2]University of Basel, Switzerland — [3]ETH Zürich, Switzerland — [4]EMPA, Switzerland — [5]PSI, Switzerland

Supramolecular control involves the selective recognition of chirality for any target assembly in order to shape e.g. the active elements within their environment. This refers equally to 3D crystal growth as well as to the field of surface-supported supramolecular assemblies. Notably, the spontaneous resolution of racemic compounds into separate enantiomeric crystals serves as an indicator for the enantioselective assembly governed by the specific intermolecular and - for surface supported assemblies - by molecule substrate interactions which can be considered as a complicating factor. Herein, we show the first example of a spontaneous chiral resolution of a helicene derivative on a Cu surface. Through STM and DFT investigations, the formation of fully segregated domains of pure enantiomers (2D conglomerate) from racemic dicyano[7]helicene were demonstrated. The propensity of the system to optimize intermolecular hydrogen bonding as well as dipolar interactions translates into chiral recognition. In addition, a discussion of the effect of chirality on the nucleation and formation of helicene chains for low coverage shall be presented.

O 89.2 Fri 10:45 A 053

STM study of molecular structures of bis(phthalocyaninato)-lutetium(III) on crystalline substrates — •Lars Smykalla, Pavel Shukrynau, and Michael Hietschold — Chemnitz University of Technology, Institute of Physics, Solid Surfaces Analysis Group, D-09107 Chemnitz, Germany

Results of the adsorption and formation of self-assembled ordered molecular structures of the double-decker phthalocyanine molecule bis(phthalocyaninato)lutetium(III) on the anisotropic metallic surface of an Ag(110) single crystal and on highly oriented pyrolytic graphite (HOPG) are reported. We used a variable temperature scanning tunneling microscope (STM) at 30 K and room temperature under ultrahigh vacuum conditions to image the molecules with submolecular resolution. The electronic properties were investigated with scanning tunneling spectroscopy and density functional theory calculations for single molecules. The observed molecular structures and scanning tunneling spectroscopy results for both different substrates are compared to gain a better understanding of the influence of the surface on the adsorbed molecules. From this we can conclude that for the molecular arrangement the molecule-molecule interactions are dominant. However, the stronger molecule-substrate interaction for metal substrates compared to the weakly interacting HOPG was found to lead to a new structure with an alternating rotation of the molecules relative to the lattice vectors.

O 89.3 Fri 11:00 A 053

Self-assembly of Tetrathiafulvalene-Fused Dipyridophenazine (TTF-dppz) analyzed by tuning fork based AFM/STM — •Sweetlana Fremy[1], Rémy Pawlak[1], Shigeki Kawai[1], Shi-Xia Liu[2], Silvio Decurtins[2], Ernst Meyer[1], and Thilo Glatzel[1] — [1]Department of Physics, University of Basel, Klingelbergstrasse 82, CH-4056 Basel, Switzerland — [2]Department of Chemistry, University of Bern, Freie Strasse 3, CH-3012 Bern, Switzerland

A main challenge of molecular electronics consists in controlling the self-assembly on a surface, which is a highly complex dynamic process with competing binding modes (molecule-surface and intermolecular interactions), driven by thermodynamic and kinetic selectivity. Here, we investigate the self assembly of TTF-dppz molecules (Tetrathiafulvalene-Fused Dipyridophenazine) on metal substrates and insulating thin films by combined tuning fork based atomic force and scanning tunneling microscopy at low temperature. The molecules are additionally functionalized with cyano-groups to yield in a better surface sticking, especially on insulating substrates. While directly after deposition on Cu(111), the molecules are disordered, post-annealing at 100°C leads to highly ordered self-assemblies of molecular wires, a network with six-fold symmetry, small crystallites and step edge decorations. Most probably the molecules decompose during the annealing, involving Cu-adatoms. The fact, that TTF-dppz molecules do not form such ordered structures on Ag(111), strengthens our presumption. Further investigations comprise the study of single molecules on thin films and the adsorption of the two single compounds dppz and TTF.

O 89.4 Fri 11:15 A 053

Supramolecular organization and subsequent interlinking of biphenyl derivatives on metal surfaces — •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, the Netherlands — [2]Department of Physics, University of Basel, Switzerland — [3]Department of Chemistry, University of Basel, Switzerland

The combination of their almost infinite structural diversity and unique self-assembly properties makes molecules ideal building blocks for tailor-made materials [1,2]. However, most of such thermodynamically controlled structures are reversible. Therefore, structures with higher stability and improved conductive properties are essential. In this work, a unique concept to control both the molecular self-assembly and the subsequent intermolecular coupling was utilized through the usage of protecting groups.

Herein, biphenyl derivatives with different protecting groups were synthesized and investigated on Ag(111) with STM and XPS before and after annealing. The protecting groups can be split off during the annealing step and the deprotected monomers were found to interlink into polymeric structures. By careful design of the organic monomers, control over reactivity and the size of polymeric structures is achieved.

[1] S. Boz et al., Angew. Chem. Int. Ed. 48 (2009) 3179

[2] J. Lobo-Checa, et al., Science. 325 (2009) 300

O 89.5 Fri 11:30 A 053

H-bonding as a tool for engineering 1D and 2D supramolecular structures on surfaces — •Mihaela Enache[1], Manfred Matena[2], Laura Maggini[3], Anna Llanes-Pallas[3], Davide Bonifazi[3], Thomas Jung[2], and Meike Stöhr[1] — [1]University of Groningen, Netherlands — [2]University of Basel, Switzerland — [3]University of Namur, Belgium

By utilizing the concepts of supramolecular chemistry, remarkable results for molecular self-assembly on surfaces have been presented. The outcome of the self-assembly process is known to be affected by the fine tuning of different parameters (such as thermal energy, ratio between different molecular units, etc.) which have a direct influence on the interplay between intermolecular and molecule-substrate interactions.

Herein, we present a scanning tunneling microscopy study demonstrating that - by choosing the recognition moieties appropriately - H-bond recognition between specially designed molecules can predictably lead to the formation of 1D and 2D structures.

Upon adsorption on Ag(111), two different molecular modules self-assemble through triple H-bonding between their complementary recognition moieties forming supramolecular architectures. Depending on the sample preparation parameters, either chain-like or porous structures can be obtained. Therefore, a well-known concept from supramolecular chemistry can be transferred for the fabrication of surface-mounted organic assemblies.

[1] Llanes Pallas et al., Angew. Chem. Int. Ed. 47 (2008) 7726

[2] Matena et al., Chem. Commun. (2009) 3525

O 89.6 Fri 11:45 A 053

The metal/ionic liquid interface: Structure formation and temperature dependent behavior of ionic liquid adlayers on Au(111) — •Benedikt Uhl, Michael Roos, and Rolf Jürgen Behm — Ulm University, Institute of Surface Chemistry and Catalysis, D-89069 Ulm, Germany

Ionic liquids (IL) are promising electrolytes in Li-Ion batteries. The behavior of the IL's at the electrode surface and the properties of the solid-liquid-interface is crucial for the performance of such electrochemical systems, but investigations on this topic are at their very beginning. In this work, we investigated the structure formation during submonolayer growth of the model systems 1-butyl-1-methylpyrrolidinium-bis(trifluoromethylsulfonyl)imide (BMP-TFSA) and 1-ethyl-3-methylimidazolium-bis(trifluoromethylsulfonyl)imide (EMIM-TFSA) on Au(111). The resulting structures were characterized with scanning tunneling microscopy (STM) under UHV conditions at temperatures between 100 K and 298 K and at varying IL coverages in the submonolayer regime. At room temperature, the adsorbed IL's form a 2D liquid. At lower temperatures, mobility is frozen and different structures appear. A 2D glassy state and various structures with long range order are detected, depending on the temperature of the substrate during the evaporation process. The 2D crystal structures are influenced by the subjacent Au(111) reconstruction pattern. In addition, the dynamics of the adlayers are investigated during continuous heating from 100 K to room temperature in order to get insight into the thermal stability of the adlayers.

O 89.7 Fri 12:00 A 053

Hierarchic Formation and Dynamics of Bi-component Supramolecular Networks — •W. Krenner[1], F. Klappenberger[1], N. Kepčija[1], E. Arras[1], Y. Makoudi[1], D. Kühne[1], S. Klyatskaya[2], M. Ruben[2,3], A. P. Seitsonen[4], and J. V. Barth[1] — [1]Physikdepartment E20, TU München — [2]Institute of Nanotechnology, Karlsruhe Institute of Technology — [3]IPCMS-CNRS UMR 7504, Université de Strasbourg — [4]Physikalisch-Chemisches Institut, Universität Zürich

In this work, the formation and dynamics of bi-component organic molecular networks providing open pores following hierarchic assembly principles are investigated via low- and variable temperature STM in UHV and DFT modeling. By co-depositing N,N' diphenyl oxalic amide (DOA) and sexiphenyl dicarbonitrile (6DC) on Ag(111), self-assembled structures are encountered where organisation depends on the stoichiometric ratio of the constituents.

All network types reflect hierarchic architectures, where similar, essential molecular binding motifs prevail. The different energetics of the individual binding motifs are assessed by theoretical simulation, showing that hierarchic assembly is driven by the strength of the respective interactions. Thereby, the experimentally observed preference of DOA-6DC binding is rationalized, accounting for the formation of mixed phases over phase segregation.

The analysis of the dynamics in the network phase with high variation in binding energies shows good accordance for the diffusion behavior expected from DFT binding energy modeling.

O 89.8 Fri 12:15 A 053

Structure and Binding of Large Molecules at Metal Surfaces: theoretical NEXAFS for Co-OEP on Ni(100) — •Chunsheng Guo[1], Lili Sun[1], Klaus Hermann[1], Christian Hermanns[2], and Wolfgang Kuch[2] — [1]Theory Department, Fritz-Haber-Institut, Berlin — [2]Inst. of Experimental Physics, Free University, Berlin, Germany

Metal octaethylporphyrins (M-OEP), $M\text{-}N_4C_20H_4(C_2H_5)_8$, adsorbed on metallic substrate are promising candidates to provide spin dependent electric transport. While experimental studies on these systems have been performed details of the adsorbate geometry and surface binding are still unclear. We have carried out density-functional theory (DFT) calculations on free Co-OEP and for Co-OEP adsorbed at Ni(100) with periodic surface models. The resulting equilibrium geometries are then applied in StoBe cluster calculations to yield theoretical C and N 1s excitation spectra of free and adsorbed Co-OEP. Experimental carbon K edge NEXAFS spectra of separate Co-OEP show a triple-peak structure which can be explained from theory by differently binding carbon. When adsorbed at Ni(100) substrate the triple-peak structure reduces to a double-peak, not yet confirmed by experiment. The measured nitrogen K edge spectra of Co-OEP, showing a double-peak structure, are also affected by the substrate. This is explained by hybridization of adsorbate final state orbitals near the nitrogen centers with 3d orbitals of the Ni substrate due to adsorbate-substrate binding. Test test Test test Test test Test test Test test Test test

Supported by SFB 658 "Molecular switches at surfaces", Berlin

O 89.9 Fri 12:30 A 053

Evaluation of Degree of Charge Transfer in Classical and Novel Donor-Acceptor Complexes Based on Tetracyanoquinodimethane by HAXPES — •Katerina Medjanik[1], Andrei Gloskovskii[2], Dmytro Kutnyakhov[1], Claudia Felser[2,3], Jean-Paul Pouget[4], Dennis Chercka[5], Martin Baumgarten[5], Klaus Müllen[5], and Gerd Schönhense[1] — [1]Inst. für Physik, Univ. Mainz — [2]Inst. für Anorg. und Anal. Chemie , Univ. Mainz — [3]MPI für Chemische Physik fester Stoffe, Dresden — [4]Université Paris-Sud, Orsay, France — [5]MPI für Polymerforschung, Mainz

Combination of the classical acceptor tetracyanoquinodimethane (TCNQ) with novel donors tetra- and hexamethoxyprene (TMP and HMP) can clarify the question about the nature and degree of charge transfer (CT) and give us the possibility to compare the results with measurements and the same conditions for the prototype system TTF-TCNQ. Hard X-ray photoemission (HAXPES) experiment has been performed at PETRA III (beamline P09) on microcrystals and thin films of HMP/TMP-TCNQ. Upon complex formation, we observed a change of the O1s and N1s spectra from a single-line spectrum to a spectrum with two distinct lines shifted by up to 2.6 eV with respect to the position of the line of the pure donors and acceptors. Peak-area analysis reveals a degree of CT of about $0.6e$. This value lies close to the CT of 2/3 for TTF-TCNQ estimated by analysis of the sulphur 2p spectra and for similar CT compounds such as NMP-TCNQ [1].

Funding DFG/TR49, Graduate School MAINZ, COMATT.

[1] J. P. Pouget et al., Phys. Rev. B 21 (1980) 486.

O 89.10 Fri 12:45 A 053

X-ray induced reversible switching of azobenzene derivatives, adsorbed on Bi(111) — •Alex Krüger, Matthias Bernien, Ch. Felix Hermanns, and Wolfgang Kuch — Freie Universität Berlin, Institut für Experimentalphysik, Arnimallee 14, 14195 Berlin

The adsorption of the photoswitch dimetacyano-azobenzene (DMC) on Bi(111) after deposition at 110 K was studied for different coverages by angle-dependent near-edge x-ray absorption fine structure (NEXAFS) spectroscopy. For the adsorption of one monolayer of molecules we find the molecules physisorbed in a nearly planar conformation parallel to the surface. By illumination with intense x rays two orders of magnitude higher in flux density than used for the NEXAFS measurements at a photon energy corresponding to the azo N 1s → LUMO transition at 399 eV, the angle dependence of the π^* resonances of N-K as well as C-K NEXAFS spectra changes significantly. The effect can be interpreted as a switching of at least 20% of the DMC molecules from the *trans* to the *cis* conformation. The process is reversible, as the NEXAFS spectra become identical to the spectra before the illumination after waiting for 1 h in darkness at 110 K, indicating a thermally induced back reaction. Using off-resonant x rays with an energy of 270 eV for the illumination, no modifications of the NEXAFS N-K and

C-K spectra were observed. A comparable effect with an even higher percentage of switched molecules occurs also in multilayers of DMC molecules on Bi(111).

This work is supported by the DFG through Sfb 658.

O 90: Metals and semiconductors: Epitaxy and growth

Time: Friday 10:30–12:30 Location: A 060

O 90.1 Fri 10:30 A 060

Role of pulse control and material parameters on submonolayer pulsed-laser depositions — Martin Mašín and •Miroslav Kotrla — Institute of Physics, Academy of Sciences of the Czech Republic, Na Slovance 2, 182 21, Praha 8, Czech Republic

Pulsed laser depositions is the promising experimental method for nanostructuring of oxide, and also metallic thin films [1]. However, its theoretical understanding on the microscopic level is still insufficient. Recently, we performed Monte Carlo simulation motivated by a Fe/Mo system to analyze the temperature dependence of island density in the case of reversible growth [2]. In this work, we present our study of the dependence of the island density on varying characteristics of pulses: different chopping frequencies, and different duration of pulses. We also compare two regimes of pulse frequency variation: with a constant average flux and with a constant pulse intensity. In the former case, we found that low frequency increases the island density highlighting the recently found anomaly in the Arrhenius plot [2]. In the latter case, we observe, in contrary, that higher frequency leads to a higher island density. Increase of pulse length causes decrease of island density, leading to molecular beam epitaxy results. Moreover, we analyzed dependence on material parameters. The increase of a diffusion barrier for monomers shifts the whole Arrhenius curve to higher temperatures, and increase of binding energy moves a position of plateaus to higher temperatures. Our results allow to optimize pulse deposition.

[1] P. O. Jubert, O. Fruchart and C. Mayer, Phys. Rev. B , 64 (2001) 115419. [2] M. Mašín, M. Kotrla: Europhys. Lett. 90 (2010) 18006.

O 90.2 Fri 10:45 A 060

Atomic structure of Fe on Ir(001) - (1x1) — •Marco Corbetta, Zhen Tian, Yiqi Q. Zhang, Alvaro Augusto Leon Vanegas, Safia Ouazi, Dirk Sander, and Jürgen Kirschner — Max Planck Institute, Halle (Saale), Germany

The correlation between structural and magnetic properties of Fe monolayers makes it a particularly interesting system to investigate the impact of lattice strain on film structure, morphology and magnetism. We study the Ir(001) - (1x1) surface by STM with a W tip obtaining atomic resolution. We then deposit 0.6 ML of Fe at 300 K and we observe a (3x3) periodicity on one layer height Fe islands at 8 K in STM constant current images. This suggests the formation of a coincidence structure where three Ir-Ir atomic distances along the [110] crystallographic direction correspond to two bcc Fe-Fe atomic distances in the same direction. The difference in length between three Ir-Ir (8.145 A) and two Fe-Fe (8.105 A) atomic distances is only +4 pm and this makes our model a reasonable proposition. After deposition of 1.2 ML of Fe we observe a (1x1) contrast by STM on the closed first Fe monolayer, in agreement with earlier studies [1]. The analysis reveals a nearest neighbour spacing of the Fe monolayer which corresponds to that of the Ir substrate. Our findings could be ascribed to a structural rearrangement within the Fe deposit with increasing Fe coverage. [1] V. Martin, W. Meyer, C. Giovanardi, L. Hammer, K. Heinz, Z. Tian, D. Sander and J. Kirschen, Phys. Rev. B 76, 205418 (2007).

O 90.3 Fri 11:00 A 060

Characterization of Pt_*x*Cu_1-x alloys on Pt(111) surfaces as model catalysts for core shell nanoparticles. — •Stephan Beckord, Albert K. Engstfeld, and R. Jürgen Behm — Ulm University, Institute of Surface Chemistry and Catalysis, D-89069 Ulm, Germany

Core-shell nanoparticles consisting of a bi- or multialloy core enclosed by a layer of a pure metal often show interesting catalytic properties. One example are PtxCu1-x alloy core Pt shell particles, which show an increased catalytic reactivity towards the oxygen reduction reaction [1] or the water gas shift reaction [2] compared to the respective monometallic particles.

To study the effect of the Pt_xCu_1-x core on the Pt shell, we prepared nanostructured bimetallic planar model surfaces under ultra high vacuum (UHV) conditions, by evaporation of Cu on a Pt(111) surface followed by annealing for (surface) alloy formation. Subsequent deposition of a Pt monolayer film results in a model system closely resembling the structure of a bimetallic core-shell nanoparticle. The resulting surfaces were characterized by scanning tunneling microscopy (STM) and auger electron spectroscopy (AES) to elucidate the composition, morphology and the distribution of the different species in the surface. From these data we will determine the dominant factors for surface alloy formation. [1] *R. Strivastava, P. Mani, N. Hahn, and P. Strasser, Angewandte Chemie, 46, 8988 (2007). [2]*J. Knudsen, A. U. Nilekar, R. T. Vang, J. Schnadt, and F. Besenbacher, J. Am. Chem. Soc. 120, 6485 (2007).

O 90.4 Fri 11:15 A 060

Taking (different) sides - Zn and Ga on different Pd-facets — •Werner Stadlmayr, Christoph Rameshan, Simon Penner, Bernhard Klötzer, and Norbert Memmel — Institute of Physical Chemistry, University of Innsbruck, Innsbruck, Austria

Pd/Zn- and Pd/Ga-catalysts have been proven to be interesting candidates for methanol-steam-reforming ($CH_3OH+H_2O \rightarrow CO_2+3H_2$)[1]. Using thin films of Zn and Ga on Pd-substrates, we investigated them regarding their alloying, structure as well as catalytic behaviour. We comment on the trends in thermal stability and give a comprehensive overview of the structural findings so far. In particular we find that both the films and alloys derived from the (110)-facets are more stable than those derived from the (111)-facets. Furthermore, Zn-films have a stronger tendency for surface alloy formation than Ga-films, while such a simple relationship does not hold for the decomposition of the alloys. Concerning catalytical properties, we show that properly prepared Pd/Zn-alloys exhibit CO_2-selectivity, while no such selectivity can be found for Pd/Ga-alloys.

[1] N. Iwasa and N. Takezawa, Top. Catal. **22**, 3-4 (2003)

O 90.5 Fri 11:30 A 060

Core shell model electrodes: Pt terminated mono- and multilayer CuPt alloys supported on Ru(0001) single crystals. — •Albert K. Engstfeld and R. Jürgen Behm — Ulm University, Institute of Surface Chemistry and Catalysis, D-89069 Ulm, Germany

Core shell particles consist of a metal A rich shell and a bi- or multialloy core, showing different catalytic activity compared to pure metal particles. An interesting example are Pt enclosed alloy particles containing Cu, Co and Pt, having a much better activity towards oxygen reduction than pure Pt.[1] The effect is mainly attributed to a change of the electronic structure of the shell due to lattice strain within the alloy core.

To study the strain effect we focus on the preparation of mono and bilayer Cu/Pt alloys on Ru(0001) single crystal surfaces under ultra high vacuum conditions, characterized by scanning tunnelling microscopy. From the atom distribution within the alloy we will discuss the dominant factors for alloy formation, in view of the different size of the atoms and difference in their intermetallic bonding. Furthermore, we will elucidate the surface segregation behaviour of Pt in the bilayer alloy during the alloying process.

[1] R. Strivastava, P. Mani, N. Hahn, and P. Strasser, Angewandte Chemie, 46, 8988 (2007)

O 90.6 Fri 11:45 A 060

Growth study: ultrathin GaN films on 6H-SiC(0001) — •Lena Neumann[1], Jürgen Gerlach[1], and Bernd Rauschenbach[1,2] — [1]Leibniz Institute of Surface Modification (IOM), D-04318 Leipzig, Germany — [2]University Leipzig, Institute of Experimental Physics II, D-04103 Leipzig, Germany

Ultrathin gallium nitride (GaN) films were deposited using the ion-beam assisted molecular-beam epitaxy (IBA-MBE) technique. The influence of the nitrogen ion to gallium atom flux ratio (I/A ratio) at different substrate temperatures during the early stages of GaN nucleation and thin film growth directly on super-polished 6H-SiC(0001) substrates was studied. The deposition process was performed by evaporation of Ga and irradiation with hyperthermal nitrogen ions from a constricted glow-discharge ion source. The GaN growth in N- and Ga-rich regimes was investigated by *in situ* reflection high energy electron diffraction (RHEED) and scanning tunnelling microscopy (STM) measurements. The results show, that the I/A ratio has a major impact on the properties of the resulting ultrathin GaN films. The growth mode, the surface roughness, the degree of GaN coverage of the substrate and the polytype mixture depend notably on the I/A ratio. At the substrate temperature of 700 °C and the I/A ratio less than 1.6 the formation of islands developed through rapid coalescence into two-dimensional growth. A three-dimensional island growth mode is favoured at lower Ga fluxes, so that the I/A ratio > 1.6. The increase of the islands diameter to height ratio with the I/A ratio increasing was observed.

O 90.7 Fri 12:00 A 060

Investigation of the three layer system MgO/Fe/GaAs(001) — •Dominique Handschak[1], Tobias Lühr[1,2], Frank Schönbohm[1,2], Sven Döhring[2], Christoph Keutner[1,2], Ulf Berges[2], and Carsten Westphal[1,2] — [1]TU-Dortmund, Experimentelle Physik I — [2]DELTA, TU-Dortmund

We report a synchrotron high-resolution x-ray photoemission (XPS) and photoelectron diffraction (XPD) study of the three layer system MgO/Fe/GaAs(001). The interface of Fe/GaAs is interesting because it is a semiconductor-ferromagnetic junction, being an interesting model system for research to spintronics. Magnesium oxide is a very efficient insulator which is used especially in TMR-components. Both interfaces have a strong influence on the efficiency of the contributing effects. In this study we report on the preparation process of the three layer system with a GaAs reconstructed surface. The structure of each layer could be clarified with core level high-resolution spectra and diffraction patterns.

O 90.8 Fri 12:15 A 060

XPD-pattern analysis of MgO/Fe/GaAs(001) by means of Genetic Algorithms — •Tobias Lühr[1,2], Dominique Handschak[1], Frank Schönbohm[1,2], and Carsten Westphal[1,2] — [1]Fakultät Physik - TU Dortmund, Otto-Hahn-Str.4, D 44221 Dortmund, Germany — [2]DELTA - TU Dortmund, Maria-Goeppert-Mayer-Str. 2, D 44227 Dortmund, Germany

Thin films of iron on gallium arsenide are of great relevance in current research. This system forms a semiconductor-ferromagnetic junction. For this reason it becomes interesting for spintronic devices. An insulating layer like magnesium oxide on this system offers the possibility of growing additional layers for technical applications (e.g. TMR-components). We investigated the three layer system MgO/Fe/GaAs(001) by means of angle-resolved photoelectron diffraction (XPD) for determining the structure of the individual layers and interfaces. For this task it is necessary to compare the experimental data sets to simulated diffraction patterns of several model structures. In the face of endless possible structures we developed a genetic algorithm that generates and optimizes such model structures in order to fit the experimental data sets. We show the functionality of the algorithm, and the results of the MgO/Fe/GaAs(001) structure determination.

O 91: [MA] Poster II

Time: Friday 11:00–14:00 Location: Poster A

O 91.1 Fri 11:00 Poster A

Inverse tunnel magnetoresistance with Mn_2VGa based magnetic tunnel junctions — •Christoph Klewe, Markus Meinert, Jan Schmalhorst, and Günter Reiss — Department of Physics, Thin Films and Physics of Nanostructures, Bielefeld University, 33501 Bielefeld, Germany

The ferrimagnetic Heusler compound Mn_2VGa is predicted to have a pseudo-gap in the majority carriers [1], which should lead to inverse tunnel magnetoresistance. We synthesized epitaxial Mn_2VGa thin films on MgO(001) substrates by dc magnetron co-sputtering, resulting in nearly stoichiometric films. XRD analysis revealed a mostly B2-ordered structure for the films deposited at substrate temperatures of 350°C, 450°C, and 550°C.

Magnetic tunnel junctions with MgO barrier and CoFe counterelectrodes were fabricated. After post-annealing at up to $T_a = 400°C$ negative TMR was obtained around zero bias, providing evidence for the inverted spin-polarization. Band structures of both electrodes were computed within the coherent potential approximation [2] and used to calculate the TMR vs. U characteristics, which are in good agreement with our experimental findings.

In addition, measurements on GMR-devices fabricated with Cu spacer layers were carried out. The current-in-plane GMR was negative as well, consistent with our TMR results.

[1] K. Özdogan, I. Galanakis, E. Sasioglu, B, Aktas, J. Phys.: Condens. Matter **18**, 2905 (2006). [2] H. Ebert, D. Ködderitzsch, J. Minar, Rep. Prog. Phys. **74**, 096501 (2011).

O 91.2 Fri 11:00 Poster A

Magnetic properties of the full Heusler compounds $Mn_{2+x}V_{1-x}Si$ — •Christian Sterwerf, Markus Meinert, Jan-Michael Schmalhorst, and Günter Reiss — Dünne Schichten und Physik der Nanostrukturen, Fakultät für Physik, Universität Bielefeld, 33501 Bielefeld, Deutschland

Half-metallic Heusler compounds have attracted much interest in the recent years because of their possible applications in spintronic devices. They provide a high spin polarization of the electrons at the Fermi level. A fully compensated half metallic ferrimagnet is ideal for spintronic devices since a vanishing magnetization leads to low stray fields and a lower energy consumption.

Thin films of the ternary full Heusler compound $Mn_{2+x}V_{1-x}Si$ were prepared by DC and RF magnetron co-sputtering on MgO (001) substrates. At $x = 0.5$ the compound has 24 valence electrons per formula unit, resulting in complete magnetic compensation according to the Slater Pauling rule $m = N - 24$.

In this work we investigate the films by means of x-ray diffraction, x-ray reflectometry, magnetometry techniques and transport measurements, especially of the anomalous Hall effect.

O 91.3 Fri 11:00 Poster A

Magneto-optical characterization of single crystalline $Co_2FeAl_{0.4}Si_{0.6}$ thin films on MgO substrates — •Ana Ruiz Calaforra[1], Andres Conca[1], Britta Leven[1], Tanja Graf[2,3], Frederick Casper[2], Claudia Felser[2,4], and Burkard Hillebrands[1] — [1]FB Physik and Landesforschungszentrum OPTIMAS, TU Kaiserslautern, 67663 Kaiserslautern, Germany — [2]Institute of Inorganic and Analytical Chemistry, Johannes Gutenberg-University Mainz, 55099 Mainz, Germany — [3]Graduate School of Excellence - Material Science in Mainz, 55099 Mainz, Germany — [4]Max Planck Institute for Chemical Physics of Solids, 01187 Dresden, Germany

The full Heusler compound $Co_2FeAl_{0.4}Si_{0.6}$ (CFAS) has been predicted to provide a 100% spin polarization with an enhanced temperature stability due to the fact that the Fermi level lies in the middle of the energy gap. Therefore, this material is a promising candidate for TMR- and GMR-devices. For this, the understanding of the magnetic properties of these compounds is of great importance. We present magneto-optical investigations on epitaxial thin CFAS films deposited on MgO (100) substrates with different seed layer materials. A magneto-optical Kerr effect setup with a rotational stage was used to study the magnetocrystalline anisotropy of the sample. An overall uniaxial anisotropy with a biaxial contribution strongly depending on the nature of the used seed layer was observed.

Support by the BMBF project MultiMag (VDI-TZ 13N9913) is acknowledged.

O 91.4 Fri 11:00 Poster A

Evolution of atomic order upon annealing in Co_2MnSi thin films probed by ^{59}Co and ^{55}Mn NMR — •Steven Rodan[1], Alexey Alfonsov[1], Sabine Wurmehl[1], Filippo Ferraro[2], Jürgen Kohlhepp[2], Bert Koopmans[2], Yuya Sakuraba[3], Bosu Subrojati[3], Koki Takanashi[3], and Bernd Büchner[1] — [1]Leibniz

Institute for Solid State and Materials Research (IFW), 01171 Dresden, Germany — [2]Eindhoven University of Technology, 5600 MB Eindhoven, Netherlands — [3]Institute for Materials Research, Tohoku University, 980-8577 Sendai, Japan

Materials with high spin polarization at the Fermi level are highly desirable for spintronics applications. Many intermetallic Heusler compounds, such as Co_2MnSi, exhibit half-metallic ferromagnetism with such large spin polarization, but this tends to depend strongly on the ordering of the atoms in the crystal lattice. Pulsed nuclear magnetic resonance (NMR) proves to be essential for identifying the type(s) of disorder present by investigating the structure locally. We performed ^{59}Co and ^{55}Mn NMR experiments on several annealed and as-cast Co_2MnSi thin films, the results of which together reveal that the atomic ordering evolves with different annealing temperatures. We compare our results with previous structural analysis which used x-ray diffraction.

O 91.5 Fri 11:00 Poster A

Direct investigation of the Co_2MnSi/MgO interface by spin-resolved photoemission — •R. Fetzer[1], J.-P. Wüstenberg[1], T. Taira[2], M. Yamamoto[2], M. Aeschlimann[1], and M. Cinchetti[1] — [1]Department of Physics and Research Center OPTIMAS, TU Kaiserslautern, Erwin-Schrödinger-Str. 46, D-67663 Kaiserslautern — [2]Graduate School of Information Science and Technology, Hokkaido University, Kita 14 Nishi 9, Sapporo 060-0814, Japan

State-of-the-art tunnelling magnetoresistance (TMR) devices based on magnetic full Heusler compounds (e.g. Co_2MnSi) as electrodes and insulating MgO as tunnelling barrier are very promising as advanced spintronic devices [1]. Understanding the spin-dependent electronic properties of Heusler/insulator interfaces is hereby of great importance for further improvement of these multilayer systems. We have studied the Co_2MnSi/MgO (100) interface by means of spin-resolved near-threshold photoemission spectroscopy. The excitation source was laser light with photon energy lower than the MgO band gap width. This allows to investigate directly the spin-dependent electronic properties of the interface as a function of the MgO thickness. We found that the interface spin polarization is positive and can be detected through MgO layers up to 20 ML. Furthermore distinct changes in crystal structure and chemical composition of the epitaxial MgO layer were observed by means of LEED and Auger electron spectroscopy when varying its thickness. We will discuss the connection between the quality of the MgO layer and the detected interface spin polarization.

[1] T.Ishikawa et al., J. Appl. Phys 103, 07A919 (2008)

O 91.6 Fri 11:00 Poster A

Spin-wave propagation in a $Co_2Mn_{0.6}Fe_{0.4}Si$ Heusler waveguide — Thomas Sebastian[1,2], •Philipp Pirro[1], Thomas Brächer[1,2], Alexander A. Serga[1], Burkard Hillebrands[1], Yusuke Ohdaira[3], Hiroshi Naganuma[3], Mikihiko Oogane[3], and Yasuo Ando[3] — [1]FB Physik und Landesforschungszentrum OPTIMAS, TU Kaiserslautern, 67663 Kaiserslautern, Germany — [2]Graduate School Material Science in Mainz, Staudinger Weg 9, 55128 Mainz, Germany — [3]Departement of Applied Physics, Tohoku University, Sendai, Japan

The class of Cobalt-based full Heusler compounds combines high Curie temperatures and spin polarizations with a lower Gilbert damping than most conventional 3d-ferromagnets [1]. These material parameters make them promising candidates in the emerging field of *magnon spintronics*. In this concept, information is transferred and processed via magnons - the excitations of the magnetic system - without flow of electronic currents. Here we present the first observation of spin dynamics in a microstructured Heusler waveguide using Brillouin light scattering microscopy. The low magnetic losses estimated by FMR measurements [2] have been confirmed by the increase of the observed propagation distances (up to 80 μm, with an exponential decay length of at least 10 μm) compared to the commonly used $Ni_{81}Fe_{19}$.

We acknowledge financial support by the *DFG Research Unit 1464: ASPIMATT.*

[1] S. Trudel, J. Phys. D: Appl. Phys. **43**, 1930001 (2010).

[2] T. Kubota, Appl. Phys. Lett. **94**, 122504 (2009).

O 91.7 Fri 11:00 Poster A

Electronic structure, magnetic and transport properties of Heusler compounds $Fe_{3-x}Mn_xSi(x = 0,..,3)$ — •Y. Shapiro[1], G. H. Fecher[1,2], S. Ouardi[1], A. Gloskovskii[1], B. Balke[1], S. Ueda[3], and C. Felser[1,2] — [1]Institute of Inorganic and Analytical Chemistry,Johannes Gutenberg - University, Mainz — [2]Max Planck Institute for Chemical Physics of Solids, Dresden — [3]NIMS Beamline Station at SPring-8, National Institute for Materials Science, Japan.

Heusler compounds are promising materials in many fields of contemporary research. The spectrum of their possible applications ranges from magnetic and magneto-mechanical materials from semiconductors, thermoelectrics to superconductors. The properties of these intermetallic compounds can be altered by changing the degree and kind of chemical order as well as by substituting one element by another.

The substitutional series of polycrystalline Heusler compounds $Fe_{3-x}Mn_xSi(x = 0,...,3)$ were synthesized and experimentally investigated with respect to their electronic and crystalline structure as well as magnetic and transport properties. The crystal structure was determined by means of x-ray diffraction. The temperature dependence of electrical resistivity, Seebeck coefficient, and thermal conductivity were investigated. Hard and soft X-ray photoelectron spectroscopy (HAXPES and MgK_α XPS) was carried out to study the details of the electronic structure and relate it to the transport properties.

O 91.8 Fri 11:00 Poster A

Transport investigations on Mn_3Si — •Frank Steckel, Regina Hermann, Christian G. F. Blum, Steven Rodan, Sabine Wurmehl, Christian Hess, and Bernd Büchner — Leibniz-Institute for Solid State and Materials Research, Dresden, Germany

We investigate the electronic and thermal transport phenomena of the itinerant antiferromagnet Mn_3Si, which has been suggested to be a prototype material for realizing half-metallic ferromagnetism with a spin density wave below 26 K. We measured the resistivity, the Hall-effect as well as the thermal conductivity and the thermopower in the temperature range from 10 K up to 300 K using single crystals. In the vicinity of the antiferromagnetic transition temperature we found clear anomalies in the transport coefficients and a large fluctuation regime which extends to temperatures much higher (up to about 150 K) than the antiferromagnetic ordering temperature.

O 91.9 Fri 11:00 Poster A

Spin calorics in ferromagnetic Heusler alloys on semiconductors — •Yori Manzke, Farshchi Rouin, Ramsteiner Manfred, and Jens Herfort — Paul-Drude-Institut für Festkörperelektronik, Hausvogteiplatz 5-7, 10117 Berlin, Germany

Recently, a spin-based counterpart to the Seebeck effect (SE) has been discovered in various ferromagnetic systems, which can potentially serve to generate spins from waste heat in future spintronic devices. In contrast to the SE, where a temperature gradient leads to a charge potential difference across a material, in the spin-based version (or SSE) a thermal gradient induces a "spin voltage", i.e. a chemical potential difference due to a spin imbalance in the material. However, the SSE is difficult to isolate due to other magnetothermal effects, and special experimental criteria must be met to eliminate such artifacts. Here, we report clear evidence of spin-induced voltages across Pt strips deposited on epitaxially grown Fe_3Si/GaAs hybrid structures. The Pt strips are intended to convert spin currents from the Fe_3Si layer into measurable voltages via the inverse spin Hall effect, while also eliminating magnetothermal artifacts. These voltages depend on the magnetization of the Fe_3Si layer and appear as a consequence of thermal gradients across the sample. Nonetheless, the spatial and temperature dependences of the spin voltages observed in our samples fundamentally differ from those of other materials systems for which the SSE has been reported. Therefore, these findings may be crucial for the understanding of the SSE.

O 91.10 Fri 11:00 Poster A

Pulsed laser deposition of thin film Heusler compounds — •Mirko Emmel, Christian Mix, and Gerhard Jakob — Institut für Physik, Johannes Gutenberg-Universität Mainz, Deutschland

Pulsed laser deposition (PLD) is a versatile technique to deposit thin films of one or more targets illuminated by a focused pulsed-laser beam. Since the energy source is located outside the chamber, the use of ultra-high vacuum is possible. Due to a stoichiometric transfer between target and substrate, PLD allows depositing all kinds of multicomponent materials. We optimized the optical elements, which resulted in higher transmission of the laser energy and a more defined laser spot on the target. At a base pressure of about 10^{-9} mbar we successfully deposited thin films of different Heusler compounds. A further advantage of a PLD system is the capability to use relatively small targets, which are not suitable for other deposition methods like sputtering. The minimum diameter of a PLD-target is defined by the spot size of the laser on the target in order to avoid ablating other material. Hysteresis loops of Co_2FeSi and Rh_2MnGe thin film showed the expected magnetic saturation values. Ellipsometry measurements of Co_2FeSi thin films were performed to determine the permittivity. This work is supported by the DFG research group ASPIMATT and the Stiftung Rheinland-Pfalz für Innovation.

O 91.11 Fri 11:00 Poster A

Magnetic resonance study of highly spin polarized compounds — •A. Alfonsov[1], S. Rodan[1], M. E. Belesi[1], S. Wurmehl[1], V. Kataev[1], F. Ferraro[2], J. T. Kohlhepp[2], H. J. M. Swagten[2], B. Koopmans[2], K. Takanashi[3], B. Subrojati[3], Y. Sakuraba[3], and B. Büchner[1] — [1]IFW Dresden, D-01169 Dresden, Germany — [2]Eindhoven University of Technology, 5600 MB Eindhoven, Netherlands — [3]Institute for Materials Research, Tohoku University, 980-8577 Sendai, Japan

Heusler alloys have attracted a considerable attention in recent years since these compounds can be halfmetallic ferromagnets. Such materials have a theoretical 100% spin polarization at the Fermi level at low temperatures, which gives them a significant potential for spintronics applications. The halfmetallicity strongly depends on the local atomic ordering. Therefore, a precise knowledge of the structural and magnetic ordering also on a local scale is crucial to control the macroscopic physical properties. To obtain this knowledge one has to call for local probe techniques. In this work we present recent nuclear magnetic resonance and electron spin resonance study of various Co-, Mn- and Fe-based Heusler compounds exhibiting different structural disorders and different magnetic ground states.

O 91.12 Fri 11:00 Poster A

Elastic properties and stability of Heusler compounds — •S. -C. Wu[1,2], S. S. Naghavi[1], G. H. Fecher[1,2], and C. Felser[1,2] — [1]Institute of Inorganic Chemistry and Analytical Chemistry, Johannes Gutenberg - University, Mainz — [2]Max Planck Institute for Chemical Physics of Solids, Dresden

The properties of Heusler compounds which are the promising thermoelectric materials are important. Various Heusler compounds are investigated with respect to their malleability and stability. By applying isotropic strain in different ways to the cubic crystal could calculate the elastic constants. The result of the cubic elastic anisotropy can be used to decide the structural stability. The behavior that Young's modulus is largest in the $\langle 111\rangle$-type directions whereas the rigidity modulus is largest in the $\langle 100\rangle$-type directions shows a direct consequence of $A_e > 1$. Zener's ratios of the most stable compounds are in the range of $1.9 < A_e < 2.7$. $A_e < 0$ is not stable and $A_e = 0$ is isotropic. More physical properties could be derived from the calculated elastic constants.

O 91.13 Fri 11:00 Poster A

Antisite disordering in new Fe-based tetragonal Heusler compounds characterised by 57Fe-Mössbauer spectroscopy — •Teuta Gasi, Vadim Ksenoofontov, Jürgen Winterlik, and Claudia Felser — Institut für Anorganische und Analytische Chemie, Johannes Gutenberg Universität, Staudinger Weg 9, 55099 Mainz, Germany

We report on magnetic properties and antisite disordering in tetragonal Heusler Compounds investigated by 57Fe-Mössbauer Spectroscopy. These materials are important because of their potential application in spintronic especially for STT (spin-transfer torque) technology, magnetocaloric or STO etc. New tetragonal Heusler compounds based on Fe and Mn were synthesized by arc-melting and characterized. 57Fe transmission and conversion electron Mössbauer spectroscopy (CEMS) was applied to explore magnetism and local surrounding of Fe atoms in bulk samples. Measurements reveal that the magnetic moments of Fe atoms in these compounds are almost vanishing, whereas in the cubic ones magnetic moments are much higher. Taking into account magnetic susceptibility measurements of Mn based compounds, one can conclude that magnetic moments of Mn atoms are mainly responsible for the bulk magnetization. The Mössbauer data support this observation.

O 91.14 Fri 11:00 Poster A

A General Phase-field Model for the Martensite Rearrangement in Ni_2MnGa — •Christian Mennerich[1], Frank Wendler[1], Marcus Jainta[1], Anna Weisshaar[1], and Britta Nestler[1,2] — [1]Karlsruhe University of Applied Sciences — [2]Karlsruhe Institute of Technology

Ferromagnetic shape memory alloys have gained major interest in the last 15 years as components in actuators and dampers, as they provide large recoverable strains at low operation cost. A multi-phase field model of Allen-Cahn type has been successfully applied to describe the microstructure rearrangement in Ni_2MnGa in the martensitic state, induced by external magnetic or strain fields. The model is based on a Helmholtz free energy density formulation and includes magnetic and elastic energy contributions. With order parameters that are related to the different eigenstrains of the twin variants and the spontaneous magnetization, the time-spatial evolution of the system is described by a set of partial differential equations. The evolution of the order parameters depends on energy contributions for twin interfaces and bulk phase states. To make the complex boundary value problem treatable, different techniques (staggered grids, geometric integration methods, Fast Fourier methods etc) are combined. In this contribution we describe the model, the discretization and numerical implementation. We present simulation results to show the general applicability of the model to the magnetic shape memory effect and stress induced martensite microstructure rearrangement.

O 91.15 Fri 11:00 Poster A

Structural and magnetic properties of zinc ferrite thin films grown by pulsed-laser deposition — •Kerstin Brachwitz[1], Marcus Jenderka[1], Andrey Timopheev[2], Alexandre Azevedo[2], Nikolai Sobolev[2], Annette Setzer[1], Pablo Esquinazi[1], Michael Lorenz[1], and Marius Grundmann[1] — [1]Institut für Experimentelle Physik II, Universität Leipzig, Germany — [2]Departamento de Fisíca and I3N, Universidade de Aveiro, Portugal

Zinc ferrite ($ZnFe_2O_4$) is a promising candidate for the application in magnetic tunnel junctions due to its ferrimagnetic properties. In this regard, we investigated the structural and magnetic properties of $ZnFe_2O_4$ thin films grown by pulsed-laser deposition on different substrates at various substrate temperatures (T_S).

X-ray diffraction measurements reveal an increasing crystalline quality of the films with increasing T_S. Epitaxial single phase $ZnFe_2O_4$ (100) thin films were observed on $SrTiO_3$ (100) substrates, whereas no symmetric $ZnFe_2O_4$ reflexes were observed for thin films deposited on r-plane sapphire independent of T_S.

Magnetic properties were studied by static magnetization and ferromagnetic resonance (FMR) measurements. All films show a strong magnetic ordering, even if the zinc ferrite spinel phase has not been detected. However, energy dispersive X-ray spectroscopy studies reveal a stoichiometric Zn/Fe ratio. FMR measurements revealed fourfold cubic magnetic anisotropy of $ZnFe_2O_4$ thin films grown on $SrTiO_3$. The values of effective magnetization and cubic anisotropy have been determined from a detailed study of the FMR spectra.

O 91.16 Fri 11:00 Poster A

Theoretical and experimental investigation of ultrathin iron fcc films — •Michael Vogel, Matthias Kronseder, Florian Freund, Georg Woltersdorf, and Christian Back — Universität Regensburg

The magnetic properties of ultrathin films are determined in essence by the magnetic anisotropy constant, magnetic moment and the exchange interaction integral. Due to the challenging experimental accessibility of these parameters and the fact that none of these parameters can be obtained separately, the combination of experimental and theoretical methods can be used [1]. Optical (MOKE) and photoemission (MCD) measurements combined with ab initio calculations (DFT-VASP) [2] leads to a full understanding of the magnetic behavior of this system. For the theoretical investigation of the interatomic exchange interactions and the magnetic moment we have modeled those as a function of the involved strain in thin films. Assuming a ferromagnetic state of thin films as demonstrated experimentally in [3], we have calculated the exchange interaction from first principles by rotating moments within specially constructed supercells, based on structural data achieved by I(V)-LEED measurements also done in [3]. In addition the exchange interactions have also been determined using a "spin-spiral" technique [4].

[1] H. L. Meyerheim et al., PRL 103, 267202 (2009) [2] G. Kresse et al., Comp. Mater. Sci. 6, 15 (1996). [3] S. Müller et al., Phys. Rev. Lett. 74, 765 (1995). [4] L.M. Sandratskii, J. Phys. Condens. Matter 3, 8565 (1993); J. Phys. Condens. Matter 3, 8587 (1993).

O 91.17 Fri 11:00 Poster A

Magnetic properties of thin iron films on strontium titanate substrates — •Armin Haase, Kay Potzger, Oskar Maciej

Liedke, and Rantej Bali — Institut für Ionenstrahlphysik und Materialforschung, Helmholtz-Zentrum Dresden-Rossendorf

In this study, the magnetic moment of thin iron films will be investigated. The methods of preparing the strontium titanate substrate surfaces for layer growth, creating near-surface defects, and growing thin iron films will be described. A procedure for surface preparation using a sequence of etching and annealing steps in an oxygen-rich environment will be introduced. The defects were created using ion implantation, and the samples were tested for defect magnetism. A magnetic moment was determined for hydrogen with the fluency of $2 \times 10^{17}\,\frac{1}{\mathrm{cm}^2}$ and the energy of 1,2 keV. Nitrogen implantation did not produce defect magnetism. In a separate process, iron layers of varying thicknesses were grown and investigated for their groth modes and magnetic properties. Finally, the steps described above were combined and repeated.

O 91.18 Fri 11:00 Poster A

Magnetic and structural properties of Fe$_{1-x}$Tb$_x$ and Fe$_{0.82-x}$Co$_{0.18}$Tb$_x$ thin films — •Birgit Hebler[1], Christian Schubert[1], Herbert Schletter[1], Florin Radu[2], Andreas Liebig[1], and Manfred Albrecht[1] — [1]Institute of Physics, Chemnitz University of Technology, D-09107 Chemnitz, Germany — [2]Hemholtz-Zentrum Berlin für Materialen und Energie, Albert-Einstein-Str.15, D-12489 Berlin, Germany

Amorphous rare earth-transition metal alloys with perpendicular magnetic anisotropy exhibit a versatile magnetic configuration making them interesting materials for exchange coupled heterostructures used in spintronic devices. We present an investigation of Fe$_{1-x}$Tb$_x$ and Fe$_{0.82-x}$Co$_{0.18}$Tb$_x$ thin films with a varying content of terbium (16 at. % < x < 30 at. %). The 20 nm thin films were prepared by magnetron co-sputtering in a UHV-chamber at room temperature. X-ray diffraction measurements and transmission electron microscopy imaging in cross-section geometry show an interdiffusion of the platinum protecting layers into the amorphous films at the interface. The temperature dependence of the magnetization reversal process was obtained by SQUID-VSM measurements in a maximum applied field of 7 T from 4 K to 400 K. Around the compensation temperature an anomalous reversal behavior was observed at higher fields, which may be assigned to a spin flop transition in the sperimagnetic configuration.

O 91.19 Fri 11:00 Poster A

Investigations of magnetism in multiferroic layer systems — •Martin Welke[1], Joachim Gräfe[1], Vasili Hari Babu[1], Remya Kunjuveettil Govind[2], Martin Trautmann[2], Francis Bern[3], Michael Ziese[3], Karl-Michael Schindler[2], and Reinhard Denecke[1] — [1]Wilhelm-Ostwald-Institut für Physikalische und Theoretische Chemie, Universität Leipzig — [2]Institut für Physik, Universität Halle — [3]Institut für Physik, Universität Leipzig

Systems with multiferroic properties are of interest for research since the 60s of the 20th century. In the starting time single crystal multiferroics were in the focus of research. Nowadays layer systems with ferroelectric and ferromagnetic components are also studied.

The work presented deals with different ferrite layers - namely Nickelferrite and Cobaltferrite - on Bariumtitanate (001). Preparation of the ferrite films was done by PLD in UHV. Subsequently they were measured by SQUID in order to obtain magnetization loops. From temperature-dependend data, there seems to be an influence of the phase transitions of Bariumtitanate on the magnetic response of the ferrite films. Altogether Nickelferrite and Cobaltferrite appear to have a small remanent magnetization.

In order to additionally characterize these materials XPS measurements were carried out. Especially the Iron to Oxygen ratio is of interest.

Furthermore XAS measurements of thick ferrite layers were taken into account.

O 91.20 Fri 11:00 Poster A

Magnetic anisotropy of strained La$_{0.7}$Sr$_{0.3}$CoO$_3$ thin films probed by XMCD — •Felix Eilers[1,2], Michael Merz[1], Dirk Fuchs[1], Hilbert von Löhneysen[1,3], Peter Nagel[1], and Stefan Schuppler[1] — [1]KIT, Institut für Festkörperphysik — [2]KIT, Fakultät für Physik — [3]KIT, Physikalisches Institut, Karlsruhe, Germany

The magnetic properties of perovskite-type La$_{1-x}$Sr$_x$CoO$_3$ have their origin in the variety of possible valence and spin states of the Co ion and in strong electronic correlations. Bulk La$_{0.7}$Sr$_{0.3}$CoO$_3$ is known to be a ferromagnetic metal below $T_C \approx 240\,\mathrm{K}$ and to exhibit large Joule magnetostriction. This motivated us to investigate a complementary magnetoelastic effect: the effect of biaxial strain on the magnetization.

La$_{0.7}$Sr$_{0.3}$CoO$_3$ thin films were grown on lattice-mismatched substrates (LaAlO$_3$ and LSAT) by pulsed laser deposition. X-ray diffraction confirmed the films to be subjected to compressive or tensile strain, respectively. Near-edge x-ray absorption fine structure (NEXAFS) and x-ray magnetic circular dichroism (XMCD) at the Co $L_{2,3}$ edge and the O K edge provided spectroscopic information on the electronic and magnetic structure. Sum rules were used to extract magnetic moments from the XMCD spectra. The difference between in-plane and out-of-plane magnetic moments was found to vary with the biaxial strain.

We gratefully acknowledge the Max Planck Institute for Intelligent Systems (E. Goering, T. Tietze, G. Schütz) for the use of their XMCD end station and the synchrotron light source ANKA for the provision of beam time.

O 91.21 Fri 11:00 Poster A

Temperature and thickness dependent sign change of the Anomalous Hall Effect in Co/Pd multilayers — •Vedat Keskin[1,2], Bekir Aktas[2], Zoe Kugler[1], Jan-Michael Schmalhorst[1], and Günter Reiss[1] — [1]Thin Films & Physics of Nanostructures, Bielefeld University, Germany — [2]Gebze Institute of Technology, Izmit, Turkey

The anomalous Hall effect (AHE) [1] was studied on ultra-thin Co/Pd multilayers, which might be a promising material for AHE based perpendicular magnetic recording technology [2]. The Co/Pd multilayers were grown on Si wafers by using conventional dc magnetron sputtering techniques. We focused on the Co thickness and temperature dependence of the AHE and the longitudinal resistivity, whereas the Pd thickness was kept constant at 1.8nm. The Co thickness was incrementally increased from 0.20nm to 0.55 nm. The AHE measurements were carried out in the temperature range of 14-330 K.Uniquely, we have observed that for a fixed temperature the polarity of the AHE changes at a certain Co thickness, the critical Co thickness decreases with increasing temperature. This behavior will be discussed with respect to the influence of extrinsic skew scattering [3]. [1] E. H. Hall, Philos. Mag. 10, 301 (1880) [2] D. Rosenblatt, M. Karpovski, and A. Gerber, Appl. Phys. Lett. 96, 022512 (2010) [3] J. Smit, Physica (Amsterdam) 24, 39 (1958).

O 91.22 Fri 11:00 Poster A

X-ray absorption and magnetic circular dichroism of perpendicular Mn$_{3-x}$Ga thin films — •Daniel Ebke, Manuel Glas, Jan Schmalhorst, Markus Meinert, Patrick Thomas, and Günter Reiss — Thin Films and Physic of Nanostructures, Bielefeld University, 33615 Bielefeld, Germany

Recently, the integration of materials with perpendicular magnetic anisotropy into magnetic tunnel junctions (MTJs) has found a lot of attraction due to the predicted lower current densities for spin torque switching and higher thermal stability. Especially, the interface of the electrodes to the tunnel barrier play a key role for the realization of MTJs with high tunneling magneto resistance (TMR) ratios. In this work, we have investigated the chemical and magnetic interface properties of perpendicular magnetized Mn$_{3-x}$Ga (x=0-1) thin films for MgO based MTJs as a function of deposition temperature and stoichiometry. The results will be compared to the corresponding magnetic bulk properties and the crystallographic ordering.

O 91.23 Fri 11:00 Poster A

Hall effect studies in ultrathin LSMO/SRO superlattices — •Francis Bern[1], Michael Ziese[1], and Ionela Vrejoiu[2] — [1]Division of Superconductivity and Magnetism, University of Leipzig, 04103 Leipzig, Germany — [2]Max Planck Institute of Microstructure Physics, 06120 Halle, Germany

A variety of ultrathin multilayer films have been produced by pulsed laser deposition. The itinerant ferromagnet SrRuO$_3$ (SRO) and the double-exchange ferromagnet La$_{0.7}$Sr$_{0.3}$MnO$_3$ (LSMO) were grown on SrTiO$_3$ (STO), both in single layers as well as in superlattices. Characterization by magnetotransport measurements indicate a structural transition due to strain in the ultrathin layers. The complex temperature dependence of the anomalous Hall coefficient suggests changes in the electronic structure and/or a conducting interfacial layer at the LSMO/SRO interface.

O 91.24 Fri 11:00 Poster A

CPP – GMR using the Heusler alloy Co$_2$FeAl$_{0.4}$Si$_{0.6}$. — •F.

Casper[1], K. Rott[2], G. Reiss[2], and C. Felser[1,3] — [1]Institute of Inorganic Chemistry and Analytical Chemistry, Johannes Gutenberg - University, Mainz, Germany — [2]Department of Physics, Bielefeld University, Bielefeld, Germany — [3]Max Planck Institute for Chemical Physics of Solids, Dresden, Germany

Large tunneling magneto resistance (TMR) values were reported from magnetic tunneling junctions (MTJs) using Heusler alloys, which indicates a high spin polarization of the electrode materials. These high spin polarized materials should also enhance current-perpendicular-to-plane giant magneto resistance (CPP GMR). Most of these experiments were performed on small MgO-substrates which are not suitable for an industrial application. We implemented the Heusler compound $Co_2FeAl_{0.4}Si_{0.6}$ (CFAS) into an industrial production. A twelve inch target is used to sputter a Cr(10)/Ag(50)/CFAS(10)/Ag(5)/CFAS(10)/Ru(8) spin valve structure on silicon and MgO wafers. The structure of the films was determined by x-ray diffraction. The film was microfabricated to form a pillars with the size of 0.2 X 0.1 μm^2 up to 1.0 X 0.4 μm^2 for the measurement of CPP-GMR. Depending on the annealing temperature the TMR ratio reaches values of 7% on MgO and 1.2% on Si wafers at room temperature. This work is supported by the Federal Ministry for Education and Research BMBF, project "'Multimag"'.

O 91.25 Fri 11:00 Poster A

Slow Relaxation Effects in CMR Manganite Films and Superlattices

— •Markus Jungbauer, Felix Koeth, Sebastian Hühn, Markus Michelmann, and Vasily Moshnyaga — I. Physikalisches Institut, Universität Göttingen

Colossal magnetoresistance (CMR) and complex magnetic/electric state close to the I. order phase (metal-insulator) transition in ferromagnetic perovskite manganites are still puzzling phenomena. We studied epitaxial films of $(La_{1-y}Pr_y)_{0.7}Ca_{0.3}MnO_3/MgO(100)$ (y=0.4-0.6) with respect to their magnetotransport and magnetooptic properties with special focus on the relaxation effects. Close to the metal-to-insulator transition temperature, T_{MI}, application of magnetic field, $B = 0 - 1\,T$, leads to a relaxation of the electrical resistivity on a timescale, $\tau \approx 100\,s$. Considering the observed temperature hysteresis of resistance and magnetization close to T_C as well as an anomalous increase of coercive field and low-field CMR in the vicinity of T_{MI} a following semi-quantitative picture of the complex magnetic state close to the phase transition was developed: the nanoscopic single-domain ferromagnetic clusters are coupled antiferromagnetically by a short-range-ordered correlated polaronic phase with a thickness of few monolayers. By growing digital $(FMM/AFMCOI)_N$ superlattices with FMM = $La_{0.7}(Ca,Sr)_{0.3}MnO_3$ and AFMCOI = $Pr_{1-x}Ca_xMnO_3$ (x=0.3-0.7) we try to reproduce and to tune this unique magnetic state with the main aim to obtain the enhanced low-field CMR close to room temperature. A financial support from EU FP7 via the Project IFOX (interfacing oxides) is acknowledged.

O 91.26 Fri 11:00 Poster A

Tailoring perpendicular anisotropy in Co/Pd multilayers by ion irradiation

— •Julia Osten[1], Peter Greene[2], Tamio Endo[3], Nobuyuki Iwata[4], Kilian Lenz[1], Kai Liu[2], and Jürgen Fassbender[1] — [1]Institute of Ion Beam Physics and Materials Research HZDR, Dresden, Germany — [2]U.C. Davis Physics Department, Davis, CA, USA — [3]Mie University, Tsu, Mie, Japan — [4]Nihon University, Funabashi, Chiba, Japan

A major obstacle towards the increase in areal magnetic recording density and the decrease in bit size is the retention of thermal stability while maintaining reasonable write fields. Materials with graded magnetic anisotropy are promising candidates to solve this problem. Here we demonstrate the approach of using post-deposition Ar-ion irradiation to tailor the perpendicular anisotropy in Co/Pd multilayer thin films. The films, with uniform as well as graded perpendicular anisotropy, were synthesized by magnetron sputtering. Based on TRIDYN simulations, different primary ion energies (1-25 keV) are chosen to achieve varying penetration depths of the ions creating a depth dependent anisotropy grading. Before and after ion irradiation, MOKE as well as magnetometry measurements were employed to detect the changes of the magnetic properties. Upon ion irradiation, the Co/Pd films exhibit reduced coercivity and remanence with increasing fluence. Higher ion energies have a more pronounced effect on reducing the perpendicular anisotropy.

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O 91.27 Fri 11:00 Poster A

Method to separate the anomalous Hall signal of different Co/Pt nanodots

— •Carsten Thönnissen[1], Alexander Neumann[1], Simon Hesse[1], Andreas Meyer[2], and Hans Peter Oepen[1] — [1]Institut für Angewandte Physik, Universität Hamburg, Germany — [2]Institut für Physikalische Chemie, Universität Hamburg, Germany

On nanosized Hall crosses (<100nm) made via electron beam lithography (EBL) nanodots are created, which can be magnetically investigated with single dot sensitivity via anomalous Hall effect (AHE). The nanodots were fabricated from thin Co/Pt films using SiO_2 particles as shadow mask for Ar^+ ion milling at 150eV [1]. Due to the fact that the number of nanodots in the sensitive area of the cross varies between one and five it is necessary to separate the signals of the different nanodots. For that purpose we use a measurement setup similar to the van der Pauw method. The DC current is sent through adjoining legs of the Hall cross and a voltage drop is measured across the other legs. The obtained signal is proportional to the current through the dot and depends on the local current direction at the position of the dot. By cyclic permutation we obtain different signal ratios which allow us to identify the individual particles. By means of micrographs taken by scanning electron microscopy we identify the position and arrangement of the dots, which is used to simulate the voltage that has to be expected for the different geometries.

[1] H. Stillrich *et al.* Adv. Funct. Mat. **18**, p76-81, (2008).

O 91.28 Fri 11:00 Poster A

Single wire and ensemble measurements on NixCo1-x nanowires for the determination of switching field distributions

— •Philip Sergelius[1], Tim Böhnert[1], Stephan Martens[1], Victor Vega Martinez[2], Kornelius Nielsch[1], and Detlef Görlitz[1] — [1]Institute of Applied Physics, University of Hamburg, Hamburg, Germany. — [2]Depto. Física, Universidad de Oviedo, Oviedo, Spain.

NixCo1-x nanowires with x varying between 0.05 and 0.77 have been synthesized by potentiostatic electrodeposition into self ordered Al2O3 Membranes (AAO) by hard anodization. The variation of the Ni:Co composition in the alloyed nanowires of appr. 20μm length, 150nm diameter and 305 nm spacing allows for a tuning of the switching field along the wire axes between 190 Oe and 400 Oe.

We performed First Order Reversal Curve (FORC) measurements on the nanowire ensembles in a VSM (Quantum Design VersaLab). The FORC analysis yields the distribution of the coercive fields for all nanowires in the membrane and the distribution of their interaction fields. Additionally, MOKE analyses utilizing a NanoMOKE2TM (Durham Magneto Optics Ltd) were performed on up to 100 singular wires of each ensemble in order to have adequate statistics for the distribution of coercivities ranging from 150 Oe to 450 Oe. The obtained coercivity distributions with widths of appr. 18 % from the FORC and MOKE measurements are discussed and compared revealing the impact of different interaction fields in the investigated templates.

O 91.29 Fri 11:00 Poster A

Investigation of the influence of dipolar interactions on the magnetic behavior of Ni nanorods

— •Florian Krämer, Philipp Bender, Andreas Tschöpe, and Rainer Birringer — Universität des Saarlandes, Saarbrücken

Ni nanorods with diameters < 42nm are expected to be uniaxial ferromagnetic single domain particles. In recent years, the magnetic properties of Ni nanorods in porous alumina templates were extensively studied. However, the investigation of characteristic magnetic properties was hampered by the large dipolar interactions (DI) due to the dense packing of the rods in the template. We synthesized Ni nanorods (D =19 nm) by current-pulsed electrodeposition of Ni into ordered porous alumina templates. The filled templates were characterized by static magnetization measurements (SMM) as a modelsystem of uniaxial ferromagnets with significant DI. Then, the nanorods were released from the templates by dissolution of the alumina in aqueous NaOH, dispersed in 20 wt% gelatine solutions @60°C and aligned paralell by an external homogenous magnetic field during gelation. These gels were also characterized by SMM as an corresponding system of uniaxial ferromagnets with negligible DI. The objective of this work was to study the influence of DI on the magnetic properties of such uniaxial ferromagnetic particles. We measured the remanence and the coercivity as a function of the angle between the rodaxis and the external field, the switching field distribution, the shape anisotropy constant and the activation volume.

O 91.30 Fri 11:00 Poster A

Magnonic modes in rectangular antidot lattices — •Jelena Panke, Benjamin Lenk, Nils Abeling, and Markus Münzenberg — I. Physikalisches Institut, Georg-August-Universität Göttingen

On the way towards spin-wave logic devices an understanding of mechanisms for the manipulation and guiding of spin waves is of crucial importance. Femtosecond laser pulses are used to optically excite (pump) and subsequently measure (probe) magnetization dynamics on timescales as long as nanoseconds. Two-dimensional arrays of antidots in a ferromagnetic film provide a periodic "potential" to the excited spin waves and induce drastic changes in the magnetization dynamics.

In the spin wave spectra of rectangular CoFeB antidot lattices different modes are observed which are influenced by the variation of material parameters (filling fraction, antidot diameter, lattice parameter). We focus on these Bloch-like modes and investigate the spin-wave population for different directions of the external field. By applying the external field along the long or short axis $a_{1,2}$ of the rectangular lattice a magnonic mode appears with a wave vector $k = \pi/a_{1,2}$ at the boundary of the first Brillouin zone for each respective direction. Therefore it is possible to tune the Bloch modes only by rotating the external field. Furthermore, band structure calculations are used to investigate the changed dispersion on the patterned media as compared to the continuous film. The periodic lattice structure induces band gaps at the zone boundary that are also sensitive to the field direction and can explain the prefered population of the magnonic modes.

O 91.31 Fri 11:00 Poster A

Influence of the dipolar interaction on the quasi-static magnetic properties of elliptical microstructures in dense packed arrays — •Andres Conca, Thomas Sebastian, Georg Wolf, Britta Leven, and Burkard Hillebrands — FB Physik und Landesforschungszentrum OPTIMAS, TU Kaiserslautern, 67663 Kaiserslautern, Germany

Elliptical magnetic structures with dimensions of a few micrometers play a crucial role in the design of magnetic field sensors and in data storage applications such as MRAM cells. The magnetic properties of such structures are mostly controlled via the shape anisotropy. In many cases, a high packing density is required. However the effect of dipolar interaction between the individual elements within the array due to stray fields can be very strong when the distances are of only a few micrometers.

We present measurements of the influence of the packing density on the coercive field H_C of elliptical elements in arrays. For this purpose, 5×5 arrays of elliptical elements were prepared with varying interelement distances. The arrays were structured using e-beam lithography from a 5 nm thick polycrystalline CoFeB thin film deposited on a Si substrate. The measurements were performed with a μMOKE setup equipped with a micro-focused HeNe-laser beam with a spotsize of 1 μm.

O 91.32 Fri 11:00 Poster A

Magnetic Films on Nanoperforated Substrates — •Carsten Schulze[1], Marco Faustini[2], Michael Grobis[3], Denys Makarov[4], David Grosso[2], and Manfred Albrecht[1] — [1]Institute of Physics, Chemnitz University of Technology, 09107 Chemnitz, Germany — [2]Laboratoire de Chimie de la Matière Condensée de Paris, Université Pierre et Marie Curie-Paris 6, CNRS, 75252 Paris Cedex 05, France — [3]San Jose Research Center, Hitachi GST, San Jose, CA 95135, USA — [4]IFW Dresden, Helmholtzstr. 20, 01069 Dresden, Germany

A study of the magnetization reversal in ferromagnetic thin films with perpendicular magnetic anisotropy deposited onto substrates with densely distributed nanoperforations is presented. The nanoperforated substrates are fabricated by a wet-chemical evaporation induced self-assembly process of block-copolymer micelles, Co/Pt multilayers are used as ferromagnetic thin films. The pinning of magnetic domain walls on the substrate-induced defects has been shown earlier [1, 2], as well as the possible application of such a system as a percolated perpendicular recording medium [3, 4].

Here, the dependence of the pinning strength on the interplay between saturation magnetization, anisotropy, domain wall width and perforation size will be discussed.

[1] D. Makarov *et al.*, *IEEE Trans. Magn.* **45** (2009) 3515.
[2] C. Schulze *et al.*, *Nanotechnology* **21** (2010) 495701.
[3] D. Suess *et al.*, *J. Appl. Phys.* **99** (2006) 08G905.
[4] M. Grobis *et al.*, *Appl. Phys. Lett.* **98** (2011) 192504.

O 91.33 Fri 11:00 Poster A

Ion beam irradiation of interlayer exchange coupled trilayers in the sub-micron regime — •Roland Neb[1], Thomas Sebastian[1], Philipp Pirro[1], Stefan Pofahl[2], Rudolf Schäfer[2], Bernhard Reuscher[3], and Burkard Hillebrands[1] — [1]TU Kaiserslautern, Landesforschungszentrum Optimas, 67663 Kaiserslautern, Germany — [2]IFW Dresden, 01069 Dresden, Germany — [3]IFOS Kaiserslautern, 67663 Kaiserslautern, Germany

Focused ion beam irradiation is a well known tool for patterning thin film media. We use this tool to pattern an antiferromagnetically coupled Fe/Cr/Fe trilayer in the micron and sub-micron regime. The irradiated areas become ferromagnetic, allowing for the creation of well-defined ferromagnetic areas in an antiferromagnetically coupled environment. The suitability of such irradiated elements for information storage was investigated. We found that if certain conditions for the patterning process are met, sub-micron elements are able not only to store information but also to be overwritten by a sufficiently high magnetic field. The resulting bit density is strongly dependent on the applied ion dose, changing by a factor of 100 in the regime of 10^{14} to 10^{16} ions/cm^2.

Financial support by the Deutsche Forschungsgemeinschaft, the Graduate School *Material Science in Mainz* and the Graduiertenkolleg 792 is gratefully acknowledged.

O 91.34 Fri 11:00 Poster A

Mechanical deformation of Dy nanocontacts in magnetic field — Marc Müller[1], •Oliver Berg[1], Christoph Sürgers[1], and Hilbert v. Löhneysen[1,2] — [1]Karlsruhe Institute of Technology, Physikalisches Institut and Center for Functional Nanostructures, D-76049 Karlsruhe — [2]Karlsruhe Institute of Technology, Institut für Festkörperphysik, D-76021 Karlsruhe

Recently, we demonstrated the reproducible tuning of the electrical conductance of Dy nanocontacts in a magnetic field by exploiting the large magnetostriction of Dy [1]. Here we report on the dependence of the contact shape on an applied magnetic field. The nanocontacts were obtained from Dy wires by the mechanically controlled break-junction technique. In zero magnetic field we find the usual variation of the conductance G vs. electrode distance x while breaking the wire mechanically, with a sequence of steps and more or less prominent conductance plateaus. From the behavior $G(x)$ we estimate the shape of the nanocontact after several cycles of mechanical deformation of the wire. We find that the final shape of the nanocontact depends on the strength and orientation of an applied magnetic field. This shaping under alternating tensile and compressive stress is attributed to the rearrangement of magnetic domains in magnetic field during formation of the nanocontact by magnetoelastic coupling.

[1] M. Müller et al., Nano Letters **11**, 547 (2011)

O 91.35 Fri 11:00 Poster A

Rolled-up tubes and cantilevers from magnetic $SrRuO_3$-$Pr_{0.7}Ca_{0.3}MnO_3$ films — Christoph Deneke[1,4], •Kathrin Dörr[2], Elisabeth Wild[3], Stefan Baunack[3], Angelo Malachias[4], and Oliver Schmidt[3] — [1]Laboratorio Nacional de Nanotecnologia, Caixa Postal 6192, Campinas, S.P., Brazil — [2]MLU Halle-Wittenberg, Halle, Germany — [3]Institute for Integrative Nanosciences, IFW Dresden, Dresden, Germany — [4]Laboratorio Nacional de Luz Sincrotron, Caixa Postal 6192, Campinas, S.P., Brazil

Three-dimensional microobjects are fabricated by the controlled release of inherently strained $SrRuO_3/Pr_{0.7}Ca_{0.3}MnO_3/SrRuO_3$ trilayers from $SrTiO_3(001)$ substrates. Cantilevers and rolled-up microtubes with a diameter of 6-8 μm are demonstrated. The etching behavior of the $SrRuO_3$ film is investigated and a selectivity of 1:9100 with respect to the $SrTiO_3$ substrate is found. The initial and final strain states of the rolled-up oxide layers are studied by x-ray diffraction on an ensemble of tubes. Relaxation of the sandwiched $Pr_{0.7}Ca_{0.3}MnO_3$ layer towards its bulk lattice parameter is observed as the major driving force for the roll-up of the trilayers. Finally, microdiffraction experiments reveal that a single object can represent the ensemble proving a good homogeneity of the rolled-up tubes.

O 91.36 Fri 11:00 Poster A

Interaction of Josephson and magnetic oscillations in Josephson tunnel junctions with a ferromagnetic layer — •Sebastian Mai, Ervand Kandelaki, Anatoly Volkov, and Konstantin Efetov — Theoretische Physik III, Ruhr-Universität Bochum, 44780

Bochum, Deutschland

We studied the dynamics of Josephson junctions with a thin ferromagnetic layer F (SFIFS junctions). In such junctions, the phase difference ϕ of the superconductors and magnetization M in the F layer are two dynamic parameters coupled to each other. We derived equations describing the dynamics of these two parameters and calculated the modified current-voltage (I-V) characteristics in the presence of a weak magnetic field (Fiske steps). We showed that the magnetic degree of freedom not only changes the form of the Fiske steps but also the overall view of the I-V curve (new peaks related to the magnetic resonance appear). We also calculated the power P absorbed in the system if a microwave radiation with an ac in-plane magnetic field is applied (magnetic resonance). The obtained formula for the power P essentially differs from the one which describes the power absorption in an isolated ferromagnetic film. In particular, this formula describes the peaks related to the excitation of standing plasma waves as well as the peak associated with the magnetic resonance.

O 91.37 Fri 11:00 Poster A

Molecular Dynamic Simulation of atomic deposition between MnAs cluster — •Andreas Rühl and Christian Heiliger — I. Physikalisches Institut, Justus Liebig University Giessen, D-35392, Germany

MnAs is a promising ferromagnetic material for magnetoelectronic devices, in particular as nano-scaled clusters, providing a great tunability concerning the shape and position. We investigate hexagonal MnAs clusters which are separated by a metal. Such structures could be produced by using a FIB (focused ion beam) two disconnect two touching MnAs clusters and to deposit a metal between them. We succesfully implemented a molecular dynamic program to simulate the atomic deposition of the metal atoms on the surface of the MnAs cluster. The necessary effective interaction potentials between the simulation participants are gained by means of a force matching method, where the effective potentials are fitted to ab initio data.

O 91.38 Fri 11:00 Poster A

Spin-resolved photoemission study of Bis(phthalocyaninato) terbium(III) (TbPc$_2$) deposited on Co/Cu(001) — •Nicolas Grossmann[1], Sabine Steil[1], Norman Haag[1], Mirko Cinchetti[1], Mario Ruben[2], and Martin Aeschlimann[1] — [1]Department of Physics and Resarch Center OPTIMAS, University of Kaiserslautern, 67663 Kaiserslautern, Germany — [2]Institut of Nanotechnology, Karlsruhe Institute of Technology, 76344 Eggenstein-Leopoldshafen

We have studied the formation of the electronic structure of the interface between an epitaxially grown Co(001) thin film and the single molecular magnet Bis(phthalocyaninato)terbium(III) (TbPc$_2$). The organic semiconductor was progressively grown on the cobalt substrate. The grown interfaces have been characterized by means of spin-resolved ultraviolet photoemission. For every growth step we have monitored the changes in the work function, the energetic position of the occupied molecular orbitals and interface states, and the changes in the cobalt spin polarization induced by interface formation. The most striking result is the presence of an occupied spin polarized hybrid interface state with a negative spin polarization, lying 0,7 eV below the Fermi level. The spin polarization of this state shows a pronounced temperature dependency. Our results agree with the recent observation of an antiferromagnetic coupling between TbPc$_2$ and a ferromagnetic metal substrate reported in [1].

[1] Gambardella et al., Phys. Rev. Lett. 107, 177205 (2011)

O 91.39 Fri 11:00 Poster A

Organic molecular beam deposition of a paramagnetic organic magnet — Sabine-Antonia Savu[1], •Reza Kakavandi[1], Indro Biswas[1], Mathias Glaser[1], Lorenzo Sorace[2], Matteo Mannini[2], Andrea Caneschi[2], Thomas Chassé[1], and Maria Benedetta Casu[1] — [1]IPTC, University of Tübingen, Tübingen, Germany — [2]LAMM, University of Florence, Florence, Italy

Nitronyl nitroxide radicals are an interesting class of organic compounds because of their magnetic properties. In this work we present a soft X-ray investigation of thin films of a pyrene derivative of the nitronyl nitroxide radical (nitpyrene), deposited onto well characterized single crystals surfaces, using strictly controlled evaporation conditions. We approach the deposition of nitpyrene using the knowledge obtained during the last years on thin film processes of organic molecules. The electronic structure and the interaction with the surface are discussed. By analyzing the attenuation of the XPS substrate signal, we find indications for island plus layer growth mode, supported by AFM measurements. We have also investigated the molecular orientation of the pyrene part versus film thickness, identifying the strength of molecule-molecule interactions versus molecule-substrate interactions by using X-ray absorption and photoemission spectroscopies.

O 91.40 Fri 11:00 Poster A

Electron Localization in a Charge Transfer Salt on Au(111) — Tobias R. Umbach[1], Isabel Fernandez-Torrente[1], •Michael H. Kleinert[1], Ricardo Rurali[2], Mats Persson[3], Jose I. Pascual[1], and Katharina J. Franke[1] — [1]Institut für Experimentalphysik, Freie Universität Berlin, Arnimallee 14, 14195 Berlin, Germany — [2]Institut de Ciencia de Materials de Barcelona, Campus de Bellaterra, 08193 Bellaterra (Barcelona), Spain — [3]The Surface Science Research Center, The University of Liverpool, L69 3BX, United Kingdom

Alkali metals are perfect candidates for varying the electronic structure in molecular environments. Acting as electron donors with a low ionization potential, they easily build charge transfer complexes under the presence of an acceptor molecule. We investigated such a charge transfer process in a monolayer of the acceptor molecule 7,7,8,8,-tetracyanoquinodimethane (TCNQ) doped with Na on a Au(111) surface, using low-temperature scanning tunneling microscopy and spectroscopy. The self-assembled Na-TCNQ phase shows a Kondo resonance centered on the cyano-terminations of the TCNQ molecules, which proves the presence of an unpaired electron in the complex. Ab initio calculations corroborate the transfer of the Na's 3s electron to the organic acceptor and reveal its localization at the cyano groups.

O 91.41 Fri 11:00 Poster A

Transport properties of novel Anthraquinone based molecular switches — •Simon Liebing[1], Torsten Hahn[1], Nadine Seidel[2], Tim Ludwig[3], and Jens Kortus[1] — [1]Institut for Theoretical Physics, TU Bergakademie Freiberg, 09596 Freiberg, Germany — [2]Institut for Organic Chemistry, TU Bergakademie Freiberg, 09596 Freiberg, Germany — [3]Institute for Theoretical Physics, TU Dresden, 01062 Dresden, Germany

Anthraquinone derivatives were recently reported to be good candidates for application as molecular switches [1]. We present a novel molecular system based on the anthraquinone-core π conjugated spacers and linkers units. The influence on the transport properties of model junctions by chemical modifications of the anthraqunine-core as well as the impact of difficult linker units is discussed. The authors show how chemical modifications can be used for Fermi level and band gap engineering. The theoretical results based on DFT [2] and NEGF [3] calculations are used to suggest further optimizations of the molecular system.

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O 91.42 Fri 11:00 Poster A

Simulation of STM images and STS spectra of Metal-Phthalocyanine molecules on different substrates - comparing the DFT/NEGF and QME approach — •Torsten Hahn[1] and Tim Ludwig[2] — [1]Institute of Theoretical Physics, TU Bergakademie Freiberg, Freiberg, Germany — [2]Institute of Theoretical Physics, TU Dresden, Dresden, Germany

STM (scanning tunneling microscopy) and STS (scanning tunneling spectroscopy) experiments are the methods of choice to study the transport characteristics of single molecules in an well defined environment [1]. Metal Phthalocyanines are known to be promising candidates for applications in molecular spintronics. The interpretation of measured STM/STS data is crucial for the understanding of material properties. We compare theoretical results obtained from DFT - NEGF (density functional theory - non equilibrium green functions formalism) [2] and QME (quantum master equation) [3] investigations and discuss their impact on the interpretation of experimental data.

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[3] Timm, Phys. Rev. B 77, 195416 (2008)

O 91.43 Fri 11:00 Poster A

Quantitative MFM on superconducting thin films — •Henry Stopfel[1], Silvia Vock[1], Tetyana Shapoval[1], Volker Neu[1], Ulrike Wolff[1], Dmytro S. Inosov[2], Silvia Haindl[1], Jan Engelmann[1], Rudolf Schäfer[1], Bernhard Holzapfel[1], and Ludwig Schultz[1] — [1]IFW Dresden, Institute for Metallic Materials, P.O. Box 270116, 01171 Dresden, Germany — [2]Max Planck Institute for Solid State Research, Heisenbergstraße 1, 70569 Stuttgart, Germany

Quantitative interpretation of magnetic force microscopy (MFM) data is a challenge, because the measured signal is a convolution between the magnetization of the tip and the stray field emanated by the sample. It was established theoretically that the field distribution just above the surface of the superconductor can be well approximated by the stray field of a magnetic monopole [1]. The description of the MFM tip, however, needs a second approximation. The temperature-dependent vortex-distribution images on a NbN thin film were fitted using two different tip models. Firstly, the magnetic tip was assumed to be a monopole that leads to the simple monopole-monopole model for the tip-sample interaction force. Performing a 2D fitting of the data with this model, we extracted λ, Δ and the vortex pinning force [2]. Secondly, a geometrical model was applied to calculate the tip-transfer-function of the MFM tip using the numerical BEM method [3].

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O 91.44 Fri 11:00 Poster A

Observation of antiferromagnetic domains using magneto-optical microscopy. — •Anna Möhn, Ingolf Mönch, Denys Makarov, Rudolf Schäfer, Oliver G. Schmidt, and Ludwig Schultz — IFW Dresden, Institute for Metallic Materials Dresden, Germany

Two different exchange biased systems were studied. Both antiferromagnetic/ferromagnetic-bilayer systems contain Py as ferromagnetic material, but one with IrMn and the other one with CoO as antiferromagnetic layer. Through the different Néel-temperatures of the antiferromagntic materials the systems show the exchange bias effect under different temperature conditions. The exchange bias effect can be used to imprint a well-defined domain pattern into the antiferromagnetic layer. To observe those imprinted antiferromagnetic domains directly we will use the Voigt effect. This quadratic magneto-optical effect is a birefringence of linearly polarized light which we observe in reflection with a wide-field Kerr microscope. Using the Voigt effect on a ferromagnet, we can see domains which differ by 90° in the axis of the magnetic moments independent of their net magnetization. The same effect is expected to be seen in an antiferromagnet if the antiferromagnetic domains are magnetized along orthogonal easy axes [1]. The required 90° domains are firstly generated as a Landau pattern in the (structured) ferromagnetic film of our bilayer systems and then imprinted to the antiferromagnetic film by cooling below the blocking temperature.

[1] Peter Oppeneer, University Uppsalla, private communication

O 91.45 Fri 11:00 Poster A

Direct Imaging of Precessional Domain Wall Propagation in Ferromagnetic Rings Induced by Circular Magnetic Fields — A. Bisig[1,2,3], •M. A. Mawass[1,4], M. Stärk[1,3], C. Moutafis[1,3], J. Rhensius[3,5], J. Heidler[2], M. Curcic[2], E. Prabu[2], M. Noske[2], M. Weigand[2], T. Tyliszczak[5], B. Van Waeyenberge[6], H. Stoll[2], G. Schütz[2], and M. Kläui[1,3,4] — [1]Paul Scherrer Institut, Villigen, Switzerland — [2]Max-Planck-Institut für Intelligente Systeme, Stuttgart, Germany — [3]Universität Konstanz, Konstanz, Germany — [4]Johannes Gutenberg-Universität Mainz, Mainz, Germany — [5]Advanced Light Source, LBNL, Berkeley, USA — [6]Ghent University, Ghent, Belgium

The controlled displacement of magnetic domain walls (DW) along magnetic nanostructures is a key prerequisite to memory storage or DW logic devices. Depending on the strength of the driving force (magnetic field or spin-polarized currents), the propagation of DW changes from simple translation to more complex precessional modes, i.e. periodic transformations of vortex DWs into transverse DWs and back during propagation. We present direct experimental visualization of the precessional motion of vortex DWs in permalloy nanorings controlled by circular fields. Employing scanning transmission x-ray microscopy (STXM) we image the propagation of a pair of vortex DWs in a stroboscopic measurement scheme. We find that the DW velocity strongly varies during the transformation processes and that the propagation and DW spin structures are highly reproducible indicating the direct observation of the Walker breakdown.

O 91.46 Fri 11:00 Poster A

Magnetic resonant scattering with Laser generated higher harmonic radiation — •Christian Weier[1], Dennis Rudolf[1], Roman Adam[1], Claus M. Schneider[1], André Kobs[2], Gerrit Winkler[2], Robert Frömter[2], Hans P. Oepen[2], Margaret M. Murnane[3], and Henry C. Kapteyn[3] — [1]Peter Grünberg Institut, Research Center Jülich, 52425, Jülich, Germany — [2]Institut für Angewandte Physik, University of Hamburg, 20355, Hamburg, Germany — [3]JILA, University of Colorado, Boulder, CO 80309-0440, USA

Laser driven higher harmonic generation has recently been used to generate extreme ultraviolet (EUV) radiation for probing magnetization dynamics of ferromagnets, element selectively, with a time resolution of few femtoseconds. EUV photons with energies of 52 eV, 61 eV and 67 eV can reach M-absorption edges of Fe, Co and Ni, respectively, what leads to a resonantly enhanced magneto-optical signal. On the other hand, there is a strong progress in imaging techniques using laser generated EUV radiation due to its low divergence and high coherence. In our experiment, we resonantly scatter EUV light from Co/Pt-multilayers forming a magnetic domain pattern. As a consequence of the magnetization dependent scattering, the amplitude of the resulting image in k-space is directly related to the average domain size. Exploring advantage of the femtosecond coherent EUV radiation, our scattering experiment gives the possibility to probe magnetization dynamics with a high temporal and spatial resolution.

O 91.47 Fri 11:00 Poster A

Switching the magnetization of nanomagnets using SP-STM — •Benjamin Ehlers, Gabriela Herzog, Johannes Friedlein, Stefan Krause, and Roland Wiesendanger — University of Hamburg, Institute of Applied Physics, Jungiusstraße 11A, 20355 Hamburg, Germany

With spin-polarized scanning tunneling microscopy (SP-STM) it is possible to manipulate the switching behavior of atomic-scale superparamagnets, using a high spin current generated between a magnetic tip and a magnetic sample. [1]

Here, current-induced magnetization switching of thermally quasistable magnetic nanoislands with a state lifetime on the order of several hours is demonstrated using SP-STM. The magnetization of an individual Fe nanoisland consisting of about 40 atoms on a W(110) surface is reversibly switched between two states by the application of short spin-polarized tunnel current pulses in the μA regime [2]. The combined action of Joule heating and spin-transfer torque during the pulse leads to a controlled reversal of the magnetization. The switching efficiency is evaluated as a function of different current pulse parameters, i.e. pulse length and amplitude, bias polarity and bias value.

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O 91.48 Fri 11:00 Poster A

Complex magnetic ground states observed in Fe nanostructures on different Ir surfaces — •Matthias Menzel[1], Kirsten von Bergmann[1], Stefan Heinze[2], Yuriy Mokrousov[3], Gustav Bihlmayer[3], Jessica Bickel[1], Jens Brede[1], Robert Wieser[1], Elena Vedmedenko[1], Stefan Blügel[3], André Kubetzka[1], and Roland Wiesendanger[1] — [1]Institut für Angewandte Physik, Universität Hamburg, 20355 Hamburg — [2]Institut für Theoretische Physik und Astrophysik, Universität Kiel, 24098 Kiel — [3]Institut für Festkörperforschung, Forschungszentrum Jülich, 52425 Jülich

The reduced symmetry and large spin-orbit interaction can give rise to complex magnetic ground states in $3d$-transition metal nanostructures on heavy element surfaces, e.g. [1]. Especially, Fe nanostructures on an Ir surface are promising candidates for non-collinear magnetic states, due to an extremely weak Heisenberg exchange [2].

Here, we present SP-STM measurements of Fe chains on the (5×1)-Ir(001) surface as well as the Fe monolayer on Ir(111) which reveal atomic-scale, non-collinear magnetic ground states in both systems [3,4]. Density functional theory calculations show that the weak Heisenberg exchange allows other interactions, as the Dzyaloshinskii-Moriya exchange or higher-order interactions, to dominate the energy landscape.

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[2] B. Hardrat *et al.*, PRB **79**, 094411 (2009).
[3] S. Heinze *et al.*, Nature Physics **7**, 713 (2011).
[4] M. Menzel *et al.*, submitted.

O 91.49 Fri 11:00 Poster A

Quantum-Mechanical Model of Spin Polarized STM — •Kolja Them, Thim Stapelfeldt, Elena Y. Vedmedenko, and Roland Wiesendanger — Institute for Applied Physics University of Hamburg Jungiusstr. 11 20355 Hamburg

Spin sensitive studies of individual magnetic ad-atoms and atomic ensembles on surfaces with spin-polarized scanning tunneling microscopy (SP-STM) have raised the necessity of a quantum-mechanical description of spin dynamics during SP-STM experiments. The quantum-mechanical treatments of STM experiments typically deal with the expectation values of observables using Gibbs ensemble averages. An SP-STM measurement, however, is a time-average of the expectation values. The lack of the time-averaging might be a reason for the fact that the theoretically predicted relaxation time on the nanosecond scale for a single spin of a magnetic adatom is at odd with the femtosecond rates measured for Fe adatoms on semiconductor surfaces. Another still unexplained finding is the extremely high switching frequency of Co atoms on Pt(111) at zero magnetic field. In the present paper we use the algebraic formulation of quantum statistical mechanics to clearly separate the thermal equilibrium Gibbs states and the time evolution of the system during SP-STM experiments. Using elaborated techniques we calculate dynamics of single quantum spins as well as magnetic ensembles at finite temperatures. We demonstrate that the relaxation times of those quantum objects on different substrates lie in the femto- or pico-second regime.

O 91.50 Fri 11:00 Poster A

Spin-transfer torque experiments on Co2MnSi/Ag/Co2MnSi (001) nanopillars — •Şaban Tirpanci[1,2], Daniel E. Bürgler[1], Yuya Sakuraba[3], Subrojati Bosu[3], Koki Takanashi[3], and Claus M. Schneider[1] — [1]Electronic Properties (PGI-6) and JARA-FIT, Forschungszentrum Jülich, Jülich, Germany — [2]GIT, Gebze, Turkey — [3]IMR, Tohoku University, Sendai, Japan

The Heusler alloy Co2MnSi (CMS) is a half-metallic ferromagnet with a Curie temperature above room temperature (RT) and high spin polarization, which in combination with Ag spacer layers yields large GMR ratios of up to 36 percent at RT [1]. Therefore, CMS is a very promising material for new spintronic devices. Fully epitaxial CMS/Ag /CMS(001) thin films are prepared by UHV magnetron sputtering [1]. Ellipsoidal nanopillars with diameters between 120 nm to 300 nm are fabricated by e-beam lithography and ion-beam etching for spin-torque measurements in current-perpendicular-plane (CPP) geometry. The two CMS layers of 20 and 5 nm thickness act as fixed and free layer, respectively, and are separated by 8 nm Ag. Previous work [1,2] is extended by performing DC and HF measurements at low temperatures in order to study the influence of the increased polarization on critical currents for current-induced switching and magnetic excitation as well as the efficiency of injection locking [3] as a prerequisite for synchronization of several spin-torque oscillators.

[1] Y. Sakuraba et al.,. Phys. Rev. B 82, 094444 (2010)
[2] R. Okura et al., Appl. Phys. Lett. 99, 052510 (2011)
[3] R. Lehndorff et al., Appl. Phys. Lett. 97, 142503 (2010)

O 91.51 Fri 11:00 Poster A

Determination and characterization of spin torque in perpendicular magnetized multilayer materials — •Tomek Schulz[1], Jan Heinen[1,2], Mathias Kläui[1,2,7], Olivier Boulle[3], Gregory Malinowsky[4], Christian Ulysse[6], Giancarlo Faini[6], Denise Hinzke[2], Henk Swagten[5], Bert Koopmans[5], and Berthold Ocker[8] — [1]Institut für Physik, Johannes Gutenberg-Universität Mainz, Germany — [2]Fachbereich für Physik, Universität Konstanz, Germany — [3]Spintec, UMR CEA/CNRS/UJF-Grenoble 1/Grenoble-INP, France — [4]Laboratoire de physique des solides, Universite Paris-sud, France — [5]Department of Applied Physics, Eindhoven University of Technology, The Netherlands — [6]CNRS, Phynano team, Laboratoire de Phtonique et de Nanostructures, Marcoussis, France — [7]SwissFEL, Paul Scherrer Institut, Villigen PSI, Switzerland — [8]Singulus Technologies AG, Kahl am Main, Germany

We report on measurements to deduce the spin torque contribution of current induced domain wall motion in out-of-plane magnetized multilayer materials. Using complementary measurement techniques such as the current-field equivalency and thermally activated domain wall hopping allow us not only to separate the torque terms on the same material, but also to gauge their accuracy and validity. The extension of these techniques to characterize novel materials reveals not only the predicted dominant non-adiabatic spin torque as in the Co/Pt multilayer nanowires, but also a dominant adiabatic torque in Co/Ni multilayer nanowires highlighting the importance of the materials composition for the acting torques.

O 91.52 Fri 11:00 Poster A

Dynamical magnetic susceptibility of nanostructures with spin–orbit coupling — •Manuel dos Santos Dias, Stefan Blügel, and Samir Lounis — Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, D-52425 Jülich, Germany

We outline a real–space linear response theory of the dynamical spin susceptibility of nanostructures, accounting for the spin–orbit interaction. The starting point is the existing formalism of time–dependent Density Functional Theory, in the Korringa–Kohn–Rostoker Green function method [1,2]. The linear response to an external time-dependent applied magnetic field transverse to the orientation of the magnetisation generates both transverse and longitudinal time-dependent spin susceptibilities, while the induced charge fluctuations introduce the screened Coulomb interaction in the problem. The breaking of the spin rotational invariance due to the spin–orbit interaction is explored, and the roles of the familiar magnetocrystalline anisotropy and the coupled spin–charge fluctuations are compared, and some examples for adatoms on simple non–magnetic surfaces are given.

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)
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O 91.53 Fri 11:00 Poster A

Imaging of magnetization reversal by spin transfer torque — •Matthias Buhl[1], Artur Erbe[1], Sebastian Wintz[1], Jörg Raabe[2], Jochen Grebing[1], Kay Potzger[1], and Jürgen Fassbender[1] — [1]Helmholtz-Zentrum Dresden-Rossendorf — [2]Swiss Light Source, Paul-Scherrer Institut

The magnetic moment of nanosized magnets is widely used for data storage in modern electronics. Integration of such magnets into larger circuits can be possible, if the read-out and the storage of data can be performed electrically. This can, for example, be achieved by using spin transfer torque for the definition of magnetic moment of a nanomagnet. Here, we demonstrate switching of a single magnetic pillar in a so-called current in plane geometry. The pillar structures are fabricated from CoFe layers using electron beam lithography on SiN membranes. The magnetization direction of the pillar is imaged using scanning transmission x-ray microscopy (STXM).

O 91.54 Fri 11:00 Poster A

Magnon dispersion relation in adiabatic spin approximation — •Christian Franz and Christian Heiliger — I. Physikalisches Institut, Justus-Liebig-Universität, Gießen, Deutschland

The adiabatic approximation is used to separate the fast electronic degrees of freedom from the slow magnetic ones. A single magnetic moment is assigned to each atom in an itinerant ferromagnet. The interaction of these moments can be described by an effective Heisenberg model.

$$H = -\sum_{i,j} J_{i,j}\vec{S}_i \cdot \vec{S}_j - \frac{g\mu_b B_0}{\hbar}\sum_{i,j} S_i^z \tag{1}$$

The exchange parameters of this model are obtained from *ab initio* calculations by applying the magnetic force theorem. The magnon dispersion and various physical parameters as the spin-wave stiffness and the Curie temperature can be determined within this model. We perform this calculations several systems and find result in good agreement with experimental and other theoretical results. This is the first step in including magnons and the electron-magnon interaction in transport calculations.

O 91.55 Fri 11:00 Poster A

Influence of pure diffusive spin currents on magnetic switching in non-local spin valves — •Björn Burkhardt[1], Helmut Körner[2,3], Piotr Laczkowski[4], Laurent Vila[4], and Mathias Kläui[1,2,3] — [1]Institut für Physik, Johannes Gutenberg Universität Mainz, 50099 Mainz, Germany — [2]Fachbereich Physik, Universität

Konstanz, 78457 Konstanz, Germany — [3]SwissFEL, Paul Scherrer Institut, 5232 Villigen PSI, Switzerland — [4]Laboratoire Nanostructure et Magnetisme, CEA/INAC, 38054 Grenoble, France

We analyzed magnetic switching processes in Permalloy stripes during injection of pure diffusive spin currents. These spin currents are created via a non-local spin valve design with aluminium as the nonmagnetic spin conduit between the stripes. By measuring the non-local spin signals as a function of temperature we find a non-montonous behavior. To determine the spin diffusion length in the aluminium conduit the distance between injection and detection stripe was varied. The depinning of domain walls assisted by pulsed pure spin currents is further studied and the spin-torque and the Joule heating effect are separated, by using the underlying symmetries of the effect.

O 91.56 Fri 11:00 Poster A

Domain Wall Manipulation with a Magnetic Tip — •Thim Stapelfeldt, Robert Wieser, Elena Y. Vedmedenko, and Roland Wiesendanger — Institute of Applied Physics and Microstructure Advanced Research Center

A theoretical concept of local manipulation of magnetic domain walls is introduced. In the proposed procedure, a domain wall is driven by a spin-polarized current induced by a magnetic tip, as used in a scanning tunneling microscope, placed above a magnetic nanostripe and then moved along its long axis with a current flowing through the vacuum barrier. The angular momentum from the spin-polarized current exerts a torque on the magnetic moments underneath the tip and leads to a displacement of the domain wall. Particularly, the manipulation of a ferromagnetic 180° transverse domain wall has been studied by means of Monte Carlo simulations. The coercivity created by defects as well as tailord pinning centers is presented as a function of the change of the exchange constant and the pinning center size, respectively.

O 91.57 Fri 11:00 Poster A

Spin caloric transport: Investigation of out-of-plane thermal gradient effects in thin film geometries — •Andreas Kehlberger, Enrique Vilanova Vidal, Gerhard Jakob, and Mathias Kläui — Johannes Gutenberg University of Mainz, Institute of Physics, Mainz

Spin caloric transport is expected to open new avenues towards low energy nanoscale spin sources. The measurement of the spin-Seebeck effect has drawn much attention to the research of thermally induced spin currents in thin film structures. In order to explain the observed amplification of signal due to the temperature of the environment, phonon enhancement of the spin caloric effect has been suggested. This magnon-phonon interaction calls for an understanding of the underlying effects of the thermal behavior of the used substrates in thin film experiments. Many thin film studies assume in-plane thermal gradients along the substrate neglecting perpendicular thermal gradients. We present studies of different measurement geometries revealing the importance of out-plane gradients, which can often not be avoided. These unexpected temperature differences lead to asymmetric thermally induced effects such as the anomalous Nernst effect, which have to be taken into account. Measurements of these effects are compared to measurements in a new optimized setup, which focuses on the minimization of the out-of-plane gradient to reveal the spin-Seebeck contribution to the signal. This work is supported by the DFG priority program SPP 1538 Spin Caloric Transport.

O 91.58 Fri 11:00 Poster A

Experimental Study of the Anisotropic Magneto-Thermopower in (113) oriented (Ga,Mn)As Thin Films — •Sibylle Meyer[1], Matthias Althammer[1], Lukas Dreher[2], Wladimir Schoch[3], Sebastian T. B. Goennenwein[1], and Rudolf Gross[1] — [1]Walther-Meißner-Institut, Bayerische Akademie der Wissenschaften, Garching, Germany — [2]Walter Schottky Institut, Technische Universität München, Garching, Germany — [3]Institut für Quantenmaterie, Universität Ulm, Ulm, Germany

In analogy to the anisotropic magnetoresistance (AMR), the thermopower of ferromagnetic materials also characteristically depends on the orientation of the magnetization vector. This anisotropic magnetothermopower (AMTP) has only scarcely been studied to date. Taking the ferromagnetic semiconductor (Ga,Mn)As with its large magneto-resistive effects as a prototype example, we have measured the evolution of both the AMR and the AMTP effects at liquid He temperatures as a function of both the orientation and the magnitude of an externally applied magnetic field. Our data show that the AMTP effect can be adequately modeled only if the symmetry of the (Ga,Mn)As crystal is explicitly taken into account. We will quantitatively compare AMR and AMTP data taken on the same (113) - oriented (Ga,Mn)As thin film with corresponding model calculations, and address the differences between the magneto-resistance and the magneto-thermopower coefficients. Financial support by DFG via SPP 1538 is gratefully acknowledged.

O 91.59 Fri 11:00 Poster A

Experimental determination of the spin mixing conductance in YIG/Pt bilayers — •Philipp Ross[1], Johannes Lotze[1], Franz D. Czeschka[1], Matthias W. Althammer[1], Mathias Weiler[1], Thomas Brenninger[1], Rudolf Gross[1,2], and Sebastian T. B. Goennenwein[1] — [1]Walther-Meißner-Institut, Bayerische Akademie der Wissenschaften, Garching, Germany — [2]Physik-Department, Technische Universität München, Garching, Germany

A spin current is a directed flow of angular momentum. Since spin currents are independent of charge motion, they can also propagate in electrical insulators. One elegant way to generate a spin current is the process of spin pumping: the magnetization of a ferromagnet is driven into resonant precession, and relaxes by emitting a spin current into an adjacent normal metal. The efficiency of the spin pumping process is dependent on the spin-mixing conductance which is in the order of 1×10^{19} m^{-2} in a variety of conducting ferromagnets [1]. We have grown insulating yttrium iron garnet (YIG) thin films on gadolinium gallium garnet substrates by pulsed laser deposition, and covered them in situ with a Pt layer. On these samples, we simulaneously recorded ferromagnetic resonance and the DC voltage generated by the inverse spin Hall effect, at different fixed temperatures between room temperature and 3 K. We find the spin-mixing conductance to be in the range from 1.2×10^{18} m^{-2} to 8×10^{19} m^{-2}, which is consistent with values measured on conductive ferromagnet/Pt interfaces. Financial support by DFG SPP 1538 is gratefully acknowledged.

[1] F. D. Czeschka *et al.*, Phys. Rev. Lett. **107**, 046601 (2011)

O 91.60 Fri 11:00 Poster A

Local charge and spin currents in magnetothermal landscapes — •Michael Schreier, Mathias Weiler, Hans Huebl, Matthias Althammer, Martin S. Wagner, Rudolf Gross, and Sebastian T. B. Goennenwein — Walther-Meißner-Institut, Bayerische Akademie der Wissenschaften, 85748 Garching, Germany

The interplay of spin currents and phonons is currently vigorously investigated, e.g., in spin Seebeck effect measurements. In such spin caloritronic experiments, homogenous temperature gradients were used to date for spin current generation. However, for a detailed understanding of the magnon-phonon interaction, a spatially resolved study of spin currents in magnetothermal landscapes appears mandatory.

We use a focused, scannable laser beam to generate a local thermal gradient along the surface normal of a thin insulating $Y_3Fe_5O_{12}$ (YIG) film grown on $Gd_3Ga_5O_{12}$. This thermal gradient gives rise to a local spin current that we electrically detect by means of the inverse spin Hall effect in a Pt thin film deposited on top of the YIG. In our room temperature experiments, we demonstrate all-electrical detection [1] and thermal manipulation of the YIG magnetic texture. We furthermore discuss the interplay of local temperature gradients, charge currents and magnetic domains also in conductive ferromagnetic thin films. Taken together, our findings open the path for local magnetothermal generation and control of spin and charge currents in ferromagnetic thin films.

This work is supported by DFG via SPP1538.

[1] M. Weiler *et al.* (2011) arXiv:1110.3981v1

O 91.61 Fri 11:00 Poster A

Realization of an experimental setup for temperature dependent measurements of the Spin Seebeck Effect — •Daniel Meier, Hanno Meyer zu Theenhausen, Jan-Michael Schmalhorst, and Günter Reiss — Thin Films and Physics of Nanostructures, Physics Department, Bielefeld University, Germany

Spin caloritronics is a growing field of research in the branch of spintronics, which combines spin, charge and heat currents. The discovery of the spin Seebeck effect (SSE) [1] gives a method for a thermal spin generator. The effect was first studied in Permalloy (Py) thin films on Sapphire substrates [1], which were partly covered by thin Pt stripes. When an in-plane temperature gradient is applied perpendicular to the Pt stripes a spin current into the Pt can be generated, which can be converted into an electromotive force via the inverse spin Hall effect. As a consequence one can measure a voltage between the ends of the

Pt stripe in a range of a few μV. The voltage size and sign depends on the position of the Pt stripe on the Py film and on the size of the temperature gradient [1].

This work presents a setup for SSE measurements at variable temperatures. It was tested on various Py/Pt samples grown on MgO and Sapphire substrates utilizing conventional photo lithography or shadow mask techniques. A high resolution of about 50nV was achieved when measuring the planar Nernst effect in the different samples.

[1] K. Uchida et al., Nature Vol. 455, 2008, 778–781

O 91.62 Fri 11:00 Poster A

Dependence of the magneto-Seebeck effect on the CoFe distribution in MgO tunnel junctions — •Jakob Walowski[1], Marvin Walter[1], Vladyslav Zbarsky[1], Anissa Zeghuzi[1], Christian Leutenantsmeyer[1], Mirco Marahrens[1], Markus Münzenberg[1], Markus Schäfers[2], Daniel Ebke[2], Günter Reiss[2], Andy Thomas[2], Patrick Peretzki[3], Michael Seibt[3], Michael Czerner[4], Michael Bachmann[4], and Christian Heiliger[4] — [1]I. Phys. Inst., Universität Göttingen — [2]Dept. of Physics, Bielefeld University — [3]IV. Phys. Inst., Universität Göttingen — [4]I. Phys. Inst., Universität Gießen

Thermally driven techniques gain more importance, as ever smaller element sizes in electronics reach exorbitantly high current densities, threatening with a breakdown of Moore's Law. Currently magnetic tunnel junctions attract a lot of attention, because they are interesting from the spinelectronic and the spincaloritronic point of view. Spin-transfer torque magnetic RAM, as well as thermal-spin-transfer torque elements are in the current discussion as future technologies.

The magneto-thermal effects in CoFeB|MgO|CoFeB tunnel junctions strongly depend on the distribution of the Co and Fe atoms within layers at the interface to the MgO barrier. Supported by theoretical calculations using the energy dependent transmission function, we present the temperature dependent Seebeck coefficients in parallel and antiparallel magnetization alignment, and the magneto-Seebeck ratio for tunnel junctions with different Co and Fe distributions.

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O 91.63 Fri 11:00 Poster A

Barrier thickness dependence of the Magneto Seebeck effect in magnetic tunnel junctions: Ab initio studies — •Michael Czerner and Christian Heiliger — I. Physikalisches Institut, Justus Liebig Universität Giessen, D-35392, Germany

The magneto Seebeck effect is the dependence of the thermopower in a magnetic tunnel junction on the relative orientation of both magnetic layers [1]. First calculations show that there is a non-trivial barrier thickness dependence of this effect [1]. Therefore, we systematically investigate the thermopower for parallel and antiparallel alignment of the magnetic leads in MgO based tunnel junctions. We show that the actual dependence on the MgO thickness also depends on the magnetic material of the leads. Our theoretical investigations are ab initio calculations based on density functional theory. In particular, we used the Korringa-Kohn-Rostoker and the non-equilibrium Green's function method to obtain the transmission function T(E). Using T(E), we calculated in linear response the transport coefficients, e.g. conductance, Seebeck coefficient, thermal conductance (electronic contribution) [2]. Additionally we study the thermopower as a function of the tilting angle between the magnetization of the two ferromagnetic leads.

[1] M. Walter, J. Walowski, V. Zbarsky, M. Münzenberg, M. Schäfers, D. Ebke, G. Reiss, A. Thomas, P. Peretzki, M. Seibt, J. S. Moodera, M. Czerner, M. Bachmann, C. Heiliger, Nature Materials 10, 742 (2011)

[2] M. Czerner, M. Bachmann, C. Heiliger, Phys. Rev. B 83, 132405 (2011)

O 91.64 Fri 11:00 Poster A

Scanning laser setup for local heat gradients in ferromagnetic micro- and nanostructures — •Florian Brandl, Haiming Yu, Thomas Rapp, and Dirk Grundler — Lehrstuhl für Physik funktionaler Schichtsysteme, Technische Universität München, Physik Department, James-Franck-Straße 1, 85748 Garching b. München, Germany

We report on the development of a scanning laser setup that allows us to generate temperature gradients locally in ferromagnetic devices. With our system we position a focused laser beam on a sample with a translation stage offering nm resolution. A pair of crossed coils provides magnetic fields in the plane of the sample of up to 100 mT. The local heating will be tested using magnetoresistance measurements on ferromagnetic micro- and nanostructures. We also plan to combine the setup with ferromagnetic resonance measurements. We acknowledge financial support through the German priority program SPP 1538 ”spin caloric transport” and the German excellence cluster ”Nanosystems Initiative Munich”.

O 91.65 Fri 11:00 Poster A

Thermomagnetic properties improved by self-organized flower-like phase separation of ferromagnetic $Co_2Dy_{0.5}Mn_{0.5}Sn$. — •Michael Schwall[1], Peter Klaer[2], Hans-Joachim Elmers[2], and Benjamin Balke[1] — [1]Institute of Inorganic Chemistry and Analytical Chemistry, Johannes Gutenberg - University, Mainz — [2]Institute of Physics, Johannes Gutenberg - University, Mainz

A thermodynamically stable phase separation of $Co_2Dy_{0.5}Mn_{0.5}Sn$ into the Heusler compound Co_2MnSn and $Co_8Dy_3Sn_4$ is induced by rapid cooling from the liquid phase. The phase separation forms an ordered flower-like structure on the microscale. The increased scattering of phonons at the phase boundaries reduces thermal conductivity and thus improves thermoelectric and spincaloric properties.

O 91.66 Fri 11:00 Poster A

Extrinsic Spin Nernst effect from first principles — •Katarina Tauber[1,2], Martin Gradhand[3], Dmitry Fedorov[1,2], and Ingrid Mertig[1,2] — [1]Max-Planck-Institut für Mikrostrukturphysik, Halle, Germany — [2]Martin-Luther-Universität Halle-Wittenberg, Halle, Germany — [3]H.H. Wills Physics Laboratory, University of Bristol, United Kingdom

Recently, a new field *“Spin Caloritronics”* [1] arose, which relates the spin degree of freedom to a temperature gradient. Within an *ab initio* approach we present a study of the *spin Nernst effect*, which describes the creation of a transversal spin current or spin accumulation due to a longitudinal temperature gradient ∇T. This effect is similar to the intensively studied spin Hall effect, where instead of ∇T an electric field is applied. Here we investigate the extrinsic skew scattering mechanism, which is dominant in the limit of dilute concentrations of substitutional alloys. Our calculations are based on a fully relativistic Korringa-Kohn-Rostoker method and a solution of the linearized Boltzmann equation. As a first application, we consider a Cu host with different impurities.

[1] G.E. Bauer, A.H. MacDonald, and S. Maekawa, Solid State Commun. 150, 459 (2010).

O 91.67 Fri 11:00 Poster A

Observation of Spin Seebeck Effect in Magnetic Semiconductor — •Ivan Soldatov, Christian Hess, Ludwig Schultz, and Rudolf Schaefer — IFW Dresden, Helmholtzstraße 20, 01069 Dresden

If a temperature gradient is applied along or perpendicular to a ferromagnetic /nonmagnetic metal interface, one can observe a pure spin current injected into the normal metal in direction perpendicular to the interface. This effect, called Spin Seebeck Effect (SSE), occupies a central role in the field of spin caloritronics, which explores the possibility of controlling spin currents by means of heat currents. In this work we investigate the SSE in a semiconducting ferromagnetic layer in Pt/GaMnAs/GaAs structures in conventional setup, purposed in pioneering work by Uchida (K. Uchida et al. Nature 455, 778 (2008)). The results include the absolute temperature dependence of the SSE dependence on the applied temperature gradient and the direction of applied magnetic field. The work is supported by the DFG-priority program Spin Caloric Transport

O 92: Invited talk (Ralph Claessen)

Time: Friday 13:15–14:00 Location: HE 101

Invited Talk O 92.1 Fri 13:15 HE 101

From surface to interface physics: Hard x-ray photoemission spectroscopy of oxide heterostructures — •Ralph Claessen — Physikalisches Institut, Universität Würzburg, Am Hubland, D-97074 Würzburg, Germany

The electronic and magnetic surface properties of transition metal oxides (TMO) often deviate from their bulk behavior due to atomic and electronic reconstructions related to the ionic nature of these materials. Such surface instabilities represent a major obstacle for studying TMO by experimental surface probes, like e.g. photoelectron spectroscopy (PES) which gives direct access to the microscopic electronic structure, but under conventional conditions is limited to an information depth of a few atomic layers only.

On the other hand, it has recently been demonstrated that the same reconstruction phenomena can also be utilized to control the *interface* in epitaxial oxide heterostructures with a polar discontinuity, opening promising perspectives for novel functionalities not present in the bulk. A prominent example is the formation of a high-mobility 2D electron system at the interface of the band insulators $LaAlO_3$ and $SrTiO_3$. In my presentation, I will discuss the interface physics of such heterostructures and show how the extension of PES to higher photon energies up to the hard x-ray regime (HAXPES) may provide useful spectroscopic information on the buried interfaces, using different heterostructure systems as examples.