

## Surface Science Division Fachverband Oberflächenphysik (O)

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### Overview of Invited Talks and Sessions

(lecture rooms HSZ 02, SCH A01, SCH A118, SCH A215, SCH A216, SCH A315, and SCH 251; Poster P2)

#### Invited Talks

O 2.1	Mon	10:15–11:00	HSZ 02	<b>Surface Science from Hours to Attoseconds: Mind the Gap</b> — •MICHAEL HORN-VON HOEGEN
O 9.1	Mon	14:00–14:45	HSZ 02	<b>Surface-confined coordination chemistry with porphyrins and phthalocyanines</b> — •J. MICHAEL GOTTFRIED
O 16.1	Tue	9:30–10:15	HSZ 02	<b>Electron Transport through Single Atoms and Molecules: an STM's View</b> — •JÖRG KRÖGER
O 23.1	Tue	14:00–14:45	HSZ 02	<b>Surfaces and Atomic Nanostructures - Model Systems for Spectroscopy of Confined Interacting Electrons</b> — •JÖRG SCHÄFER
O 28.1	Wed	9:30–10:15	HSZ 02	<b>Catalytic Autothermal Reforming of Renewable Fuels at Millisecond Times</b> — •LANNY SCHMIDT
O 35.1	Wed	14:00–14:45	HSZ 02	<b>Engineering surfaces, interfaces and structural phases to tailor magnetic properties</b> — •JÜRGEN FASSBENDER
O 43.1	Thu	9:30–10:15	HSZ 02	<b>Measuring spin polarization vectors with ARPES</b> — •JÜRGEN OSTERWALDER, HUGO DIL, FABIAN MEIER, JORGE LOBO-CHECA, LUC PATTHEY, VLADIMIR N. PETROV
O 50.1	Thu	14:00–14:45	HSZ 02	<b>Si-based spintronics from first principles</b> — •MAHBUBE HORTAMANI
O 61.1	Fri	10:15–11:00	HSZ 02	<b>First-principles approaches towards organic film growth</b> — •CLAUDIA AMBROSCH-DRAXL, PETER PUSCHNIG, DMITRII NABOK
O 68.1	Fri	13:30–14:15	HSZ 02	<b>Surface Structure Analysis – Present Status and Future</b> — •KLAUS HEINZ
O 69.1	Fri	14:15–15:00	HSZ 02	<b>Transient Electronic Structure and Insulator-to-Metal Transitions Probed by Time-resolved Photoemission Spectroscopy</b> — •MARTIN WOLF

#### Invited talks of the joint symposium SYAI

See SYAI for the full program of the Symposium.

SYAI 1.1	Thu	15:00–15:30	SCH 251	<b>Insights and Progress in Density Functional Theory</b> — PAULA PAULA MORI-SANCHEZ, ARON COHEN, •WEITAO YANG
SYAI 1.2	Thu	15:30–16:00	SCH 251	<b>Quasiparticle energy calculations in a new light: from defects in semiconductors to the <i>f</i>-electron challenge</b> — •PATRICK RINKE
SYAI 1.3	Thu	16:00–16:30	SCH 251	<b>LDA+DMFT approach to excitations spectrum in Half-Metallic Ferromagnets</b> — •ALEXANDER LICHTENSTEIN
SYAI 1.4	Thu	17:00–17:30	SCH 251	<b>Insight and prediction of material properties from ab initio calculations of electronic excitations</b> — •LUCIA REINING, MATTEO GATTI, RALF HAMBACH, CHRISTINE GIORGETTI
SYAI 1.5	Thu	17:30–18:00	SCH 251	<b>Local excitations in strongly interacting charge-transfer insulators: Frenkel excitons within TD-LDA+<i>U</i> and strong coupling theory</b> — •WEI KU
SYAI 1.6	Thu	18:00–18:30	SCH 251	<b>Electron tunneling and transport at molecular junctions</b> — •ROBERTO CAR

## Sessions

O 1.1–1.3	Sun	16:00–18:30	HSZ 04	<b>Tutorial (Walter Pfeiffer, Christoph Lienau, Michael Bauer)</b>
O 2.1–2.1	Mon	10:15–11:00	HSZ 02	<b>Invited Talk (Michael Horn-von Hoegen)</b>
O 3.1–3.7	Mon	11:15–13:00	SCH A01	<b>Oxides and insulators I</b>
O 4.1–4.7	Mon	11:15–13:00	SCH A118	<b>Metal substrates: Adsorption of organic / bio molecules I</b>
O 5.1–5.7	Mon	11:15–13:00	SCH A215	<b>Nanostructures at surfaces: Wires, tubes</b>
O 6.1–6.7	Mon	11:15–13:00	SCH A216	<b>Electronic structure I</b>
O 7.1–7.7	Mon	11:15–13:00	SCH A315	<b>Semiconductor substrates</b>
O 8.1–8.5	Mon	11:15–12:45	SCH 251	<b>Focused Session: Epitaxial Graphene I</b>
O 9.1–9.1	Mon	14:00–14:45	HSZ 02	<b>Invited Talk (J.Michael Gottfried)</b>
O 10.1–10.7	Mon	15:00–16:45	SCH A01	<b>Oxides and insulators II</b>
O 11.1–11.7	Mon	15:00–16:45	SCH A118	<b>Metal substrates: Adsorption of organic / bio molecules II</b>
O 12.1–12.6	Mon	15:00–16:30	SCH A215	<b>Nanostructures at surfaces: Dots, particles, clusters I (magnetic)</b>
O 13.1–13.7	Mon	15:00–16:45	SCH A216	<b>Electronic structure II</b>
O 14.1–14.7	Mon	15:00–16:45	SCH A316	<b>Organic, polymeric, biomolecular films – also with absorbates I</b>
O 15.1–15.5	Mon	15:00–16:30	SCH 251	<b>Focused Session: Epitaxial Graphene II</b>
O 16.1–16.1	Tue	9:30–10:15	HSZ 02	<b>Invited Talk (Jörg Kröger)</b>
O 17.1–17.10	Tue	10:30–13:00	SCH A01	<b>Oxides and insulators III</b>
O 18.1–18.9	Tue	10:30–12:45	SCH A118	<b>Metal substrates: Adsorption of organic / bio molecules III</b>
O 19.1–19.9	Tue	10:30–12:45	SCH A215	<b>Nanostructures at surfaces: Arrays</b>
O 20.1–20.10	Tue	10:30–13:00	SCH A216	<b>Nano-optics of metallic and semiconducting nanostructures (time resolved)</b>
O 21.1–21.6	Tue	10:30–12:00	SCH A316	<b>Methods: Electronic structure theory I</b>
O 22.1–22.8	Tue	10:30–13:00	SCH 251	<b>Focused Session: Epitaxial Graphene III</b>
O 23.1–23.1	Tue	14:00–14:45	HSZ 02	<b>Invited Talk (Jörg Schäfer)</b>
O 24.1–24.5	Tue	15:00–16:15	SCH A01	<b>Methods: Molecular simulations and statistical mechanics</b>
O 25.1–25.5	Tue	15:00–16:15	SCH A118	<b>Surfaces and films: forces, structure and manipulation</b>
O 26.1–26.7	Tue	15:00–16:45	SCH A215	<b>Nanostructures at surfaces: Dots, particles, clusters II (SPM)</b>
O 27.1–27.122	Tue	18:30–21:00	P2	<b>Poster Session I (Methods: Scanning probe techniques; Methods: Atomic and electronic structure; Methods: Molecular simulations and statistical mechanics; Oxides and Insulators: Clean surfaces; Oxides and Insulators: Adsorption; Oxides and Insulators: Epitaxy and growth; Semiconductor substrates: Clean surfaces; Semiconductor substrates: Epitaxy and growth; Semiconductor substrates: Adsorption; Nano-optics of metallic and semiconducting nanostructures; Electronic structure; Methods: Electronic structure theory; Methods: other (experimental); Methods: other (theory); Solutions on surfaces; Epitaxial Graphene; Surface order interface magnetism; Phase transitions; Time-resolved spectroscopies)</b>
O 28.1–28.1	Wed	9:30–10:15	HSZ 02	<b>Invited Talk (Lanny Schmidt)</b>
O 29.1–29.9	Wed	10:30–12:45	SCH A01	<b>Nanostructures at surfaces: preparation</b>
O 30.1–30.10	Wed	10:30–13:00	SCH A118	<b>Metal substrates: Adsorption of organic / bio molecules IV</b>
O 31.1–31.8	Wed	10:30–12:30	SCH A216	<b>Nano-optics of metallic and semiconducting nanostructures (theory)</b>
O 32.1–32.8	Wed	10:30–12:30	SCH A315	<b>Surface or interface magnetism</b>
O 33.1–33.6	Wed	10:30–12:00	SCH A316	<b>Methods: Electronic structure theory II</b>
O 34.1–34.8	Wed	10:30–13:00	SCH 251	<b>Focused Session: Epitaxial Graphene IV</b>
O 35.1–35.1	Wed	14:00–14:45	HSZ 02	<b>Invited Talk (Gaede Prize) (Jürgen Fassbender)</b>
O 36.1–36.7	Wed	15:00–16:45	SCH A01	<b>Particles and clusters</b>
O 37.1–37.10	Wed	15:00–17:30	SCH A118	<b>Metal substrates: Adsorption of organic / bio molecules V</b>
O 38.1–38.10	Wed	15:00–17:30	SCH A216	<b>Nano-optics of metallic and semiconducting nanostructures (experiments I)</b>
O 39.1–39.10	Wed	15:00–17:30	SCH A315	<b>Metal substrates: Solid-liquid interfaces</b>
O 40.1–40.10	Wed	15:00–17:30	SCH A316	<b>Methods: Scanning probe techniques I</b>
O 41.1–41.10	Wed	15:00–17:30	SCH 251	<b>Ab-initio approaches to excitations in condensed matter I</b>

O 42.1–42.126	Wed	17:45–20:30	P2	Poster Session II (Nanostructures at surfaces: arrays; Nanostructures at surfaces: Dots, particles, clusters; Nanostructures at surfaces: Other; Nanostructures at surfaces: Wires, tubes; Metal substrates: Adsorption of O and/or H; Metal substrates: Clean surfaces; Metal substrates: Adsorption of organic/bio molecules; Metal substrates: Solid-liquid interfaces; Metal substrates: Adsorption of inorganic molecules; Metal substrates: Epitaxy and growth; Heterogeneous catalysis; Surface chemical reactions; Ab-initio approaches to excitations in condensed matter; Organic, polymeric, biomolecular films– also with adsorbates; Particles and clusters)
O 43.1–43.1	Thu	9:30–10:15	HSZ 02	Invited Talk (Jürg Osterwalder)
O 44.1–44.10	Thu	10:30–13:00	SCH A118	Metal substrates: Adsorption of organic / bio molecules VI
O 45.1–45.10	Thu	10:30–13:00	SCH A215	Heterogeneous catalysis
O 46.1–46.10	Thu	10:30–13:00	SCH A315	Time-resolved spectroscopies I
O 47.1–47.8	Thu	10:30–12:30	SCH A316	Methods: Scanning probe techniques II
O 48.1–48.7	Thu	10:30–13:00	HSZ 02	Focused Session: Spin-Orbit Interaction at Surfaces: From the Rashba Effect to Topological States of Matter I
O 49.1–49.12	Thu	10:30–13:30	SCH 251	Ab-initio approaches to excitations in condensed matter II
O 50.1–50.1	Thu	14:00–14:45	HSZ 02	Invited Talk (Mahbube Hortamani)
O 51.1–51.12	Thu	16:15–19:15	SCH A01	Surface chemical reactions I
O 52.1–52.17	Thu	15:00–19:15	SCH A118	Metal substrates: Adsorption of organic / bio molecules VII
O 53.1–53.14	Thu	15:00–18:30	SCH A215	Nanostructures at surfaces: Dots, particles, clusters III
O 54.1–54.14	Thu	15:00–18:30	SCH A216	Nano-optics of metallic and semiconducting nanostructures (experiments II)
O 55.1–55.5	Thu	15:00–16:15	SCH A315	Time-resolved spectroscopies II
O 56.1–56.17	Thu	15:00–19:15	SCH A316	Metal substrates: Epitaxy, growth and adsorbates
O 57.1–57.12	Thu	15:00–19:00	HSZ 02	Focused Session: Spin-Orbit Interaction at Surfaces: From the Rashba Effect to Topological States of Matter II
O 58	Thu	15:00–18:30	SCH 251	SYAI: Ab-initio approaches to excitations in condensed matter
O 59	Thu	19:30–20:00	HSZ 02	General Meeting of the Surface Science Division
O 60.1–60.4	Thu	20:00–21:00	HSZ 02	Post Deadline Session followed by Surface Science "get-together"
O 61.1–61.1	Fri	10:15–11:00	HSZ 02	Invited Talk (Claudia Ambrosch-Draxl)
O 62.1–62.7	Fri	11:15–13:00	SCH A01	Surface chemical reactions II
O 63.1–63.7	Fri	11:15–13:00	SCH A118	Semiconductor substrates: Adsorption
O 64.1–64.6	Fri	11:15–12:45	SCH A215	Metal substrates: Adsorption of inorganic molecules
O 65.1–65.7	Fri	11:15–13:00	SCH A315	Time-resolved spectroscopies III
O 66.1–66.6	Fri	11:15–12:45	SCH A316	Organic, polymeric, biomolecular films – also with adsorbates II
O 67.1–67.6	Fri	11:15–12:45	SCH 251	Ab-initio approaches to excitations in condensed matter III
O 68.1–68.1	Fri	13:30–14:15	HSZ 02	Invited Talk (Klaus Heinz)
O 69.1–69.1	Fri	14:15–15:00	HSZ 02	Invited Talk (Martin Wolf)

## Annual General Meeting Surface Science Division

Thursday 19:30–20:00 HSZ 02

- Report of the Chairman of the DPG Surface Science Division
- Miscellaneous

## Notes

Poster Sessions O27 (Tuesday, 18:30–21:00) , O42 (Wednesday, 17:45–20:30) in room P2.

Post Deadline Session O60 on Thursday 20:00–21:00, in HSZ 02, followed by the Surface Science "get-together".

**O 1: Tutorial (Walter Pfeiffer, Christoph Lienau, Michael Bauer)**

Time: Sunday 16:00–18:30

Location: HSZ 04

**Tutorial** O 1.1 Sun 16:00 HSZ 04  
**Ultrafast Nanooptics: Bringing Ultimate Time Resolution to the Nanoscale** — ●WALTER PFEIFFER — Fakultät für Physik, Universität Bielefeld, 33615 Bielefeld, Germany

The coherent broadband optical excitation of nanostructures forms the basis of the emerging field of "ultrafast nanooptics". In metallic nanostructures and hybrid nanostructures, electromagnetic excitations tend to be highly localized and strongly enhanced. The coherent excitation of such nanostructures by ultrafast light pulses adds the temporal degree of freedom and allows for controlling the spatiotemporal properties of these nanolocalized fields. The spatio-temporal evolution of such optical near-field distributions could play a key role in a variety of important applications across the disciplines, including the realization of novel laser structures, the exploitation of optical nonlinearities for ultrasensitive chemical and biological probing, and the development of enhanced single-photon sources for quantum communication.

Starting from the fundamentals of nanooptics and ultrafast optics this introductory lecture will provide an overview of recent progress in the field of "ultrafast nanooptics".

15 min. break.

**Tutorial** O 1.2 Sun 16:55 HSZ 04  
**Ultrafast Nano-Optics: Applications in Nano-Science** — ●CHRISTOPH LIENAU — Institut für Physik, Carl von Ossietzky Universität Oldenburg, 26129 Oldenburg, Germany

Ultrafast nano-optics is a comparatively young and rapidly growing field of research aiming at probing, manipulating and controlling ultrafast optical excitations on nanometer length scales. The ability to control light on nanometer length and femtosecond time scales opens up exciting possibilities for probing dynamic processes in nanostructures in real time and space. This tutorial gives a brief introduction into the experimental tools of this emerging field and discusses recent progress in ultrafast nano-optics.

We specifically discuss how ultrafast nano-optical techniques can be used to (i) visualize light propagation in novel photon waveguides, (ii) probe and manipulate coherent optical excitations in individual and

dipole-coupled pairs of quantum dots, (iii) probe the dynamics of surface plasmon polariton excitations in metallic nanostructures, (iv) generate novel nanometer-sized ultrafast light and electron sources and (v) to reveal the optical interaction between excitons and surface plasmon polaritons in hybrid metal-semiconductor nanostructures. The results will indicate that combining light localization on nanometer-length and femtosecond time scales carries significant potential for realizing novel optoelectronic devices such as ultrafast nano-optical switches or surface plasmon polariton amplifiers and lasers.

15 min. break.

**Tutorial** O 1.3 Sun 17:50 HSZ 04  
**Near-field Dynamics Probed with Time-Resolved PEEM** — ●MICHAEL BAUER — IEAP, Christian-Albrechts-Universität zu Kiel, Kiel, Germany

Photoemission Electron Microscopy (PEEM) in combination with non-linear photoemission has recently attracted considerable attention due to its high sensitivity to light-induced collective (plasmonic) electron excitations in nanoscale objects at a lateral resolution in the 10 nm regime. A highly promising aspect in this context is the potential of two-photon PEEM to be performed in a time-resolved stroboscopic mode enabling real-time experiments at a temporal resolution in the femtosecond-regime. This allows one to monitor for instance the spatio-temporal dynamics of the local near-field associated with the plasmon mode.

This paper gives an overview of some recent results to exemplify the potential of the PEEM technique in this field. The focus is set on the investigation of periodic and random assemblies of silver nanoparticles in interaction with femtosecond light fields. Aspects, such as the imaging of local near fields [1] and the local field enhancement [2], plasmon dynamics [3], and the manipulation of local near-fields using coherent control schemes [4] will be addressed.

[1] L.I. Chelaru et al., Phys. Rev. B 73, 115416 (2006), L. Douillard et al., Nanoletters 8, (2008) 935 [2] M. Chinchetti et al., Phys. Rev. Lett. 95 (2005) 257403 [3] A. Kubo et al., Nanoletters 5 (2005) 1123 [4] M. Aeschlimann et al., Nature 446 (2007) 301

**O 2: Invited Talk (Michael Horn-von Hoegen)**

Time: Monday 10:15–11:00

Location: HSZ 02

**Invited Talk** O 2.1 Mon 10:15 HSZ 02  
**Surface Science from Hours to Attoseconds: Mind the Gap** — ●MICHAEL HORN-VON HOEGEN — Experimentelle Physik, Universität Duisburg-Essen, 47048 Duisburg

Energy dissipation plays a major role for many processes in nature. Energy transfer on a femto- to nano-second time scale is important for chemical reactions, laser ablation, nanoscale heattransport, plasmonics or strongly driven phase transitions. In my group such dynamic processes are studied within the collaborative research center SFB 616 "Energy Dissipation at Surfaces". I will present examples for the ultrafast electron dynamics in nano structures or layers of organic

semiconductors upon fs-laser excitation by means of fs-time resolved photo electron emission microscopy (PEEM). The excitation, propagation, interference and dissipation of surface plasmon polariton waves in selforganised Ag-nanostructures is lively imaged with sub-fs temporal resolution in the PEEM. The dynamics of structural changes at surfaces upon excitation with a fs-laser pulse is studied on the ps-time scale by time resolved electron diffraction in reflection geometry (RHEED). With this technique strongly driven phase transitions in adsorbate systems on Si surfaces could be studied far away from equilibrium. Utilizing the Debye Waller effect the cooling of vibrational excitations in adsorbate systems or the nanoscale heat transport through a heterofilm interface is observed on the ps-time scale.

**O 3: Oxides and insulators I**

Time: Monday 11:15–13:00

Location: SCH A01

O 3.1 Mon 11:15 SCH A01  
 **$(\sqrt{3}\times\sqrt{3})R30^\circ$  Superstructure in CoO(111) Surfaces** — ●WOLFGANG MEYER, KERSTIN BIEDERMANN, MATTHIAS GUBO, LUTZ HAMMER, and KLAUS HEINZ — Lehrstuhl für Festkörperphysik, Universität Erlangen-Nürnberg, Staudtstr. 7, 91058 Erlangen

CoO(111) films of thicknesses 10-150 Å were prepared by using a Ir(100)-(1×1) surface as a support. At all thicknesses they exhibit a  $(\sqrt{3}\times\sqrt{3})R30^\circ$  superstructure with respect to the hexagonal unit

cell of CoO(111). The latter is slightly distorted below the thickness of about 15 Å (due to the films' accommodation to the quadratic unit cell of the Ir substrate) but relaxes to ideal hexagonal symmetry at larger thickness. Thereby, however, the in-plane lattice parameter only gradually approaches that of bulk CoO (3.012 Å) – at a thickness of about 150 Å it is still (but only) 0.6% above that.

Though the  $(\sqrt{3}\times\sqrt{3})R30^\circ$  structure reversibly transforms to a (1×1) phase with temperature increasing beyond 50°C it must be con-

considered as the CoO films' ground state structure. As the thick films exhibit a lattice parameter rather close to that of bulk CoO(111) one can assume that the  $(\sqrt{3}\times\sqrt{3})R30^\circ$  termination is intrinsic to CoO(111). This makes the crystallography of the surface even more interesting and, in the light of that, we have investigated it by quantitative LEED and atomically resolved STM. It turns out that the CoO(111) surface is metallic and terminated by a wurtzite-type stacking of layers (as retrieved earlier [1]), whereby the atoms within the unit cell undergo a layer dependent buckling or trimerization.

[1] W. Meyer et al., *Phys. Rev. Lett.* **101** (2008) 016103

O 3.2 Mon 11:30 SCH A01

**First-Principles Study of the Growth Kinetics of 1D Pd Islands on SnO<sub>2</sub>** — ●ALEXANDER URBAN and BERND MEYER — Interdisziplinäres Centrum für Molekulare Materialien (ICMM), Friedrich-Alexander-Universität Erlangen-Nürnberg

The vapor deposition of Pd on a reduced SnO<sub>2</sub>(101) surface leads to the formation of one-dimensional (1D) nanowires. Scanning tunneling microscopy reveals the growth of islands with a monoatomic height and a width of 5 Å and a length of up to 350 Å [1]. Nanowires and 1D conductors are potential building blocks of nanoscale devices. For the design of nanowires with specific properties it is essential to fully understand the atomistic processes that lead to this for metal oxide substrates unusual overlayer growth. In order to gain insight into the energetics and the kinetics of the growth of Pd islands on SnO<sub>2</sub>(101) surfaces, the system has been studied by first-principles DFT slab calculations [1] as well as by kinetic Monte-Carlo (kMC) simulations. It is found that a pronounced 1D diffusion, combined with a strong interaction of Pd with the surface Sn atoms and the lack of stable binding sites at the sides of the nanowires are responsible for the formation of the 1D islands.

[1] K. Katsiev, M. Batzill, U. Diebold, A. Urban, and B. Meyer, Growth of One-Dimensional Pd Nanowires on the Terraces of a Reduced SnO<sub>2</sub>(101) Surface *Phys. Rev. Lett.* **98** (2007) 186102

O 3.3 Mon 11:45 SCH A01

**Interface formation and thin film growth of single crystalline Bi(111) on the NaCl(100) surface** — ●THOMAS PAYER, FRANK MEYER ZU HERINGDORF, and MICHAEL HORN-VON HOEGEN — Universität Duisburg-Essen, Duisburg, Germany

Starting from the clean and atomically flat NaCl(100) surface [1] we studied the interface formation and the thin film growth of Bi at room temperature using LEED, AFM and TED. The initial few layers of Bi grow layer by layer showing a diffraction pattern identical to the one observed from the clean NaCl surface indicating that the first nanometer of Bi grows in the NaCl lattice. Subsequently an epitaxial, (111)-oriented film grows on top of this wetting layers. Due to the nearly perfect 7:10 epitaxial ratio of lattice constants the film grows in domains up to micrometer size with a very low defect density and a roughness that can be reduced below 1nm rms by a short anneal at 100°C. Subsequent to film growth the free standing Bi membranes could be obtained by dissolving the NaCl substrate in water. Such membranes are mechanically stable down to 20 nm thickness.

[1] Appl. Phys. Lett. **93**, 093102 (2008)

O 3.4 Mon 12:00 SCH A01

**Ultrathin titanium oxide films grown on Pt<sub>3</sub>Ti(111): Electronic and structural characterization** — ●SÉVERINE LE MOAL, MARCO MOORS, CONRAD BECKER, and KLAUS WANDEL — Institute of Physical and Theoretical Chemistry, University of Bonn, Wegelerstr. 12, D-53115 Bonn, Germany

As TiO<sub>2</sub>-supported platinum is a well-known catalyst, e.g. for CO hydrogenation, the formation of titanium oxides on Ti-Pt alloy surfaces raises much interest. In this work the electronic and structural properties of ultrathin titanium oxide films grown on a Pt<sub>3</sub>Ti(111) single crystal have been investigated by ultraviolet photoelectron spectroscopy (UPS) and low energy electron diffraction (LEED) as a function of oxygen pressure ( $10^{-8}$  to  $10^{-5}$  mbar), oxygen exposure (up to 9000 L) and oxidation temperature (300 to 1000 K). For low oxygen exposures (below  $\sim 200$  L) and above 800 K, a quasi-hexagonal structure ( $a = 3.35$  Å,  $b = 3.25$  Å,  $\alpha = 124^\circ$ ) with two domains rotated by  $8^\circ$  with respect to each other prevails. Upon oxidation at higher exposures and above 900 K a hexagonal structure ( $a = 3.20$  Å) with two domains rotated by  $8^\circ$  with respect to each other is predominantly observed. In this case the  $p(2\times 2)$  structure attributed to the Pt<sub>3</sub>Ti(111) substrate is no longer present, indicating a possible segregation of titanium to the subsurface. Despite the variety of ordered structures, which have

been found for different oxidation conditions, no significant differences in the shape of the valence band spectra have been observed.

O 3.5 Mon 12:15 SCH A01

**Investigation of ultra-thin Chromium layers on Titanium Dioxide by resonant photoemission** — ●SEBASTIAN MÜLLER and DIETER SCHMEISSER — Brandenburgische Technische Universität Cottbus, Konrad-Wachsmann-Allee 17, 03046 Cottbus

Oxide supported metal films and clusters offer interesting properties with a wide range of possible applications. In this context, Titanium Dioxide is chosen as a model substrate due to its simple electronic structure with a  $d^0$  configuration. We study the interaction of ultrathin Chromium films deposited on TiO<sub>2</sub> film with focus on the modifications of the valence band and band gap region. Normal photoemission in bulk and surface sensitive modes as well as resonant photoemission at the Cr 2p and Ti 2p edges are used to distinguish the different Cr 3d and Ti 3d contributions to the valence band. In the initial step we find to gap states of distinct character with a sharp resonance of the Cr 3d related state at the Cr 2p edge. With increasing layer thickness we observe that this resonance extends to about 20 eV below the Fermi-Energy. Datasets of valence band spectra measured around the Cr 2p edge show 2 resonant mechanisms in this case i.e. a participator channel for the 3d state accompanied by a spectator channel at fixed kinetic energy.

O 3.6 Mon 12:30 SCH A01

**Thin iron oxides on corundum - Raman and XRD investigations** — ●ALEXANDER M. GIGLER<sup>1,2</sup>, MAIKE LÜBBE<sup>1</sup>, ROBERT W. STARK<sup>1,2</sup>, and WOLFGANG MORITZ<sup>1</sup> — <sup>1</sup>Sect. Crystallography, LMU-München, D-80333 München — <sup>2</sup>Center for Nanoscience (CeNS), LMU-München, D-80799 München

Iron oxides are a material of great interest as oxidation catalyst [1], for styrene synthesis [2], for corrosion processes [3], as gas sensing material [4]. For its initial growth, a complicated behavior has been supposed including faceting [5], interface expansion [6], or formation of different iron oxide phases such as an additional metastable FeO like iron oxide phase by LEED measurements [7]. We report on the formation of magnetite (Fe<sub>3</sub>O<sub>4</sub>) and hematite (Fe<sub>2</sub>O<sub>3</sub>) on corundum (Al<sub>2</sub>O<sub>3</sub>) as observed by XRD and Raman spectroscopy. Magnetite appears independently from the substrate temperature during evaporation and cannot be removed by post-annealing in an oxygen atmosphere. The temperature range for formation of hematite was 400°C to 500°C. For 300°C, only magnetite can be observed, since growth of hematite is inhibited by the slow activation kinetics at the surface causing a lack of oxygen. For 600°C, the partial pressure of oxygen is too low for hematite growth and the phase-diagram is in favor of magnetite.

[1] G. Samsonov, *The Oxide Handbook* (1973). [2] M. Muhler, *J. of Catalysis* **138**, 413 (1992). [3] S.J. Oh, *Hyperfine Int.* **112**, 59 (1998). [4] M. Ivanovskaya, *Sens. and Act. B* **93**, 422 (2003). [5] S.I. Yi, *Surf. Sci.* **443**, 212 (1999). [6] T. Fujii, *Surf. Sci.* **366**, 579 (1996). [7] S. Gota, *PRB* **60**, 14387 (1999).

O 3.7 Mon 12:45 SCH A01

**Oxygen-deficient cobalt oxide monolayer on Ir(100)-(1x1)** — ●CHRISTINA EBENSPERGER, MATTHIAS GUBO, WOLFGANG MEYER, LUTZ HAMMER, and KLAUS HEINZ — Lehrstuhl für Festkörperphysik, Universität Erlangen-Nürnberg, Staudtstr. 7, 91058 Erlangen

When cobalt of slightly less than a monolayer deposited on Ir(100)-(1x1) is oxidized under oxygen-deficient conditions a new ultrathin cobalt-oxide is formed. It exhibits a (3x3) superstructure on the substrate which can be transformed reversibly into an oxygen-rich c(10x2) structure as described in ref. [1].

The crystallographic structure of the new oxide was determined by quantitative LEED using an exceptionally large data base of more than 12.000 eV. Excellent agreement between experimental and model intensities was achieved (Pendry R-factor: 0.16). The analysis reveals an extremely oxygen-deficient oxide consisting of eight cobalt and only five oxygen ions per (3x3) unit cell with the oxygen located on top of iridium atoms. Four oxygen ions 3-fold coordinated to cobalt are grouped symmetrically around one oxygen ion which in turn is 4-fold coordinated to cobalt. The cobalt ions are closer to the substrate than the oxygen ions, yet not as much as expected from thin cobalt films on iridium. The iridium atoms with oxygen ions on top are displaced by 0.1 Å into the top Ir layer.

The findings of the LEED analysis are corroborated by STM investigations. Depending on the tunnelling conditions either oxygen or the underlying substrate is imaged.

[1] C. Giovanardi et al., Phys.Rev.B 74 (2006) 125429

**O 4: Metal substrates: Adsorption of organic / bio molecules I**

Time: Monday 11:15–13:00

Location: SCH A118

O 4.1 Mon 11:15 SCH A118

**Molecule-substrate interactions of a strong charge-transfer molecule** — •DANIEL WEGNER<sup>1</sup>, STEPHANE BEDWANI<sup>2</sup>, ALAIN ROCHEFORT<sup>2</sup>, and MICHAEL F. CROMMIE<sup>1</sup> — <sup>1</sup>University of California at Berkeley and Lawrence Berkeley National Laboratory, Berkeley, USA — <sup>2</sup>Ecole Polytechnique de Montreal, Canada

Molecules containing multiple cyano groups such as tetracyanoethylene (TCNE) or tetracyanoquinodimethane (TCNQ) represent the archetype of strong electron acceptors. These molecules play a vital role in charge-transfer complexes and metal-organic coordination networks. Potential applications range from nanoscopic templating to molecular electronics and molecule-based magnetism. However, there is still a general lack of information on the properties of these molecules in contact with a conducting surface (e.g., the metallic leads of a single-molecule junction). We have performed scanning tunneling microscopy experiments and first-principles density functional theory calculations of the adsorption of TCNE on the Cu(100) surface. By comparing the experimental results with two different adsorption models, we show that the molecular self-assembly is caused by a strong structural modification of the Cu(100) surface rather than the formation of a coordination network via diffusing Cu adatoms. Surface atoms become highly buckled, and the chemisorption of TCNE is accompanied by a partial charge transfer due to a bonding-backbonding process.

O 4.2 Mon 11:30 SCH A118

**Perpendicular Interaction between Donor and Acceptor Molecules** — GAYANI PERERA<sup>1</sup>, RYOTA MISHIMA<sup>1,2</sup>, and •SAW-WAI HLA<sup>1</sup> — <sup>1</sup>Ohio University, Physics and Astronomy Department, Athens, Ohio 45701, USA. — <sup>2</sup>Division of Material Physics, Graduate School of Engineering Science, Osaka University, Japan.

The capability to modify the electronic properties of materials by the interaction between donor and acceptor molecules plays a significant role in molecular electronics. Formation of molecular charge transfer complexes have been observed for different donor acceptor system in a lateral configuration [1]. Here, we present the structural and electronic properties of decamethylmanganocene (Mn(C5Me5)2) and 7,7,8,8-tetracyanoquinodimethane (TCNQ) molecules on a Au(111) surface at 4.6K using low temperature scanning tunneling microscopy to investigate the perpendicular interaction between the molecules. The molecular complexes are formed by depositing Mn(C5Me5)2 on predeposited TCNQ on Au(111) surface. TCNQ formed well ordered self assembled domains of molecules. Perpendicular interaction between the Mn(C5Me5)2 and TCNQ were determined by means of conductance tunneling spectroscopy. This work is supported by the Ohio University BNNT, National Science Foundation NSF-DMR 0304314, NSF-PIRE: OISE 0730257, and the United States Department of Energy, DE-FG02-02ER46012 grants. [1] F. Jackel, U.G.E. Perera, V. Iancu, K.-F. Braun, N. Koch, J.P. Rabe and S.-W. Hla, Phys. Rev. Lett. 100 (2008) 126102.

O 4.3 Mon 11:45 SCH A118

**Layer growth and desorption kinetics of organic acceptor molecules on Au(111)** — PAUL FRANK<sup>1</sup>, NORBERT KOCH<sup>2</sup>, RALPH RIEGLER<sup>3</sup>, KLAUS MÜLLEN<sup>3</sup>, and •ADOLF WINKLER<sup>1</sup> — <sup>1</sup>Institute of Solid State Physics, Graz University of Technology, Graz, Austria — <sup>2</sup>Institute of Physics, Humboldt University Berlin, Germany — <sup>3</sup>Max Planck Institute of Polymer Research, Mainz, Germany

The layer growth and desorption kinetics of the organic acceptor molecules hexaazatriphenylene-hexacarbonitrile (HAT-CN) on Au(111) surfaces has been studied by TDS, XPS and AFM. Ultra-thin films of HAT-CN show a quite unexpected thermal stability. The first two layers are wetting the surface. They desorb at 460 K (2nd layer) and 610 K (1st layer), respectively. For higher initial coverage a layer like film forms at and below room temperature, which transforms into a Stranski-Krastanov film upon heating at ca. 400 K. Interestingly, during this transformation also the 2nd wetting layer is incorporated into the nascent islands which then desorb at a higher temperature of ca. 490 K. At even higher initial coverage eventually the 1st mono-

layer becomes incorporated into the islands during heating and all the molecules desorb already at ca. 500 K. This shows that the two wetting layers are meta-stable and depend on the initial coverage and the temperature. The reason for this unusual behavior can be identified by the evaluation of the desorption spectra for the individual desorption peaks. It turns out that the desorption energies for all layers are rather similar, but that the pre-exponential factors (in particular for the 1st layer) differ by many orders of magnitude.

O 4.4 Mon 12:00 SCH A118

**Electronic Structure of the Hexaketo- and Hexamethoxy-Substituted Coronene Nanographenes on Au** — •MEDJANIK K.<sup>1</sup>, NAGHAVI S.<sup>2</sup>, RIEGER R.<sup>3</sup>, KUTNYAKHOV D.<sup>1</sup>, NEPLJKO S.A.<sup>1</sup>, SCHÖNHENSE G.<sup>1</sup>, ALIJANI V.<sup>2</sup>, FELSER C.<sup>2</sup>, BAUMGARTEN M.<sup>3</sup>, and MUELLEN K.<sup>3</sup> — <sup>1</sup>Institut für Physik, Universität Mainz — <sup>2</sup>Institute for Analytic and Anorganic Chemistry Univ. Mainz — <sup>3</sup>Max-Planck-Institute for Polymer Research, Mainz

The electronic structure of the donor hexamethoxycoronene and the acceptor coronene-hexaone adsorbed on gold surfaces has been studied by UPS. There substituted nanographenes are synthesized by a novel route described in [1]. A special evaporation system has been developed that is suitable for milligram amounts of evaporant materials. The electronic structure of the keto- and methoxy-species is substantially different because the ligands strongly influence the aromatic system. The keto-species exhibits a significant energetic level shift in the first monolayer with the HOMO being shifted by 1.5 eV towards lower binding energies. The transition from monolayer to multilayer is accompanied by a characteristic variation of the work function that exhibits a sharp minimum. The methoxy species, in contrast, shows constant peak positions throughout the coverage range (along with a continuous drop of the work function) but already for thin layers strong charging sets in. An ab-initio calculation (Gaussian03) has been performed that shows good agreement.

Funded by DFG through Transregio SFB TRR 49

[1] R. Rieger et al., Chem. Eur. J. 14 (2008) 6322

O 4.5 Mon 12:15 SCH A118

**Electronic structure of FeTPC on Cu(111) vs Cu(100) investigated with STM and STS** — •STEFAN KUCK, LEONID LICHTENSTEIN, GERMAR HOFFMANN, and ROLAND WIESENDANGER — Institute of Applied Physics, University of Hamburg, Hamburg, Germany

The investigation of organic molecular systems on metallic surfaces is of great interest due to the manifold applications derived from this combination. However, complications arise from the hybridization of molecule and substrate states at the molecule-substrate interface. Here we locally address the interface of corrole molecules and copper surfaces. In a recent STM study we could show the influence of the substrate on the geometry of iron triphenylcorrole (FeTPC) molecules inducing a bending into a saddle conformation [1]. Molecules are completely asymmetric on the copper substrate which results in a very peculiar electronic structure. We present the influence of the different facets of the copper substrate on the appearance of molecular orbitals spatially resolved in maps of differential conductance.

[1] S. Kuck et al., J. Am. Chem. Soc. 2008, 130, 14072

O 4.6 Mon 12:30 SCH A118

**Ring opening reaction of spiropyran on a Au(111) surface** — •MARTEN PIANTEK, CRISTINA NAVIO, ALEX KRÜGER, MATTHIAS BERNIEN, JORGE MIGUEL, and WOLFGANG KUCH — Institut für Experimentalphysik, Freie Universität Berlin

Molecules that exhibit a photon-induced reversible transition between two isomeric states entail an enormous potential for applications in electronics, photonics, and computing. 1',3',3'-trimethyl-6-nitro-spiro[chromene-2,2'-indole](BIPS) undergoes such a photochromic process involving a heterolytic cleavage of the C–O bond in the pyran ring which goes along with a drastic change of the molecular electronic properties. In the gas phase, in solution, and in the crystalline form, this ring opening/closing mechanism is well understood.

Here we present a temperature-dependent adsorption study of one monolayer of BIPS on a Au(111) single crystal surface. By means of angle-dependent near edge X-ray absorption fine structure (NEXAFS) and X-ray photoemission spectroscopy (XPS) we obtained information about the adsorption geometry and the electronic properties. The simulation of NEXAFS by means of DFT calculations was used for the interpretation of the experimental data. We find that the BIPS molecules deposited at 150 K are in the closed-ring configuration. While the illumination with UV-light had no effect on the monolayer, during heating the sample up to 330 K the molecules transform to the ring opened configuration. Since we did not find a back transformation by cooling back to 150 K, the opened-ring geometry is the preferred conformation on the the surface, in contrast to gas phase and solution.

O 4.7 Mon 12:45 SCH A118

**Electron induced conformational changes of an imine-based molecular switch on a Au(111) surface** — ●CHRISTIAN LOTZE<sup>1</sup>, NILS HENNINGSSEN<sup>1</sup>, KATHARINA FRANKE<sup>1</sup>, GUNNAR SCHULZE<sup>1</sup>, YING LUO<sup>2</sup>, RAINER HAAG<sup>2</sup>, and JOSE IGNACIO PASCUAL<sup>1</sup> — <sup>1</sup>Inst. f. Experimentalphysik, Freie Universität Berlin, Germany — <sup>2</sup>Inst. f. organische Chemie, Freie Universität Berlin, Germany

Azobenzene-based molecules exhibit a cis-trans configurational photoisomerisation in solution. Recently, the adsorption properties of azobenzene derivatives have been investigated on different metal surfaces in order to explore the possible changes in the film properties induced by external stimuli. In azobenzene, the diazo-bridge is a key group for the isomerization process. Its interaction with a metal surface is dominated through the N lone-pair electrons [1], which reduces the efficiency of the conformational change. In order to reduce the molecule-surface interaction, we explore an alternative molecular architecture by substituting the diazo-bridge (-N=N-) of azobenzene by an imine-group (-N=CH-). We have investigated the imine-based compound para-carboxyl-di-benzene-imine (PCI) adsorbed on a Au(111) surface. The carboxylic terminations mediates the formation of strongly bonded molecular dimers, which align in ordered rows preferentially following the fcc regions of the Au(111) herringbone reconstruction. Low temperature scanning tunneling microscopy was used to induce conformational changes between trans and cis state of individual molecules in a molecular monolayer. [1] N. Henningsen, R. Rurali, K. J. Franke, I. Fernández-Torrente, and J. I. Pascual, Appl. Phys. A 93, 241 (2008)

## O 5: Nanostructures at surfaces: Wires, tubes

Time: Monday 11:15–13:00

Location: SCH A215

O 5.1 Mon 11:15 SCH A215

**Playing pinball with atoms** — ●AMIRMEHDI SAEDI, ARIE VAN HOUSLET, RAOUL VAN GASTEL, BENE POELSEMA, and HAROLD ZANDVLIET — University of Twente, Enschede Netherlands

The feasibility of controlling an atomic scale mechanical device by an external electrical signal has been demonstrated [1]. On a Pt modified Ge(001) surface, a switching motion of pairs of dimers is induced by electrons that are directly injected into the atoms with a scanning tunneling microscope tip. By precisely controlling the tip current and distance we make two atom pairs behave like the flippers of an atom-sized pinball machine. This atomic scale mechanical device can reside in six different configurations which enables the system to exhibit up to five distinct flipping modes.

[1]. A. Saedi, A. van Houselt, R. van Gastel, B. Poelsema and H.J.W. Zandvliet, accepted for publication in Nano Lett.

O 5.2 Mon 11:30 SCH A215

**High temperature growth of Ag-nanowires on bare Si(001)** — ●SIMON SINDERMANN, DIRK WALL, MICHAEL HORN-VON HOEGEN, and FRANK-JOACHIM MEYER ZU HERINGDORF — Department of Physics and Center for Nanointegration Duisburg-Essen

Self-organized Ag-islands on bare Si(001) grow in various shapes. Amongst others, quasi 1-dimensional nanowires can be observed with a fixed width of a few hundred nanometers while their length can expand up to tens of micrometers. To specify the conditions and processes leading to nanowire-formation, the growth was examined at elevated temperatures (800K - 1000K) by Photo-Emission Electron Microscopy (PEEM). From the experimental data we determined the ratio of the number of nanowires over the number of all other islands and observed that this ratio increases exponentially with an activation energy of about 1.4eV [1]. Another important parameter to nanowire-growth is the vicinity of the surface. On 4° vicinal samples all nanowires are aligned along the step edges in  $[1\bar{1}0]$  direction, whereas we find nanowire in two directions ( $[110]$  and  $[1\bar{1}0]$ ) on flat Si(001). Due to previous experimental results, this observation can be explained by the anisotropy of diffusion which increases quickly from 0° to reach the maximum at 4° [2].

[1] D. Wall, S. Sindermann, M. Horn-von Hoegen, and F.-J. Meyer zu Heringdorf; J. P.:Cond. Matt. (submitted)

[2] D. Wall, K. R. Roos, M. Horn-von Hoegen, and F.-J. Meyer zu Heringdorf; Mater. Res. Soc. Symp. Proc. 1088E; 1088-W05-04 (2008)

O 5.3 Mon 11:45 SCH A215

**Self-Organized Atomic Gold Nanowires on Ge(001) Revealed by Scanning Tunneling Microscopy** — ●CHRISTIAN BLUMENSTEIN, SEBASTIAN MEYER, JÖRG SCHÄFER, and RALPH CLAESSEN — Physikal. Institut, Universität Würzburg, 97074 Würzburg

Atomic nanowires have become objects of intense research, as they host a wealth of physical phenomena not encountered in three-dimensional solids. They are synthesized by self-organization of metal adatoms on suitable semiconducting substrates that guide chain formation. Thus far, examples for quasi one-dimensional (1D) systems have been found where the Fermi surface hosts a charge density wave (CDW). This can be observed below room temperature in systems on Si(111) or high-index variants thereof. However, the ease of CDW condensation points at still significant coupling to the second dimension. In the search for better defined 1D systems, we have identified self-organized Au-induced chains on Ge(001) which grow in a long-range  $c(8 \times 2)$  phase and exhibit metallic behavior. In using scanning tunneling microscopy, we find that the wires are spaced by several Ge lattice constants, while their electron density is strictly confined laterally [1]. In turn, the metallic charge cloud is spread out very evenly in chain direction, as seen for a large range of bias values. Such exceptional degree of confinement may open a pathway to study non-Fermi liquid physics. The talk will review the various structural ingredients of this exceptional 1D electron system.

[1] J. Schäfer et al., Phys. Rev. Lett. 101, in press (Dec. 2008).

O 5.4 Mon 12:00 SCH A215

**Magnetism versus formation of transition-metal chains in break junctions** — ●ALEXANDER THIESS<sup>1,2</sup>, YURIY MOKROUSOV<sup>1,2</sup>, STEFAN HEINZE<sup>2</sup>, and STEFAN BLÜGEL<sup>1</sup> — <sup>1</sup>Institut für Festkörperforschung und Institute for Advanced Simulation, Forschungszentrum Jülich, 52545 Jülich, Germany — <sup>2</sup>Institute of Applied Physics, University of Hamburg, 20355 Hamburg, Germany

One of the pressing issues in break junction (BJ) experiments is the experimental search for evidence of magnetism in suspended monoatomic transition-metal (TM) chains [1]. Our strategy to tackle this question is a theoretical analysis of the most fundamental and transparent quantity of these systems: the probability for successful chain creation itself. On the basis of *ab initio* calculations both including and excluding spin-polarization of 3d, 4d and 5d TM chains we developed a model describing chain formation in BJs [2]. Contrasting the different probabilities of forming non-magnetic or magnetic chains, we find that emerging magnetism suppresses the tendency to chain formation. Comparing our results to existing experiments may serve as a proof that even 5d chains in BJs are magnetic.

[1] C. Untiedt, D.M.T Dekker, D. Djukic, J.M. van Ruitenbeek, Phys. Rev. B 69, 081401 (2004)

[2] A. Thiess, Y. Mokrousov, S. Blügel, S. Heinze, Nano Letters 8, 2144 (2008)

O 5.5 Mon 12:15 SCH A215

**Dysprosium silicide nanowires on Si(557)** — ●MARTIN FRANZ<sup>1</sup>, MARTINA WANKE<sup>1</sup>, MATTHIAS VETTERLEIN<sup>1</sup>, GERD PRUSKIL<sup>1</sup>,

CHRISTOPHER PROHL<sup>1</sup>, BRITTA HÖPFNER<sup>1</sup>, FLORIAN GENZ<sup>1</sup>, PETAR STOJANOV<sup>2</sup>, ERIC HUWALD<sup>2</sup>, JOHN RILEY<sup>2</sup>, and MARIO DÄHNE<sup>1</sup> — <sup>1</sup>Institut für Festkörperphysik, Technische Universität Berlin, D-10623 Berlin, Deutschland — <sup>2</sup>School of Physics, La Trobe University, Bundoora, VIC 3086, Australia

The structural and electronic properties of self-assembled nanowires on the Si(557) surface have been studied using scanning tunneling microscopy (STM) and angle-resolved photoemission spectroscopy (ARPES) using a toroidal electron analyser. The Si(557) surface is a vicinal Si(111) surface with a miscut angle of 9.5° that facets into (111) and (112) terraces. Different types of nanowires are grown depending on the Dy coverage. At submonolayer coverages, thin semimetallic nanowires with one-dimensional band structure are grown. In contrast, the nanostructures forming at monolayer and multilayer dysprosium coverages exhibit a very different behavior. At these preparation conditions broad nanowires are grown on the Si(111) facets of the Si(557) surface, consisting of DySi<sub>2</sub> in the monolayer case and Dy<sub>3</sub>Si<sub>5</sub> in the multilayer case. A two-dimensional metallic band structure is observed which is similar to the corresponding ones of the dysprosium silicides on Si(111). This project was supported by the DFG, project number Da 408/11.

O 5.6 Mon 12:30 SCH A215

**Silicon overgrowth of rare earth silicide nanowires on Si(001)** — ●MATTHIAS VETTERLEIN, MARTINA WANKE, MARTIN FRANZ, and MARIO DÄHNE — Institut für Festkörperphysik, Technische Universität Berlin, D-10623 Berlin, Deutschland

The overgrowth of rare earth silicide nanowires on the Si(001) surface by silicon has been investigated by STM. Free standing broad silicide nanowires present interesting properties such as a one-dimensional metallicity along the wires. Due to this metallicity the self assembled

nanowires may be used e.g. as nano-interconnects in advanced chip designs. To prevent oxidation and destruction of the nanowires under ambient conditions a suitable capping is required. For this purpose, silicon is an ideal capping material because of its perfect lattice match with the substrate. To the best of our knowledge we present for the first time silicon capping experiment of rare earth silicide nanowires. Our STM results show that capping with small amounts of silicon does not destroy the wires. After further annealing the wires are still present under the silicon cap layer. This indicates the feasibility of nanowire capping by silicon. This project was supported by the DFG, project number Da 408/11.

O 5.7 Mon 12:45 SCH A215

**Periodic LDOS modulations in self-organized bi-atomic chains** — ●MATTHIAS MENZEL, KIRSTEN VON BERGMANN, ANDRÉ KUBETZKA, and ROLAND WIESENDANGER — Institut für Angewandte Physik, Universität Hamburg, Jungiusstr. 11, 20355 Hamburg

The (5×1)-reconstructed Ir(001) surface is an ideal template for the self-organized formation of one-dimensional nanostructures [1]. In this reconstruction, which exists in two rotational domains, the topmost layer forms trenches along the ⟨110⟩-directions of the surface. We used this property of the surface to grow bi-atomic Fe chains at room temperature which we investigated by means of low temperature scanning tunneling microscopy (STM) and spectroscopy (STS).

In maps of the differential conductance ( $dI/dU$ ), which is proportional to the local density of states (LDOS), the Fe chains exhibit various different periodic modulations of the LDOS along the chain axis. Those oscillations are commensurate with respect to the atomic distance in the Fe chains and we observe modulations of two, three and four times the atomic distance. The modulations are found to be non-dispersive in energy and they do not depend on the chain length. [1] L. Hammer *et al.*, Phys. Rev. B, **67**, 125422 (2003)

## O 6: Electronic structure I

Time: Monday 11:15–13:00

Location: SCH A216

O 6.1 Mon 11:15 SCH A216

**Electron Dynamics of Quantum-Well States in Pb Nanocrystals** — ●I-PO HONG, CHRISTOPHE BRUN, FRANÇOIS PATTHEY, and WOLF-DIETER SCHNEIDER — École Polytechnique Fédérale de Lausanne, Institut de Physique des Nanostructures, CH-1015 Lausanne, Switzerland

Electrons confined in a thin metal film occupy discrete electronic eigenstates known as quantum well states (QWS). As a function of film thickness, the electronic density of states is modulated in an oscillatory manner when a QWS passes through the Fermi level, affecting many of the physical and chemical properties of a thin film. Here we use low-temperature scanning tunneling microscopy and scanning tunneling spectroscopy to study the quasiparticle linewidth of the QWS in Pb nanocrystals on Si(111)-7×7 and on Pb-√3×√3/Si(111). An analysis of the QWS linewidth within a model which accounts for the tunneling process and electron reflection at the Pb-Si and Pb-vacuum interfaces, allows us to determine quantitatively the QWS quasiparticle lifetime, including defect and interface scattering, electron-phonon interaction, and electron-electron interaction.

We acknowledge financial support of the Swiss National Science Foundation.

O 6.2 Mon 11:30 SCH A216

**The Two-Dimensional Electron System Au/Ge(111) Studied by Angle-Resolved Photoemission** — ●PHILIPP HÖPFNER<sup>1</sup>, MAIK HESSMANN<sup>1</sup>, JÖRG SCHÄFER<sup>1</sup>, CARSTEN ENDERLEIN<sup>2</sup>, THOMAS BRAUN<sup>2</sup>, CHRISTIAN BLUMENSTEIN<sup>1</sup>, SEBASTIAN MEYER<sup>1</sup>, KARSTEN HORN<sup>2</sup>, and RALPH CLAESSEN<sup>1</sup> — <sup>1</sup>Physikal. Institut, Universität Würzburg, 97074 Würzburg — <sup>2</sup>Fritz-Haber-Institut, 14195 Berlin

Two-dimensional electron systems (2DES) at surfaces offer high potential for studying correlation effects. Adsorbed metals on (111) semiconductor substrates provide intriguing realizations of a 2DES by forming (√3×√3) reconstructions with metal coverage (Sn, Pb, Au etc.) not exceeding one monolayer. Electron-electron interaction is assumed to play an important role. Examples include Sn/Ge(111) as a rather highly correlated system which even exhibits a Mott-Hubbard transition. In particular, the choice of metal species and substrate will

affect orbital character and overlap. By this means, it should be possible to tailor the correlation strength, and to thus understand the mechanisms behind it. Here we explore the little studied noble metal adsorbates by addressing the Au/Ge(111)-(√3×√3) system. Angle-resolved photoelectron spectroscopy (ARPES) reveals a metallic character, and for the first time provides an account of the Fermi surface topology. In addition, ARPES determination of the band dispersion reveals electron- and hole-like bands. Their behavior and the effective masses are suggestive of a less correlated electron system, thereby reflecting the tunability of the electronic interactions in a monolayer 2DES.

O 6.3 Mon 11:45 SCH A216

**Valence level bands and Fermi surface of decagonal Al-Cu-Co** — WOLFGANG THEIS<sup>1</sup>, JAN HUGO DIL<sup>2</sup>, AJAY SHUKLA<sup>3</sup>, JEONGWON KIM<sup>3</sup>, HOON KOH<sup>4</sup>, ELI ROTENBERG<sup>4</sup>, PETER GILLE<sup>5</sup>, and ●KARSTEN HORN<sup>2</sup> — <sup>1</sup>Fachbereich Physik, FU Berlin, D — <sup>2</sup>Fritz Haber Institute of the MPG, Berlin, D — <sup>3</sup>UGC-DAE-CSR, Indore, India — <sup>4</sup>ALS, Lawrence Berkeley Lab, USA — <sup>5</sup>Dpt. Geosciences, LMU Munich, D

Valence electronic states in quasicrystals seem to defy the concept of Bloch states because of the absence of translational periodicity. However, this may not necessarily preclude the existence of delocalized electronic states in quasicrystals, since critical electronic states which fall off with a power law may exist, and evidence for delocalized states has been found in quasicrystals in the region of the deeper valence bands. For an analysis of the transport properties of quasicrystals an investigation of the region near the Fermi level is important, however, Here we examine the s-p-derived electronic structure of decagonal Al-Cu-Co in this region using angle-resolved photoemission. These states are accessible in Al-Cu-Co because, unlike in Al-Ni-Co, the d bands are well removed and do not interfere. We find that the electronic structure can be well represented by parabolic dispersing bands in a region of about 1 eV below the Fermi level. The data are analyzed within a model that uses a subset of specific reciprocal lattice vectors, and that provides a consistent description of the photoemission intensity distribution and the dispersion of the observed state signatures.

O 6.4 Mon 12:00 SCH A216

**Interplay between electronic states and structure during Au faceting** — ●FREDERIK SCHILLER<sup>1</sup>, MARTINA CORSO<sup>2</sup>, JAVIER CORDÓN<sup>3</sup>, JAVIER GARCÍA DE ABAJO<sup>4</sup>, and ENRIQUE ORTEGA<sup>1,2,3</sup> — <sup>1</sup>Unidad de Física de Materiales CSIC/UPV, Manuel Lardizábal 3, E-20018 San Sebastián, Spain — <sup>2</sup>DIPC, Manuel Lardizábal 4, E-20018 San Sebastián, Spain — <sup>3</sup>Dpto. Física Aplicada I, Universidad del País Vasco, Plaza Oñate 2, E-20018 San Sebastián, Spain — <sup>4</sup>Instituto de Óptica-CSIC, Serrano 121, E-28006 Madrid, Spain

Au(111) vicinal surfaces are characteristic examples of two-phase segregation or faceting. Between  $\sim 4^\circ$  and  $9.5^\circ$  miscut, the surface exhibits hill-and-valley structures formed by bunches of relatively wide ( $d_w \sim 36\text{-}41$  Å) and narrow ( $d_n \sim 14$  Å) terraces. The evolution of surface electronic states in such a faceted system is followed using a curved crystal. Beyond  $4^\circ$  the surface state splits into distinct  $d_w$  and  $d_n$  bands. Our analysis suggests the crucial role of surface states in defining the characteristic  $d_w$  and  $d_n$  sizes during Au faceting.

O 6.5 Mon 12:15 SCH A216

**The influence of reconstruction on the surface state of Au(110)** — ●ANDREAS NUBER<sup>1</sup>, MITSU HARU HIGASHIGUCHI<sup>2</sup>, FRANK FORSTER<sup>1</sup>, PETER BLAHA<sup>3</sup>, KENYA SHIMADA<sup>4</sup>, and FRIEDRICH REINERT<sup>1,5</sup> — <sup>1</sup>Experimentelle Physik II, Universität Würzburg, Am Hubland, D-97074 Würzburg, Germany — <sup>2</sup>Graduate School of Science, Hiroshima University, Higashi-Hiroshima 739-8526, Japan — <sup>3</sup>Institute of Materials Chemistry, Vienna University of Technology, Getreidemarkt 9/165, A-1060 Vienna, Austria — <sup>4</sup>Hiroshima Synchrotron Radiation Center, Hiroshima University, Higashi-Hiroshima 739-0046, Japan — <sup>5</sup>Forschungszentrum Karlsruhe, Gemeinschaftslabor für Nanoanalytik, D-76021 Karlsruhe, Germany

We present high-resolution angle-resolved photoelectron spectroscopy on Au(110). The unreconstructed surface shows a Shockley-type surface state at  $E_0 = 590$  meV whereas on the  $(2 \times 1)$  missing-row reconstructed surface no such surface state below  $E_F$  can be detected [1]. We performed relativistic LDA calculations which agree well with our experimental data. Adsorption of 1 ML Ag on the  $(2 \times 1)$  reconstructed surface results in a destruction to a  $(1 \times 1)$  surface structure and a Shockley state appears at  $E_0 = 475$  meV. Shifting down the surface state from just above to below  $E_F$  by Na adsorption allowed to extrapolate a binding energy on the reconstructed surface of  $E_0 = -120$  meV above the Fermi level.

[1] A. Nuber *et al.* Phys. Rev B **78**, 195412 (2008).

O 6.6 Mon 12:30 SCH A216

**PE and IPE study of the surface electronic structure of Y(0001)** — ●SEBASTIAN D. STOLWIJK<sup>1</sup>, MICHAEL BUDKE<sup>1</sup>, KRISTIAN M. DÖBRICH<sup>2</sup>, and MARKUS DONATH<sup>1</sup> — <sup>1</sup>Physikalisches Institut, Westfälische Wilhelms-Universität Münster — <sup>2</sup>Fachbereich Physik, Freie Universität Berlin

Yttrium and gadolinium are isoelectronic elements with respect to their valence bands but differ in their magnetic properties due to the additional 4f electrons in Gd. Therefore, Y may be viewed as paramagnetic model for ferromagnetic Gd. A comparative study of the electronic structure of Y and Gd promises to reveal electronic properties that are directly linked to ferromagnetism.

For more than 20 years, differences in the photoemission spectra of Y(0001) obtained from single-crystalline bulk samples and thin films grown on W(110) have remained an unsolved puzzle. Our recent study on the (0001) surface of a single-crystalline yttrium bulk sample shows that most of the spectral features arise due to impurities such as carbon, chlorine, oxygen and hydrogen [1]. In order to develop a consistent picture of the surface electronic structure of Y(0001), we compare direct and inverse-photoemission results from single-crystalline yttrium bulk samples and ultrathin films, particularly with regard to the surface state close to the Fermi level. These results are discussed in view of data obtained for Gd.

[1] M. Budke, J. S. Correa, and M. Donath, Phys. Rev. B **77**, 161401(R) (2008)

O 6.7 Mon 12:45 SCH A216

**Y(0001) bulk crystal - An adequate substrate for the growth of Gd(0001) films?** — MICHAEL BUDKE, TOBIAS ALLMERS, ●KAREN ZUMBRÄGEL, and MARKUS DONATH — Physikalisches Institut, Westfälische Wilhelms-Universität Münster

With a negligible lattice mismatch and identical crystal structure, Y commends itself as the ideal substrate for Gd thin film growth. We report on the growth, magnetism and electronic structure of Gd(0001) films grown on a Y(0001) bulk crystal in comparison with films grown on W(110). By combining scanning tunneling microscopy, low-energy electron diffraction, magneto-optical Kerr-effect measurements, as well as direct and inverse photoemission in one ultra-high vacuum system, we are able to provide a detailed characterization of the obtained films. As one of the main criteria we discuss the appearance of the surface state near the Fermi energy. Our results show that although bulk Y crystals suffer from naturally occurring impurities, they are nevertheless a good alternative to W(110) substrates for the growth of Gd.

## O 7: Semiconductor substrates

Time: Monday 11:15–13:00

Location: SCH A315

O 7.1 Mon 11:15 SCH A315

**Electronic structure of the cleaved non-polar GaN(1100) surface** — ●P. LÖPTIEN<sup>1</sup>, M. BERTELLI<sup>1</sup>, M. WENDEROTH<sup>1</sup>, R.G. ULBRICH<sup>1</sup>, A. RIZZI<sup>1</sup>, J. MALINDRETOS<sup>1</sup>, M.C. RIGHI<sup>2</sup>, A. CATELLANI<sup>3</sup>, A. FERRETTI<sup>2</sup>, and L.C. SAMOS<sup>2</sup> — <sup>1</sup>IV. Phys. Inst., Univ. Göttingen, Germany — <sup>2</sup>Dip. Fisica, Modena, Italy — <sup>3</sup>CNR, Parma, Italy

The non-polar GaN(1100) surface ( $m$ -plane) has recently gained importance due to the demonstration of high-efficiency LEDs and LDs. A thorough microscopic understanding of this surface is therefore of great interest. Up to now the existence of surface states within the bandgap at the  $\bar{\Gamma}$  point of the Brillouin zone is an open question. We performed cross-sectional scanning tunneling microscopy and spectroscopy (XSTM/XSTS) and ab initio DFT-LDA simulations of this surface. Our calculations suggest an unreconstructed surface and no surface state bands inside the gap at  $\bar{\Gamma}$ . The Ga derived empty surface state band is found to be degenerate with the CB minimum. In experiment, the unintentionally n-doped GaN(0001) samples grown by HVPE were thinned to  $\sim 100$  nm. They were cleaved in UHV along the  $m$ -plane and measured in-situ at room temperature. The experiments confirmed clearly the unreconstructed surface. The current measured by STS at different voltages can be explained with tip-induced band bending (TIBB). Conduction band states are addressed both at positive and negative bias voltages. This is confirmed by a simulation with a one-dimensional Poisson equation solver. We conclude that the Fermi-level is not pinned on clean cleaved surfaces. It follows that the bandgap has no intrinsic surface states at the  $\bar{\Gamma}$  point of the BZ.

O 7.2 Mon 11:30 SCH A315

**Impurity induced charge density oscillations in the  $\pi$ -bonded chains of the Si(111)-2 $\times$ 1 surface** — ●KAROLIN LÖSER<sup>1</sup>, MARTIN WENDEROTH<sup>1</sup>, THOMAS K. A. SPAETH<sup>1</sup>, JENS K. GARLEFF<sup>2</sup>, and RAINER G. ULBRICH<sup>1</sup> — <sup>1</sup>IV. Phys. Inst., Georg-August Univ. Göttingen, Germany — <sup>2</sup>PSN, Eindhoven University of Technology, the Netherlands

The  $\pi$ -bonded chain in the Si(111)-2 $\times$ 1 reconstructed surface behaves in many respects like a quasi 1-d electronic system. Investigating such chains in P-doped Si with a low-temperature STM (6-8 K) we found extended 1-d electronic contrast induced by the substitutional Phosphorus atom. The presence of the point defect modifies the electronic properties of the chains and causes localization of electron density. The contrast feature occurs at a bias voltage of about -0.5 V and has a length of 10 nm. Depending on the lattice site of the P-atom, it is confined to either one or two neighbouring  $\pi$ -bonded chains.

STS data on the  $\pi$ -bonded chains show a Coulomb Gap in the differential tunneling conductance at  $E_F$ . The Coulomb Gap has a width of up to 150 meV, depending linearly on the reciprocal length of undisturbed chain. The Coulomb Gap vanishes for undisturbed chain lengths of several hundred nm. We recently succeeded in preparing large surface areas ( $> 600$  nm)<sup>2</sup> without steps or domain boundaries cutting the chains. Scanning these areas we discovered that the P-atoms induce long range spatial oscillations of the LDOS along the  $\pi$ -bonded chains in addition to the well-known LDOS-feature. These oscillations have a wavelength of about 15 nm at a bias voltage of -0.5

V.

O 7.3 Mon 11:45 SCH A315

**Epitaxial growth of micrometer-sized Cu-pyramides on Silicon** — ●SUSANNE SEYFFARTH and HANS-ULRICH KREBS — Institut für Materialphysik, Universität Göttingen, Friedrich-Hund-Platz 1, 37077 Göttingen

Studying the morphology of thin metallic films is very important regarding the properties of these films. Therefore thin Cu films on Si(111) and Si(100) substrates were prepared using pulsed laser deposition (PLD) in ultra high vacuum. At elevated substrate temperatures above 200 °C epitaxial growth of three dimensional pyramides with edge lengths of about five micrometers and heights up to 500 nanometers is observed using scanning electron microscopy (SEM) and atomic force microscopy (AFM). The base area of these islands is a triangle for Si(111) and a square for Si(100) depending on the orientation of the substrate. Epitaxial relationships with the Si substrates were studied using x-ray diffraction analysis (XRD). Furthermore periodic alignments of the pyramidal islands was achieved. The shape of the pyramidal islands was influenced by alloying Ni during deposition process. Additionally the decomposition of the Cu-islands was examined.

O 7.4 Mon 12:00 SCH A315

**MOVPE preparation of Si(100) surfaces for III-V hetero epitaxy** — ●HENNING DÖSCHER, PETER KLEINSCHMIDT, SEBASTIAN BRÜCKNER, ANJA DOBRICH, CHRISTIAN HÖHN, and THOMAS HANNAPPEL — Helmholtz-Zentrum Berlin für Materialien und Energie, Glienicker Str. 100, 14109 Berlin

The epitaxial growth of III-V semiconductors on silicon substrates is a major challenge for the integration of opto- and micro-electronic devices. But still, there is little experience in the preparation of the crucial Si(100) surface with metal-organic vapor phase epitaxy (MOVPE) and the respective interfaces to III-V materials.

In many ways the applied process environment common for the optoelectronic industry differs from the ultra high vacuum (UHV) conditions typical in surface science - e.g. by the distinct presence of hydrogen as precursor residue and as process gas. For the desired growth of polar materials on non-polar substrates, the hetero-interface represents a source of highly corruptive anti-phase disorder. Ideally, this effect may be suppressed by the preparation of a completely double-stepped substrate surface with only one reconstruction domain.

Here, the preparation of clean Si(100) surfaces by MOVPE growth is investigated with regard to the requirements of hetero-epitaxial GaP growth. A contamination free transfer mechanism to UHV enabled X-ray photoelectron spectroscopy (XPS), low energy electron diffraction (LEED), scanning tunnelling microscopy (STM) and Fourier-transform infrared spectroscopy (FTIR) characterization of the prepared surfaces, while reflectance anisotropy spectroscopy (RAS) was applied in-situ.

O 7.5 Mon 12:15 SCH A315

**Ge nanoisland growth on the In/Si(112)-"(3.5 × 1)"surface** — ●MORITZ SPECKMANN, THOMAS SCHMIDT, JAN INGO FLEGE, TORSTEN WILKENS, and JENS FALTA — Institute of Solid State Physics, University of Bremen, 28359 Bremen

In this work we investigated the adsorption of In on Si(112) and the subsequent growth of Ge islands using a variety of different surface sensitive techniques. The unstable Si(112) surface consists of (111)- and (337)-like facets in  $[1\bar{1}0]$  direction (Baski et al., PRL, **74** (1995) 956). The surface is smoothened due to the adsorption of metals, such as Ga or In (Snijders et al., PRB, **72** (2005) 125343).

In LEED images we find an incommensurate "(3.5 × 1)"reconstruction for the In/Si(112) surface. We determine the number and the positions of the In atoms inside one unit cell using XPS

and X-Ray Standing Waves (XSW). With these results it is, for the first time, possible to propose a structural model based on direct structural data.

By means of Low Energy Electron Microscopy (LEEM) and Photoemission Electron Microscopy (PEEM) we monitored the growth of Ge on the In/Si(112) surface. First a smooth wetting layer is formed and after a few MLs islands start to grow. The observed islands are triangularly shaped with a longer edge along the  $[110]$  direction. The island density is higher compared to the growth on bare Si(112). Moreover no arrangement or preferential direction is visible for Ge islands on the bare Si(112) surface. The corresponding LEED patterns reveal a  $(4 \times 1)$  reconstruction with additional facet spots which are attributed to the Ge islands.

O 7.6 Mon 12:30 SCH A315

**Structural properties of sub-monolayer InAs coverages on GaAs(001)** — ●CHRISTOPHER PROHL, BRITTA HÖPFNER, JAN GRABOWSKI, HOLGER EISELE, and MARIO DÄHNE — Institute of Solid State Physics, Technical University Berlin, Germany

Even if InAs/GaAs is the model system for III-V-semiconductor quantum dots, the growth and dot formation is still not understood in detail. In this work, we investigated low InAs coverages in the sub-monolayer range to understand the growth of InAs on GaAs and to receive a databasis, also for further investigation of quantum dots and their capping. Molecular beam epitaxy (MBE) was used to prepare different samples with increasing sub-monolayer InAs-coverages on a GaAs(001) wafer. The growth was performed on both As-rich reconstructions, the  $c(4 \times 4)$  and the  $\beta 2(2 \times 4)$ . Using in-situ scanning tunneling microscopy (STM) with atomic resolution, the formation of an InAs/GaAs- layer was investigated step by step, from the clean GaAs surface up to about one monolayer coverage of InAs. It was found that InAs first grows directly on boundaries of different  $c(4 \times 4)$  domains. Further on, it then sticks to the hollow sites of perfectly  $c(4 \times 4)$  reconstructed areas of GaAs(001). Continuing growth leads to a complete monolayer but with a new reconstruction for both the  $c(4 \times 4)$  and the  $\beta 2(2 \times 4)$  reconstructed surface. The authors thank K. Jacobi and the MPG for providing the experimental set-up. This work was supported by project Da 408/12 of the DFG.

O 7.7 Mon 12:45 SCH A315

**Structural properties of the InAs/GaAs system before and after quantum dot formation.** — ●BRITTA HÖPFNER, CHRISTOPHER PROHL, JAN GRABOWSKI, HOLGER EISELE, and MARIO DÄHNE — Institute of Solid State Physics, Technical University Berlin, Germany

The structure of the wetting layer prior to quantum dot formation and the shape of just formed quantum dots are of high interest for the understanding of the quantum dot growth mechanisms. To understand growth and properties of InAs layers on GaAs step by step a molecular-beam epitaxy-system (MBE) including reflection high energy electron diffraction (RHEED) and attached scanning-tunneling microscopy (STM) was used. In this work, GaAs(001) surfaces covered with increasing InAs coverages beginning with about one monolayer up to the formation of quantum dots were prepared. In order to study the influence of the surface reconstruction on the growth, both As-rich GaAs(001)  $c(4 \times 4)$  and  $\beta 2(2 \times 4)$  reconstructed surfaces were used. Atomically resolved STM images of different coverages and an analysis of the growth behavior will be presented. Structural changes during closing of the first monolayer will be shown.

The authors thank K. Jacobi and the MPG for providing the experimental set-up. The work was supported by project Da 408/12 of the DFG.

## O 8: Focused Session: Epitaxial Graphene I

Time: Monday 11:15–12:45

Location: SCH 251

### Topical Talk

O 8.1 Mon 11:15 SCH 251

**Atmospheric pressure graphitization of SiC: a route towards wafer-size graphene films** — K.V. EMTSEV<sup>1</sup>, A. BOSTWICK<sup>2</sup>, K. HORN<sup>3</sup>, J. JOBST<sup>1</sup>, G.L. KELLOG<sup>4</sup>, L. LEY<sup>1</sup>, J.L. MCCHESENEY<sup>2</sup>, T. OHTA<sup>4</sup>, S.A. RESHANOV<sup>1</sup>, J. RÖHRL<sup>1</sup>, E. ROTENBERG<sup>2</sup>, A.K. SCHMID<sup>5</sup>, D. WALDMANN<sup>1</sup>, H.B. WEBER<sup>1</sup>, and ●TH. SEYLLER<sup>1</sup> —

<sup>1</sup>FAU Erlangen-Nürnberg — <sup>2</sup>Advanced Light Source, USA — <sup>3</sup>FHI Berlin — <sup>4</sup>Sandia National Laboratories, UAS — <sup>5</sup>National Center for Electron Microscopy, USA

Graphene, a single monolayer of  $sp^2$ -bonded carbon, is a very unique 2-dimensional electron gas system with electronic properties fundamentally different to other 2DEG systems [1]. A manifold of applications

has already been suggested, which requires a uniform, ordered growth of graphene on an insulating substrate. The growth of graphene on insulating silicon carbide (SiC) surfaces by high-temperature annealing in vacuum [2] was proposed for the development of graphene-based electronics [3]. However, vacuum decomposition of SiC yields graphene layers with small grains. We have investigated the growth of graphene on SiC(0001) in an argon atmosphere [4] which produces monolayer graphene films with significantly improved morphology and carrier mobility. The new growth process establishes a method for the synthesis of graphene films on a technologically viable basis. [1] A.H. Castro Neto, et al., arXiv:0709.1163v2. [2] A. Charrier, et al., J. Appl. Phys. 92 (2002) 2479. [3] C. Berger et al., J. Phys. Chem. B 108 (2004) 19912; C. Berger, et al., Science 312 (2006) 1191. [4] K.V. Emtsev, et al., arXiv:0808.1222v1.

O 8.2 Mon 11:45 SCH 251

**Atomic Hole Doping of Graphene** — ●ISABELLA GIERZ<sup>1</sup>, CHRISTIAN RIEDL<sup>1</sup>, ULRICH STARKE<sup>1</sup>, CHRISTIAN AST<sup>1</sup>, and KLAUS KERN<sup>1,2</sup> — <sup>1</sup>Max-Planck-Institute for Solid State Research, D-70569 Stuttgart, Germany — <sup>2</sup>Institut de Physique des Nanostructures, Ecole Polytechnique Federale de Lausanne, CH-1015 Lausanne, Switzerland

Graphene is an excellent candidate for the next generation of electronic materials due to the strict two-dimensionality of its electronic structure as well as the extremely high carrier mobility. A prerequisite for the development of graphene based electronics is the reliable control of the type and density of the charge carriers. While gating has been successfully demonstrated, the development of reliable chemical doping methods turns out to be a real challenge. In particular hole doping is an unsolved issue. Here we show by angle-resolved photoemission spectroscopy (ARPES) that atomic doping of an epitaxial graphene layer on a silicon carbide substrate with bismuth, antimony or gold presents effective means of p-type doping. Bismuth and antimony are only able to reduce the substrate induced n-type doping of epitaxial graphene. Gold adatoms, however, shift the Dirac point into the unoccupied states. In combination with the intrinsic n-type character of epitaxial graphene on SiC, the charge carriers can be tuned from electrons to holes, without affecting the conical band structure.

O 8.3 Mon 12:00 SCH 251

**Molecular Hole Doping and Band Structure Engineering of Epitaxial Graphene on SiC** — ●CAMILLA COLETTI, CHRISTIAN RIEDL, DONG SU LEE, KLAUS VON KLITZING, JURGEN H. SMET, and ULRICH STARKE — Max-Planck-Institut für Festkörperforschung, Heisenbergstr. 1, 70569 Stuttgart

In view of its intriguing two-dimensional electron gas properties, graphene is a promising host material for next-generation electronics. In particular, graphene epitaxially grown on silicon carbide (SiC), offers realistic prospects for electronic device implementation. However, the intrinsic n-type doping and the consequent metallic nature of these epitaxial layers badly accommodate in conventional electronics. We show, via angle resolved ultraviolet photoelectron spectroscopy (ARUPS) and Raman analysis, how monolayer and few layer epitaxial graphene can be rendered truly semiconducting by functionalizing the graphene surface with the strong electron acceptor tetrafluorotetracyanoquinodimethane (F4-TCNQ). We also report how, in the case of bilayer graphene, the molecular layer influences the details of the band structure thus suggesting the possibility for band gap engineering. We provide via X-ray photoelectron spectroscopy (XPS) and va-

lence band investigations a complete characterization of this charge transfer complex. Furthermore, by demonstrating air stability and the feasibility of implementation via wet chemistry we show that the F4-TCNQ/graphene heterostructure is extremely appealing for future, carbon based electronic applications.

O 8.4 Mon 12:15 SCH 251

**Electronic excitations in epitaxial graphene layers grown on SiC(0001)** — ●THOMAS LANGER<sup>1,2</sup>, HERBERT PFNÜR<sup>1</sup>, CHRISTOPH TEGENKAMP<sup>1</sup>, HANS WERNER SCHUMACHER<sup>2</sup>, and UWE SIEGNER<sup>2</sup> — <sup>1</sup>Institut für Festkörperphysik, Leibniz Universität Hannover, Appelstrasse 2, D-30167 Hannover, Germany — <sup>2</sup>Physikalisch-Technische Bundesanstalt, Bundesallee 100, D-38116 Braunschweig, Germany

Transport measurements on epitaxial graphene require flat and large-scale graphene layers to apply electrical contacts. For this purpose growth of graphene on SiC(0001) has been studied with spot profile analysis low energy electron diffraction (SPA-LEED) and has been controlled and correlated in addition with X-ray photoelectron spectroscopy (XPS). The lateral (H(S)-analysis) and vertical (G(S)-analysis) roughness of different prepared SiC samples has been investigated as a function of graphene layers. Only the buffer and the first graphene layer show almost no additional roughening within the transfer width (200 nm) after graphitization process. The influence of interfaces on the loss function of epitaxial graphene layers has been studied further by means of electron energy loss spectroscopy (EELS). Electronic transitions and plasmon losses are sensitive to the interface. The collective in-plane excitations show a characteristic blueshift after graphitization, while single electron transitions with dipole moments along the surface normal are suppressed for the buffer layer. These characteristics can be used to distinguish between the buffer layer and intact graphene layers on top.

O 8.5 Mon 12:30 SCH 251

**Raman Spectra of Epitaxial Graphene on SiC and of Epitaxial Graphene Transferred to SiO<sub>2</sub>** — DONG SU LEE, ●CHRISTIAN RIEDL, BENJAMIN KRAUSS, KLAUS VON KLITZING, ULRICH STARKE, and JURGEN H. SMET — Max-Planck-Institut für Festkörperforschung, Heisenbergstr. 1, 70569 Stuttgart

Raman spectra were measured for epitaxial graphene grown on SiC and compared to those obtained for epitaxial graphene successfully transferred from SiC to SiO<sub>2</sub> [1]. The number of layers for graphene on SiC(0001) was preassigned by angle-resolved ultraviolet photoemission spectroscopy (ARUPS) [2]. The Raman spectra of epitaxial graphene show significant differences as compared to micromechanically cleaved graphene obtained from highly oriented pyrolytic graphite crystals. The G peak is found to be blue-shifted, presumably due to charge doping from the substrate. The 2D peak does not exhibit any obvious shoulder structures, but it is much broader and almost resembles a single-peak even for multilayers. However, the linewidth of the 2D peak is found to be an unambiguous fingerprint to identify the number of layers for graphene on SiC(0001). A comparison of the Raman data obtained for graphene on SiC(0001) with data for epitaxial graphene transferred to SiO<sub>2</sub> reveals that both the G peak blue-shift and the 2D peak lineshape of a single-peak are clearly due to the SiC substrate. The increased linewidth of the 2D peak however stems from the graphene structure itself and not from the substrate.

[1] D. S. Lee et al., Nano Letters, DOI: 10.1021/nl802156w.

[2] C. Riedl et al., Appl. Phys. Lett. **93**, 033106 (2008).

## O 9: Invited Talk (J.Michael Gottfried)

Time: Monday 14:00–14:45

Location: HSZ 02

### Invited Talk

O 9.1 Mon 14:00 HSZ 02

**Surface-confined coordination chemistry with porphyrins and phthalocyanines** — ●J. MICHAEL GOTTFRIED — Lehrstuhl für Physikalische Chemie II, Universität Erlangen-Nürnberg, Germany

Surface-confined coordination chemistry focuses on structure and reactivity of adsorbed metal complexes, which are promising candidates for novel heterogeneous catalysts and sensors with well-defined, uniform active sites. If the complexes possess vacant coordination sites, the substrate surface can directly interact with the metal center and influence its electronic structure. In this context, porphyrins, phthalocya-

nines, and other tetrapyrroles with their planar, four-fold coordination environment are especially versatile ligands and their transition metal complexes are well suited for the chemical functionalization of surfaces. This lecture gives an overview of recent advances in the field of surface chemistry and physics of metallotetrapyrroles. In particular, the following aspects will be addressed: (1) Self-assembly and intramolecular conformation, (2) Surface-confined synthesis by direct metalation, (3) Electronic interaction between metal center and substrate, and (4) Electronic and structural effects of the axial coordination of small molecules to the metal centers.

## O 10: Oxides and insulators II

Time: Monday 15:00–16:45

Location: SCH A01

O 10.1 Mon 15:00 SCH A01

**Ultrathin cobalt oxide-cobalt interface films** — ●MATTHIAS GUBO, CHRISTINA EBENSPEGER, WOLFGANG MEYER, LUTZ HAMMER, and KLAUS HEINZ — Lehrstuhl für Festkörperphysik, Universität Erlangen-Nürnberg, Staudtstr. 7, 91058 Erlangen

The deposition of 1.75 monolayers of cobalt on the unreconstructed Ir(100)-(1×1) surface at liquid nitrogen temperature and under oxygen-poor conditions leads – after annealing at about 670 K – to a well ordered c(4×2) superstructure.

The crystallographic structure of this phase was determined by quantitative low-energy electron diffraction (LEED) whereby an excellent agreement between experimental and calculated I(E)-curves was achieved (Pendry R-factor: 0.17). The resulting model reveals that the film is made up by two atomic layers whereby the layer above the substrate consists exclusively of cobalt, i.e. is a metallic layer which however is strained due to epitaxial misfit. All oxygen atoms reside in the second, outermost layer. It is similar to a (compressed) rocksalt-type CoO(100) plane, however with cobalt vacancies in a c(4×2) periodic arrangement equivalent to a Co:O stoichiometry of 3:4. This is consistent with atomically resolved STM images, whereby cobalt ions of the oxide layer are imaged. The same two-dimensional c(4×2) oxide can also be grown on thicker cobalt films on Ir(100) by post-oxidation at 320 K. The interface between the ultrathin cobalt oxide and metallic cobalt is possibly relevant for magnetoelectronic devices.

O 10.2 Mon 15:15 SCH A01

**Growth and atomic structure of epitaxial ultrathin BaTiO<sub>3</sub> films on Pt(100)** — ●STEFAN FÖRSTER, MICHAEL HUTH, ANKE HÖFER, KARL-MICHAEL SCHINDLER, and WOLF WIDDRA — Martin-Luther-Universität Halle-Wittenberg, Halle, Germany

Ultrathin BaTiO<sub>3</sub>(100) films were grown by radio frequency-assisted magnetron sputtering on Pt(100) at room temperature using a Ar/O<sub>2</sub> gas mixture at a pressure of  $2.5 \times 10^{-3}$  mbar. The growth exhibits high reproducibility with respect to film thickness and composition. The Ba/Ti stoichiometry as determined by XPS can be controlled via the gas pressure and the Ar/O<sub>2</sub> ratio during deposition. The long-range order of films with perfect BaTiO<sub>3</sub> stoichiometry can be improved by post annealing in  $1 \times 10^{-4}$  mbar O<sub>2</sub> at 1000 K. These films show sharp BaTiO<sub>3</sub>(100)-(1×1) diffraction spots in LEED which allow a LEED-IV analysis in the range of 20 - 400 eV. STM measurements for a 5 ML film reveal a smooth topography with small islands in the top layer. By annealing in oxygen at temperatures above 1050 K a stoichiometric BaTiO<sub>3</sub>(100)-(4×4) structure is formed.

O 10.3 Mon 15:30 SCH A01

**Long-range ordered manganese oxide bilayer on Pt(111): An in-vivo STM, STS and LEED study at elevated temperatures** — ●BENJAMIN BOCHMANN, STEFFEN SACHERT, CHRISTIAN HAGEDORF, and WOLF WIDDRA — Martin-Luther-Universität Halle-Wittenberg, Halle, Germany

Growth as well as atomic structure of ultrathin epitaxial manganese oxide films on Pt(111) have been studied using STM, STS and LEED. The films have been prepared by reactive Mn deposition in an oxygen atmosphere of  $10^{-8}$  to  $10^{-6}$  mbar. STM measurements performed during growth (in-vivo) at elevated temperatures (400-600 K) reveal three different well-ordered monolayer structures depending on preparation conditions with MnO, Mn<sub>3</sub>O<sub>4</sub> and MnO<sub>2</sub> stoichiometry. Only the MnO monolayer is thermally stable up to 1100 K and long time stable. The others will be reduced slowly by gaseous carbon monoxide. For manganese oxides bilayers, again three different long-range ordered structures are observed depending on the oxygen content similar as in the monolayer. The MnO(001)-like bilayer is less stable than the MnO monolayer. Heating to 780 K in UHV leads to a reorganization of the MnO(001)-like bilayer and the formation of two new uniaxially reconstructed structures with different corrugation heights. All bilayer structures and films up to six layers thickness exhibit characteristic STS spectra in the 1 - 6 eV range.

O 10.4 Mon 15:45 SCH A01

**Preparation and investigation of NdGaO<sub>3</sub>(110) surfaces** — ●RASUOLE DIRSYTE<sup>1</sup>, JUTTA SCHWARZKOPF<sup>1</sup>, JENS LIENEMANN<sup>2</sup>, MARCO BUSCH<sup>2</sup>, HELMUT WINTER<sup>2</sup>, and ROBERTO FORNARI<sup>1,2</sup> —

<sup>1</sup>Leibniz Institute for Crystal Growth, Max Born Straße 2, D - 12489 Berlin, Germany — <sup>2</sup>Department of Physics, Humboldt University, Newtonstraße 15, D - 12489 Berlin, Germany

Atomically smooth, single terminated surfaces are required for the controlled and epitaxial growth of oxide films. NdGaO<sub>3</sub> is one of the promising substrates for the epitaxial growth of superconducting, ferroelectric, dielectric, and magneto-resistive materials, due to its chemical and structural compatibility. The preparation conditions of NdGaO<sub>3</sub> wafers were optimised by changing the annealing temperature and time in order to obtain surfaces with an atomically smooth step-and-terrace structure. After preparation of a regularly stepped surface the substrates were exposed to different oxygen-argon atmospheres at fixed substrate temperature of 730°C in order to simulate the thermal conditions met before starting the MO-CVD growth process. The annealing in pure argon atmosphere leads to total degradation of the step-and-terrace structure, while the surface structure could be preserved in argon/oxygen mixture with low oxygen content (2 %). The surface roughness as well as the width of the terraces and the height of the steps was measured by AFM in contact mode. The termination of NdGaO<sub>3</sub>(110) surface was determined by the means of proton- and electron-induced AES.

O 10.5 Mon 16:00 SCH A01

**C-AFM characterization of high-k dielectric films grown by molecular beam deposition** — ●PETER DUDEK, JAREK DABROWSKI, GRZEGORZ KOZLOWSKI, GRZEGORZ LUPINA, GUNTHER LIPPERT, and HANS-JOACHIM MÜSSIG — IHP, Im Technologiepark 25, 15236 Frankfurt (Oder) / Germany

Very thin high-k dielectric films (thickness below 10 nm, dielectric constant k around 100) deposited on metallic electrodes are of particular interest for dynamic random access memories (DRAM). High capacitance density of storage capacitors must be accompanied by extremely low leakage currents: leakage should not exceed about  $10^{-8}$  A/cm<sup>2</sup> at bias around 0.5 V. This study uses conductive atomic force microscopy (C-AFM) to investigate microscopic aspects of electron transport across group-II hafnate and zirconate films deposited by MBE. Typically, most leakage is confined to nano-sized „hot spots”. Analysis of hot spot IV characteristics, including their statistical distribution, provides insight into leakage mechanisms. This analysis is guided by quantum-mechanical simulations for trap-assisted tunnelling and ab initio calculations for the formation energies and electronic structures of point defects. Among the effects discussed in this work is local resistivity switching. We also present the first data obtained for dielectric perovskite films with intentional admixture of TiO, whereby the influence of substrate electrode (TiN, Ru, or Pt) is considered.

O 10.6 Mon 16:15 SCH A01

**Wavefunction-based ab-initio results for the adsorption of N<sub>2</sub>O on CeO<sub>2</sub> surfaces** — CARSTEN MÜLLER<sup>1</sup>, ●BEATE PAULUS<sup>2</sup>, and KERSTI HERMANSSON<sup>1</sup> — <sup>1</sup>Department of Materials Chemistry, The Angstrom Laboratory, Uppsala University, Lägerhyddsvägen 1, 75121 Uppsala, Sweden — <sup>2</sup>Institut für Chemie und Biochemie, Freie Universität Berlin, Takustr. 3, 14195 Berlin

For the ab-initio description of the adsorption process on surfaces it is necessary to model all interactions on the same theoretical footing. The standard density functional methods have their difficulties with describing dispersion forces. But especially for the physisorption, where no covalent bonds are formed between the adsorbant and the surface these interactions are essential. They can only well described with wavefunction based correlation methods like coupled-cluster methods. With the method of increments [1] it is possible to apply these wavefunction based correlation methods to extended systems and absorption processes on surfaces [2]. Here we apply the method to the adsorption of N<sub>2</sub>O on the CeO<sub>2</sub> 111 surface in different adsorption structures. Due to the partitioning of the correlation part of the adsorption energy according to localized orbital groups, it is possible to discuss the individual contributions to the binding. Therefore, the method of increments yields not only highly accurate results for the adsorption energy, but also gain information about the chemical binding on surfaces.

[1] B. Paulus, Phys. Rep. 428, 1 (2006).

[2] C. Müller, B. Herschend, K. Hermansson and B. Paulus, J. Chem.

Phys. 128, 214701 (2008).

O 10.7 Mon 16:30 SCH A01

**Adsorption of CO on TiO<sub>2</sub>(110): A first principles study** — ●MATTHIAS MEHRING and THORSTEN KLÜNER — Theoretical Chemistry, Carl von Ossietzky University of Oldenburg, 26111 Oldenburg, Germany

Titania plays an important role in materials science. It serves as heterogeneous catalyst, photocatalyst, or corrosion protective coating [1]. The wide field of photochemistry, and photodesorption, sparked the interest of theoretical and experimental research. Photodesorption can be described as a prototype of a huge group of non-adiabatic surface reactions [2] like simple rotational and vibrational excitations of small molecules or photodiffusion. These reactions could be a basis for pho-

ton driven molecular switches or molecular rotors [2].

The present study provides an insight into adsorption process of CO from a rutile surface, which is modeled by a finite cluster approach embedded in a field of point charges. The smallest cluster model which describes the system with sufficient accuracy is a Ti<sub>9</sub>O<sub>18</sub> cluster [3], in our case we use a cluster model of the type Ti<sub>15</sub>O<sub>30</sub>. The adsorption of CO on the relaxed rutile surface serves as first step to study the desorption mechanism. Therefore it is necessary to compute potential energy surfaces of the electronic ground state and excited states involved in the desorption process.

In this work, we present first results on CO interacting with TiO<sub>2</sub>(110). The calculated potential energy surfaces will pave the way for a detailed microscopic understanding of surface photochemistry of this important adsorbate-substrate system.

## O 11: Metal substrates: Adsorption of organic / bio molecules II

Time: Monday 15:00–16:45

Location: SCH A118

O 11.1 Mon 15:00 SCH A118

**Molecular chemistry at surfaces: Ring opening reaction of Spiropyran molecules on a metal surface** — ●GUNNAR SCHULZE, MARTEN PIANTEK, CRISTINA NAVÍO, JORGE MIGUEL, MATTHIAS KOCH, FELIX LEYSSNER, KATHARINA J. FRANKE, PETRA TEGEDER, WOLFGANG KUCH, and JOSE IGNACIO PASCUAL — Inst. für Experimentalphysik, Freie Universität Berlin, Arnimallee 14, 14195 Berlin

The ring-opening reaction of spirocyan (SP) to the merocyanine (MC) form is a reversible photochromic process in solution. The interest in this basic reaction stems from the different properties of each isomer, regarding to structure (SP is chiral), electrical dipole moment (MC has a large dipole) and electronic structure (MC is coloured). In solution SP is the thermally stable isomer. Here, we report that on a metal surface, MC turns out to be more stable. We investigate the thermally induced ring-opening transition from the organic photo switch 6-nitro-spiropyran to its merocyanine isomer on a Au(111) surface by means of low temperature scanning tunnelling microscopy (STM), scanning tunnelling spectroscopy (STS) and force-field simulations. In submonolayer coverages, each isomer presents a very distinct behaviour in terms of electronic properties and structure of the self-assembled molecular domains. Once that the merocyanine domains are created by thermal activation, they remain stable, suggesting that the interaction of the conjugated planar backbone with the metal surface helps to stabilize this isomer. The ring opening reaction can be also induced by local electric currents conducted through the molecule by the STM tip.

O 11.2 Mon 15:15 SCH A118

**Manipulation of conjugated molecular chains on Au(111)** — ●LEIF LAFFERENTZ<sup>1</sup>, FRANCISCO AMPLE<sup>2</sup>, HAO YU<sup>3</sup>, STEFAN HECHT<sup>3</sup>, CHRISTIAN JOACHIM<sup>2</sup>, and LEONHARD GRILL<sup>1</sup> — <sup>1</sup>Institut für Experimentalphysik, Freie Universität Berlin, Arnimallee 14, 14195 Berlin — <sup>2</sup>Nanosciences Group, CEMES-CNRS, 31055 Toulouse, France — <sup>3</sup>Institut für Chemie, Humboldt-Universität zu Berlin, Brook-Taylor-Str. 2, 12489 Berlin

The goal of molecular electronics is to utilize individual molecules as components in electronic devices. These units have to be linked by conducting connections. To achieve this, two conditions have to be met: First, the connections have to be robust while allowing efficient charge transfer. Furthermore, it is necessary to gain a basic understanding of the charge transport, which requires the ability to measure the current through single molecule junctions.

Solidly connected molecular structures of predetermined architecture could be produced with our method of on-surface synthesis [1]. In this way, conjugated chains with lengths of up to over 100 nm were formed from dibromoterfluorene (DBTF) molecules on a Au(111) surface. The chains are characterized and manipulated by means of low-temperature scanning tunneling microscopy (STM). It will be shown that it is possible to lift part of individual chains off the surface employing vertical manipulation with the STM tip, which opens the exciting possibility to measure currents through this molecular junction.

[1] L. Grill, M. Dyer, L. Lafferentz, M. Persson, M. V. Peters, and S. Hecht, *Nature Nanotech.* 2, 687 (2007)

O 11.3 Mon 15:30 SCH A118

**STM investigation of imine-based molecular switches on Au(111)** — ●JOHANNES MIELKE<sup>1</sup>, YING LUO<sup>2</sup>, RAINER HAAG<sup>2</sup>, and LEONHARD GRILL<sup>1</sup> — <sup>1</sup>Institut für Experimentalphysik, Freie Universität Berlin, Arnimallee 14, 14195 Berlin — <sup>2</sup>Institut für Chemie und Biochemie - Organische Chemie, Freie Universität Berlin, Takustr. 3, 14195 Berlin

In the field of molecular electronics, molecular switches are highly relevant because they can control the conductance. Switches based on azobenzene molecules have attracted large interest in the last years. A very similar molecular switch can be created by replacing the functional azo group by an imine group, which does not considerably alter the electronic structure of the molecule and conserves the capability of undergoing a reversible trans-cis isomerisation. Such processes have already been studied in solution and the gas phase but not on surfaces.

In this work, imine molecules with four tert-butyl groups were adsorbed on Au(111) and their adsorption and switching behaviour were studied using a low temperature STM. The molecules were found to form two types of ordered islands and an interesting irreversible switching behaviour was observed when looking at their temperature dependence, because the number of trans isomers was reduced upon heating of the sample.

O 11.4 Mon 15:45 SCH A118

**Reversible breaking and forming of a metal-ligand bond by STM: PVBA and Cu adatoms on Cu(111)** — ●ROBIN OHMANN, LUCIA VITALI, and KLAUS KERN — Max-Planck-Institute for Solid State Research, Stuttgart, Germany

Controlling functional properties at the atomic scale is interesting for fundamental research and is a key for creating smaller operational units for computational devices. Recently, strong attention is focused on surface-adsorbed atoms and molecules, which undergo reversible positional or conformational changes. Here, we used 4-[trans-2-(pyrid-4-yl-vinyl)] benzoic acid (PVBA) molecules, which were deposited in ultra high vacuum (UHV) via molecular beam epitaxy on a Cu(111) surface and measured with a scanning tunneling microscope operating at low temperature (6 K). Single PVBA molecules and self-assembled dimers, which are bond together by a Cu atom in the center, are predominantly observed. Although the single molecules show a stable configuration, for the dimers we found that the tunneling current oscillates between two values above a threshold voltage. This random telegraph noise has been investigated as a function of tip-sample distance, applied voltage and lateral position of the tip. By measuring the topography at well defined conditions, we were able to image both states of the dimer and ascribe their origin to a ligand in contact with and detached from the central metal atom.

O 11.5 Mon 16:00 SCH A118

**Stilbene - a molecular switch on surfaces** — ●THORSTEN ULRICH KAMPEN<sup>1,3</sup>, PHILIPP MARTIN SCHMIDT-WEBER<sup>1</sup>, RALPH PÜTTNER<sup>2</sup>, CHRISTINE KOLCZEWSKI<sup>1</sup>, KLAUS HERMANN<sup>1</sup>, and KARSTEN HORN<sup>1</sup> — <sup>1</sup>Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, Germany — <sup>2</sup>Freie Universität Berlin, Institut für Experimentalphysik, Berlin, Germany — <sup>3</sup>SPECS GmbH, Berlin, Germany

We have investigated the potential of Stilbene as a molecular switch on surfaces. In this study, Si(100) and Cu(110) serve as exemplary semi-

conductor and metal substrates. Using the StoBe software package and performing NEXAFS measurements on the cis and trans isomers in the gas phase, both isomers are clearly identified by the lineshape of the resonances. NEXAFS investigations, aided by the results from photoelectron spectroscopy, showed that the interaction of the orbitals at the C=C bridge of stilbene with the substrate atoms has a direct influence on the isomerisation process. The isomerisation requires an excitation into the unoccupied bridge orbitals. On Si(100), the bonding of the molecules to the surface takes place via this C=C bridge thereby inhibiting the isomerisation. On Cu(110) adsorbate-substrate bonding does not involve the C=C bridge, and therefore does not inhibit the isomerisation. For different coverages cis-to-trans isomerisation with an overall conversion of about 25% is possible.

O 11.6 Mon 16:15 SCH A118

**Structure microscopy attributed to hydrogen** — ●CHRISTIAN WEISS, RUSLAN TEMIROV, OLGA NEUCHEVA, SERGEY SOUBATCH, and FRANK STEFAN TAUTZ — Institut für Bio und Nanosysteme (IBN-3) and JARA-Fundamentals of Future Information Technology

Condensation of H<sub>2</sub> (D<sub>2</sub>) leads to ultra-high geometrical resolution in low temperature scanning tunneling microscopy. This has been shown for different molecular adsorbates on different metallic surfaces [1]. Geometrical resolution in this context means that ring-structures in which carbon atoms in many organic molecules are arranged can be clearly identified. Strong non-linear behavior in conductance spectra

appears simultaneously with high resolution images, when hydrogen is condensed to the tunnelling junction. In this contribution we analyze the relation between spectroscopic features and imaging contrast to elucidate the specific feature that is responsible for the improved resolution. References: [1] R Temirov, S Soubatch, O Neucheva, A Lassise, and F S Tautz 2008 New. J. Phys 10 053012

O 11.7 Mon 16:30 SCH A118

**Inelastic electron tunneling spectroscopy in single C<sub>60</sub> junctions: the role of energy level alignment** — ●KATHARINA J. FRANKE, GUNNAR SCHULZE, and JOSE IGNACIO PASCUAL — Freie Universität Berlin, Berlin, Germany

Inelastic scattering of electrons has important implications in transport through single molecule junctions as it leads to heating effects [1]. Here, we measure the inelastic tunneling spectra (IETS) of C<sub>60</sub> molecules adsorbed on different metal surfaces in order to identify the molecular vibrations playing a role in transport close to the Fermi level. We find that the alignment of the lowest unoccupied molecular orbital (LUMO) has an important effect on the detection of molecular vibrations. When the LUMO exhibits a small tail crossing the metal's Fermi level, we are able to observe all eight H<sub>g</sub> modes, exhibiting a strong coupling to the LUMO. The inelastic signal is further analyzed along the transition from the tunneling to the contact regime.

[1] G. Schulze, et al., Phys. Rev. Lett. 100, 136801 (2008)

## O 12: Nanostructures at surfaces: Dots, particles, clusters I (magnetic)

Time: Monday 15:00–16:30

Location: SCH A215

O 12.1 Mon 15:00 SCH A215

**Correlation of shape and magnetic anisotropy of mass-filtered Fe and FeCo alloy nanoparticles supported by W(110)** — ARMIN KLEIBERT<sup>1</sup>, ●FURKAN BULUT<sup>2</sup>, KERSTIN GEBHARDT<sup>3</sup>, WOLFGANG ROSELLEN<sup>3</sup>, DANIELA SUDFELD<sup>4</sup>, JOHANNES PASSIG<sup>1</sup>, JOACHIM BANSMANN<sup>2</sup>, KARL-HEINZ MEIWES-BROER<sup>1</sup>, and MATHIAS GETZLAFF<sup>3</sup> — <sup>1</sup>Institut für Physik, Universität Rostock, Germany — <sup>2</sup>Institut für Oberflächenchemie und Katalyse, Universität Ulm, Germany — <sup>3</sup>Institut für Angewandte Physik, Universität Düsseldorf, Germany — <sup>4</sup>Institut für Experimentalphysik, Universität Duisburg-Essen, Germany

Magnetic clusters and nanoparticles are promising candidates for many future applications. Understanding and controlling their magnetic anisotropy energy (MAE) is important, particularly when attempting, e.g., to overcome the so-called superparamagnetic limit in high density storage devices. In the present work we study shape and interface related contributions to the MAE of supported nanoparticles. For this purpose mass-filtered Fe and FeCo nanoparticles have been deposited onto a bare W(110) surface. The structure and shape of the nanoparticles were determined by *ex situ* high resolution transmission electron microscopy. *In situ* scanning tunneling microscopy yields evidence for a partial flattening of the supported particles. Magnetization curves reveal a magnetic hard axis perpendicular to the surface. The observed MAE is compared to model calculations on shape and interface anisotropy contributions of flattened nanoparticles.[1]

[1] A. Kleibert *et al.*, J. Phys.: Condens. Matter **20**, 445005 (2008).

O 12.2 Mon 15:15 SCH A215

**Ultra-high dense array of magnetic quantum dots on a self-assembled nanostructured template** — ●LAURA FERNÁNDEZ<sup>1</sup>, MARTINA CORSO<sup>2</sup>, MAXIM ILYN<sup>3</sup>, FREDERIK SCHILLER<sup>4</sup>, and JOSÉ ENRIQUE ORTEGA<sup>1,2,4</sup> — <sup>1</sup>Departamento de Física Aplicada I, Universidad del País Vasco, San Sebastián, Spain — <sup>2</sup>DIPC, San Sebastián, Spain — <sup>3</sup>Física de Materiales, Universidad del País Vasco, San Sebastián, Spain — <sup>4</sup>Unidad de Física de Materiales, Centro Mixto CSIC-UPV/EHU, San Sebastián, Spain

The growth of magnetic nanoparticles on surfaces by auto-organization processes represents a flexible and powerful alternative to obtain high-density, patterned magnetic storage media. Here, we report on the growth of a dense array of Co quantum dots on a previously designed template formed by the Moiré surface structure, which allows the achievement of dot areal densities that overcome the boundary of 1 Teradots/inch<sup>2</sup>. The structural properties of the template and the tunability of the quantum dot array have been thoroughly explored by

Scanning Tunneling Microscopy at several deposition temperatures and different Co coverage. The magnetic response of the Co quantum dots has been investigated by vibrating sample magnetometry, showing an uniaxial out-of-plane anisotropy and soft magnetic behaviour at 300 K.

O 12.3 Mon 15:30 SCH A215

**Ferromagnetism of magnetic nanodot ensembles promoted by substrate-mediated interaction** — ●PAVEL A. IGNATIEV<sup>1</sup>, NIKOLAY N. NEGULYAEV<sup>2</sup>, ALEXEY S. SMIRNOV<sup>3</sup>, LARISSA NIEBERGAL<sup>1</sup>, ALEXANDER M. SALETSKY<sup>3</sup>, and VALERI S. STEPANYUK<sup>1</sup> — <sup>1</sup>Max-Planck-Institut für Mikrostrukturphysik, Weinberg 2, D-06120 Halle, Germany — <sup>2</sup>Physics Department, Martin-Luther-University Halle-Wittenberg, 06099 Halle, Germany — <sup>3</sup>Faculty of Physics, Moscow State University, 119899 Moscow, Russia

Recent experimental studies evidenced collective ferromagnetic behavior with high Curie temperatures in Fe nanodots assemblies created on Cu(111) surfaces by means of buffer layer assisted growth [1,2]. It was suggested that a substrate-mediated indirect RKKY-like exchange interaction between Fe dots was responsible for the magnetic order [2].

Here we present combined ab initio and kinetic Monte Carlo (kMC) investigations of the magnetic ordering in ensembles of Fe nanodots embedded in noble metal (Cu, Ag, Au) substrates. Exchange interactions in considered systems are calculated fully ab initio by means of the Korringa-Kohn-Rostoker Green's function method. kMC simulations based on this ab initio input revealed the ferromagnetic ordering in the ensemble of Fe nanodots.

[1] J. P. Pierce et al., Phys. Rev. Lett. 92, 237201 (2004).

[2] M. A. Torija et al., Phys. Rev. Lett. 95, 257203 (2005).

O 12.4 Mon 15:45 SCH A215

**Structural and Magnetic Properties of Fe and Co Clusters on Alumina/Ni<sub>3</sub>Al(111)** — ●ANDREAS BUCHSBAUM<sup>1</sup>, MAURIZIO DE SANTIS<sup>3</sup>, HELIO TOLENTINO<sup>3</sup>, GEORG KRESSE<sup>2</sup>, MICHAEL SCHMID<sup>1</sup>, and PETER VARGA<sup>1</sup> — <sup>1</sup>Inst. f. Allg. Physik, TU Wien, Austria — <sup>2</sup>Faculty of Physics, CMS, University of Vienna, Austria — <sup>3</sup>Institute Neel, CNRS Grenoble, France

The structure of the  $\approx 5$  Å thick aluminum oxide on Ni<sub>3</sub>Al(111), which has been solved recently, exhibits holes at the corner of the ( $\sqrt{67} \times \sqrt{67}$ )R12.2° unit cell, reaching down to the metal substrate [1]. Therefore, the ultrathin oxide film, forming a nanomesh with a 4.1 nm lattice, is a perfect template for growing highly regular arranged metal clusters. Pd atoms trapped in the corner holes, create metallic nucleation sites, where Fe as well as Co clusters can nucleate and form

a well-ordered hexagonal arrangement on the oxide nanomesh [1]. We have studied the morphology of the Fe and Co clusters and applied different methods to determine the orientation of the clusters. For Fe we found cluster growth in either bcc[110] or bcc[100] direction, depending on the deposition temperature and for Co we found close-packed planes on top of the clusters and random stacking of fcc and hcp planes. As the cluster size is limited to  $< 4$  nm, pure Fe and Co clusters are superparamagnetic at temperatures where the Ni<sub>3</sub>Al substrate is paramagnetic, i.e., the blocking temperature  $T_B$  of the clusters is below the Curie temperature of the substrate  $T_C$ . For ferromagnetic clusters, materials with higher anisotropy are required.

[1] M. Schmid et. al., Phys. Rev. Lett. 99, 196104 (2007).

O 12.5 Mon 16:00 SCH A215

**Probing the Magnetism of Nanostructures buried in Metallic Surfaces: an *Ab-Initio* Study** — ●OLEG O. BROVKO and VALERI S. STEPANYUK — Max-Planck-Institut für Mikrostrukturphysik, Weinberg 2, D-06120 Halle, Germany

For a long time it has been known, that the apparent transparency of metallic surfaces for electronic states can be utilized to detect and study buried nanostructures. We show that it is as well possible to

study the magnetic properties of nanostructures buried up to 20Å deep in metallic surfaces. Our *ab-initio* calculations reveal the possibility of detecting magnetic properties of 3d atoms and small clusters embedded into a metallic surface and even determining the magnetic coupling between them.

O 12.6 Mon 16:15 SCH A215

**Utilizing the Quantum Confinement on Islands for Exchange Interaction Tailoring: an *Ab-Initio* Study** — ●OLEG O. BROVKO and VALERI S. STEPANYUK — Max-Planck-Institut für Mikrostrukturphysik, Weinberg 2, D-06120 Halle, Germany

Vacuum barriers at island borders inevitably confine the surface electrons to the island's geometry. Electron density redistribution which arises from such a confinement can have a substantial effect on the magnetic interaction of impurities adsorbed on top of the island. Our *ab-initio* calculations for 3d adatoms adsorbed on islands clearly demonstrate that by varying the island's size it is possible to tailor the surface-state-mediated exchange interactions of adatoms at separations ranging from several angstroms to several nanometers. By deliberate choice of the islands size the exchange coupling can be enhanced, weakened or even reversed.

## O 13: Electronic structure II

Time: Monday 15:00–16:45

Location: SCH A216

O 13.1 Mon 15:00 SCH A216

**Self-assembled arrays of molecular quantum resonators** — ●FLORIAN KLAPPENBERGER<sup>1</sup>, DIRK KÜHNE<sup>1</sup>, WOLFGANG KRENNER<sup>1</sup>, IÑAKI SILANES<sup>2</sup>, ANDRES ARNAU<sup>2</sup>, JAVIER GARCÍA DE ABAJO<sup>3</sup>, SVETLANA KLYATSKAYA<sup>4</sup>, MARIO RUBEN<sup>4</sup>, and JOHANNES BARTH<sup>1</sup> — <sup>1</sup>Physik Department E20, TU München, Germany — <sup>2</sup>Departamento de Física de Materiales and Unidad de Física de Materiales, E-20018 San Sebastian, Spain — <sup>3</sup>Instituto de Óptica CSIC, Serrano 121, 28006 Madrid, Spain — <sup>4</sup>Institute of Nanotechnology, Forschungszentrum Karlsruhe, Karlsruhe, Germany

Confinement of Ag(111) surface state electrons by self-assembled, periodic, two-dimensional, nanoporous networks is studied by means of low-temperature scanning tunneling microscopy/spectroscopy and electronic structure calculation. We compare the case of a purely organic, hydrogen bonded Kagomé network constructed from dicarbonitrile-sexiphenylene molecules with the case of a Co-directed assembly of a metal-organic honeycomb network of the same molecule featuring a pore size of 24 nm<sup>2</sup>. Both network types induce resonance states within the cavities with varying lateral electronic density distribution. The spectroscopic features of the resonances together with our analysis employing a boundary element method based on Greens functions indicate finite reflection at the boundaries of the cavities, thus transmission through the pore boundaries allows interaction of electrons in neighboring resonators. By the choice of the network we can steer the pore shape and size and hence engineer the electronic properties of the functionalized surface.

O 13.2 Mon 15:15 SCH A216

**Temperature dependent quasiparticle renormalization in nickel metal** — ●RUSLAN OVSYANNIKOV, JAIME SÁNCHEZ-BARRIGA, JÖRG FINK, and HERMANN A. DÜRR — Helmholtz Zentrum Berlin, BESSY II, Albert-Einstein-Strasse 15, D-12489 Berlin, Germany

One of the fundamental consequences of electron correlation effects is that the bare particles in solids become 'dressed', i.e. they acquire an increased effective mass and a lifetime. We studied the spin dependent quasiparticle band structure of Ni (111) with high resolution angle resolved photoemission spectroscopy. At low temperatures (50 K) a renormalization of quasiparticle energy and lifetime indicative of electron-phonon coupling is observed in agreement with literature [1]. With increasing temperature we observe a decreasing quasiparticle lifetime at the Fermi level for all probed minority spin bands as expected from electron phonon coupling. Surprisingly the majority spin states behave differently. We actually observe a slightly increased lifetime at room temperature. The corresponding increase in Fermi velocity points to a temperature dependent reduction of the majority spin quasiparticle renormalization.

[1] M. Higashiguchi et al., Phys. Rev. B 72, 214438 (2005)

O 13.3 Mon 15:30 SCH A216

**Modulated spin polarization in nanostructures** — ●SEBASTIAN WEDEKIND, HIROFUMI OKA, GUILLEMIN RODARY, DIRK SANDER, and JÜRGEN KIRSCHNER — Max-Planck-Institut für Mikrostrukturphysik, Weinberg 2, D-06120 Halle(Saale)

Deposition of 0.7 ML Co onto the clean Cu(111) surface at room temperature leads to the formation of triangular two atomic layers high Co islands. We study the electronic properties of these nano islands by scanning tunneling microscopy (STM) and spectroscopy (STS) at 7 K. We observe pronounced spatial modulation patterns in the local density of states (LDOS) within the islands due to electron confinement. We explore the magnetic properties of the very same islands by spin-polarized STM and STS in a magnetic field of up to 4 T. Our spin-polarized measurements in field clearly identify the parallel and anti-parallel spin orientation states of tip and sample [1]. This enables us to measure the spatial distribution of the spin polarization within single Co islands. We find that the spin polarization is spatially modulated. Our results are discussed in view of recent theoretical predictions [2].

[1] G. Rodary, S. Wedekind, D. Sander, and J. Kirschner, JJAP (in press)

[2] L. Niebergall, V. S. Stepanyuk, J. Berakdar, and P. Bruno, PRL **96**, 127204 (2006)

O 13.4 Mon 15:45 SCH A216

**Surface reconstruction and energy gap of superconducting V<sub>3</sub>Si(001)** — ●NADINE HAUPTMANN, MICHAEL BECKER, JÖRG KRÖGER, and RICHARD BERNDT — Institut für Experimentelle und Angewandte Physik, Christian-Albrechts-Universität zu Kiel, D-24098 Kiel, Germany

Scanning tunneling microscopy of the superconductor V<sub>3</sub>Si(001) reveals a yet unknown surface reconstruction which is most likely induced by carbon. We suggest a structural model for the reconstructed surface, which is consistent with experimental data obtained by scanning tunneling microscopy and Auger electron spectroscopy. Superconductivity of the reconstructed sample persists as monitored by scanning tunneling spectroscopy of the superconducting energy gap. Financial support by the DFG is gratefully acknowledged.

O 13.5 Mon 16:00 SCH A216

**Engineering the band line up of Si(111) and organic semiconductors by -CH<sub>3</sub>, -H and -GaSe termination** — ●THOMAS MAYER<sup>1</sup>, RALF HUNGER<sup>2</sup>, ANDREAS KLEIN<sup>1</sup>, and WOLFRAM JAEGERMANN<sup>1</sup> — <sup>1</sup>TU-Darmstadt Fachbereich Materialwissenschaften — <sup>2</sup>now Solibro GmbH Thalheim

We report on the variation of the Si(111) ionization energy induced by surface dipoles of -CH<sub>3</sub>, -H, and -GaSe terminations. Photoelectron spectroscopy is used to determine the experimental dipoles which are

compared to model calculations applying simple geometric and electronegativity arguments. The position of the vacuum level within bulk Si is derived to be 5.12 eV above the valence band maximum. In addition the variation of the band line up of Si(111) towards PTCDA and ZnPc is measured. While for -CH<sub>3</sub> and -H terminations the Anderson model applies, for GaSe termination an additional interface dipole is induced. We relate this dipole to a varied molecule orientation.

O 13.6 Mon 16:15 SCH A216

**Symmetry Analysis of Tunnel Current Eigenchannels** — ●MARTYNA POLOK<sup>1</sup>, DMITRY FEDOROV<sup>1</sup>, STEVEN WALCZAK<sup>1,2</sup>, PETER ZAHN<sup>1</sup>, and INGRID MERTIG<sup>1,2</sup> — <sup>1</sup>Martin-Luther-Universität Halle, Institut für Physik, D-06099 Halle, Germany — <sup>2</sup>Max-Planck-Institut für Mikrostrukturphysik, Weinberg 2, D-06120 Halle, Germany

Thanks to advances in Scanning Tunneling Microscopy (STM) it is now possible to probe both the electronic and magnetic properties of surfaces. We present an ab initio study of a tip approaching a Cu(001) surface decorated with a single Cu or Co adatom.

Electronic transport is calculated using the Kubo linear response theory in the Baranger and Stone formalism. This description is equivalent to the Landauer language, where conductance is understood as a sum over all transmission eigenchannels.

For a magnetic system additional channels created by the *3d* electrons can cause an increase in the tunnel current. The transmission amplitude of the eigenchannels depends on the overlap between those valence orbitals available at the Fermi energy  $\epsilon_F$ . A detailed study of the local density of states shows that in the case of magnetic adatoms this is a spin dependent effect. For the investigated systems the major-

ity spin current is dominated by electrons with spherically symmetric orbitals in the plane perpendicular to the transport direction (*z*), these are the *s*, *p<sub>z</sub>*, and *d<sub>z<sup>2</sup></sub>* orbitals. For the minority spin channel electrons with asymmetric orbitals, *p<sub>x</sub>*, *p<sub>y</sub>*, *d<sub>xz</sub>*, and *d<sub>yz</sub>*, dominate at the Fermi energy and therefore determine the current distribution.

O 13.7 Mon 16:30 SCH A216

**Electron and Phonon Density of States of HOPG by Scanning Tunnelling Spectroscopy** — ●NORBERT MAURER, CARSTEN TRÖPPNER, and M. ALEXANDER SCHNEIDER — Lehrstuhl für Festkörperphysik, Universität Erlangen-Nürnberg, Staudtstr. 7, 91058 Erlangen

Motivated by the current interest in few-layer graphene and the widespread use of graphite as substrate we investigated the electronic structure of highly ordered pyrolytic graphite (HOPG) by low-temperature Scanning Tunnelling Spectroscopy in liquid Helium at 4.2K.

We find that the main features of the differential conductance (*dI/dV*) signal can perfectly be explained by a total density of states calculation as e.g. obtained from a TB-fit to the graphite band structure [1]. However, some of these features induce a structure in the second derivative (*d<sup>2</sup>I/dV<sup>2</sup>*) signal. Hence both, first and second derivative signals have to be evaluated carefully to extract signatures of inelastic excitations [2]. We discuss the spatial dependence of electronic and inelastic contributions to the tunnelling conductance at step edges and within the HOPG unit cell.

[1] A. Grüneis, et al., arXiv:0808.1467v2 [cond-mat.mtrl-sci] [2] L. Vitali, et al., Phys. Rev. B **69**, 121414 (2004)

## O 14: Organic, polymeric, biomolecular films – also with absorbates I

Time: Monday 15:00–16:45

Location: SCH A316

O 14.1 Mon 15:00 SCH A316

**Reactive Adsorption effects on ordered Bis-terpyridine networks** — ●THOMAS WALDMANN<sup>1</sup>, DANIELA KÜNZEL<sup>2</sup>, ACHIM BREITRUCK<sup>1</sup>, HARRY E. HOSTER<sup>1</sup>, AXEL GROSS<sup>2</sup>, and R. JÜRGEN BEHM<sup>1</sup> — <sup>1</sup>Institute of Surface Chemistry and Catalysis, Ulm University, D-89069 Ulm, Germany — <sup>2</sup>Institute of Theoretical Chemistry, Ulm University, D-89069 Ulm, Germany

We tested the influence of H<sub>2</sub>, O<sub>2</sub> and CO interaction with ordered networks of a Bis-terpyridine derivative (2,4'-BTP)[1,2] on Au(100), Ag(111) and Graphite (HOPG) surfaces using Video-STM (1 frame/s). Under UHV conditions[3,4] as well as in solution[1,2], the molecules form ordered networks on the single crystalline surfaces. Upon interaction with reactive gases, new structures are formed. The STM images are compared with DFT and MP2 calculations of the molecules in the gas phase.

[1] U.Ziener et al., Chem.Eur.J. **8**, 951, 2002

[2] C. Meier et al., J.Phys.Chem.B **109**, 21015, 2005

[3] H.E. Hoster et al., Langmuir **23**, 11570, 2007

[4] M.Roos et al., Phys. Chem. Chem. Phys. **9**, 5672, 2007

O 14.2 Mon 15:15 SCH A316

**Stranski-Krastanov growth of Sexithiophene and para-sexiphenyl on Cu(110)-(2x1)O** — ●LIDONG SUN<sup>1</sup>, GÜNTHER WEIDLINGER<sup>1</sup>, MARIELLA DENK<sup>1</sup>, RICHARD DENK<sup>1</sup>, MICHAEL HOHAGE<sup>1</sup>, PETER ZEPPENFELD<sup>1</sup>, STEPHEN BERKEBILE<sup>2</sup>, GEORG KOLLER<sup>2</sup>, FALKO.P. NETZER<sup>2</sup>, and MICHAEL.G. RAMSEY<sup>2</sup> — <sup>1</sup>Institute of Experimental Physics, Johannes Kepler University Linz, Austria — <sup>2</sup>Institute of Physics, Karl-Franzens University Graz, Austria

The initial stage of Sexithiophene (6T) and para-sexiphenyl (p-6P) growth on Cu(110)-(2x1)O has been investigated by in-situ reflectance difference spectroscopy (RDS) and scanning tunneling microscopy (STM). For both organic molecules, the optical response of the thin films shows a strong anisotropy indicates that the molecules are lying down on the surface with their long axis parallel to the [001] direction of the Cu(110) surface. Furthermore, the RD spectra of the growing films reveal systematic changes with increasing of film thickness reflecting a clear evolution of the absorption spectrum from a single molecule like to molecular crystal exciton. The observed evolution of the optical anisotropy also clearly shows that both 6T and p-6P thin films follow a Stranski-Krastanov growth mode with two ML thick wetting layers. Corresponding STM investigation on the morphology of 6T and p-6P

thin films of up to two monolayers confirms the conclusion deduced from RDS results.

O 14.3 Mon 15:30 SCH A316

**Experimental and theoretical NEXAFS investigations of metalloporphyrin films** — ●NORMAN SCHMIDT<sup>1</sup>, CHRISTIAN HUB<sup>1</sup>, WOLFGANG HIERINGER<sup>2</sup>, THOMAS STRUNSKUS<sup>3</sup>, and RAINER FINK<sup>1</sup> — <sup>1</sup>Univ. Erlangen, Physikalische Chemie II, Erlangen, Germany — <sup>2</sup>Univ. Erlangen, Theoretische Chemie, Erlangen, Germany — <sup>3</sup>C.-A.-Univ. Kiel, Lehrstuhl für Materialverbunde, Kiel, Germany

Metallo-porphyrins are well-known as electron donors in photoinduced electron transfer processes and for their semiconducting properties. They are used as, e.g., dyes, sensitizers, catalysts and in various organo-electronic devices. For improved device design and performance, more detailed knowledge about film morphology and related electronic structure is necessary. In the present study, the electronic structure of thick films of (H<sub>2</sub>, Mn, Fe, Co, Zn, Sn)-tetraphenylporphyrins on Au-plated Si-wafers was investigated using NEXAFS spectroscopy. The obtained N 1s spectra reflect modifications in the electronic structure of the central metal ion interacting with the nitrogen donor functions of the porphyrin ring. Furthermore, the orientation of ultrathin and thick films of ZnTPP and SnTTBPP(OH)<sub>2</sub> (TTBPP=tetra(p-tert.butylphenyl)porphyrin) on an Ag(100) single crystal was studied by angle-dependent NEXAFS spectroscopy. In thin films, the porphyrin frame is lying almost flat on the surface, while the phenyl ligands are twisted by about 60 degrees with respect to the surface plane. Corroborating high-level TD-DFT calculations were used to allow more detailed interpretation of the experimental data (this project is funded by the DFG within SFB 583, TP C9).

O 14.4 Mon 15:45 SCH A316

**Controlled formation of axially bonded Co-phthalocyanine dimers** — XIN GE<sup>1</sup>, CARLOS MANZANO<sup>1</sup>, ●RICHARD BERNDT<sup>1</sup>, LENNART T. ANGER<sup>2</sup>, FELIX KÖHLER<sup>2</sup>, and RAINER HERGES<sup>2</sup> — <sup>1</sup>Institut für Experimentelle und Angewandte Physik, Christian-Albrechts-Universität, D-24098 Kiel — <sup>2</sup>Otto Diels-Institut für Organische Chemie, Christian-Albrechts-Universität, D-24098 Kiel

STM is used to laterally move single Co-Phthalocyanine (CoPc) molecules on an ordered CoPc layer and to investigate the electronic states of the resulting structures. DFT calculations show that an axial Co-Co bond is formed from the *d<sub>z<sup>2</sup></sub>* orbitals when molecules are

positioned almost vertically on top of each other. This leads to a substantial increase of the conductance of the molecular center at negative bias. The results demonstrate the critical importance of precisely controlling the molecular environment when investigating conductances. Moreover, the results show that axial bonding may be used to achieve three-dimensional molecular architectures on a surface and that STM can be used as a powerful tool to elucidate the nature of unusual chemical bonding modes. Financial support via SFB 677 is gratefully acknowledged.

O 14.5 Mon 16:00 SCH A316

**The Effect of Different Substituents on the Surface Composition of Ionic Liquids - An ARXPS study (interchanged with O 14.6)** — •CLAUDIA KOLBECK<sup>1</sup>, KEVIN ROBERT JOHN LOVELOCK<sup>1</sup>, TILL CREMER<sup>1</sup>, NATALIA PAAPE<sup>2</sup>, PETER WASSERSCHIED<sup>2,3</sup>, and HANS-PETER STEINRÜCK<sup>1,3</sup> — <sup>1</sup>Lehrstuhl für Physikalische Chemie II, Egerlandstr. 3, 91058 Erlangen — <sup>2</sup>Lehrstuhl für Chemische Reaktionstechnik, Egerlandstr. 3, 91058 Erlangen — <sup>3</sup>Erlangen Catalysis Resource Center (ECRC)

A molecular understanding of ionic liquid (IL) surfaces is essential in order to explain related macroscopic properties such as surface tension. Due to their low vapour pressure ILs, i.e., molten salts with melting points below 100 °C, can be studied employing surface science techniques under ultra-high vacuum conditions. Angle resolved X-ray photoelectron spectroscopy (ARXPS) was used to investigate the change in surface composition of imidazolium based ionic liquids (ILs) by systematic variation of non-functionalised and functionalised groups attached to the molecules. For [C<sub>n</sub>MIm][Tf<sub>2</sub>N] (n = 2-16) with saturated carbon chains of different length as substituents of the imidazolium cation, a surface enrichment of the chains was clearly observed for n ≥ 4. Enrichment of the aliphatic carbon also occurs for alkyl groups attached to the anion as observed for [C<sub>2</sub>MIm][C<sub>8</sub>OSO<sub>3</sub>].<sup>[1]</sup> Poly(ethyleneglycol)ether functionalities introduced in the cation chain, however, lead to a stoichiometric surface composition, and, thus, to no enrichment of the chains.<sup>[2]</sup>

[1] K. R. J. Lovelock et al., submitted to *J. Phys. Chem. B*.

[2] C. Kolbeck et al., *Langmuir* **2008**, 24, 9500.

O 14.6 Mon 16:15 SCH A316

**Surface Composition and Electronic Structure of Ionic Liquids - Influence of the anion (interchanged with O 14.5)** — •TILL CREMER<sup>1</sup>, CLAUDIA KOLBECK<sup>1</sup>, KEVIN ROBERT JOHN LOVELOCK<sup>1</sup>, FLORIAN MAIER<sup>1</sup>, NATALIA PAAPE<sup>2</sup>, PETER STEFFEN SCHULZ<sup>2</sup>, PETER WASSERSCHIED<sup>2</sup>, and HANS-PETER STEINRÜCK<sup>1</sup> — <sup>1</sup>Lehrstuhl für Physikalische Chemie II, Egerlandstr. 3, 91058 Erlangen — <sup>2</sup>Lehrstuhl für Chemische Reaktionstechnik, Egerlandstr. 3,

91058 Erlangen

Ionic Liquids (ILs) are a new class of solvents exhibiting unique physico-chemical properties. They are promising candidates for many applications in electrochemistry, synthesis, separation and lubrication technologies, and catalysis. For many of these processes knowledge of the interface, e.g. the IL-vacuum interface is of fundamental value. Due to their extremely low vapour pressure IL surfaces can be investigated under ultra high vacuum conditions such as X-ray photoelectron spectroscopy (XPS). In an extended angle resolved XPS (ARXPS) study, the near surface region of a wide range of 1-octyl-3-methylimidazolium based Ionic Liquids (ILs) was investigated. While for all IL surfaces enhancement of the alkyl chain was observed by ARXPS, the level of alkyl enhancement was found to be significantly dependent on the nature of the anion. Moreover, careful analysis of the fine structure of the C 1s region resulted in observation of an anion-dependent difference in relative binding energy positions for chemically different carbon species present in the imidazolium cation. These shifts were compared and correlated to <sup>1</sup>H- and <sup>13</sup>C-NMR measurements. This work was supported by the DFG through SPP 1191 "Ionic Liquids".

O 14.7 Mon 16:30 SCH A316

**In-situ EC-STM studies on the influence of halide anions on structure and reactivity of Dibenzylviologen on Cu(100)** — •KNUD GENTZ<sup>1</sup>, PETER BROEKMANN<sup>2</sup>, and KLAUS WANDEL<sup>1</sup> — <sup>1</sup>Institute of Physical and Theoretical Chemistry, Bonn University — <sup>2</sup>University of Bern

Copper has become a focus of research activities over the last two decades due to its use as interconnect material in microchip design. Nitrogen-containing cationic organic molecules have been studied as additives for the so-called copper damascene process. In the present investigation the structures and reactivity of a Dibenzylviologen (DBV) layer adsorbed on a bromide-modified Cu(100) surface have been studied by in-situ electrochemical STM and will be compared to the results on the chloride-modified substrate and the related Diphenylviologen (DPV). N,N'-dibenzyl-4,4'-bipyridinium molecules (Dibenzylviologen, DBV) spontaneously adsorb on a halide-modified Cu(100)-surface, forming distinctive patterns, which have been characterized by in-situ Scanning Tunneling Microscopy. Depending on the adsorption potential a striped phase, a cavitand phase and an amorphous phase have been identified. Cyclic Voltammetry indicates that even more processes take place on the surface, because if the potential is decreased beyond a range of fully reversible processes, an irreversible surface phase formation is observed at -450 mV vs. RHE. This surface phase passivates the surface against adsorption of the dicationic phase, so the charge reversal of the interface in the outer Helmholtz layer seems to be reduced.

## O 15: Focused Session: Epitaxial Graphene II

Time: Monday 15:00–16:30

Location: SCH 251

### Topical Talk

O 15.1 Mon 15:00 SCH 251

**Structure and Growth of Epitaxial Graphene on SiC: a New Platform for Carbon Electronics** — •EDWARD CONRAD — The Georgia Institute of Technology, Atlanta, Georgia 30332-0430, USA

The use of epitaxial graphene as a platform for carbon electronics hinges on a number of properties of graphene: growth, structure and transport. While graphene grown on both the Si-face and C-face of SiC are possible alternatives for device materials, I will show in this talk that C-face graphene currently offers the most immediate advantages to graphene device growth and fabrication. I will show how transport properties of C-face graphene make growth problems such as controlling thickness or uniformity much less relevant than on Si-face graphene. LEEM, PEEM, x-ray diffraction and transport measurements will be presented to elucidate the unique structure of C-face graphene films. I will also review new work on how to passivate charge transport between the SiC and the graphene.

O 15.2 Mon 15:30 SCH 251

**Effects of periodic potentials in graphene** — •ERVAND KANDELAKI, SAM SHALLCROSS, and OLEG PANKRATOV — Lehrstuhl für Theoretische Festkörperphysik, Staudtstr. 7-B2, 91058 Erlangen

For epitaxial graphene grown on the Si-face of SiC one expects a covalent bonding<sup>[1]</sup> and hence a significant impact of the substrate on the

properties of graphene. Density-functional *ab initio* calculations<sup>[2]</sup> as well as experimental data<sup>[3]</sup> reveal the emergence of the long-periodic  $6\sqrt{3} \times 6\sqrt{3}$  superstructure in the first carbon layer which plays the role of a buffer layer and does not possess graphene's characteristic spectrum. This superstructure generates a long-periodic perturbation then transmitted to a second "genuine graphene" layer. The large scale and complexity of the system invites the use of a continuum approximation to model the low energy excitation spectrum. The appropriate effective Hamiltonian is thus the Dirac-Weyl Hamiltonian with an additional periodic potential. We investigate the electronic spectrum of this effective Hamiltonian via the Korringa-Kohn-Rostocker method which is widely used for Schrödinger particles in a periodic potential. The main benefit of this method is the separation of the geometrical part, given by periodicity of the external potential, from the single-site scattering problem. The latter can be solved for any cylindrically symmetric potential. The impact upon the spectrum of various parameters such as potential periodicity, perturbation amplitude, and single-site scatterer type are discussed. [1] A. Mattausch and O. Pankratov, *Phys. Rev. Lett.* **99**, 076802 (2007). [2] S. Kim *et al.*, *Phys. Rev. Lett.* **100**, 176802 (2008). [3] C. Riedl *et al.*, *Phys. Rev. B* **76**, 245406 (2007).

O 15.3 Mon 15:45 SCH 251

**An *ab initio* study of graphene buffer layers on SiC** —

•STEPHAN HENSEL, MICHEL BOCKSTEDTE, and OLEG PANKRATOV — Lst. Theoretische Festkörperphysik, Universität Erlangen-Nürnberg, Staudtstr 7B2, 91058 Erlangen

Silicon Carbide enables the growth of few layer graphene by thermal sublimation of silicon. Graphene layers with disparate properties are formed on (0001) and (000 $\bar{1}$ ) surfaces.<sup>1–4</sup> On (0001)-SiC a  $6\sqrt{3} \times 6\sqrt{3}$  buffer layer forms, which serves as a template for subsequent aligned layers.<sup>1,2</sup> On (000 $\bar{1}$ )-SiC, in contrast, carbon layers are mutually rotated being practically decoupled from each other and hence possessing individual Dirac spectra.<sup>3</sup> The distinction manifests itself in the presence (Si-termination) or absence (C-termination) of covalent graphene-SiC bonding in XPS.<sup>4</sup> With ab initio methods we analyzed the bonding of graphene on SiC (0001) and (000 $\bar{1}$ ) surfaces. We consider a tractable  $5 \times 5$  model that allows for low strain and the turbostratic registry of graphene. The calculations demonstrate clearly the distinct bonding features on the two surfaces. While covalent graphene-substrate bonds are present for almost all atoms on the Si-terminated surface, such bonding is absent for as much as 50% of the carbon atoms on the C-terminated face.

[1] T. Ohta *et al*, Science **313**, 951 (2006)

[2] C. Riedl *et al*. Phys. Rev. B **76**, 245406 (2007).

[3] J. Hass *et al*, Phys. Rev. Lett. **100**,125504 (2008).

[4] K.V. Emtsev *et al*, Phys. Rev. B **77**, 155303 (2008).

O 15.4 Mon 16:00 SCH 251

**Dynamical properties of cubic and hexagonal silicon carbide from Si-rich to C-rich reconstructions up to graphene formation** — •JUERGEN A. SCHAEFER and ROLAND J. KOCH — Institut für Physik and Institut für Mikro- und Nanotechnologien, Technische Universität Ilmenau, P. O. Box 100565, 98684 Ilmenau, Germany

Using high resolution electron energy loss spectroscopy (HREELS) in conjunction with low energy electron diffraction (LEED) and X-ray

induced photoelectron spectroscopy (XPS), we have studied the vibrational properties of cubic SiC (001) and hexagonal SiC (0001) surface reconstructions from Si-rich to C-rich SiC surfaces, and up to graphene formation in the hexagonal case. Upon sequential annealing from 30 K up to 1500 K, the coupling between the longitudinal optical phonons, the so called Fuchs-Kliwer phonons, and the carrier plasmons that originate from the presence of bulk dopants and / or from the layered semimetallic character of graphene and few layer graphene (FLG), drastically influence the HREELS-spectra. It seems that the latter graphitic layer is essentially unperturbed by the substrate underneath. The measured phonon dispersion strongly resembles that of graphite.

O 15.5 Mon 16:15 SCH 251

**Graphene nanomembranes excited by ac voltages of an STM** — •TORGE MASHOFF<sup>1</sup>, VIKTOR GERINGER<sup>1</sup>, TIM ECHTERMEYER<sup>2</sup>, MAX LEMME<sup>2</sup>, MARCUS LIEBMANN<sup>1</sup>, MARCO PRATZER<sup>1</sup>, and MARKUS MORGENSTERN<sup>1</sup> — <sup>1</sup>II. Institute of Physics, RWTH-Aachen University and JARA-FIT, 52074 Aachen — <sup>2</sup>Advanced Microelectronic Center Aachen (AMICA), AMO GmbH, 52074 Aachen

We investigate graphene monolayers deposited on a SiO<sub>2</sub> surface using scanning tunneling microscopy (STM) at ultra-high vacuum and temperatures of 5 K. Depending on the tunneling-voltage it is possible to lift nanometer-sized areas of the partly freely suspended flake by a few 100 pm while still achieving stable STM-measurements. From I(U) and I(z)-spectroscopy data we determine mechanical properties of the nanomembrane such as pretension and Young's modulus using a model of a parallel-plate capacitor and a clamped circular membrane. These data are in good agreement with previous measurements using atomic force microscopy. Application of an ac voltage leads to oscillations of the nanomembrane which are detected by strongly nonlinear in-phase current oscillations.

## O 16: Invited Talk (Jörg Kröger)

Time: Tuesday 9:30–10:15

Location: HSZ 02

### Invited Talk

O 16.1 Tue 9:30 HSZ 02

**Electron Transport through Single Atoms and Molecules: an STM's View** — •JÖRG KRÖGER — Christian-Albrechts-Universität zu Kiel, D-24098 Kiel, Germany

Two electron transport regimes will be considered. One regime is characterised by electrons tunnelling through a vacuum barrier with currents of the order of 1 nA. Engineering of a molecular switch on surfaces and vibrational spectroscopy of a single atom serve as examples for state-of-the-art experiments performed in the tunnelling regime.

In the other transport regime currents in the microampère range are used. At these elevated currents a single-atom or single-molecule contact is formed with the tip of the microscope and electrons are transported ballistically through the junction. Contact spectroscopy of single atoms, the quantized conductance of magnetic atoms, and the dependence of single-molecule conductance on the molecule orientation between the contacting electrodes are highlights of this rather unconventional use of a scanning tunnelling microscope. Financial support by the DFG through SFB 668 and SFB 677 is acknowledged.

## O 17: Oxides and insulators III

Time: Tuesday 10:30–13:00

Location: SCH A01

O 17.1 Tue 10:30 SCH A01

**Oxygen adatoms at SrTiO<sub>3</sub>(001): A density-functional theory study** — •HANNES GUHL<sup>1</sup>, WOLFRAM MILLER<sup>1</sup>, and KARSTEN REUTER<sup>2</sup> — <sup>1</sup>Institut für Kristallzüchtung, Max-Born-Str. 2, D-12489 Berlin, Germany — <sup>2</sup>Fritz-Haber-Institut der Max-Planck-Gesellschaft, Faradayweg 4-6, 14195 Berlin, Germany

Apart from its use in photo-catalytic and sensing applications, the SrTiO<sub>3</sub>(001) surface is also receiving increasing attention as a suitable substrate material for thin film growth. For the latter context the numerous reported surface reconstructions, partly in sensitive dependence of the applied annealing temperature, indicate a complex surface kinetics, which needs to be understood and controlled when aiming at growth experiments tailored to the atomic-scale. As a first step in this direction we carry out density-functional theory calculations addressing the energetics and electronic properties of adsorbed oxygen atoms at both regular terminations of SrTiO<sub>3</sub>(001). With the bonding at the SrO-termination in general stronger than at the TiO<sub>2</sub>-termination, we find in both cases that the most stable adsorption site does not correspond to the one expected from a continuation of the perovskite lattice. Instead, the ad-atom forms a strong bond to a surface oxygen

atom that is reminiscent of the oxygen-oxygen bond in SrO<sub>2</sub>. Mapping the potential energy surface for lateral adatom motion away from the stable site, the obtained diffusion barriers are about 0.8 eV in the isolated ad-atom limit. This suggests that, at least at the studied ideal terminations, oxygen mobility is not a major bottleneck under typical growth conditions.

O 17.2 Tue 10:45 SCH A01

**Adsorption of benzoic acids on NaCl surface** — •WEI CHEN<sup>1</sup>, CHRISTOPH TEGENKAMP<sup>1</sup>, HERBERT PFNÜR<sup>1</sup>, and THOMAS BREDOW<sup>2</sup> — <sup>1</sup>Institut fuer Festkörperphysik, Leibniz Universität Hannover, Hannover, Germany — <sup>2</sup>Institut für Physikalische und Theoretische Chemie, Universität Bonn, Bonn, Germany

The adsorptions of benzoic acid (BA) and its OH-substituted derivatives, salicylic acid (SA) and para-salicylic acid (p-SA) on NaCl surfaces have been investigated by periodic DFT. On NaCl(100) these molecules bond to the surface weakly with binding energies of around 0.4 eV (in the absence of van der Waals interaction), through the electrostatic interaction between oxygen and surface sodium. The band gap is reduced to the HOMO-LUMO separation of the adsorbate (4.86 eV for SA). In existence of surface anion vacancy, the unpaired electron

localized in the vacancy transfers to the molecules after adsorption. As a result the LUMO of the adsorbate is partially occupied. Larger increase of adsorption energies have been found due to stronger bonding between oxygen and sodium, as well as the interaction between the transferred unpaired electron over the benzene ring and surface sodium. On (001)-like step site, it shows a stronger binding than on NaCl (100) surface, with adsorption energies of around 0.8 eV, whereas the electronic structure remains similar. On (011)-like step site the adsorption energy further increases to about 1.0 eV. Interestingly, due to the 1.5 eV upward shift of 2p state from step edge Cl atoms, the band gap is effectively reduced (2.97 eV for SA). Implication of these results to the contact charging effect will be discussed.

O 17.3 Tue 11:00 SCH A01

**Correlation between bonding geometry and band gap states at organic-inorganic interfaces: catechol on rutile TiO<sub>2</sub>(110)** — ●ANNABELLA SELLONI<sup>1</sup>, JIAN-GUO WANG<sup>1</sup>, SHAO-CHUN LI<sup>2</sup>, PETER JACOBSON<sup>2</sup>, XUE-QING GONG<sup>1</sup>, and ULRIKE DIEBOLD<sup>2</sup> — <sup>1</sup>Department of Chemistry, Princeton University, Princeton NJ 08544 — <sup>2</sup>Department of Physics, Tulane University, New Orleans, LA 70118 (USA)

Adsorbate-induced band gap states in semiconductors are of particular interest due to the potential of increased light absorption and photoreactivity. A combined theoretical and experimental (STM, photoemission) study of the molecular-scale factors involved in the formation of gap states in TiO<sub>2</sub> is presented. Using the organic catechol on rutile TiO<sub>2</sub>(110) as a model system it is found that the bonding geometry strongly affects the molecular electronic structure. At saturation catechol forms an ordered 4 × 1 overlayer. This structure is attributed to catechol adsorbed on rows of surface Ti atoms with the molecular plane tilted from the surface normal in an alternating fashion. In the computed lowest-energy structure one of the two terminal OH groups at each catechol dissociates and the O binds to a surface Ti atom in a monodentate configuration, while the other OH group forms a H-bond to the next catechol neighbor. Through proton exchange with the surface this structure can easily transform into one where both OH groups dissociate and the catechol is bound to two surface Ti in a bidentate configuration. Only bidentate catechol introduces states in the band gap of TiO<sub>2</sub>.

O 17.4 Tue 11:15 SCH A01

**Understanding the Accuracy of Density-Functional Theory Exchange-Correlation Functionals for Adsorption at Ionic Substrates: Water on salt and some other examples** — ●BO LI<sup>1</sup>, ANGELOS MICHAELIDES<sup>1,2</sup>, and MATTHIAS SCHEFFLER<sup>1</sup> — <sup>1</sup>Fritz-Haber-Institut der Max-Planck-Gesellschaft, Faradayweg 4-6 Berlin, Germany — <sup>2</sup>London Centre for Nanotechnology and Department of Chemistry, University College London, London UK

The interaction of water with salt (NaCl) is of widespread importance. Although numerous theoretical studies have been reported (see Ref. [1] and references therein), none has provided a reliable estimate of the strength of the bond between water and NaCl(001). Moreover, the adsorption energies predicted by density-functional theory (DFT) range from 0.2 to 0.7 eV/H<sub>2</sub>O depending on exchange-correlation (xc) functional. Here, we address this through a set of second order Møller-Plesset perturbation theory and coupled cluster calculations on a series of Na<sub>x</sub>Cl<sub>x</sub> (x= 5 to 25) clusters to arrive at a reliable estimate of the H<sub>2</sub>O adsorption energy on NaCl(001). This is then used to *understand* the performance of a range of xc functionals in treating this and related adsorption systems. Further, through symmetry-adapted perturbation theory the relative importance of electrostatics, covalency, and van der Waals forces in water adsorption on ionic substrates is unraveled.

[1] A. Verdager, G. M. Sacha, H. Bluhm, and M. Salmeron, Chem. Rev. **106**, 1478 (2006).

O 17.5 Tue 11:30 SCH A01

**Theoretical evidence for mixed adsorption of water on Fe<sub>3</sub>O<sub>4</sub>(001)** — ●NARASIMHAM MULAKALURI<sup>1,2</sup>, ROSSITZA PENTCHEVA<sup>1</sup>, MARIA WIELAND<sup>1</sup>, WOLFGANG MÖRITZ<sup>1</sup>, and MATTHIAS SCHEFFLER<sup>2</sup> — <sup>1</sup>Section Crystallography, Dept. for Earth and Environmental Sciences, University of Munich — <sup>2</sup>Fritz-Haber-Institut der MPG, Berlin

The interaction of water with a mineral surface is a fundamental process towards understanding surface reactivity. Based on density functional theory (DFT) calculations we investigate the adsorption of wa-

ter and its influence on the electronic properties and surface reconstruction of Fe<sub>3</sub>O<sub>4</sub>(001). Starting from a single water molecule per ( $\sqrt{2} \times \sqrt{2}$ )R45° unit cell, we vary the concentration and configuration of water and hydroxyl groups. The surface phase diagram compiled within the framework of *ab-initio* thermodynamics indicates that a clean wave-like distorted bulk termination (*modified* B-layer) [1] is favorable over a substantial range of O<sub>2</sub> and H<sub>2</sub>O partial pressures, but competes with a B-layer with oxygen vacancies in the oxygen poor limit. Such vacancies can promote dissociation of isolated water molecules. With increasing pressure in the gas phase there is a crossover to a mixed molecular and dissociative adsorption mode. A quantitative low energy electron diffraction (LEED) analysis confirms two distinct Fe-O-distances. DFT and LEED results indicate a suppression of the ( $\sqrt{2} \times \sqrt{2}$ )R45°-reconstruction.

[1] R. Pentcheva et al., Phys. Rev. Lett. **94**,126101 (2005).

O 17.6 Tue 11:45 SCH A01

**Tailoring the adsorption properties of SiO<sub>2</sub> thin films** — ●JAN-FREDERIK JERRATSCH, NIKLAS NILIUS, and HANS-JOACHIM FREUND — Fritz-Haber-Institut der MPG, D14195 Berlin, Germany

An ultra-thin silica film grown on Mo(112) can be chemically modified by inserting Li atoms into the nano-pores of the oxide material. The Li becomes cationic upon incorporation and considerably reduces the silica/Mo work function by creating a positive surface dipole. The smaller work function facilitates charge transfer processes from the Mo support into adsorbates on the surface. The hence negatively charged ad-species have a much larger binding energy due to Coulomb interactions with the support. This principle is demonstrated for gold deposited onto Li/silica/Mo(112) using a low temperature STM. Whereas single Au atoms and small clusters are anchored on the Li-modified surface, they are unable to bind to the pristine oxide film.

O 17.7 Tue 12:00 SCH A01

**Structure of CO<sub>2</sub> adsorbed on the KCl(100) single crystal surface** — ●JOCHEN VOGT, MILICA HADNADIEV, and HELMUT WEISS — Chemisches Institut der Otto-von-Guericke-Universität Magdeburg, Universitätsplatz 2, 39106 Magdeburg, Germany

Self-organization phenomena in two dimensions are a hallmark of systems with weak molecule-surface interaction in gas adsorption. On insulator single crystal surfaces, such systems can be ideally studied experimentally, e. g. by means of polarization infrared spectroscopy (PIRS) and low-energy electron diffraction (LEED). On the KCl(100) surface at a temperature of 80 K, the first layer of carbon dioxide grows in three different phases: firstly a lattice-gas, secondly a disordered phase at submonolayer coverage, which thirdly undergoes a phase-transition to a highly ordered ( $6\sqrt{2} \times \sqrt{2}$ )R45° structure, if the CO<sub>2</sub> partial pressure exceeds a critical temperature-dependent value. So far, not much was known about the structure of the 237 Å<sup>2</sup> unit cell of the high-order phase which in absolute terms offers place for up to 14 inequivalent CO<sub>2</sub> molecules. Total energy minimizations and Monte Carlo Simulations based on pair-potentials favor a structure containing 12 inequivalent molecules. Using a vibrational exciton approach, simulated infrared spectra based on this structure are in very satisfactory agreement with experimental IR spectra. According to theory, 10 molecules are stabilized on the surface due to a predominant molecule-molecule interaction, while only two molecules are "pinned" onto the surface at sites with favorable molecule-surface interaction. This might explain the rapid aging of the structure observed in the experiments.

O 17.8 Tue 12:15 SCH A01

**An Azobenzene Derivate on NaCl/Ag(111): Surface Structure, Molecule Adsorption, and Electron-Induced Switching** — ●ALI SAFIEI, JÖRG HENZL, and KARINA MORGENSTERN — Leibniz University of Hannover, Institute of Solid State Physics, Appelstraße 2, 30167 Hannover

Thin NaCl films on metallic substrates offer the possibility of investigating the conformational, mechanical and electronic structure and thus functionalities of molecules with low coupling to the substrate. We first studied the growth of NaCl islands by scanning tunnelling microscopy and spectroscopy on the clean Ag(111) surface. On this surface the islands grow epitaxially in double layers, are atomically flat and nearly defect-free. Spectroscopic dI/dV measurements show that the surface state of Ag on NaCl double layer is shifted to higher energies than on the pure Ag(111) surface. Amino-nitro-azobenzene molecules (ANA) are adsorbed on the NaCl islands at very low temperatures. We found the trans-configuration of ANA on the ultra-thin insulating layers and realized a reversible switching process by electron-induced

manipulation. In contrast to the switching processes on Au(111) [1], these conformational changes resemble the trans-cis isomerisation of the ANA molecule in the gas phase. The reason is that the molecules on NaCl islands are less coupled to the substrate. The shift of the surface state of Ag on NaCl, the switching process and the energy barrier of the reversible switching will be discussed in this talk.

[1] Jörg Henzl, Michael Mehlhorn, Heiko Gawronski, Karl-Heinz Rieder, Karina Morgenstern, *Angew. Chem. Int.* 45 (2006) 603-606.

O 17.9 Tue 12:30 SCH A01

**The resonant x-ray absorption coefficient by diffraction peak widths** — ●VICTOR SOLTWISCH, YEVGEN GOLDSHTEYN, ENRICO SCHIERLE, DETLEF SCHMITZ, and EUGEN WESCHKE — Helmholtz-Zentrum Berlin für Materialien und Energie

The (010) structural reflection of multiferroic DyMnO<sub>3</sub> was measured for photon energies across the *M*<sub>5</sub> absorption edge of Dysprosium by resonant soft x-ray diffraction. It is found that the width of this diffraction peak exactly tracks the x-ray absorption spectrum obtained from the same sample by measurement of the total electron yield (TEY). While such a connection has been anticipated, we provide a direct experimental proof. The method is more bulk sensitive than TEY and avoids the problem of self absorption present in fluorescence-yield data. Furthermore, it provides an excellent tool for measurements of

the absorption coefficient in insulators at low temperatures or in strong magnetic fields.

O 17.10 Tue 12:45 SCH A01

**Ferroelectric domain structures on BaTiO<sub>3</sub>(100) observed by Laser-excited PEEM** — ●ANKE HÖFER, KLAUS DUNCKER, STEFAN FÖRSTER, and WOLF WIDDRA — Martin-Luther-Universität Halle-Wittenberg, Halle, Germany

The ferroelectric domain structure at a single crystal BaTiO<sub>3</sub>(100) surface is imaged by photoelectron emission microscopy (PEEM) using a fully tunable femtosecond laser source. For a BaTiO<sub>3</sub>(100) surface which is prepared under UHV conditions by sputtering and annealing in an oxygen atmosphere, at room temperature a stripe like domain pattern is observed with high contrast aligned in the high symmetry [100] direction of the substrate. The PEEM pattern is explained by sequences of 90°-a-c domains.

Wavelength-dependent images with UV excitation in the range of 290 - 330 nm show a varying domain contrast and allow the determination of the local photoemission threshold for one ferroelectric domain. For higher laser pulse energies and for wavelengths below the onset of one-photon photoemission, two-photon PEEM images show the ferroelectric domain structure as well.

## O 18: Metal substrates: Adsorption of organic / bio molecules III

Time: Tuesday 10:30–12:45

Location: SCH A118

O 18.1 Tue 10:30 SCH A118

**Probing Orientation and Conformation of  $\alpha$ -Helix and  $\beta$ -Sheet Model Peptides on Self-Assembled Monolayers with SFG and NEXAFS Spectroscopy** — ●TOBIAS WEIDNER, JULIA APTE, LARA J. GAMBLE, and DAVID G. CASTNER — National ESCA and Surface Analysis Center for Biomedical Problems, University of Washington, Seattle, USA

Understanding the interaction of proteins and peptides with engineered surfaces from first principles is essential for the design of biomaterials applications. In this study we characterized amphiphilic  $\alpha$ -helix and  $\beta$ -strand model peptides on self-assembled monolayers (SAMs) on Au in situ using sum frequency generation (SFG) spectroscopy and ex situ using near edge X-ray absorption fine structure (NEXAFS) spectroscopy. The  $\alpha$ -helix peptide is a 14-mer and the  $\beta$ -strand is a 15-mer composed of hydrophilic lysine (K) and hydrophobic leucine (L) residues. SAMs having either carboxylic acid or methyl terminal groups were used as charged and hydrophobic model surfaces, respectively. SFG peptide spectra on methyl SAMs exhibited peaks near 2965 cm<sup>-1</sup> and 2875 cm<sup>-1</sup> related to ordered leucine side chains. A relative phase of 0 rad for both peptides showed, that the leucines were oriented towards the interface. Features near 3200 cm<sup>-1</sup> and 3400 cm<sup>-1</sup> related to bound water were also observed. The spectra on carboxylic acid SAMs were dominated by a peak near 3300 cm<sup>-1</sup>, indicating substantial lysine-surface interactions. The linear dichroism of the amide  $\pi^*$  orbital near 400.1 eV observed in the NEXAFS spectra proves the peptides are oriented parallel to the interface on both SAMs.

O 18.2 Tue 10:45 SCH A118

**Irradiation-promoted exchange reaction as a tool for Chemical Lithography** — NIRMALYA BALLAV<sup>1</sup>, ANDREAS TERFORT<sup>2</sup>, and ●MICHAEL ZHARNIKOV<sup>1</sup> — <sup>1</sup>Angewandte Physikalische Chemie, Universität Heidelberg, D-69120 Heidelberg, Germany — <sup>2</sup>Institut für Anorganische und Analytische Chemie, Goethe-Universität Frankfurt, 60438 Frankfurt, Germany

The development of novel approaches for the fabrication of nanostructures and, in particular, chemical and biological patterns is an important technological and scientific challenge. One of the perspective methods applies a modification of chemisorbed monomolecular films - self-assembled monolayers (SAMs), which are well-ordered 2D-assemblies of long-chain molecules attached to a suitable substrate. A flexible molecular architecture of the SAM constituents allows one to use a wide range of substrates, whereas the molecular size of these constituents makes SAMs an ideal platform for the fabrication of micro- and nanostructures. We present here a new approach for the fabrication of chemical patterns with aliphatic SAMs as templates. The

approach relies upon electron beam or X-ray lithography, but requires much lower patterning dose as compared to already available methods. The technique is based on so-called irradiation-promoted exchange reaction (IPER) between the primary SAM template and potential molecular substituent and can utilize a broad variety of commercially available molecules. The preparation of chemical patterns occurs similar to photography: in the first step the pattern is written by electrons, and in the second step it is developed in the solution of the substituent.

O 18.3 Tue 11:00 SCH A118

**Embedded dipoles in monomolecular films: physical and electronic structure effects** — ●MICHAEL ZHARNIKOV<sup>1</sup>, ORLANDO M. CABARCOS<sup>2</sup>, TOBIAS WEIDNER<sup>1</sup>, SUNDARARAJAN UPPLI<sup>2</sup>, LINDA S. DAKE<sup>3</sup>, and DAVID L. ALLARA<sup>2</sup> — <sup>1</sup>Angewandte Physikalische Chemie, Universität Heidelberg, Im Neuenheimer Feld 253, D-69120 Heidelberg, Germany — <sup>2</sup>Department of Chemistry and the Materials Research Institute, Pennsylvania State University, University Park, PA 16802, USA — <sup>3</sup>Department of Physics, Utica College, Utica, NY 13502, USA

Ester moiety was imbedded into the molecular chain of alkanethiolate self-assembled monolayers (SAMs) on Au(111), with the length of the segments below and above the ester moiety being varied. The bottom segments of the alkyl chain were found to be better ordered than the upper ones. The presence of the ester moiety leads to the formation of a strong electric dipole layer with a component of 1.05 Debye normal to the surface. This dipole layer exhibits a strong electrostatic effect on the XPS spectra in which the C 1s photoelectron kinetic energies are consistently shifted by 0.85 eV between the top and bottom alkyl chain segments, regardless of relative lengths. This shift correlates, within error, with the value of 0.81 eV predicted via classical electrostatics due to the presence of the ester dipole layer. Overall, these data show that SAMs assembled from molecules with appropriately selected internal groups can be used to prepare internally layered structures with highly controlled electrical characteristics and further demonstrate that simple XPS shifts in core level energies can be used to derived accurate molecular dipole values in structured thin films.

O 18.4 Tue 11:15 SCH A118

**Differences in Self Assembly of Linear Dicarboxylic Acids** — ●CHRISTOPH HEININGER<sup>1</sup>, LORENZ KAMPSCHULTE<sup>1,2</sup>, MARKUS LACKINGER<sup>1</sup>, and WOLFGANG HECKL<sup>1,2</sup> — <sup>1</sup>Ludwig-Maximilians-University and Center for NanoScience, Theresienstrasse 41, 80333 München — <sup>2</sup>Deutsches Museum, Museumsinsel 1, 80538 München

Self-assembly at the liquid solid interface into two-dimensionally ordered supramolecular structures of three aromatic dicarboxylic acids; 2,6-naphthalenedicarboxylic acid (NDA), 4,4\*-biphenyldicarboxylic acid (BPDA), and 4,4\*-stilbenedicarboxylic acid

(SDA) is studied by scanning tunneling microscopy. The structure of the compounds is very similar and consists of two interconnected aromatic moieties and functionalization through two carboxylic groups in linear configuration. For all molecules, ordered monolayers were observed on a graphite substrate, and the resulting structures can be described as a dense packing of one-dimensionally hydrogen-bonded rows. Concerning the stability of the adsorbate layers, the average domain size, and the degree of order, distinct differences were noticed. Supported by density functional theory (DFT) calculations, these differences are analyzed and explained as a consequence of molecular structure, adsorption geometry, and adsorption energy.

O 18.5 Tue 11:30 SCH A118  
**N,N'-di(n-butyl)quinacridone monolayer on Ag(110): a DFT study with semiempirical dispersion corrections** — ●JÖRN-HOLGER FRANKE<sup>1</sup>, VASILE CACIUC<sup>2</sup>, LIFENG CHI<sup>1</sup>, and HARALD FUCHS<sup>1</sup> — <sup>1</sup>Physikalisches Institut, WWU Münster, Germany — <sup>2</sup>Forschungszentrum Jülich, Germany

We studied the adsorption of N,N'-di(n-butyl)quinacridone (DBQA) on Ag(110) by DFT including semiempirical dispersion corrections. 4 different adsorption geometries are studied, the most stable one showing a binding of molecular oxygen to first layer Ag atoms and butyl chains folded away from the substrate. The charge redistribution upon adsorption is governed by charge donation to the molecular LUMO and the push-back effect, yielding a lowering of calculated work functions by up to 0.85 eV. The semi-empirical dispersion corrections introduce a large non-site specific binding energy gain for all configurations and induce an approach of the molecule to the substrate for weakly bound ones.

[1] J.-H. Franke, V. Caciuc, L.F. Chi, and H. Fuchs, PRB, 78, 165432

O 18.6 Tue 11:45 SCH A118  
**Chemical versus van der Waals Interaction: The Role of the Heteroatom** — ●NICOLAE ATODIRESEI, VASILE CACIUC, PREDRAG LAZIĆ, and STEFAN BLÜGEL — Institut für Festkörperforschung (IFF), Forschungszentrum Jülich, 52425 Jülich, Germany

We performed first-principles calculations aimed to investigate the role of an heteroatom like N in the chemical and the long-range van der Waals (vdW) interactions for a flat adsorption of several  $\pi$ -conjugated molecules on the Cu(110) surface. To evaluate the dispersion effects we used an *ab initio* as well as a semiempirical method. A key result of our study is that a state of the art investigation of the bonding mechanism leading to a flat molecule-substrate adsorption geometry requires the use of both methods to correctly describe the geometry, the electronic structure and the correlation effects of the molecule-surface interface. Our study reveals that the molecule-surface vdW interactions involve not only  $\pi$ -like orbitals which are perpendicular to the molecular plane but also  $\sigma$ -like orbitals delocalized in the molecular plane.

Ref.

1. N. Atodiresei, V. Caciuc, H.-J. Franke and S. Blügel, Phys. Rev. B **78**, 045411 (2008).

2. N. Atodiresei, V. Caciuc, P. Lažic, and S. Blügel, arXiv:0811.3082.

O 18.7 Tue 12:00 SCH A118  
**Theoretical Investigation of Bis(terpyridine)-based Surface Structures** — ●DANIELA KÜNZEL and AXEL GROSS — Institute for Theoretical Chemistry, Ulm University, D-89069 Ulm, Germany

Ordered organic layers of bis(terpyridine)-derived molecules (BTPs) adsorbed on graphite show a number of interesting properties that can easily be varied by slight modifications of the system such as the coverage [1]. In order to understand this dependence, structures of 3,3'-BTP and 2,4'-BTP on graphite were investigated using density functional theory (DFT) and several force field methods such as COMPASS, UFF, CVFF and Dreiding.

These calculations confirm that the formation of weak C-H...N hy-

drogen bonds controls the self-assembled adsorption of BTP molecules into ordered surface structures. Modifications with different surface coverages and surface structures can be obtained, depending on BTP isomer and adsorption conditions. In addition, chemical modifications of the adsorbate molecules and their consequences on structure formation have been addressed.

Due to its large cavities, the hexagonal structure of 3,3'-BTP is of special interest. These cavities can be used as a template for the adsorption of guest molecules such as phthalocyanine derivatives. At room temperature, the guest molecules can rotate within the cavities, as both STM experiments and force field calculations of the rotational barriers demonstrate [1]. Furthermore, the dependence of the rotational barriers on the size of the guest molecules will be discussed.

[1] C. Meier *et al.*, Angew. Chem. Int. Ed. **47**, 3821 (2008).

O 18.8 Tue 12:15 SCH A118  
**First-principles and semi-empirical van der Waals studies of pyridine and thymine on the Cu(110) surface** — ●V. CACIUC<sup>1</sup>, N. ATODIRESEI<sup>1</sup>, P. LAZIĆ<sup>1</sup>, J.-H. FRANKE<sup>2</sup>, Y. MORIKAWA<sup>3</sup>, and S. BLÜGEL<sup>1</sup> — <sup>1</sup>Institut für Festkörperforschung, Theorie I, Forschungszentrum Jülich, D-52425 Jülich, Germany — <sup>2</sup>Physikalisches Institut, Westfälische Wilhelms Universität Münster, Wilhelm-Klemm-Str. 10, D-48149 Münster, Germany — <sup>3</sup>The Institute of Scientific and Industrial Research, Osaka University, 8-1 Mihogaoka, Ibaraki Osaka, 567-0047 Japan

We performed density functional calculations aimed to investigate the adsorption geometry and bonding mechanism of a single pyridine (C<sub>5</sub>H<sub>5</sub>N) and thymine (C<sub>5</sub>H<sub>6</sub>N<sub>2</sub>O<sub>2</sub>) molecule on the Cu(110) surface. In the ground state, the pyridine molecule adsorbs with its molecular plane perpendicular to the substrate and is oriented along the [001]-direction while the thymine is aligned along the [1 $\bar{1}$ 0]-direction. For this adsorption configuration, the bonding mechanism of these molecules involves a strong hybridization between the highest occupied molecular orbitals (HOMOs) and the *d*-states of the substrate. However, when the molecular plane is parallel to surface, the long-range van der Waals interactions play an important role on both the molecule-surface geometry and the adsorption energy. Their specific role was analyzed by means of a semi-empirical and the seamless methods. In particular, for a planar configuration, the inclusion of the dispersion effects can dramatically change the character of the adsorption process from physisorption to chemisorption.

O 18.9 Tue 12:30 SCH A118  
**Molecular Switches at Surfaces: The Role of Van Der Waals Interactions** — ●ERIK MCNELLIS, JOERG MEYER, and KARSTEN REUTER — Fritz-Haber-Institut, Faradayweg 4-6, 14195 Berlin

Molecules that by external stimuli may be reversibly switched between different defined states are envisioned as a key component of a future molecular nanotechnology. For the latter, it is particularly the molecular function when the switch is stabilized at a solid surface that is of key interest. Using density-functional theory (DFT) with a gradient-corrected (GGA) functional we carry out a detailed characterization of the metastable structures of the prototypical molecular switch azobenzene at close-packed coinage metal surfaces. We obtain a range of switch-surface interactions that goes from weak physisorption at Au(111) to a reversal in the stability of the gas-phase cis and trans molecular conformations at Cu(111). In view of the known inadequacies of present-day GGA functionals in the description of long-range van der Waals interactions, we check on these findings considering corrections from semi-empirical pair potential schemes. While corrections to the gradient are small enough to leave adsorbate geometries essentially unchanged, the obtained adsorption energy corrections are substantial, in certain cases significantly altering the pure DFT picture. We discuss this, and the discomforting differences obtained between the employed semi-empirical schemes in the greater context of molecular adsorption at metal surfaces.

## O 19: Nanostructures at surfaces: Arrays

Time: Tuesday 10:30–12:45

Location: SCH A215

O 19.1 Tue 10:30 SCH A215

**Fabrication of periodic templates on Si: from nanometer to micrometer scale** — ●CHRISTIAN PFAHLER<sup>1</sup>, FABIAN ENDERLE<sup>1</sup>, ACHIM MANZKE<sup>1</sup>, STEFAN WIEDEMANN<sup>1</sup>, ALFRED PLETTL<sup>1</sup>, PAUL ZIEMANN<sup>1</sup>, EYK SCHREIBER<sup>2</sup>, ULRICH ZIENER<sup>2</sup>, and KATHARINA LANDFESTER<sup>2</sup> — <sup>1</sup>Institut für Festkörperphysik, Universität Ulm, D-89069 Ulm — <sup>2</sup>Institut für Organische Chemie III, Universität Ulm, D-89069 Ulm

Colloidal polystyrene (PS) particles either pure or loaded with a metal precursor are used to generate nanomasks on Si and SiO<sub>2</sub>. The latter ones were prepared by emulsion techniques [1,2]. Dip-coating a pre-treated substrate permits the deposition of monolayers over areas up to ten square millimeters.

Isotropic etching in oxygen plasmas reduces the diameter of the pure particles continuously down to 50 nm and the emulsion colloids to hybrid particles with 20-50 nm, respectively. Typical starting values in both cases are 300 nm. Additional annealing further reduces the Pt particles to diameters between 6-14 nm.

Using this set of particles as a mask for anisotropic reactive ion etching (RIE), arrays of pillars and pores can be fabricated with variable distance and size from 10 nm up to the classical colloidal lithography scale.

[1] A. Manzke et al., *Adv. Mater.* **19**, 1337 (2007).

[2] E. Schreiber et al., *Chem. Mater.* submitted (2008).

O 19.2 Tue 10:45 SCH A215

**UTAM-synthesized large-scale regular arrays of surface patterns of 0-d and 1-d nanostructures** — ●YONG LEI, STEFAN OSTENDORP, and GERHARD WILDE — Institut für Materialphysik, Westfälische Wilhelms-Universität Münster, Wilhelm-Klemm-Str. 10, 48149 Münster, Germany

Here we report an UTAM surface nano-patterning fabrication system in synthesizing large-scale regular arrays of 0-D (dots) and 1-D (wires and tubes) surface nanostructures. Different metallic and semiconductor nanodots were fabricated on silicon and sapphire substrates using an ultra-thin alumina membrane (UTAM) as the evaporation mask. The diameter, spacing, shape, and even the crystalline structures of the synthesized surface nano-patterns are adjustable and hence resulting in tunable physical properties of these nano-patterns. A nanoporous silicon oxide surface structure with embedded metallic oxide nano-dots can be realized by oxidizing the metallic nanodots. Using the UTAM-prepared Au nanodots as the catalysts, regular ZnO nanowire arrays were prepared using the CVD process. A unique type of rectangular cross-section ZnO nanowires with a layered structure was also obtained. These layered ZnO nanowires exhibit strong yellow photoluminescence, which is unusual compared to the green photoluminescence of the conventional CVD-prepared ZnO nanowires. The mechanism of this yellow photoluminescence is closely related to the layered structures of the nanowires. These yellow luminescent ZnO nanowires could be used as an excellent component of some optical devices such as flat displays.

O 19.3 Tue 11:00 SCH A215

**Ion beam pattern formation on Si(001) with and without codeposition** — ●SVEN MACKO and THOMAS MICHELY — II. Physikalisches Institut, Universität zu Köln, Germany

Si(001) is sputtered with ion fluences  $> 10^{22}$  ions/m<sup>2</sup> and at angles  $\vartheta = 0^\circ - 83^\circ$  with respect to the surface normal. Sputtering was performed under UHV conditions with a differentially pumped and scanning fine focus ion source. The chamber pressure rose to  $\approx 9 \times 10^{-8}$  mbar during erosion and great care was exercised to sputter the Si sample only. At room temperature for  $\vartheta = 0^\circ - 45^\circ$  no pattern formation was observed. To the contrary, rough starting surfaces smoothened. For flat starting surfaces the roughness remained below 3 Å. The observed absence of roughness partly agrees and partly disagrees with observations in the literature. We tested the effect of codeposition, either through physical vapor phase deposition or sputter deposition. At room temperature, with ion fluences  $> 5 \times 10^{21}$  ions/m<sup>2</sup>, Mo sputter codeposition leads to regular, concentration dependent patterns of dots and ripples. At elevated temperatures also other codeposited materials give rise to large surface roughness.

O 19.4 Tue 11:15 SCH A215

**Substrate effect on supramolecular self-assembly: from semiconductors to metals** — ●TAKAYUKI SUZUKI<sup>1</sup>, THERESA LUTZ<sup>1</sup>, DIETMAR PAYER<sup>1</sup>, NIAN LIN<sup>1,2</sup>, STEVEN TAIT<sup>1,3</sup>, GIOVANNI COSTANTINI<sup>1,4</sup>, and KLAUS LERN<sup>1,5</sup> — <sup>1</sup>MPI for Solid State Res., Heisenbergstr. 1, 70569 Stuttgart — <sup>2</sup>Dept. of Phys., The Hong Kong Univ. of Sci. Technol., Clear Water Bay, Kowloon, HK — <sup>3</sup>Dept. of Chem., Indiana Univ., Bloomington, 47405 IN — <sup>4</sup>Dept. of Chem., Univ. of Warwick, Coventry, CV4 7AL — <sup>5</sup>IPN, EPFL, 1015 Lausanne

Terephthalic acid (TPA) deposited on Si(111)-7×7, Si(111)- $\sqrt{3} \times \sqrt{3}$ -Ag and Ag(111) has been studied as a model system to understand how much passivated semiconductor surfaces differ from semiconductor and metal surfaces in respect to supramolecular self-assembly. By scanning tunneling microscopy it is found that TPA molecules do not form any ordered supramolecular structure on the pristine semiconductor surface, due to a strong molecule-substrate interaction. On the contrary, TPA has a weaker interaction with Si(111)- $\sqrt{3} \times \sqrt{3}$ -Ag, leading to the formation of an ordered supramolecular layer stabilized by carboxyl hydrogen bonds. These structures are very similar to the supramolecular layer of TPA formed on Ag(111), indicating that the two substrates behave similarly in respect to the adsorption of functional organic molecules. However, the deposition of Fe on the TPA layers on Si(111)- $\sqrt{3} \times \sqrt{3}$ -Ag does not induce the formation of metal-organic frameworks which, on the contrary, readily develop on Ag(111). The origins of this difference are probably the particular electronic properties and reactivity of the two substrates.

O 19.5 Tue 11:30 SCH A215

**Sub-wavelength patterning of organic monolayers via non-linear processing with single femtosecond laser pulses** — ●NILS HARTMANN<sup>1</sup>, STEFFEN FRANZKA<sup>1</sup>, JÜRGEN KOCH<sup>2</sup>, ANDREAS OSTENDORF<sup>2</sup>, and BORIS N. CHICHKOV<sup>2</sup> — <sup>1</sup>Fachbereich Chemie and Center for Nanointegration Duisburg-Essen (CeNIDE), Universität Duisburg-Essen (UDE), Universitätsstraße 5, 45117 Essen — <sup>2</sup>Laser Zentrum Hannover e. V., Hollerithallee 8, 30419 Hannover

Femtosecond laser patterning of octadecylsiloxane monolayers on quartz glass at a wavelength of 800 nm, pulse lengths  $< 30$  fs and ambient conditions has been investigated. Due to its optical band gap of 8.5 eV, quartz glass represents an ideal platform for femtosecond laser processing of silane-based monolayers via nonlinear absorption processes. Selective decomposition of the coating with single laser pulses at sub-wavelength resolution can be achieved over a wide range of fluences from 4.2 down to 3.1 J/cm<sup>2</sup>. In particular, at a 1/e laser spot diameter of 1.8 microns, structures with a width of 250 nm and below were fabricated. This opens up a facile route towards laser fabrication of transparent templates with chemical structures down into the sub-100 nm regime [1]. Such templates represent promising platforms for biotechnological applications, e. g. biosensor arrays and microfluidic chips.

1. N. Hartmann, S. Franzka, J. Koch, B. N. Chichkov, A. Ostendorf, *Appl. Phys. Lett.* **92** (2008) 223111.

O 19.6 Tue 11:45 SCH A215

**Electrocatalysis on Nanostructured Surfaces: Electrochemical Behaviour of Ir(210)** — ●KHALED SOLIMAN, FELICE SIMEONE, LUDWIG KIBLER, and TIMO JACOB — Institut für Elektrochemie, Universität Ulm, 89069 Ulm

Recently it was found that Ir(210) transforms to a nanostructured surface morphology with three-sided nanopyramids after oxygen adsorption and annealing in ultra high vacuum (UHV) [1]. Motivated by this work we envisaged to prepare such nanofaceted surfaces outside a UHV system. We could show that faceted Ir(210) can indeed be prepared by inductive heating in presence of an inert atmosphere, which contains traces of oxygen [2]. Such surfaces are of interest for electrocatalysis. In order to characterize Ir(210) cyclic voltammetry (CV) and STM measurements were carried out. In our CV-curves of faceted Ir(210) in sulfuric acid a characteristic needle-like peak appeared, which serves as indicator for the presence and quality of the nanofacets. The STM images showed a typical structure of faceted Ir(210) surface, which could be explained by theoretical calculations employing density functional theory and thermodynamic considerations [3]. Finally, we performed first studies on the electrocatalytic

behaviour of planar and nanofaceted Ir(210).

[1] I. Ermanoski, C. Kim, S. P. Kelty, T. E. Madey, *Surf. Sci.*, **596**, 89 (2005). [2] K. A. Soliman, F. C. Simeone and L. A. Kibler, *Electrochem. Comm.*, **11**, 31 (2008). [3] P. Kaghazchi, F. C. Simeone, K. A. Soliman, L. A. Kibler, T. Jacob, *Faraday Discuss.*, **140**, 69 (2008).

O 19.7 Tue 12:00 SCH A215

**Photoluminescence quenching of PS and its use as template to confine R6G** — ●PUSHPENDRA KUMAR<sup>1</sup>, MANASH GHOSH<sup>1</sup>, PETER LEMMENS<sup>1</sup>, FRANK LUDWIG<sup>2</sup>, and MEINHARD SCHILLING<sup>2</sup> — <sup>1</sup>IPKM, TU Braunschweig, Germany — <sup>2</sup>EMG, TU Braunschweig, Germany

The different chemical treatment including Ag nanoparticle deposition was carried out on the electrochemically formed mesoporous silicon (PS) to investigate the PL quenching of PS and its further use as a porous template to confine the rhodamine 6G (R6G). For all states of preparation of PS sample, PL and UV/VIS transmission spectroscopy was measured. In the final state the complete quenching of PL was observed. From our transmission measurements we concluded that the quenching of PL is attributed to a fundamental disruption of the luminescence mechanism. R6G is then confined to PL quenched PS sample. The blue shift in the R6G PL peak is observed compare to bulk R6G. The shift in R6G peak is attributed to a confining effect.

O 19.8 Tue 12:15 SCH A215

**Towards covalently bonded supramolecular networks - substrate induced polymerisation in 2D** — ●HERMANN WALCH, RICO GUTZLER, GEORG EDER, WOLFGANG M. HECKL, and MARKUS LACKINGER — Center for NanoScience (CeNS) und Sekt. Kristallographie, LMU München, Theresienstr. 41, 80333 München

Hydrogen-bonds as stabilizing intermolecular links for supramolecular self-assembly and the influence of the substrate have extensively been investigated. Compared to hydrogen bonded structures, metal-coordination networks were found to be more stable due to increased interaction strength. However, in terms of network stability it is desired to introduce covalent intermolecular bonds. The main challenge is to still maintain ordered growth despite the irreversibility of the bonds. While 3D covalent organic frameworks (COFs) are widely investigated, little is known about surface supported 2D COFs. So far, the prepara-

tion of covalently bonded molecular aggregates on surfaces is limited to a few molecules and close-packed structures. Here, we report on the formation of 2D COFs from a halogen substituted polyaromatic compound on Ag(110) and Cu(111) surfaces. Interestingly, on HOPG(001) the same compound forms non-covalently bonded networks which are stabilized by halogen-hydrogen bonds, whereas on metal surfaces the formation of covalent networks is observed. This illustrates that for this compound the substrate is not only an epitaxial template but can also act as a catalyst for the formation of covalent bonds. Experiments were carried out with a Scanning Tunnelling Microscope (STM) at room temperature under ultrahigh vacuum conditions.

O 19.9 Tue 12:30 SCH A215

**Temperature-induced phase transition in self-assembled supramolecular monolayers** — ●RICO GUTZLER<sup>1</sup>, THOMAS SIRTLL<sup>1</sup>, MICHAEL SCHMITTEL<sup>2</sup>, WOLFGANG M. HECKL<sup>1,3</sup>, and MARKUS LACKINGER<sup>1</sup> — <sup>1</sup>Center for NanoScience (CeNS) and Ludwig-Maximilians-University — <sup>2</sup>University Siegen — <sup>3</sup>Deutsches Museum

We present self-assembled molecular monolayers at the liquid-solid interface, whose morphology can be switched reversibly between two crystallographically different structures by heating above a temperature threshold. At room temperature, STM experiments reveal a non-densely packed six-fold honeycomb pattern at the interface between solution and graphite. The solute molecule with C<sub>3</sub> symmetry and carboxyl-terminated lobes adsorbs in a planar manner when dissolved in nonanoic acid. In this adsorption geometry, all of the three carboxylic groups are involved in two-fold intermolecular hydrogen bonds. Raising the temperature of the sample induces a phase transition which is accompanied by a substantial change in the monolayer morphology. The rearrangement results in a row structure comprised of densely packed, nearly upright standing molecules. The reversibility is demonstrated by subsequent cooling to room temperature which yields the original hexagonal monolayer. This unambiguously proves that the room temperature structure is not only a kinetically trapped metastable state which is just converted to the thermodynamically equilibrium structure by supplying thermal energy. Since in the row structure one carboxylic group per molecule points off the surface, the phase transition is accompanied by a change in surface affinity.

## O 20: Nano-optics of metallic and semiconducting nanostructures (time resolved)

Time: Tuesday 10:30–13:00

Location: SCH A216

O 20.1 Tue 10:30 SCH A216

**Analytic solution to optimal control of plasmon propagation in nanostructures** — ●PHILIP TUCHSCHERER<sup>1</sup>, CHRISTIAN REWITZ<sup>1</sup>, DMITRI V. VORONINE<sup>1</sup>, F. JAVIER GARCÍA DE ABAJO<sup>2</sup>, WALTER PFEIFFER<sup>3</sup>, and TOBIAS BRIXNER<sup>1</sup> — <sup>1</sup>Institut für Physikalische Chemie, Universität Würzburg, Am Hubland, 97074 Würzburg, Germany — <sup>2</sup>Instituto de Optica, CSIC, Serrano 121, 28006 Madrid, Spain — <sup>3</sup>Fakultät für Physik, Universität Bielefeld, Universitätsstr. 25, 33516 Bielefeld, Germany

Localization and adaptive control of optical near-fields using polarization-shaped laser pulses have previously been demonstrated theoretically and experimentally. Spatial localization and ultrafast switching of near-fields has a wide range of potential applications such as space-time resolved 'nano-femto' spectroscopy, quantum information processing, and nanoplasmonic devices.

We have now found an analytic solution to the problem of optimal control of plasmon propagation direction. The contrast between energy deposition at two particular locations within a nanostructure array can be manipulated with amplitude and polarization-shaped laser pulses.

Optimal fields from this deterministic approach are found to agree well with those from evolutionary optimization. Apart from the contrast of local energy deposition, nonlinear signals are also controlled by compressing the near fields at the desired site.

The analytic approach gives insight into the mechanisms involved and presents a way to simplify and improve experiments.

O 20.2 Tue 10:45 SCH A216

**Dephasing of Optical Magnetism in Magnetic Photonic Crystals** — ●MICHAEL GEISELMANN<sup>1,2</sup>, TOBIAS UTIKAL<sup>1,2</sup>, MARKUS LIPPITZ<sup>1,2</sup>, and HARALD GIESSEN<sup>1</sup> — <sup>1,4</sup>Physikalisches Institut, Universität Stuttgart, Germany — <sup>2</sup>Max Planck Institut für Festkörper-

forschung, Stuttgart, Germany

We investigate the time dynamics of optical magnetism in a magnetic photonic crystal. The structure consists of gold cut-wire pairs with a magnesium fluoride spacer on top of a HfO<sub>2</sub> slab waveguide. In the cut-wire pair structure, a symmetric and an antisymmetric plasmonic mode can be optically excited. The antisymmetric mode is regarded as a magnetic resonance. With the correct grating period the magnetic resonance in the wires can be coupled to the photonic mode, which is excited in the slab waveguide. In the strong coupling regime, a polaritonic system is formed, termed a magnetic plasmon polariton. In the experiment we study its femtosecond time dynamics using a nonlinear third-harmonic autocorrelation technique. We find that due to the coupling to the waveguide mode the dephasing of the system can be drastically prolonged up to 60 fs. To the best of our knowledge, this is the first experimental demonstration of temporally resolved magnetism in a magnetic photonic crystal.

O 20.3 Tue 11:00 SCH A216

**Ultrafast dephasing of the surface plasmon polaritons in metallic nanoparticles: Influence of the chemical environment** — ●MARTIN WORTMANN, NILS BORG, FRANK HUBENTHAL, and FRANK TRÄGER — Institut für Physik und Center for Interdisciplinary Nanostructure Science and Technology – CINSaT, Universität Kassel, Heinrich-Plett-Straße 40, D-34132 Kassel

It is well known that intrinsic size effects for metal nanoparticles have a significant influence on the electron dynamics and lead to a reduction of the dephasing time of the surface plasmon resonance. To take this effect into account, the parameter  $A$  has been introduced, which quantifies the influence of all independent damping contributions  $A_i$ , with  $A = \sum A_i$  (Matthiessen law). Although theoretically well understood, an exact knowledge of  $A$  as well as a microscopic understanding of the

involved processes, in particular of the chemical surrounding, are still lacking.

In this contribution we present first results on the influence of an inhomogeneous chemical environment on the  $A$ -parameter. We have investigated silver nanoparticles supported on sapphire and quartz substrates. The obtained  $A$ -parameters amount to  $A_{\text{sap}} = 0,20$  nm/fs and to  $A_{\text{qua}} = 0,54$  nm/fs, respectively. The latter value is higher, because quartz induces chemical damping. A subsequent coverage of the samples with  $\text{SO}_2$  opens a second damping channel and the  $A$ -parameters increase. Interestingly, for both  $\text{SO}_2$  covered samples the  $A$ -parameter is the same and amounts to  $A = 1,76$  nm/fs. This leads to the conclusion, that the two different damping channels are not independent.

O 20.4 Tue 11:15 SCH A216

**Enhancing optical near-fields in nanoantennas via shaped ultrashort laser pulses** — ●CHRISTIAN REWITZ<sup>1</sup>, PHILIP TUCHSCHORER<sup>1</sup>, DMITRI V. VORONINE<sup>1</sup>, ANDREAS REISERER<sup>1</sup>, JER-SHING HUANG<sup>2</sup>, BERT HECHT<sup>2</sup>, and TOBIAS BRIKNER<sup>1</sup> — <sup>1</sup>Institut für Physikalische Chemie, Universität Würzburg, Am Hubland, 97074 Würzburg, Germany — <sup>2</sup>Nano-Optics and Biophotonics Group, Department of Experimental Physics 5, University of Würzburg, Am Hubland, 97074 Würzburg, Germany

Femtosecond laser pulse shaping has been developed into an efficient tool for the manipulation of interference phenomena on the nanoscale. We show that this technique can be applied to tailor the ultrafast temporal response of the strongly confined and enhanced optical near-fields in the feed gap of resonant optical antennas.

Using finite-difference time-domain (FDTD) simulations followed by Fourier transformation, we obtain the impulse response of a nanostructure in the frequency domain, which allows obtaining its temporal response to any arbitrary pulse shape.

Additionally to this deterministic approach, an adaptive scheme involving an evolutionary algorithm can be used to obtain the optimal spectral phase that pre-compensates for the dispersion induced by the antennas. Comparing deterministic and adaptive results allows for a better understanding of plasmonic resonances in nanostructures. The presented control mechanisms will be of importance for experiments involving light-induced processes in nanometer-scale volumes.

O 20.5 Tue 11:30 SCH A216

**Ultrafast Coherent Control of Third-Harmonic Generation in Plasmonic Nanostructures** — ●TOBIAS UTIKAL<sup>1,3</sup>, MARK I. STOCKMAN<sup>1,2</sup>, ALBERT P. HEBERLE<sup>1</sup>, MARKUS LIPPITZ<sup>3</sup>, and HARALD GIESSEN<sup>1</sup> — <sup>1</sup>4. Physikalisches Institut, Universität Stuttgart — <sup>2</sup>Department of Physics and Astronomy, Georgia State University, USA — <sup>3</sup>MPI für Festkörperforschung, Stuttgart

We present a new technique to coherently control ultrafast nonlinear plasmonic effects on a nanometer scale. By using a nonlinear four-photon process (third-harmonic generation) our detection is not limited to the local optical intensity in the system, but additionally supports phase information. The nanostructure under investigation consists of a 1-D gold wire grating on top of a dielectric slab waveguide. The coupling of particle plasmons, optically excited in the wires, to photonic waveguide modes leads to plasmon-polaritonic eigenstates, characterized by long dephasing times, whose dynamics can be coherently controlled on a femtosecond timescale. In the experiment one polaritonic eigenstate is excited by a first sub-8 fs laser pulse (start pulse). A subsequent second pulse (control pulse) follows the start pulse after a few tens of femtoseconds. Dependent on the exact phase delay, the control pulse either stops the polariton oscillation or re-excites it again. A third pulse (probe pulse), which is aligned at a small angle to the start and control pulse, is continuously shifted in time. Photons of the probe pulse together with photons of the start and control pulse create a nonlinear third-harmonic signal depending on the coherently controlled polarization of the polariton.

O 20.6 Tue 11:45 SCH A216

**Subwavelength spatio-temporal control of the local excitation of metal nanostructures** — MARTIN AESCHLIMANN<sup>1</sup>, MICHAEL BAUER<sup>5</sup>, ●DANIELA BAYER<sup>1</sup>, TOBIAS BRIKNER<sup>3</sup>, STEFAN CUNOVIC<sup>2</sup>, FRANK DIMLER<sup>3</sup>, ALEXANDER FISCHER<sup>1</sup>, JAVIER GARCÍA DE ABAJO<sup>4</sup>, VIKTOR MYROSHNYCHENKO<sup>4</sup>, WALTER PFEIFFER<sup>2</sup>, MARTIN ROHMER<sup>1</sup>, CHRISTIAN SCHNEIDER<sup>1</sup>, FELIX STEEB<sup>1</sup>, CHRISTIAN STRÜBER<sup>2</sup>, and DMITRI V. VORONINE<sup>3</sup> — <sup>1</sup>University of Kaiserslautern, Germany — <sup>2</sup>University of Bielefeld, Germany — <sup>3</sup>Ludwigs-Maximilian-Universität, Würzburg, Germany — <sup>4</sup>CSIC, Madrid, Spain — <sup>5</sup>University of Kiel, Germany

Using time-resolved two-photon photoemission electron microscopy we demonstrate simultaneous spatial and temporal control of nanooptical fields. Based on the recent demonstration of ultrafast adaptive near field optics, we now investigate directly the temporal evolution of the local excitation by spatially resolved cross correlation measurements. Planar silver nanostructures manufactured by e-beam lithography are excited by polarization shaped pump pulses and the corresponding local excitation is probed by a time-correlated probe excitation using circularly polarized laser pulses. The time-resolved cross correlation traces for different regions of the nanostructure show a clear variation of their relative intensities. This confirms that the polarization-shaped incident laser pulse does indeed switch between two different excitation patterns within a time scale that can be controlled almost freely and is limited only by the spectral bandwidth of the used coherent light source. First spatio-temporal control experiments will be shown.

O 20.7 Tue 12:00 SCH A216

**Femtosecond Surface Plasmon Characterisation on Nanostructured Surfaces** — ●JOSE FRANCISCO LOPEZ-BARBERA, BRIAN ASHALL, FERGAL O'REILLY, and DOMINIC ZERULLA — University College Dublin, School of Physics, Dublin 4, Ireland.

Latest developments in ultrafast pulses have presented new opportunities for the investigation of surface plasmon polaritons (SPPs) on the sub 20 fs time scale. We have extended the characterization of the resonant photon-SPP coupling processes on smooth surfaces as presented in [1], emphasising the excitation, propagation, and temporal and spectral responses of the SPPs.

Broadening these studies, we have characterized the same processes using SPP excitation on metallic coated nanostructures of specific surface symmetry and tuneability. As expected, the nanostructured samples show different temporal characteristics which are attributed to their more complex propagation mechanisms. Furthermore, using our tuneable plasmonic structures [2] we present the influences of the tuneability of such systems on the temporal characteristics of the SPPs.

[1] S. E. Yalcin et al., Appl. Phys. Lett. 93, 101103 (2008).

[2] Stephanie Rehwald, Michael Berndt, Frank Katzenberg, Stephan Schwieger, Erich Runge, Klaus Schierbaum, and Dominic Zerulla, Phys. Rev. B 76, 085420 (2007).

O 20.8 Tue 12:15 SCH A216

**Surface plasmon polariton - exciton interaction in semiconductor-metal hybrids and dye-metal systems** — ●STEPHAN SCHWIEGER<sup>1</sup>, PARINDA VASA<sup>2</sup>, CHRISTOPH LIENAU<sup>2</sup>, and ERICH RUNGE<sup>1</sup> — <sup>1</sup>Technische Universität Ilmenau, 98693 Ilmenau, Germany — <sup>2</sup>Carl von Ossietzky Universität Oldenburg, 26129 Oldenburg, Germany

Surface plasmons polaritons (SPPs) are optical excitations that are confined to a metal surface and coupled to far-field radiation, e.g., by a periodic nanowire array. The interaction of SPPs and excitons in semiconductor quantum wells (QW) [P. Vasa et. al., PRL, 101, 116801 (2008)] or in a dye layer is investigated. The coupling strength is estimated for different systems and band structures of the coupled modes are calculated. A band gap at the exciton resonance energy is found for the dye system, which indicates strong coupling energies. In the semiconductor system, we predict an efficient energy transfer from excitons to SPPs and a clear enhancement of the SPP life time and propagation length for optimized parameters.

O 20.9 Tue 12:30 SCH A216

**Ultrafast optical nonlinearities in hybrid metal-J-aggregate nanostructures** — ●PARINDA VASA<sup>1</sup>, ROBERT POMRAENKE<sup>1</sup>, STEPHAN SCHWIEGER<sup>2</sup>, ERICH RUNGE<sup>2</sup>, and CHRISTOPH LIENAU<sup>1</sup> — <sup>1</sup>Carl von Ossietzky Universitaet, Institut fuer Physik, 26111 Oldenburg, Germany — <sup>2</sup>Technische Universitaet Ilmenau, Institut fuer Physik, 98684 Ilmenau, Germany.

We report the first measurement of an ultrafast optical nonlinearity resulting from the strong interaction between Surface Plasmon Polaritons (SPPs) excited on a gold grating and excitons in a J-aggregated cyanine dye. The hybrid metal-J-aggregate nanostructure is fabricated by spin coating the dye solution on a gold grating fabricated using a focused ion beam. The hybrid structures are characterized using far-field linear reflectivity as well as photoluminescence measurements and exhibit enhanced SPP-exciton coupling in the linear optical regime. The nonlinearity is investigated by low-temperature, angle-resolved, ultrafast pump-probe spectroscopy with 20-fs-time resolution. The strong coupling results in a significant shift in the response wavelength and

changes in the response time of the third order nonlinearity of the dye exciton are observed. Specifically, we observe, under certain resonance conditions, extremely strong, more than tenfold changes of the radiative lifetime of the dye exciton due to its coupling to SPP. Such a strong ultrafast nonlinear interaction between metal and excitons will be of key importance to amplify SPP excitations in such hybrid structures.

O 20.10 Tue 12:45 SCH A216

**Coherent exciton-surface plasmon polariton coupling in hybrid metal-J-aggregate** — ●ROBERT POMRAENKE<sup>1</sup>, PARINDA VASA<sup>1</sup>, STEPHAN SCHWIEGER<sup>2</sup>, ERICH RUNGE<sup>2</sup>, and CHRISTOPH LIENAU<sup>1</sup> — <sup>1</sup>Carl von Ossietzky Universitaet, Institut fuer Physik, 26111 Oldenburg, Germany — <sup>2</sup>Technische Universitaet Ilmenau, Institut fuer Physik, 98684 Ilmenau, Germany.

Understanding and manipulating the interactions between quantum emitters and Surface Plasmon Polaritons (SPPs) is the key to design-

ing and implementing novel nano-optical devices such as nano-lasers or ultrafast optical switches. Here, we report the observation of a greatly enhanced coherent coupling between Surface Plasmon Polaritons (SPPs) excited on a metal grating and excitons in a J-aggregated cyanine dye. The hybrid metal-semiconductor nanostructure is fabricated by spin coating the dye solution on a gold grating fabricated using a focused ion beam. The structure is designed to maximize the radiative interaction between the two excitations which is probed by low-temperature, angle-resolved, far-field reflectivity and photoluminescence measurements. As a result of the strong interaction between the two resonances, coupled SPP-exciton polariton modes following hybrid dispersion relations are formed. The experimental results are explained within a phenomenological, coupled oscillator model. Such a strong interaction can be used to significantly alter the optical response of an organic semiconductor or to design novel hybrid devices.

## O 21: Methods: Electronic structure theory I

Time: Tuesday 10:30–12:00

Location: SCH A316

O 21.1 Tue 10:30 SCH A316

**Embedding based order-N implementation of the FLAPW method** — ●FRANK FREIMUTH<sup>1,2</sup>, DANIEL WORTMANN<sup>1,2</sup>, and STEFAN BLÜGEL<sup>1,2</sup> — <sup>1</sup>Institut für Festkörperforschung, Forschungszentrum Jülich, 52425 Jülich, Germany — <sup>2</sup>Institute for Advanced Simulation, Forschungszentrum Jülich, 52425 Jülich, Germany

The Full-potential Linearized Augmented Plane Wave (FLAPW) method is known to set the standard for precision among the *ab initio* density functional theory codes. On the other hand, the computational effort of the FLAPW method is high and increases cubically with system size, making the applicability to large systems difficult.

In this talk we will discuss a Green-function (GF) based implementation of the FLAPW method suitable for the calculation of thick layered systems. Using the embedding method the layers may be calculated individually and joined together subsequently. The overall computational cost increases linearly with the number of layers. Our order-N GF implementation of the FLAPW method is able to fully replace the standard Bloch-function based implementation of the FLAPW method. Furthermore, the embedding concept allows to extend the applicability of the FLAPW framework to non-periodic infinite systems, e.g. surfaces and interfaces. Due to the high flexibility of the GF method general boundary conditions are easily imposed, e.g. the non-equilibrium situation arising in tunnel junctions under finite bias.

Besides the theoretical description of the method we give proof of evidence by presenting a set of applications for film, surface and transport calculations.

O 21.2 Tue 10:45 SCH A316

**Scalar relativistic schemes for all-electron DFT with atom-centered basis functions** — PAULA HAVU, ●VOLKER BLUM, and MATTHIAS SCHEFFLER — Fritz-Haber-Institut der Max-Planck-Gesellschaft, D-14195 Berlin, Germany

Numeric atom-centered orbitals are an efficient, accurate basis choice for all-electron electronic structure theory [1]. For seamless efficiency and accuracy, a one-component (two with spin) Schrödinger-like equation is computationally most convenient, but for most elements ( $Z \gtrsim 30$ ), relativistic effects arising near the nucleus cannot be ignored. Dirac's equation can simply be rewritten in a "scalar-relativistic" (one-component) form, but with a separate Hamiltonian for each eigenstate. For some paradigm test systems [e.g., the Au dimer; CO adsorption on Pt(111)], we here benchmark the accuracy of a hierarchy of scalar-relativistic schemes that circumvent the state dependence: (i) the unsatisfactory "zero-order regular approximation" (ZORA), which simply neglects the state dependence; (ii) a restriction of ZORA to only the atomic center of each basis function ("atomic ZORA") and (iii) a perturbative rescaling of all ZORA eigenvalues ("scaled ZORA" [2]), which both recover geometries and binding energies within a few 10 meV of benchmark full-potential linearized augmented plane wave [FP-(L)APW] calculations; and (iv) a separate, exact treatment of all non-overlapping core states, which then necessitates only small further (scaled) ZORA-like approximations to the extended semicore and valence states. [1] V. Blum *et al.*, *Comp. Phys. Comm.*, accepted (2008). [2] E. van Lenthe *et al.*, *J. Chem. Phys.* **101**, 9783 (1994).

O 21.3 Tue 11:00 SCH A316

**RPA atomization energies of extended systems** — ●JUDITH HARL and GEORG KRESSE — Universität Wien, Austria

Density functional theory (DFT) applying the local density or generalized gradient approximation (LDA, GGA) leads to bond length errors of the order of 1 % and atomization energies are not reproduced with chemical accuracy. Furthermore, the (semi-)local LDA and GGA do not properly account for long-range van der Waals interactions.

Therefore, the adiabatic connection fluctuation dissipation theorem (ACFDT), which provides in principle an exact expression for the correlation energy, has received increased interest in the recent years (e.g., [1]-[3]). In the present work, we evaluate lattice constants and atomization energies of molecules and extended systems within the ACFDT framework applying the random phase approximation (RPA).

The RPA energy includes the exact exchange energy and a compatible correlation energy that also accounts for long-range van der Waals interactions. We found that the rare-gas solids Ne, Ar, and Kr are well described within the RPA and the correct long-range  $1/V^2$  volume dependence is reproduced. For insulators and metals, covalent and ionic bonded systems, RPA lattice constants are found to deviate on average by only 0.25 % from experiment. Atomization energies, however, are throughout too small ( $\approx 0.2$  eV/atom) and the mean error remains close to the results obtained with DFT-PBE.

[1] F. Furche, *Phys. Rev. B* **64**, 195120 (2001). [2] A. Marini, P. García-González, A. Rubio, *Phys. Rev. Lett.* **96**, 136404 (2006) [3] J. Harl, G. Kresse, *Phys. Rev. B* **77**, 045136 (2008)

O 21.4 Tue 11:15 SCH A316

**Real-Space DFT for Molecules on Surfaces** — ●PAUL BAUMEISTER<sup>1</sup>, TOMOYA ONO<sup>2</sup>, DANIEL WORTMANN<sup>1</sup>, and STEFAN BLÜGEL<sup>1</sup> — <sup>1</sup>Institut für Festkörperforschung, Forschungszentrum Jülich, 52425 Jülich, Germany — <sup>2</sup>Department of Precision Science and Technology, Osaka University, Suita, Osaka 565-0871, Japan

We present a real-space code for density functional calculations that has been newly developed in Osaka and Jülich. Exploiting that most operations needed for electronic structure calculation are intrinsically local, the tasks on a real-space grid can be very efficiently parallelized by a domain decomposition scheme. In combination with iterative solvers, this favours the performance and scaling behaviour for large system sizes on massively parallel machines. So far our calculations have been based on the pseudopotential approach. Recently, the norm-conserving pseudopotentials have been replaced by the projector augmented wave (PAW) method proposed by Blöchl[1]. In order to save computational costs and to increase the accuracy, the double grid technique[2] is implemented to enable reasonably coarse grids.

The grid-based method is unrestricted with respect to boundary conditions, i.e. any combination of periodic and isolated boundary conditions can be selected which is well suited for calculating single molecules, wire structures and surface (film) setups without the usage of a super cell. We present the equilibrium structure of terephthalic acid adsorbed to a Cu(111) surface.

[1] P. E. Blöchl, *PRB* **50**, 17953 (1994)

[2] T. Ono, and K. Hirose, *PRL* **82**, 5016 (1999)

O 21.5 Tue 11:30 SCH A316

**Adsorption of Super-heavy Elements on a Au(111)** — ●JOSEF ANTON and TIMO JACOB — Institut für Elektrochemie, Uni Ulm, 89081 Ulm

Understanding the physical properties and the catalytic behavior of super-heavy elements is certainly an interesting but also challenging topic [1]. The major problems are connected with the rather short life time of these elements ( $\leq 1$  s), resulting in very limited experiment times (before the nucleus decays) on only one atom at a time. While most standard techniques of 'traditional' chemistry are not applicable, gas-phase thermo-chromatography is one of the few remaining [1]. In this method the adsorption site of the super-heavy element is measured on a gold-covered detector whose endings are kept at different temperatures.

In order to achieve an accurate theoretical description of the super-heavy elements and their adsorption on the detector surface, the electrons of the systems have to be treated fully-relativistically. We used our four-component DFT code [2,3] to determine the adsorption energies of the elements 112 and 114 and their homologues, mercury and lead respectively, on Au(111) at various surface sites. Besides discussing these results, more general trends as well as a comparison to available experimental data will be given.

[1] *The Chemistry of Superheavy Elements*, Ed. M. Schädel, Kluwer Academic Publishers, Dordrech (2003).

[2] J. Anton, B. Fricke, E. Engel, *Phys. Rev. A*, **69**, 012505 (2004).

[3] V. Pershina, J. Anton, T. Jacob, *Phys. Rev. A*, **78**, 032518 (2008).

O 21.6 Tue 11:45 SCH A316

**Massive parallelization of the KKR Green-function method for large scale ab-initio calculations** — ●ALEXANDER THIESS, RUDOLF ZELLER, and STEFAN BLÜGEL — Institut für Festkörperforschung and Institute for Advanced Simulation, Forschungszentrum Jülich, 52545 Jülich, Germany

Recent experimental progress in the analysis of oxide interfaces reveals the importance of complex defects arising from local disorder or oxygen vacancies on transport and magnetic properties of the system [1]. For a theoretical treatment by density-functional calculations large unit cells containing thousands of atoms are unavoidable. As existing density-functional methods are usually restricted to a few hundreds of atoms in the unit cell, we have developed an algorithm based on the KKR Green-function method capable of treating geometries consisting of several thousands of inequivalent atoms. We combine the advantages of the screened KKR formalism and an iterative solution of the Dyson equation [2] with the new generation of massively parallelized computers to obtain a parallelization over the number of atoms in the unit cell. Calculations of test systems with up to 4096 atoms in the unit cell show that our algorithm scales efficiently on the Jülich BlueGene computer JUGENE [3] for several thousands of processors.

[1] A. Ohtomo, H. Y. Hwang, *Nature* **427**, 423 (2004)

[2] R. Zeller, *J. Phys.: Condens. Matter* **20**, 294215 (2008)

[3] <http://www.fz-juelich.de/jsc/jugene>

## O 22: Focused Session: Epitaxial Graphene III

Time: Tuesday 10:30–13:00

Location: SCH 251

### Topical Talk

O 22.1 Tue 10:30 SCH 251

**Structural and electronic properties of graphene on Ru(0001)** — ●SEBASTIAN GÜNTHER — Department Chemie, Ludwig-Maximilians-Universität München, Butenandtstr. 11, 81377 München, Germany

STM on clean and Au covered graphene on Ru(0001) revealed a surprisingly large apparent height corrugation of 0.8-1.2 Å within the unit cell of the imaged moiré structure with a size of  $\sim (11 \times 11)$  Ru lattice spacings. Up to then graphene was thought to be a rather flat 2-dim network, weakly interacting with metal substrates. In order to understand whether graphene can form a strongly corrugated layer on a transition metal substrate and what type of interaction between carbon and substrate is formed, we performed ARPES measurements, SXRD and a LEED I(V) analysis. In ARPES strong electronic interaction between C and Ru could be evidenced by the observation of a large gap of the graphene pi-band at the K-point of the Brillouin zone. Further details of the electronic structure were found and will be discussed. The geometric configuration of the g-Ru(0001) was addressed by SXRD and LEED I(V) measurements. SXRD proved that in fact the periodic moiré consists of a much larger unit cell of  $(25 \times 25)$  g on  $(23 \times 23)$  Ru size with a superimposed  $(2 \times 2)$  symmetry. Crystal truncation rod data indicated pronounced buckling of the underlying Ru atoms evidencing strong interaction of C and Ru atoms. Finally, a LEED I(V) analysis proved both the large height modulation of the graphene layer of  $\sim 1.5$  Å as well as strong vertical and lateral atom displacements in the underlying Ru layers.

### Topical Talk

O 22.2 Tue 11:00 SCH 251

**Unraveling the strong interaction between graphene monolayer and Ru(0001) : a DFT-based STM and STS study** — ●MARIE-LAURE BOCQUET and BIN WANG — Laboratoire de Chimie, Ecole Normale Supérieure de Lyon, Lyon, France

In this talk, I will refer to recently published experimental Scanning Tunneling Microscopy experiments resolving the  $(12 \times 12)C / (11 \times 11)$  Ru Moiré superstructure and will propose a detailed comparison with large-scale ab initio periodic calculations.

I will show that, in contrast to expectations, the measured electronic corrugation of the Moiré pattern mainly originates from a geometric buckling of the graphene sheet of 1.5 Å, induced by alternating weak and strong chemical interactions with Ru. This finding holds when considering smaller  $((10 \times 10)$  Ru) and larger  $((12 \times 12)$  Ru) coincidence structures in the calculations. The chemical bonding in the strong

contact regions, leads to three recently measured properties nicely reproduced by the calculations :

- the STM transparence of carbon atoms directly above surface Ru atoms;
- the asymmetry between low- and high- lying carbon electronic states probed by STS spectroscopy ;
- the considerable band gap opening in the graphene states.

Finally I will review similar studies of graphene monolayer on various metal surfaces which allow us to classify the metals in two separate classes, one in which graphene is chemisorbed and one in which it is physisorbed.

O 22.3 Tue 11:30 SCH 251

**Adsorption of organic molecules on C/Ru(0001) - a combined STM and TPD study** — ●MICHAEL ROOS, HARRY E. HOSTER, and R. JÜRGEN BEHM — Institute of Surface Chemistry and Catalysis, Ulm University, D-89069 Ulm, Germany

Bis(terpyridine)derivatives (BTP) form highly ordered hydrogen bonded 2D networks on graphite (HOPG) at both the solid/liquid [1,2] and the solid/gas [3,4] interface. These structures depend on the positions of the N-Atoms, which can be varied in the synthesis [1,2]. As recently found by temperature programmed desorption (TPD), the high translational and rotational mobility of BTP molecules on HOPG gives rise to a distinct entropic stabilization of the first monolayer. In this talk, we will show that this mobility is reduced when the HOPG substrate is replaced by a graphene monolayer on Ru(0001) with its Moiré-like corrugation [5]. As will be shown for two different BTP isomers, this lower mobility becomes apparent both in the 2D structures and in the desorption rates of the resulting adlayers.

[1] C. Meier et al., *J. Phys. Chem. B* **109**, 21015 (2005).

[2] C. Meier et al., *Angew. Chem. Int. Ed.* **47**, 3821 (2008).

[3] H. E. Hoster et al., *Langmuir* **23**, 11570 (2007).

[4] A. Breittrück et al., *Surf. Sci.* **601**, 4200 (2007).

[5] S. Marchini et al., *Phys. Rev. B* **76**, 075429 (2007).

O 22.4 Tue 11:45 SCH 251

**Novel 1 nm thin carbon nanosheets** — ●ANDREY TURCHANIN<sup>1</sup>, ANDRE BEYER<sup>1</sup>, CHRISTOPH T. NOTTBOHM<sup>1</sup>, XIANGHUI ZHANG<sup>1</sup>, RAINER STOSCH<sup>2</sup>, ALLA SOLIGUBENKO<sup>3</sup>, JOACHIM MAYER<sup>3</sup>, PETER HINZE<sup>2</sup>, THOMAS WEIMANN<sup>2</sup>, and ARMIN GÖLZHÄUSER<sup>1</sup> — <sup>1</sup>Fakultät für Physik, Universität Bielefeld, 33615 Bielefeld — <sup>2</sup>Physikalisch-Technische Bundesanstalt, 38116 Braunschweig —

<sup>3</sup>Gemeinschaftslabor für Elektronenmikroskopie, RWTH Aachen, 52074 Aachen

We present a route for the fabrication of novel ultrathin ( $\sim 1$  nm) carbon films and membranes, whose electrical behavior can be tuned from insulating to conducting. Self-assembled monolayers of biphenyls are cross-linked by electrons, detached from the surfaces and subsequently pyrolyzed. This transformation was characterized by a variety of complementary spectroscopic and microscopic techniques. Above 1000K, the cross-linked aromatic monolayer forms a mechanically stable graphitic phase consisting of nanosize patches of graphene. The transition is accompanied by a drop of the sheet resistivity from  $\sim 10^8$  to  $10^2$  k $\Omega$ /sq and a mechanical stiffening of the nanomembranes from  $\sim 10$  to 50 GPa. The technical applicability of the nanosheets is discussed.

- [1] W. Geyer et al, Appl. Phys. Lett. 75, 2401 (1999)
- [2] W. Eck et al, Adv. Mater., 17, 2583 (2005)
- [3] A. Turchanin et al, Appl. Phys. Lett., 90, 053102 (2007)
- [4] C. T. Nottbohm et al, Ultramicroscopy, 108, 88 (2008)

O 22.5 Tue 12:00 SCH 251

**In-situ Raman spectroscopy and In-situ optical microscopy of graphene growth on polycrystalline nickel** — ●STEFAN THIELE<sup>1</sup>, MARIO HOFMANN<sup>1</sup>, KYEONG-JAE LEE<sup>1</sup>, HOOTAN FAHRHAT<sup>1</sup>, ALFONSO REINA<sup>1</sup>, JUERGEN A. SCHAEFER<sup>2</sup>, and JING KONG<sup>1</sup> — <sup>1</sup>Department of Materials Science and Engineering, Department of Electrical Engineering and Computer Sciences, Massachusetts Institute of Technology, Cambridge, Massachusetts 02139, USA — <sup>2</sup>Institut für Physik and Institut für Mikro- und Nanotechnologien, Technische Universität Ilmenau, P. O. Box 100565, 98684 Ilmenau, Germany

Due to our experience in nanotube growth, two modes of graphene growth on polycr. Ni should be possible [1]. It is possible that graphene growth is starting immediately after hydrocarbon gas injection [2] similar to the carbon nanotube growth or carbon atoms could dissolve into nickel and graphene is only growing when the carbon is precipitating out of the nickel during the cool down [3]. We used In-situ Raman spectroscopy and In-situ optical microscopy to investigate the large area graphene growth on polycrystalline nickel substrates [1] to proof one of the above theories. For the period of our growth process at high temperatures no Raman signal of graphene was detected. During the cool down process we observed an increasing film growth in the temperature range of 800- 900°C and subsequently a rising Raman signal, which is not changed significantly at lower temperatures. Further details will be discussed at the conference. [1] A. Reina et al., Nanoletters, in press, [2] Qingkai Yu et al., APL 93, 113103 (2008), [3] S. Moshkalyov et al., Mat. Sci. Eng. B 112, 147 (2004)

O 22.6 Tue 12:15 SCH 251

**Ambient pressure CVD grown and transferred graphene: STM and UPS study** — ●ROLAND J. KOCH<sup>1,2</sup>, ALFONSO REINA<sup>1</sup>, JUERGEN A. SCHAEFER<sup>2</sup>, and JING KONG<sup>1</sup> — <sup>1</sup>Department of Materials Science and Engineering, Department of Electrical Engineering and Computer Sciences, Massachusetts Institute of Technology, Cambridge, Massachusetts 02139, USA — <sup>2</sup>Institut für Physik and Institut für Mikro- und Nanotechnologien, Technische Universität Ilmenau, P. O. Box 100565, 98684 Ilmenau, Germany

We used polycrystalline nickel as a substrate to synthesize few layer graphene (FLG) via Chemical Vapor Deposition (CVD). These sam-

ples have been analyzed using scanning tunneling microscopy (STM) and ultra violet photoelectron spectroscopy (UPS). In addition, the FLG transferred to other Ni and Si/SiO<sub>2</sub> samples were characterized. Large Moiré patterns have been observed by STM on both, the transferred and the not transferred samples, indicating a stacking disorder between first and second graphene layer. This is in line with results of FLG grown on SiC by Si sublimation [Varchon et al., Phys. Rev. B 77, 165415 2008]. The UPS measurements show a strong correlation of the quality and structure of the graphene films and a final state effect above vacuum level.

O 22.7 Tue 12:30 SCH 251

**Synthesis and characterization of graphite monolayers on Ni (111)- and polycrystalline Ni-surfaces** — KATHARINA KLOECKNER, ROLAND J. KOCH, SYED-IMAD U. AHMED, and ●JUERGEN A. SCHAEFER — Institut für Physik and Institut für Mikro- und Nanotechnologien, Technische Universität Ilmenau, P. O. Box 100565, 98684 Ilmenau, Germany

To understand the fundamental surface science related properties of two different substrate surfaces, Ni (111) and polycrystalline Ni, adsorption experiments of CO and propene (C<sub>3</sub>H<sub>6</sub>) are investigated. Since the adsorption of CO on metal surfaces has been studied very intensively in the past, a very thorough characterization of the different surfaces studied in this contribution is possible. Simultaneously, CO adsorption is a good reference for residual gas adsorption, which is dominated by CO. Propene has been chosen to study the catalytic dehydrogenation on nickel as well as graphene formation. Different stages of interaction were controlled via High Resolution Electron Energy Loss Spectroscopy (HREELS) and X-ray Photoelectron Spectroscopy (XPS).

O 22.8 Tue 12:45 SCH 251

**Electronic structure of the graphene twist bilayer** — ●SAM SHALLCROSS<sup>1</sup>, SANGEETA SHARMA<sup>2</sup>, and OLEG PANKRATOV<sup>1</sup> — <sup>1</sup>Lehrstuhl für Theoretische Festkörperphysik, Staudtstr. 7-B2, 91058 Erlangen — <sup>2</sup>Institut für Theoretische Physik, Freie Universität Berlin, Arnimallee 14, D-14195 Berlin, Germany

While the Bernal stacked AB graphene bilayer has received great attention, this represents only one degree of freedom between graphene layers, i.e., the translational degree of freedom. It has recently been realized that the rotational degree of freedom between such layers is in many instances of great importance, e.g. in explaining the single layer graphene type behaviour for graphene layers grown on the C-face of SiC [1,2]. We shall explore this degree of freedom between graphene layers via the simple prototype of the "graphene twist bilayer". This analysis, based on a simple application of Diophantine algebra, leads to the conclusion that such systems may either (i) become *completely* electronically decoupled for some  $\theta < \theta_0$ , or, (ii) decouple only in *specific regions* of the Brillouin zone. Using a standard tight-binding technique, we thoroughly explore the graphene twist bilayer, and establish that this system belongs to class (ii), and decouples only in the vicinity of the Dirac point, but that this decoupling occurs for all rotation angles. We consider the small angle limit and show that in this limit the Dirac spectrum has a considerably damped Fermi velocity, and exists only in a much reduced energy window.

[1] J. Hass et al., Phys. Rev. Lett., 100:125504, 2008. [2] S. Shallcross, S. Sharma, and O. A. Pankratov, Phys. Rev. Lett., 101:056803, 2008.

## O 23: Invited Talk (Jörg Schäfer)

Time: Tuesday 14:00–14:45

Location: HSZ 02

### Invited Talk

O 23.1 Tue 14:00 HSZ 02

**Surfaces and Atomic Nanostructures - Model Systems for Spectroscopy of Confined Interacting Electrons** — ●JÖRG SCHÄFER — Physikal. Institut, Universität Würzburg, Germany

Low-dimensional systems defined on surfaces and by self-organized nanostructures provide a new gateway to study electronic interactions. This intimately pertains to quasiparticles intertwined with elementary excitations, the role of confined electron systems and touches the regime of non-Fermi liquid physics. Quasiparticle dynamics can be detected directly in photoemission spectra. In the last years, this method has been extended beyond phonons to include coupling to spin exci-

tations. Regarding dimensional confinement, one-dimensional (1D) systems may be susceptible to charge density waves with energy gaps. Yet less known effects such as fluctuations and unusual many-body states can also be unveiled.

Very recently, self-organized atomic nanowires have been identified where the 1D confinement reaches its ultimate limit [1, 2]. We will review the unique properties of such chains grown on semiconductor templates. In novel Au-induced chains, tunneling data reveal that metallic charge is delocalized in 1D direction. Yet laterally it is confined to atomic dimensions, thereby establishing a 1D electron liquid as not reported before [2]. The talk presents an overview of the

state-of-the-art of spectroscopy on surface electron systems, including a perspective for exotic physics.

- [1] A. A. Stekolnikov *et al.*, PRL **100**, 196101 (2008).  
 [2] J. Schäfer *et al.*, PRL **101**, in press (2008), Editors' Suggestion.

## O 24: Methods: Molecular simulations and statistical mechanics

Time: Tuesday 15:00–16:15

Location: SCH A01

O 24.1 Tue 15:00 SCH A01

**Optimal Control of Dissipative Wave Packet Dynamics** — ●ERIK ASPLUND and THORSTEN KLÜNER — Institut für Reine und Angewandte Chemie, Carl von Ossietzky Universität Oldenburg, Germany

Light interacting with atoms and molecules is not only a source of information about the atoms and molecules studied, it can also initiate charge and energy transfer processes, i.e. chemical reactions. If excitation, excited state dynamics and relaxation all happen on the same time scale, a theoretical approach is required, which allows for a faithful description not relying on a separation of time scales. This can be done within the framework of the Surrogate Hamiltonian approach [1]. In this approach, a quantum system is separated into a primary system and a bath. The primary system is then explicitly immersed in the bath which acts as a dissipative environment. A theoretical tool for the design of laser pulses to transfer an initial state to a final state is optimal control theory (OCT) [2]. Besides the traditional final-time control algorithms, there exist methods to also handle time-dependent control targets [3,4]. To gain control of a dissipative system, time-dependent OCT is combined with the Surrogate Hamiltonian method. It is shown that an effective control of a dissipative system is possible.

References: [1] Roi Baer, and Ronnie Kosloff, J. Chem. Phys. **106**, 8862 (1997). [2] Wusheng Zhu, Jair Botina, and Herschel Rabitz, J. Chem. Phys. **108**, 1953 (1997). [3] Yukiyoishi Ohtsuki, Gabriel Turinici, and Herschel Rabitz, J. Chem. Phys. **120**, 5509 (2004). [4] I. Serban, J. Werschnik, and E. K. U. Gross, Phys. Rev. A **71**, 053810 (2005).

O 24.2 Tue 15:15 SCH A01

**First-principles study of the vibrational relaxation of the H stretching on Ge(100): Isotope effects** — ●SUNG SAKONG and PETER KRATZER — Fachbereich Physik, Universität Duisburg-Essen, Duisburg, Germany

The vibrational energy of covalently bonded adsorbates is dissipated to several smaller energy quanta (adsorbate vibrations and phonons) on semiconductor surfaces, when the vibrational energy is smaller than the gap. Then, electronic dissipation is precluded and the relaxation proceeds through slower channels of the coupling between vibrations and vibration-phonon interaction. Within the weak vibration-phonon coupling regime, this slow relaxation process can be described by the first-order perturbation theory using a potential energy surface obtained from first-principles calculations (J. Chem. Phys. **129**, 174702 (2008)). Using this framework, we analyze the vibrational relaxation of the H-Ge stretching on Ge(100) surface. Because of the small energy of Ge phonons, the downward transitions from the H stretch mode require at least two phonons to satisfy energy conservation. Most interestingly, the relaxation of the H stretching becomes up to five times faster at a heterogeneously saturated dimer using H and D, as observed in SFG experiments. The weak interaction between H and D within a dimer opens relaxation channels that require only one phonon for the transition instead of two phonons. Transitions mediated by fewer phonons corresponds to lower order expansion terms of the vibrational potential, thus these channels systematically make a larger contributions to the relaxation process and lead to a faster vibrational lifetime.

O 24.3 Tue 15:30 SCH A01

**Correlation energy of two-dimensional systems: toward non-empirical and universal modeling** — ●S. PITTALIS<sup>1,3</sup>, E. RASANEN<sup>2,3</sup>, C. PROETTO<sup>1,3</sup>, and E.K.U. GROSS<sup>1,3</sup> — <sup>1</sup>Institut fuer Theoretische Physik, Freie Universitaet Berlin, Arnimallee 14, D-14195 Berlin, Germany — <sup>2</sup>Nanoscience Center, Department of Physics, Uni-

versity of Jyväskylä, FIN-40014 Jyväskylä, Finland — <sup>3</sup>European Theoretical Spectroscopy Facility (ETSF)

The capability of density-functional theory to deal with the ground-state of correlated systems depends on the accuracy of functionals developed for the exchange and correlation energies. Most of the approximations developed so far have focused on three-dimensional systems. Such efforts for two-dimensional (2D) systems have been relatively scarce despite the rapidly increasing experimental and theoretical interest in 2D structures such as semiconductor heterostructures, quantum-Hall systems, graphene, and various types of quantum dots. Here we derive a correlation-energy functional for 2D systems by modeling the correlation-hole functions in such a way that they satisfy a set of exact properties. We find very encouraging results for a wide range of correlation energies covering several few-electron quantum dots with and without external magnetic field, having different spin-polarizations and current densities.

O 24.4 Tue 15:45 SCH A01

**Cluster expansion formalism for adsorbate-induced surface segregation** — ●TOBIAS KERSCHER and STEFAN MÜLLER — Universität Erlangen-Nürnberg, Lehrstuhl für Theoretische Physik 2, Staudtstr. 7, D-91058 Erlangen

The segregation profile of alloy surfaces can strongly depend on the presence of adsorbates. We present the development of a model cluster expansion in the framework of the computer code UNCLE [1] to address adsorption on binary alloy surfaces. In principle, we realize this by the combination of two binary cluster expansions: both occupied and unoccupied adsorbate sites as well as the individual chemical species of the alloy are considered. Density functional calculations provide the energetics for the construction of the position-dependent interactions. Supported by Deutsche Forschungsgemeinschaft

- [1] D. Lerch *et al.*, to be submitted to Mod. Simul. Mater. Sci. Eng.  
 [2] S. Müller *et al.*, Appl. Phys. A. **82**, 415 (2006).

O 24.5 Tue 16:00 SCH A01

**Liquid drop plus shell corrections model for deformed atomic cluster on the surface** — ●VERONIKA DICK<sup>1</sup>, DORIN POENARU<sup>1,2</sup>, RADU GHERGHESCU<sup>1,2</sup>, ILEANA PLONSKI<sup>1,2</sup>, ANDREY LYALIN<sup>1</sup>, ANDREY SOLOV'YOV<sup>1</sup>, and WALTER GREINER<sup>1</sup> — <sup>1</sup>Frankfurt Institute for Advanced Studies (FIAS), J.W. Goethe Universität, Ruth-Moufang-Str. 1, 60438 Frankfurt am Main, Germany — <sup>2</sup>Horia Hulubei National Institute of Physics and Nuclear Engineering (IFIN-HH), PO Box MG-6, 077125 Bucharest-Magurele, Romania

In the present work we adapt a simple liquid drop model (LDM) for description of stability and shape deformation of atomic clusters deposited on a surface. We investigate the role of cluster-surface interaction in the plastic deformation of the clusters deposited on a surface. We present the atomic cluster on the substrate like an oblate spheroidal cap. Analytical relationships for the deformation-dependent liquid drop model energies of oblate, prolate semi-spheroidal atomic clusters and oblate spheroidal cap have been obtained.

A superdeformed prolate hemispheroid is the most stable hemispheroidal shape within LDM. It is also the shape with maximum degeneracy of quantum states of the hemispheroidal harmonic oscillator used to compute the shell and pairing corrections. The microscopic corrections as well as total deformation energy show parabolic valley and ridges of the potential energy surfaces in the plane (deformation, number of atoms). The ground state and isomeric state deformation of clusters of various sizes depends on the interplay between the minima of LDM and shell correction energies.

## O 25: Surfaces and films: forces, structure and manipulation

Time: Tuesday 15:00–16:15

Location: SCH A118

O 25.1 Tue 15:00 SCH A118

**Understanding surface energies of transition metals with density-functional theory** — ●ALOYSIUS SOON, MARTIN FUCHS, and MATTHIAS SCHEFFLER — Fritz-Haber-Institut der MPG, Berlin, Germany

Determining index-specific surface energies of metals is, to date, still a non-trivial task, both experimentally and theoretically. Density-functional theory (DFT) calculations within the local-density approximation (LDA) for exchange-correlation (XC) have provided understanding of qualitative trends. Yet, absolute surface energies, in particular of *d*-metals still exhibit significant uncertainties related to the description of XC: gradient corrected functionals (GGA) which improve over the LDA for other properties often predict less accurate surface energies. This calls for a careful (re-)analysis of XC effects on surface energies, including non-local exchange and/or correlation.

Here we analyze the surface energies of 4*d*-metals with modern GGA functionals (PBEsol, AM05, developed to better describe bulk solids and (jellium) surfaces than the LDA and previous GGAs), using the all-electron FHI-aims code.<sup>1</sup> Relating the bulk cohesive energy and surface energy via a bond-cutting model we find that the modern GGAs can indeed correct the poorer results of the usual PBE-GGA but worsen the bulk cohesive energies of 4*d*-metals. In addition, we consider hybrid XC functionals (B3LYP, PBE0, and HSE03), using a cluster correction scheme,<sup>2</sup> and discuss the effects of including exact exchange on the calculated surface energies. 1. <http://www.fhi-berlin.mpg.de/aims/>; 2. Q.-M. Hu *et al.*, Phys. Rev. Lett. **98**, 176103 (2007); **99**, 169903(E).

O 25.2 Tue 15:15 SCH A118

**Energetics, electronic structure, and packing density of the Ir, Pt, and Au(100) surface reconstructions by all-electron DFT** — ●PAULA HAVU<sup>1</sup>, VILLE HAVU<sup>1</sup>, PATRICK RINKE<sup>1,2</sup>, VOLKER BLUM<sup>1</sup>, and MATTHIAS SCHEFFLER<sup>1,2</sup> — <sup>1</sup>Fritz-Haber-Institut der Max-Planck-Gesellschaft, D-14195 Berlin, Germany — <sup>2</sup>University of California at Santa Barbara, CA 93106, USA

Among fcc metals, only the late-5*d* transition metals Ir, Pt, and Au rearrange by quasihexagonal reconstructions on the nominally quadratic (100) surface structure. However, Ir reconstructs in one direction only [(5×1)], while Au(100) and Pt(100) rearrange in *both* lateral directions with large unit cells, often characterized as (5×*N*) (*N* ≥ 20 in the experimental literature). Elucidating the exact packing density and energetics have been the focus of many experiments, but theory has so far been relegated to either (5×1) approximants, or simplified empirical potentials. Using *N* = 1, 10, 15, 20, 25, 30 supercell models (up to 786 atoms/cell) and the FHI-aims code [1], we here show how all-electron density-functional theory (DFT) captures the energetics, electronic structure, and lateral packing densities of all three surfaces for different local-density and generalized gradient approximations. Remarkably, the effect of the 2D reconstruction [(5×*N*) instead of (5×1)] on the surface energy is nearly an order of magnitude bigger for Au than for Pt. DFT captures quantitatively the energetically rather subtle difference in packing densities, which is slightly higher for Au than Pt, consistent with experiment [2]. [1] V. Blum *et al.*, Comp. Phys. Comm., accepted (2008). [2] V. Jahns *et al.*, Surf. Sci. **430**, 55 (1999).

O 25.3 Tue 15:30 SCH A118

**Melting of two-dimensional adatom superlattices stabilized by long-range electronic interactions** — ●N. N. NEGULYAEV<sup>1</sup>, V. S. STEPANYUK<sup>2</sup>, L. NIEBERGALL<sup>2</sup>, P. BRUNO<sup>2,3</sup>, M. PIVETTA<sup>4</sup>, M. TERNES<sup>4,5</sup>, F. PATTHEY<sup>4</sup>, and W.-D. SCHNEIDER<sup>4</sup> — <sup>1</sup>Fachbereich Physik, Martin-Luther-Universität, D06099 Halle, Germany — <sup>2</sup>Max-Planck-Institut für Mikrostrukturphysik, D06120 Halle, Germany — <sup>3</sup>European Synchrotron Radiation Facility, F38043 Grenoble, France — <sup>4</sup>Ecole Polytechnique Federale de Lausanne, CH1015 Lausanne, Switzerland — <sup>5</sup>IBM Research Division, Almaden Research Center, San Jose, CA 95120, USA

According to the KTHNY theory [1], a true 2D solid melts to liquid

via intermediate phase, named hexatic.

Here we report on a combined experimental and theoretical study of the solid to liquid phase transition of 2D Ce adatom superlattices on Cu(111) and Ag(111) noble metal surfaces. Variable temperature STM measurements and DFT calculations elucidate the formation of the Ce superlattice, while kinetic Monte Carlo simulations describe the temperature dependent Ce adatom coordination within this 2D system [2]. Although the Ce superlattice is stabilized by long-range interactions mediated by surface-state electrons, the substrate atomic potential hinders the existence of the hexatic phase [2]. These results are in agreement with the melting behavior of a 2D lattice in the presence of a 'fine mesh' substrate potential [1].

[1] D.R. Nelson and B.I. Halperin, Phys. Rev. B **19**, 2457 (1979).

[2] N.N. Negulyaev *et al.*, Phys. Rev. Lett., submitted.

O 25.4 Tue 15:45 SCH A118

**Second order phase transition and critical fluctuations in a quasi-1D system: Br/Pt(110)** — ●MICHAEL CORDIN<sup>1</sup>, BARBARA LECHNER<sup>1</sup>, ALEXANDER MENZEL<sup>1</sup>, ERMALD BERTEL<sup>1</sup>, CESARE FRANCHINI<sup>2</sup>, RAINALDO ZUCCA<sup>2</sup>, and JOSEPH REDINGER<sup>2</sup> — <sup>1</sup>Institute for Physical Chemistry, University of Innsbruck, Austria — <sup>2</sup>Center for Computational Materials Science, Vienna University of Technology, Austria

Deposition of 0.5 monolayers (ML) of Bromine on Pt(110) results in a c(2x2)-Br/Pt(110) structure with almost perfect long-range order at 300 K. Upon cooling this structure to 50 K a reversible, apparent "inverse" order-disorder transition is observed. On a nearly defect-free surface the c(2x2) structure decays into striped c(2x2) and (2x1) domains. The resulting stripe pattern exhibits typical hallmarks of critical behaviour, i.e. a scale-free domains-in-domains structure. We therefore conclude that there is a continuous phase transition between the (2x1) and the c(2x2) structure and the disorder at 50 K is due to the proximity of the critical temperature. The conclusion is supported by DFT calculations, which place the (2x1) as the stable groundstate 17 meV below the c(2x2) structure (at 0 K). Even very small defect concentrations lead to the appearance of a third structural element at 50 K, namely a local (3x2) unit mesh[1]. Possible origins of the continuous phase transition will be discussed.

[1] E. Dona *et al.*, Phys. Rev. Lett. **98**, 186101 (2007).

O 25.5 Tue 16:00 SCH A118

**Surface reconstruction of clean bcc-Fe{110}: a quasi-hexagonal top-layer with periodic height modulation** — ●TOYO KAZU YAMADA<sup>1,2</sup>, HIDETOSHI TAMURA<sup>2</sup>, MOTOYUKI SHISHIDO<sup>2</sup>, TOSHIKAZU IRISAWA<sup>2</sup>, LUKAS GERHARD<sup>1</sup>, WULF WULFHEKEL<sup>1</sup>, and TADASHI MIZOGUCHI<sup>2</sup> — <sup>1</sup>Physikalisches Institut, Universität Karlsruhe, Wolfgang-Gaede-Straße 1, 76131 Karlsruhe, Germany — <sup>2</sup>Faculty of Science, Gakushuin University, 1-5-1 Mejiro, Toshima 171-8588, Tokyo, Japan

In general every surface has stress due to a symmetry break. When the stress overcomes the elastic limit, the surface reconstructs. There have been found surface reconstructions on only several metal surfaces. So far, no surface reconstruction was reported on the Fe surface. Iron is an important popular ferromagnetic metal which has been widely used since the ancient age in practical applications owing to its strength and abundance. We use Fe single crystals made by a chemical vapor deposition technique, which include no impurities in bulk and give us an extremely clean surface.

We found a new surface reconstruction on the {110} plane of bcc Fe-whisker single crystals. Atomically-resolved STM images showed a quasi-hexagonal atomic array with mesoscopic-range periodic height modulation of about 1/3 of an atomic step. This height modulation was found to be a result of an interference between the quasi-hexagonal top-layer and the sub-surface bcc-Fe{110} layer. Details of the atomic structure as well as local density of states of this new reconstruction are presented.

## O 26: Nanostructures at surfaces: Dots, particles, clusters II (SPM)

Time: Tuesday 15:00–16:45

Location: SCH A215

O 26.1 Tue 15:00 SCH A215

**Quantum well states in two-dimensional gold clusters** — XIAO LIN<sup>1</sup>, ●NIKLAS NILIUS<sup>1</sup>, HANS-JOACHIM FREUND<sup>1</sup>, MICHAEL WALTER<sup>2</sup>, PENTTI FRONDELIUS<sup>2</sup>, KAROLINA HONKALA<sup>2</sup>, and HANNU HÄKKINEN<sup>2</sup> — <sup>1</sup>Fritz-Haber Institut der MPG, D14195 Berlin, Germany — <sup>2</sup>Department of Physics, University of Jyväskylä, FI-40014 Finland

The electronic structure of ultra-small Au clusters on thin MgO/Ag(001) films is analyzed by scanning tunneling spectroscopy and density functional theory. The clusters exhibit two-dimensional quantum well states, whose shapes resemble the eigenstates of a 2D electron gas confined in a parabolic potential. From the HOMO and LUMO symmetries, the electron filling and charge state of particular clusters are determined. In accordance to a DFT charge-analysis, the aggregates accumulate a number of excess electrons due to charge transfer from the support. Monitoring the HOMO-LUMO gap as a function of cluster size, the transition from non-metallic to metallic Au behavior is deduced for clusters containing 70-100 atoms.

O 26.2 Tue 15:15 SCH A215

**Fluorescence Enhancement by Increase of Spontaneous Emission Rate between Two Metal Nanoparticles** — ●PHILLIP OLK<sup>1</sup>, THOMAS HÄRTLING<sup>1</sup>, MARC TOBIAS WENZEL<sup>1</sup>, PETRA MELA<sup>2</sup>, MARTIN MÖLLER<sup>2</sup>, and LUKAS M. ENG<sup>1</sup> — <sup>1</sup>Institut für angewandte Photophysik, TU Dresden, 01062 Dresden — <sup>2</sup>DWI an der RWTH Aachen e.V., 52056 Aachen

Small metal nanoparticles are known to be suitable for nano-optical experiments due to the enhanced electric fields in their very vicinity. We show here that coupling of very small gold particles of 12 nm in diameter to a 80 nm particle attached to a scanning fibre probe affects the fluorescence signal of a surrounding fluorescent immersion medium dramatically.

By comparison of our experimental result to calculations based on the multiple multipole method we exclude multiple causes for the increased fluorescence signal: locally enhanced fields of the excitation light, re-orientation of the fluorescent dipoles, enhanced scattering efficiencies, or an increase of the metal's auto-fluorescence can be ruled out. Instead, we ascribe the increased fluorescence signal to an influence of the nanoparticles on the *emission* behaviour of the dye.

O 26.3 Tue 15:30 SCH A215

**Finite size effects in isolated superconducting clusters of Pb-An STM study** — IVAN BRIHUEGA<sup>1</sup>, ●SANGITA BOSE<sup>1</sup>, MIGUEL MORENO UGEDA<sup>1,2</sup>, CHRISTIAN H. MICHAELIS<sup>1</sup>, and KLAUS KERN<sup>1,3</sup> — <sup>1</sup>Max-Planck-Institut für Festkörperforschung, Heisenbergstrasse 1, D-70569 Stuttgart, Germany — <sup>2</sup>Univ. Autonoma Madrid, Dept. Fis. Mat. Condensada, E-28049 Madrid, Spain. — <sup>3</sup>Institut de Physique des Nanostructures, Ecole Polytechnique Fédérale de Lausanne, CH-1015 Lausanne, Switzerland.

We report on the evolution of superconductivity in isolated Pb nanoparticles grown in situ probed by Scanning tunneling spectroscopy (STS). We observe a gradual decrease of the superconducting energy gap (D) with reduction in particle size which is accompanied by a simultaneous increase in the quasiparticle lifetime broadening (G). Superconductivity gets completely destroyed at small particle sizes which are consistent with the Anderson criterion. Our results also show that for these small particles the evolution of T<sub>c</sub> is mainly governed by the quantum size effects (QSE).

O 26.4 Tue 15:45 SCH A215

**Interaction of the STM tip with adatoms on metal surfaces:**

**ab initio study** — ●KUN TAO<sup>1</sup>, VALERI S STEPANYUK<sup>1</sup>, and PATRICK BRUNO<sup>2</sup> — <sup>1</sup>Max-Planck Institute of Microstructure Physics, Weinberg 2, 06120 Halle, Germany — <sup>2</sup>European Synchrotron Radiation Facility BP 220, F-38043 Grenoble Cedex, France

Using first-principles calculations based on the density functional theory, we investigate interaction of the STM tip with magnetic adatoms on metal surfaces. We perform calculations in the fully relaxed geometries for the tip and the substrate. Both interactions with nonmagnetic and magnetic tips are studied. We concentrate on 3d transition metal adatoms supported on Cu(001) and Cu(111) surfaces. The exchange interaction of the magnetic tip with 3d transition metal adatoms supported on Cu(001) surface is discussed. Our results indicate that the spin direction of the magnetic adatoms can be manipulated by approaching the tip to the substrate. The interplay between the structure relaxations and the electronic properties of the junction is revealed.

O 26.5 Tue 16:00 SCH A215

**Two level conductance fluctuations investigated with LT-STM** — ●ALEXANDER SPERL, JÖRG KRÖGER, and RICHARD BERNDT — Christian-Albrechts-Universität zu Kiel, D-24098 Kiel, Germany

Single silver atoms adsorbed on a Ag(111) surface were contacted with the tip of a cryogenic scanning tunneling microscope. At small tip-atom distances we observe fluctuations of the junction conductance between two levels. These two-level fluctuations depend on the applied voltage between tip and sample. An analysis of this behavior will be presented. Funding by the Deutsche Forschungsgemeinschaft through SPP 1153 is acknowledged.

O 26.6 Tue 16:15 SCH A215

**Linewidth of a Cesium Adatom Resonance on Ag(111)** — ●MARTIN ZIEGLER<sup>1</sup>, JÖRG KRÖGER<sup>1</sup>, RICHARD BERNDT<sup>1</sup>, ANDREI BORISOV<sup>2,3</sup>, and JEAN-PIERRE GAUYACQ<sup>2,3</sup> — <sup>1</sup>Christian-Albrechts-Universität zu Kiel, D-24098 Kiel, Germany — <sup>2</sup>CNRS, Laboratoire des Collisions Atomiques et Moléculaires, UMR 8625, Bâtiment 351, 91405 Orsay Cedex, France — <sup>3</sup>Université Paris-Sud, Laboratoire des Collisions Atomiques et Moléculaires, UMR 8625, Bâtiment 351, 91405 Orsay Cedex, France

Single Cs atoms adsorbed on Ag(111) induce a resonance appearing just below the threshold of the quasi-two-dimensional Shockley-type surface state continuum. Spectroscopic analysis using a cryogenic scanning tunneling microscope and theoretical modeling are used to identify the importance of the various contributions to the linewidth and to the decay of the resonance: resonant charge transfer, inelastic transitions, and adsorbate vibrations perpendicular to the surface. *Financial support by the Deutsche Forschungsgemeinschaft through SFB668 is acknowledged.*

O 26.7 Tue 16:30 SCH A215

**Local electronic properties of individual nanostructures on the boron nitride nanomesh** — ●CHRISTIAN H. MICHAELIS, SANGITA BOSE, IVAN BRIHUEGA, and KLAUS KERN — Max-Planck-Institut für Festkörperforschung, Heisenbergstraße 1, 70569 Stuttgart

We present the final development of a home-built sub-Kelvin STM which operates in ultra high vacuum conditions, is equipped with a 14 Tesla magnet and has a base temperature of 0.9 K. We have used this low temperature STM for the spectroscopic study of isolated nanostructures and molecules on top of a boron nitride ultrathin insulating spacer on Rh(111). This combination offers the unique possibility of investigating the local electronic properties of atomic-scale structures with ultimate energy resolution. As examples we will discuss magnetic and superconducting metal clusters and functional organic molecules.

**O 27: Poster Session I (Methods: Scanning probe techniques; Methods: Atomic and electronic structure; Methods: Molecular simulations and statistical mechanics; Oxides and Insulators: Clean surfaces; Oxides and Insulators: Adsorption; Oxides and Insulators: Epitaxy and growth; Semiconductor substrates: Clean surfaces; Semiconductor substrates: Epitaxy and growth; Semiconductor substrates: Adsorption; Nano- optics of metallic and semiconducting nanostructures; Electronic structure; Methods: Electronic structure theory; Methods: other (experimental); Methods: other (theory); Solutions on surfaces; Epitaxial Graphene; Surface order interface magnetism; Phase transitions; Time-resolved spectroscopies)**

Time: Tuesday 18:30–21:00

Location: P2

O 27.1 Tue 18:30 P2

**Design of an XSTM head for low temperature high magnetic field studies of III-V heterostructures** — ●BRUNO CHILIAN, JENS WIEBE, and ROLAND WIESENDANGER — Institute of Applied Physics, University of Hamburg, Germany

With the ultimate goal of future spintronic applications, dilute magnetic semiconductors like Mn doped GaAs have been heavily studied because of the possibility to tune their magnetic properties and thereby control the charge carrier's spin degree of freedom. However, a detailed understanding of how the local moments of magnetic impurities couple has yet to be achieved.

One technique which combines the power of atomic scale characterization with the ability to probe deeply buried impurities in MBE grown samples is cross sectional scanning tunneling microscopy (XSTM). However, few instruments have demonstrated the ability to provide atomic scale spectroscopic capability of such systems with high energy resolution. Here, we describe a homebuilt STM head which can be utilized in UHV conditions in a 300mK 14T environment.

To be able to locate the MBE grown layer of interest on the cleaved wafer surface, our STM head is capable of coarse XY sample movement. Its small diameter fits into the narrow bore of the 14 T superconducting magnet in our 300 mK facility. While constituting one of the main design challenges, the compact build simultaneously ensures mechanical stability, thereby promoting low noise levels.

O 27.2 Tue 18:30 P2

**A STM with a scan width from 500 microns down to sub-nanometers** — ●FATIH KALKAN and KARINA MORGENSTERN — Institut für Festkörperphysik, Gottfried Wilhelm Leibniz Universität Hannover, Appelstr. 2, D-30167 Hannover, Germany

The scanning tunnelling microscope (STM) is a very powerful tool for exploring the atomic-scale realm of surfaces, and for investigating adsorbate-surface interactions. However, for imaging, e.g. of prestructured surfaces, it would be desirable to bridge the gap between optical spectroscopy and the usual STM scan width. We have constructed a room temperature STM, which has the special ability of scanning with two different scan widths from the optical region down to atomic resolution. We have realised it with two different stages: The first one is a commercial Piezo stage which gives us the possibility of scanning an area up to  $500 \times 500 \mu\text{m}^2$ . The second one is a custom-built beetle type STM which scans from several microns down to atomic resolution. This newly designed STM with its wide scan width will allow us to connect the results from atomic-sized structures to the large-scale environment for prestructured surfaces.

O 27.3 Tue 18:30 P2

**Characterization of Epitaxial Layers of Organic Molecules by Three-Dimensional Force- and Dissipation-Spectroscopy** — ●GERNOT LANGEWISCH, DANIEL BRAUN, HARALD FUCHS, and ANDRE SCHIRMEISEN — CeNTech (Center for Nanotechnology) and Institute of Physics, University of Münster, Germany

Thin films of  $\pi$ -conjugated organic molecules are of high relevance for organic semiconductor applications. A widely studied organic semiconductor is 3,4,9,10-perylenetetracarboxylic-dianhydride (PTCDA). We applied non-contact atomic force microscopy in ultrahigh vacuum to investigate PTCDA deposited on Ag(111) by molecular beam epitaxy. Single PTCDA-molecules, arranged in the herringbone structure, were resolved in the topography scans. By site-specific force and dissipation versus distance measurements three-dimensional maps of tip-sample forces and dissipation with submolecular resolution were obtained. These maps are interpreted with respect to mechanical relaxation processes of the individual molecules.

O 27.4 Tue 18:30 P2

**Controlled Atmosphere High Temperature SPM for electrochemical measurements** — ●NILS OHMER<sup>1</sup>, MOGENS MOGENSEN<sup>1</sup>, BJØRN JOHANSEN<sup>1</sup>, and TORBEN JACOBSEN<sup>2</sup> — <sup>1</sup>Fuel Cells and Solid State Chemistry Division, Risø National Laboratory for Sustainable Energy, DTU, DK-4000 Roskilde, Denmark. — <sup>2</sup>Department of Chemistry, Technical University of Denmark, DK-2800 Lyngby, Denmark.

The Controlled Atmosphere High Temperature Scanning Probe Microscope (CAHT-SPM) works in principle like a normal AFM, but makes it possible to take, additional to the topography images, electrical images at the same time and at temperatures of up to 800 °C in a controlled atmosphere. Furthermore it is possible to use the tip as a working electrode to perform electrochemical impedance measurements at selected points. This poster provides information about the set up of the CAHT-SPM, in-house-made probes for electrical measurements at high temperatures and some results of measurements at 650 °C.

O 27.5 Tue 18:30 P2

**Development of a combined AFM-STM for measurements under transport conditions and at low temperatures** — ●JAN RAPHAEL BINDEL, MARCUS LIEBMAN, and MARKUS MORGENSTERN — II. Physikalisches Institut B, RWTH Aachen and JARA-FIT, Otto-Blumenthal-Straße, 52074 Aachen

We present a microscope combining atomic force (AFM) and scanning tunneling microscopy (STM) capabilities using a tuning fork. The device allows the investigation of a sample by AFM and to take STM images on spots of interest.

To use the full scope of the microscope, it is equipped with an  $xy$  drive which has a traverse path of 2 mm x 2 mm. Furthermore, the microscope can operate in two different modes, the AFM-STM constellation which makes it possible to apply a gate voltage on the sample and the pure STM mode, in which four point transport measurements can be done simultaneously with scanning.

The whole concept allows the usage in ultra high vacuum (UHV), at low temperatures down to 300 mK and in magnetic fields up to 14 T. Therefore, it has a compact symmetric design with a diameter of only 30 mm, which guarantees stability and high resonance frequencies. First test measurements of the microscope are presented.

O 27.6 Tue 18:30 P2

**Force-field spectroscopy on KBr(001): Experiment and simulation** — ●KAI RUSCHMEIER<sup>1</sup>, ANDRÉ SCHIRMEISEN<sup>1</sup>, and REGINA HOFFMANN<sup>2</sup> — <sup>1</sup>Physikalisches Institut, Westfälische Wilhelms-Universität Münster and Center for Nanotechnology (CeNTech), 48149 Münster, Germany — <sup>2</sup>Physikalisches Institut and DFG-Center for Functional Nanostructures, Universität Karlsruhe, 76128 Karlsruhe, Germany

An atomic force microscope (AFM) is capable of imaging the surface of insulating samples with atomic precision by scanning an atomically sharp tip over the surface. Furthermore, the force field representing the spatial orientation and magnitude of the force acting between the AFM probe and the sample surface can be measured by force field spectroscopy. These measurements depend on the respective sample atoms but also crucially on the particular tip structure and material.

We compare force field measurements on KBr(001) at room temperature with atomistic simulations for two individual tip configurations, a  $\text{K}^+$ - and a  $\text{Br}^-$ -terminated tip, assuming that the tip was contaminated with sample material during the experiments [1]. The 2-dimensional force fields were obtained at two different sample positions: along the corrugation maxima and almost halfway between the

corrugation maxima and minima. We find good agreement between our measurements and simulations for the  $K^+$ -terminated tip for both sample positions confirming a previous analysis [2].

- [1] R. Hoffmann *et al.*, Phys. Rev. Lett. **92**, 146103 (2004).  
 [2] K. Ruschmeier *et al.*, Phys. Rev. Lett. **101**, 156102 (2008).

O 27.7 Tue 18:30 P2

**Indium microsoldering of graphene on silicon dioxide substrate** — ●ANN-KATRIN MICHEL<sup>1</sup>, VIKTOR GERINGER<sup>1</sup>, TIM ECHTERMEYER<sup>2</sup>, MARCUS LIEBMANN<sup>1</sup>, and MARKUS MORGENSTERN<sup>1</sup> — <sup>1</sup>II. Physikalisches Institut, RWTH Aachen and JARA-FIT, Otto-Blumenthal-Straße, 52074 Aachen — <sup>2</sup>Advanced Microelectronic Center Aachen (AMICA), Otto-Blumenthal-Straße 25, 52074 Aachen

Electron beam lithography is the standard method to produce electrical contacts for nanostructures made e.g. from graphene. A major disadvantage of this method is, apart from high costs, the contamination of the sample due to the residual photoresist. This problem gets even more severe, if scanning probe techniques are applied. Therefore, a more simple technique to make ohmic contacts to graphene without contamination is desirable and has been developed recently [1].

We reproduced this method by designing a setup for microsoldering of graphene flakes on silicon dioxide with multiple indium solder contacts. Mobility measurements on graphene samples using four point indium contacts have been used to characterize the contacts. Moreover, we describe the application to scanning tunneling microscopy (STM) of the microsoldered graphene samples.

- [1] C. Ö. Girit and A. Zettl, Appl. Phys. Lett. **91**, 193512 (2007)

O 27.8 Tue 18:30 P2

**Controlled nanoparticle manipulation along defined vector pathways** — ●MICHAEL FELDMANN, DIRK DIETZEL, and ANDRÉ SCHIRMEISEN — Institute of Physics and Center for Nanotechnology, University of Münster, Germany

Manipulation of nanoparticles with an atomic force microscope (AFM) is a very promising approach to measure friction of nanoscale objects with well defined contact area. For example, the phenomenon of frictional duality was revealed for Sb nanoparticles on graphite in vacuum [1]. However, so far the manipulation was performed during conventional image scanning with a commercial AFM control unit [2]. To optimize the control over the manipulation process a new AFM control system has been developed. This system enables AFM tip translations along arbitrary programmable vector pathways while allowing to select distinct control parameters like normal force and velocity for each single vector. Due to the systems ability to simultaneously record the lateral force along the x axis, it is thus possible to conduct nanotribological experiments with individually chosen nanoparticles in a highly controlled and reproducible fashion.

- [1] Dietzel *et al.*, Phys. Rev. Lett., **101**, 125505 (2008)  
 [2] Dietzel *et al.*, J. Appl. Phys., **102**, 84306 (2007)

O 27.9 Tue 18:30 P2

**Nanoscale charge transport measurements using a multi-tip scanning tunneling microscope** — PHILIPP JASCHINSKY, JAKOB WENSORRA, MIHAIL ION LEPSA, and ●BERT VOIGTLÄNDER — Institute of Bio- und Nanosystems (IBN) and JARA-Fundamentals of Future Information Technology, Forschungszentrum Jülich, D-52425 Jülich, Germany

We demonstrate the ability of a multi-tip scanning tunneling microscope (STM) combined with a scanning electron microscope (SEM) to perform charge transport measurements on the nanoscale. The STM tips serve as electric probes that can be precisely positioned relative to the surface nanostructures using the SEM control and the height reference provided by the tunneling contact. The tips work in contact, noncontact, and tunneling modes. We present vertical transport measurements on nanosized GaAs/AlAs resonant tunneling diodes and lateral transport measurements on the conductive surface of 7x7 reconstructed Si(111). The high stability of the double-tip STM allows nondestructive electrical contacts to surfaces via the tunneling gaps. We performed two-point electrical measurements via tunneling contacts on the Si(111)(7x7) surface and evaluated them using a model for the charge transport on this surface.

O 27.10 Tue 18:30 P2

**s-SNOM from IR to the THz with tuned scatterers** — ●HANS-GEORG VON RIBBECK<sup>1,2</sup>, MARC TOBIAS WENZEL<sup>1</sup>, and LUKAS MATTHIAS ENG<sup>1</sup> — <sup>1</sup>Institute of applied photo physics, TU Dresden, Germany — <sup>2</sup>Forschungszentrum Dresden-Rossendorf, Dresden, Ger-

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Here we present a scattering near-field optical microscope (s-SNOM) set-up established at the free-electron laser source (FEL) at the Forschungszentrum Dresden-Rossendorf. This microscope is capable to perform optical observations at nanometer scale resolution over the full wavelength range of the FEL, i.e. 3 to 250 micron (1.2 to 100 THz). Furthermore, the optical resolution governed by the near-field interaction between tip and sample and the signal-to-noise ratio is enhanced by specially designed, optically resonant probes. This ultimately results in a much better spatial confinement achieving a resolution preferably of  $\lambda/1000$  for the THz region. Also, coupling both a resonant tip and sample will lead to giant polaritonic resonances. Finally the described setup will grant access to new areas of nanoscale applications, such as observing the optical behavior of strained and mixed silicon structures, high-Tc superconductors, single quantum dots, and superlattices at THz frequencies.

Basis to our approach is the recent work [1] where an optical confinement of the near field in z-direction was achieved through tuned scatterers in the form of metallic nanoparticles (MNPs) attached to the AFM tip, serving as non-resonant antennas. Tunability in the THz range will be achieved through geometrically tuned metal wires [2].

O 27.11 Tue 18:30 P2

**High Order Field Emission Resonances on W(110) and Fe/W(110) studied by Scanning Tunneling Spectroscopy** — ●ANIKA EMMENEGGER, STEFAN KRAUSE, ANDRÉ KUBETZKA, GABRIELA HERZOG, and ROLAND WIESENDANGER — Institute of Applied Physics, University of Hamburg, Jungiusstr. 11, 20355 Hamburg, Germany

Above metal surfaces a Rydberg-like series of states exists close to the vacuum level due to the potential well created by the attractive image potential and the surface projected bulk band gap [1]. In scanning tunneling microscopy (STM) experiments these so-called image-potential states (IPS) experience a Stark Shift [2], hence they are often called field emission resonances in this context.

Neglecting the influence of the image potential, a simple triangular potential model can be applied to determine the effective electric field in the constant current spectroscopy of IPS [3]. Whereas commercial STM electronics typically provide a maximum gap voltage of 10 V, we present scanning tunneling spectra of field emission resonances above the W(110) and Fe/W(110) surface up to the order of  $n=30$  and voltages up to 20 V. The results will be discussed in terms of electric field determination, revealing that the assumption of a constant electric field is only applicable to voltages exceeding 10 V.

- [1] U. Thomann *et al.*, Phys. Rev. B **61**, 16163 (2000).  
 [2] S. Crampin, Phys. Rev. Lett. **95**, 46801 (2005).  
 [3] J. H. Coombs and J. K. Gimzewski, J. of Microsc. **125**, 841 (1988).

O 27.12 Tue 18:30 P2

**Microscopically high speed friction measurements** — ●FENGZHEN ZHANG<sup>1</sup>, OTHMAR MARTI<sup>1</sup>, STEFAN WALHEIM<sup>2</sup>, and THOMAS SCHIMMEL<sup>2,3</sup> — <sup>1</sup>Institute of Experimental Physics, Ulm University, 89069 Ulm — <sup>2</sup>Forschungszentrum Karlsruhe — <sup>3</sup>University of Karlsruhe

Quartz crystals have been found to be the best substrates for the Atomic Force Microscopy (AFM) high speed friction measurements. To prove the oscillation of the quartz crystals, we prepared Fischer Patterns on the surface. During the oscillation of the quartz crystals, the topographies of the Fischer Pattern show clearly the oscillation information (in tapping mode AFM). The result of the comparison of the friction under different oscillation speeds and after oscillation will be discussed. We will also present the measurement data of friction at high speeds of surfaces without and with adsorbed monolayers.

O 27.13 Tue 18:30 P2

**Non-contact Atomic Force Spectroscopy using Field Ion Microscope characterized Tips** — ●JENS FALTER<sup>1</sup>, DANIEL-ALEXANDER BRAUN<sup>1,2</sup>, UDO SCHWARZ<sup>4</sup>, HENDRIK HÖLSCHER<sup>3</sup>, ANDRÉ SCHIRMEISEN<sup>1,2</sup>, and HARALD FUCHS<sup>1,2</sup> — <sup>1</sup>Physikalisches Institut, Universität Münster, Germany — <sup>2</sup>CeNTech, Münster, Germany — <sup>3</sup>IMT, Forschungszentrum Karlsruhe, Germany — <sup>4</sup>Department of Mechanical Engineering, Yale University, New Haven, USA

Although atomic force microscopy (AFM) is a tool for resolving surfaces with atomic resolution, the underlying contrast mechanisms is not yet fully understood. Beyond imaging this technique is capable

to measure the interaction potential of tip and sample atoms in force spectroscopy experiments. What remains completely unknown is the atomic scale configuration of the tip. One method which allows determining the configuration of the probing tip apex with atomic precision is the field ion microscope (FIM). We present a home-built ultrahigh vacuum system, which combines these two microscopy techniques. The AFM head [1] is capable to operate at liquid helium temperatures and the force sensor is based on a tuning fork system [2]. The tuning fork concept allows to chose a material for the tip, which is suitable for FIM operation. A home build tip-holder is used for the in-situ tip exchange between the two microscopes. First results of both microscopy methods correlate the force spectroscopy curves from the AFM with the tip apex radii obtained from the FIM analysis.

[1] B. Albers et al., Rev. Sci Instrum. 79 033704 (2008)

[2] F.J. Giessibl, Appl. Phys. Lett. 76 1470 (2000)

O 27.14 Tue 18:30 P2

**Scanning Tunneling Spectroscopy at the [110]-[1 $\bar{1}$ 0] Cleaved Edge of GaAs** — S. SIEWERS, M. WENDEROTH, L. WINKING, P. KLOTH, and R. G. ULBRICH — IV. Phys. Inst. Georg-August-Universität Göttingen

We report the first cross-sectional scanning tunneling spectroscopy (STS) study of zincblende [110]-[1 $\bar{1}$ 0] cleaved edges with atomic resolution. The samples were prepared in-situ by a double cleavage procedure applied to  $6 \cdot 10^{18} \text{ cm}^{-3}$  Si-doped GaAs in UHV. In edge-approaching scans and for positive sample bias we observed a monotonically decreasing tunnel current within a few tens of nm from the edge. For negative bias we found the onset of this decrease within a few nm from the edge, followed by a considerable increase directly at the edge. Comparing these observations with scans over charged defects embedded in plane surfaces, we conclude that the edge contains a negative line charge density. The data suggests that the observed effect is not simply caused by tip-induced band bending and screening of bulk states confined within the  $90^\circ$ -edge geometry. Spectroscopic measurements on edges support the concept of a negatively charged quasi-1d electronic state localized along the edge. It is laterally confined within  $\sim 2$  lattice constants and is clearly observed in the local density of states derived from the STS data. To estimate the absolute value of its charge density we simulated the shape and spatial extension of the screening cloud of a negative line charge located at the center of the "quarter-space" geometry. By adjusting this potential to the spectroscopic data we find a line charge density of  $\sim 0.7$  electrons per unit cell.

O 27.15 Tue 18:30 P2

**Frictional properties of a mesoscopic contact with engineered surface roughness** — JOHANNES SONDHAUSS<sup>1</sup>, HARALD FUCHS<sup>1,2</sup>, and ANDRÉ SCHIRMEISEN<sup>1,2</sup> — <sup>1</sup>Institute of Physics, University of Münster, Münster, Germany — <sup>2</sup>Center for Nanotechnology (CeN-Tech), University of Münster, Münster, Germany

Friction force microscopy (FFM) is a standard tool to measure friction down to atomic scales. In this work, we use FFM to investigate the influence of interface roughness of mesoscopic contacts on friction, where both sliding partners, tip and sample, have precisely engineered properties. We use a focused ion beam (FIB) to modify commercial cantilevers in order to firmly attach spherical titanium particles with diameters between 4 and 15  $\mu\text{m}$ . As sample we produce groove-like patterns on a silicon surface with the FIB with a lattice periodicity ranging from 1 to 9  $\mu\text{m}$  and a depth of 25 nm. The average friction force was measured systematically for different tip radii as a function of load and lattice periodicity of the sample grooves. For the 5  $\mu\text{m}$  tip the maximum friction force was found where the geometry of the spherical tip and the lattice are commensurate. These findings highlight the importance of surface structure on tribological properties of mesoscale contacts.

O 27.16 Tue 18:30 P2

**SFM manipulation techniques applied to graphene** — STEFAN EILERS, TOBIAS LIEBIG, and JÜRGEN P. RABE — Humboldt-Universität zu Berlin

The properties of graphene render it a promising candidate for future generation electronic devices. For the investigation of properties and possible applications or devices structuring and manipulation techniques are needed. Thinness, flexibility and flatness make it possible to apply SFM techniques to single or multilayer graphene well known from using with molecules on graphite. Here, some effects produced by a SFM tip are demonstrated. First, manipulation of graphene itself is shown, in detail sawing were a gap and a nanoribbon is produced and

manipulating parts of graphene without destruction. In both cases the manipulation is started on SiO<sub>2</sub> substrate and kept in contact with it while moving the SFM tip. It appears that the graphene can only be desorbed and turned when the manipulation is done near an edge of graphene or when the graphene piece is small enough because there the adsorption force between graphene and the substrate is smaller than the force to break the bonds in graphene. Second, adsorption and manipulation of DNA on an amphiphile interlayer is presented. The interlayer is needed to make sure that the DNA is mobile enough to be manipulated. It appears that a force can be found large enough to manipulate DNA but to small to damage the graphene.

O 27.17 Tue 18:30 P2

**Development of a Scanning Tunneling Microscope for measurements below 100mK** — MAXIMILIAN ASSIG, FABIAN ZINSER, WOLFGANG STIEPANY, ANDREAS KOCH, PETER ANDLER, 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 setups and measurement techniques, which can break through instrumental limitations and open new areas in measurement accuracy. Scanning Tunneling Microscopy (STM) is a technique for probing the electronic structure of single adsorbed atoms and nanostructures at surfaces with atomic resolution. As the energy resolution increases with decreasing temperature, cooling the STM below 100mK results in an energy resolution which is better than  $24\mu\text{eV}$ . To achieve this goal, we want to connect a home-built STM to the mixing chamber of a custom-designed bottom-loading dilution cryostat. Tip and sample can be transferred directly from the preparation chamber into the STM without breaking the ultra high vacuum (UHV), which allows *in situ* sample preparation. Measurements can be performed in high magnetic fields of 14T perpendicular and 500mT parallel to the sample surface. We present design and concept of the STM as well as milestones in the project realization.

O 27.18 Tue 18:30 P2

**Eddy current microscopy** — BENEDICT KLEINE BUSSMANN, TINO ROLL, MARION MEIER, and MARIKA SCHLEBERGER — Universität Duisburg-Essen, Fachbereich Physik, Lotharstrasse 1, D-47048, Germany

We present eddy current microscopy [1] measurements on geometrically confined conductive structures on insulating substrates. The principle of eddy current microscopy is as follows: A magnetic tip of an Atomic Force Microscope oscillates above a sample and induces eddy currents in the conducting areas of the sample due to the time-dependent magnetic field they are exposed to. This leads to an electromagnetic interaction between the sample and probe: Thus, according to Lenz's rule a damping of the oscillation occurs and leads to a contrast in the phase and/or dissipation signal [2,3]. By using the well established technique of AFM this method can thus be used to perform conductivity measurements on submicron scale without any need to contact the sample (like for example four-point-probe techniques). We will present measurements we recently performed under ambient conditions as well as in situ measurements.

[1] B. Hoffmann, R. Houbertz, and U. Hartmann, Appl. Phys. A: Mater. Sci. Process. 66, S409 \*1998\*.

[2] T. Roll, M. Meier, S. Akcöltekin, M. Klusmann, H. Lebius and M. Schleberger Conductive nanodots on the surface of irradiated CaF<sub>2</sub> phys. stat. sol. (RRL) 2, 209 (2008) [3] Tino Roll, Marion Meier, Ulrich Fischer and Marika Schleberger Distance dependence of the phase signal in eddy current microscopy Thin Solid Films 516, 8630 (2008)

O 27.19 Tue 18:30 P2

**Detecting resonant modes of plasmon-polaritons and phonon-polaritons using a NSThM** — DAVID HELLMANN, ACHIM KITTEL, and ULI F. WISCHNATH — EHF, Fak. V, Physik, Carl von Ossietzky Universität Oldenburg

With a Near-field Scanning Thermal Microscope (NSThM) the heat transfer between a sample and a probe can be measured [1,2]. The NSThM combines a STM tip with a coaxial thermocouple sensor and, thus, can collect data concerning the heat transfer a few nm above the scanned surface along with usual STM maps. Evanescent thermal radiation has been investigated recently by De Wilde et al. at larger sample-tip distances (200 nm to some  $\mu\text{m}$ ) [3]. The authors find resonant modes of surface plasmon-polaritons and phonon-polaritons on certain structures. Subject of this study are NSThM measurements on structures where such resonances can be expected. With the NSThM

it is possible to investigate the influence of those resonant modes on the heat transfer in the direct vicinity of the samples surface in the range from about 1 nm to a few tens of nanometers.

Literature [1] A. Kittel et al., PRL 95, 224301 (2005) [2] U. Wischnath, RSI 79, 073708 2008 [3] Y. De Wilde et al., Nature Vol 444, 7.12.2006, p.740-743

O 27.20 Tue 18:30 P2

**Near-field Scanning Thermal Microscope: From temperature to heat flow** — ●LUDWIG WORBES, ULI F. WISCHNATH, and ACHIM KITTEL — Universität Oldenburg EHF EPKOS

The Near-field Scanning Thermal Microscope (NSThM) developed in our group combines the function of a normal STM with the ability to use the scanning probe as a thermocouple temperature sensor [1].

By operating in UHV in our experiment the heat transfer mechanism is restricted to radiative transfer in contrast to other SThM devices. The radiative transfer is dominated by evanescent modes of the thermal electromagnetic field for small distances. The heat transfer mediated by these modes between sample and sensor has been calculated using different theoretical approaches.

In order to compare the theoretical predictions with the experiment, we need to know the relation between the measured thermovoltage and the heat flow. This is up to now done by calculating the thermal conductivity of the tip based on the geometry and material properties. Here we present a calibration procedure based on measuring the heat flow through a bridge structure, whose thermal conductivity is easier to quantify. We use the so called  $3\omega$  method, using the bridge as a heater and as a resistive temperature sensor at the same time.

[1] U. F. Wischnath, J. Welker, M. Munzel, and A. Kittel, Rev. Sci. Instrum. 79, 073708 (2008).

O 27.21 Tue 18:30 P2

**A Novel Scanning Tunneling Potentiometry Setup with Microvolt Resolution** — ●T. DRUGA<sup>1</sup>, M. WENDEROTH<sup>1</sup>, M. A. SCHNEIDER<sup>2</sup>, and R. G. ULBRICH<sup>1</sup> — <sup>1</sup>IV. Phys. Inst., Georg-August-Universität Göttingen — <sup>2</sup>Lehrstuhl für Festkörperphysik Univ. Erlangen-Nürnberg

In Scanning Tunneling Potentiometry (STP) the tunneling tip is used as a weakly coupled voltage probe to determine the spatial variation of the electrochemical potential due to a lateral surface current or temperature difference between tip and sample. We have developed a potentiometric technique based on a standard STM setup allowing to measure the local potential with  $\mu\text{V}$  and Angstrom resolution. Unlike recent implementations [1,2] that use alternating voltages as transport fields or for controlling the tip sample distance similar to the scheme suggested by Murali and Pohl [3] our STP method uses DC-voltages only. Hence it not only allows standard STS being conducted in parallel but also ensures correct assignment of the energy of tunneling electrons. Further advantages of our technique is that (i) the sample bias for the topography can be chosen independently from the potentiometry and (ii) the potential can be mapped simultaneously for reverse current directions. It has been implemented in both a room temperature and low temperature STM-setup. The performance is demonstrated by measuring local transport fields on  $\text{Si}(111)\sqrt{3} \times \sqrt{3}$ -Ag and thermovoltage maps on Ag(111). This work was supported by the DFG as part of SFB 602 Tp A7. [1] Rev. Sci. Int. 79, 083704 (2008) [2] Rev. Sci. Int. 79, 073904 (2008) [3] Appl. Phys. Lett. 48, 514 (1986)

O 27.22 Tue 18:30 P2

**Studies towards Tip Enhanced Raman Scattering with Scanning Capability** — ●SETH WHITE<sup>1,2</sup>, MORITZ BRENDEL<sup>1</sup>, PETER LEMMENS<sup>1</sup>, DIETRICH WULFERDING<sup>1</sup>, and VLADIMIR GNEZDILOV<sup>1,3</sup> — <sup>1</sup>IPKM, TU Braunschweig, Germany — <sup>2</sup>MPI-FKF, Stuttgart, Germany — <sup>3</sup>ILTP, Kharkov, Ukraine

Tip- and surface-enhanced Raman scattering methods combined with scanning probe microscopy should enable precision measurements on finely structured samples while simultaneously providing local topographical information. A single etched Au[1,2] nano-apex scanning tip could thus be used both for scanning probe investigation and micro-Raman signal enhancement in one instrument. Samples with molecular scale structuring such as impregnated nano-porous silica and alumina are of particular interest in our studies.

[1] Ren et al. (2004), Rev. of Sci. Inst. 75, 4, April 2004

[2] Anderson, Pike (2002), Rev. of Sci. Inst. 73, 3, March 2002

O 27.23 Tue 18:30 P2

**Mechanical and electronic characterization of individual single-walled carbon nanotubes by scanning probe microscopy** — ●MARTIN BOHRISCH, FLORIAN SZILLAT, PHILIPP ZEIGER-MANN, HANS KLEEMANN, and BERND SCHRÖTER — Universität Jena, Institut für Festkörperphysik, Max-Wien-Platz 1, 07743 Jena, Deutschland

The selective growth of carbon nanotubes with particular structural and electronic properties is a prerequisite to utilize them in electronic and sensor devices. Single-walled carbon nanotubes were grown by catalyst-assisted chemical vapor deposition on insulating substrates. A horizontal alignment in predefined directions has been achieved by a growth on single-crystalline substrates like sapphire. Scanning electron microscopy is used to observe the orientation of the nanotubes. The high purity of the nanotubes is demonstrated by x-ray photoelectron and raman spectroscopy. Scanning probe techniques are utilized to determine mechanical and electronic properties of individual carbon nanotubes. The influence of the substrate-nanotube interaction on the radial deformation of single-walled carbon nanotubes was examined by contact atomic force microscopy (AFM). Electrical measurements were done by conductive AFM.

O 27.24 Tue 18:30 P2

**New scan mode for the NSThM** — ●LARS HOELZEL, ULI F. WISCHNATH, and ACHIM KITTEL — Energy and Semiconductor Research Laboratory - University of Oldenburg

The near-field scanning thermal microscope (NSThM)[1] is able to measure the thermal flux between a sharp tip of a STM and a heated or cooled sample surface under ultra-high vacuum conditions. Hence, the main contribution is mediated by evanescent electro-magnetic fields. Up to now the heat flux was investigated in scanning tunnelling mode of the STM on which the NSThM is based on [2]. While the tunnelling current decays on a short length scale the heat flux decays on a roughly ten times larger length scale. First data achieved by a new scanning mode are presented in this contribution. This mode employs a control loop which keeps the heat current constant. Therefore, it is possible to investigate the influence of the surface morphology on the heat flux at larger distances.

[1] Uli F. Wischnath et al., Rev. Sci. Instrum. 79, 073708 (2008)

[2] Achim Kittel et al., Appl. Phys. Lett. 93, 193109 (2008)

O 27.25 Tue 18:30 P2

**Infrared antennas for near-field microscopy and enhanced near-field spectroscopy** — ●THOMAS TAUBNER<sup>1,2</sup>, MARK BRONGERSMA<sup>2</sup>, and JON SCHULLER<sup>2</sup> — <sup>1</sup>I. Physikalisches Institut, RWTH Aachen, Germany — <sup>2</sup>Department of Material Science, Stanford University, USA

Scattering-type near-field optical microscopy (s-SNOM) relies on the scattering of light at a sharp metallic tip to obtain images with a resolution independent of the wavelength. The use of infrared light enables the acquisition of spectroscopic information on a samples chemical, structural and electronic properties at nanoscale resolution. Currently, the main limitation of this technique comprises of the low signals that demand tunable laser sources and restrict the spectral range of operation.

We present new concepts to increase the sensitivity of IR near-field spectroscopy in order to apply s-SNOM over a broader spectral range in the mid-IR. We suggest to employ resonantly enhanced near-fields of metallic nanostructures: The optical properties of materials of such structures can be tuned by changing their size to create optical antennas that concentrate light into tiny, subwavelength volumes. Specifically, we investigate the antenna properties of modified, metal-coated AFM tips in order to enable high-resolution near-field microscopy with increased sensitivity. We also show that the near-field probing process can be enhanced by suitable substrates, increasing both signals and contrasts in infrared s-SNOM when probing thin sample layers.

O 27.26 Tue 18:30 P2

**Ab initio investigation of the  $\text{LiNbO}_3(0001)$  surface** — ●SIMONE SANNA<sup>1</sup>, ALEXANDER V. GAVRILENKO<sup>2</sup>, and WOLF GERO SCHMIDT<sup>1</sup> — <sup>1</sup>Lehrstuhl für Theoretische Physik, Universität Paderborn, 33095 Paderborn, Germany — <sup>2</sup>Norfolk State University, Center for Materials Research, 700 Park Avenue Norfolk, VA 23504 USA

Lithium niobate (LN) is frequently used for various (nonlinear) optical and acoustic applications. While traditional applications mainly exploit LN bulk properties, more recently the (microscopic) surface and interface properties of LN have become important (1). Therefore the

understanding and analysis of LN surfaces and interfaces is indispensable to optimise and fully implement LN based devices. Unfortunately up to date very little information is available about the LN surfaces and their structure on atomic level (2). We present here an *ab initio* simulation of ferroelectric LN (0001) surfaces with different stoichiometry based on density functional theory within the generalised gradient approximation. This approach was recently shown to yield reliable structures and energies for bulk LN both in its paraelectric and ferroelectric phase (3). We discuss the stability of a series of candidate structures with varying stoichiometry and surface reconstructions in dependence of the chemical environment. The effect of the dipole corrections and of the cell size on the total local potential and on the electronic and structural properties of the surfaces are shown in detail.

(1) G. Namkoong *et al.*, Appl. Phys. Lett. 87 (2005), 171107.  
 (2) S. V. Levchenko *et al.*, Phys. Rev. Lett. 100 (2008) 256101.  
 (3) W. G. Schmidt *et al.*, Phys. Rev. B 77 (2008), 035106.

O 27.27 Tue 18:30 P2

**Auger spectroscopy of the ion neutralization at epitaxial transition metal surfaces** — ●CHRISTIAN TUSCHE and JÜRGEN KIRSCHNER — MPI für Mikrostrukturphysik, D-06120 Halle, Germany

The neutralization of ground state  $\text{He}^+$  at a metal surface proceeds by Auger neutralization, emitting an Auger electron from the conduction band of the metal. In ion-neutralization-spectroscopy (INS), developed by Hagstrum [1], the distribution of emitted electrons is related to the surface density of states (DOS). In contrast,  $\text{He}^{++}$  neutralization starts with a double electron capture into the outer He-2s and -2p shells, forming double excited  $\text{He}^{**}$ . Subsequent auto-ionization (AI) emits a He-KLL Auger electron from the projectile.

We prepared clean surfaces of the transition metals Mn, Fe, and Ni by epitaxial growth on a W(110) substrate.  $\text{He}^+$  and  $\text{He}^{++}$  ions ( $E_{kin} \leq 30\text{eV}$ ) were scattered at the clean surface and after adsorption of sub-monolayers of carbon, oxygen, or caesium. INS provides detailed information on changes of the work-function and electronic structure. All adsorbates are found to reduce the number of electrons emitted close to the Fermi energy. In the  $\text{He}^{**}$  AI decay we observe a changed spectral weight of *triplet* and *singlet* terms with adsorbate coverage, like reported before by Busch *et al.* [2]. Our experiments give evidence that this can be related to the adsorbate induced changes in the DOS. We hope that our experiments will stimulate detailed theoretical studies of the electron transfer processes in ion-neutralization.

[1] Hagstrum: Phys. Rev. **150**, p. 495-515 (1966)

[2] Busch, Wethekam, Winter: : Phys. Rev. A **78**, 010901 (2008)

O 27.28 Tue 18:30 P2

**Ar gas discharge lamp with heated LiF window: A monochromatized light source for photoemission** — MICHAEL BUDKE, ●ALEXANDER WITTKOWSKI, and MARKUS DONATH — Westfälische Wilhelms-Universität Münster, 48149 Münster, Deutschland

We present a simple, inexpensive, and highly effective method for monochromatizing the vacuum ultraviolet light emitted from an Ar gas discharge for use, e.g., in photoemission experiments [1]. By using a slightly heated window of LiF acting as low-pass filter, the emission spectrum of the Ar gas discharge is reduced to the Ar line at 11.62 eV (106.7 nm). The performance of the low-pass filter is demonstrated by photoemission measurements on Cu(111). Furthermore, we compare our light source with an unmonochromatized He gas discharge, which represents the most widely used laboratory photon source in photoemission.

[1] M. Budke and M. Donath, Appl. Phys. Lett. 92, 231918 (2008)

O 27.29 Tue 18:30 P2

**High-resolution electron gun for inverse photoemission** — ●ANNA ZUMBÜLTE, THOMAS SAERBECK, and MARKUS DONATH — Physikalisches Institut, Westfälische Wilhelms-Universität Münster, 48149 Münster

Inverse photoemission (IPE) is an applied method to investigate the unoccupied part of the electronic structure above the Fermi level. The setup of such an experiment consists of an electron gun and a detection system for photons. A high energy and angle resolution is necessary for a k-resolved separation of as many electronic states as possible in the spectra. Therefore the improvement of the setup components is always an object. State-of-the-art setups achieve an energy resolution of about 150 meV and an angular resolution of  $2^\circ$ - $5^\circ$  [1].

We present a spin-polarized electron gun with comparable energy resolution and an improved angular resolution. It consists of a GaAs photoemitter combined with a toroidal  $90^\circ$  electrostatic deflector act-

ing as monochromator. With this we achieve an energy resolution of 150 meV to 250 meV, depending on the current. Measurements of the beam profile indicate a low divergence that can be verified by IPE spectra of Cu (111). Here, the intensity ratio between the two surface states observed at normal incidence is an indicator of the angular resolution. In our case, measurements show a divergence smaller than  $2^\circ$ .

[1] M. Budke *et al.*, Rev. Sci. Instrum. 78, 113909 (2007)

O 27.30 Tue 18:30 P2

**Simulation of photoelectron diffraction at high kinetic energies** — ●AIMO WINKELMANN<sup>1</sup>, CHARLES S. FADLEY<sup>2,3</sup>, and JAVIER GARCIA DE ABAJO<sup>4</sup> — <sup>1</sup>Max Planck Institut für Mikrostrukturphysik, Halle, Germany — <sup>2</sup>Department of Physics, University of California Davis, Davis, CA 95616, USA — <sup>3</sup>Materials Sciences Division, Lawrence Berkeley National Laboratory, Berkeley, CA 94720, USA — <sup>4</sup>Instituto de Optica – CSIC, Serrano 121, 28006 Madrid, Spain

The theoretical modelling of x-ray photoelectron diffraction (XPD) with hard x-ray excitation of up to 20 keV energy is discussed using the dynamical theory of electron diffraction [1]. Via calculations for diamond and silicon it is demonstrated that the dynamical theory explains available current data for kinetic energies around 1 keV very well. The XPD patterns for energies above about 1 keV are dominated by Kikuchi bands which are created by the dynamical scattering of electrons from lattice planes. The origin of the intensity distribution in such bands is discussed from the point of view of atomic positions in the unit cell. The profiles and positions of the element-specific photoelectron Kikuchi bands are found to be sensitive to lattice distortions and the position of impurities or dopants with respect to lattice sites. These results thus suggest several future uses of such hard XPD for studies of the bulk structure of complex materials. The dynamical calculations are compared to results from a cluster model that is more often used to describe lower-energy XPD.

[1] A. Winkelmann, C.S. Fadley, F.J. Garcia de Abajo  
 New J. Phys. **10** (2008) 113002

O 27.31 Tue 18:30 P2

**(SP)VLEED: A spin-polarized very-low-energy electron-diffraction experiment** — ●KATHRIN WULFF, ULRICH BURGBACHER, ANKE B. SCHMIDT, and MARKUS DONATH — Physikalisches Institut, Westfälische Wilhelms-Universität Münster

The shape of the surface-barrier potential at conductive surfaces dictates the appearance and spin dependence of surface states. Currently, parameterized polynomials are incorporated in theoretical calculations to connect the Coulomb-like asymptotic regime far from the surface to the bulk muffin-tin zero. In intensity versus energy profiles  $I(V)$  of elastically scattered electrons fine structures appear, which are sensitive to the shape of the surface-barrier potential [1]. So far, spin-polarized low-energy electron-diffraction measurements on W(100) have already shown a strong spin dependence of the  $I(V)$  profiles due to spin-orbit interaction [2].

We present a new experimental setup for spin-polarized very-low-energy electron-diffraction (SP-VLEED) measurements to investigate the spin dependence of the surface-barrier potential of ferromagnets. Spin-polarized electrons emitted from a GaAs photocathode are directed onto the sample with a variable angle of incidence and with energies in the range of 0 to 50 eV. The specular reflected intensity is measured as a function of the primary-electron energy with a retarding field analyser. To access certain crystallographic axes, the sample can be rotated around an azimuthal axis.

[1] R.O. Jones, P.J. Jennings, Surf. Sci. Reports **9** (1988) 165.

[2] E.G. McRae, D.T. Pierce, Phys. Rev. B **24** (1981) 4230.

O 27.32 Tue 18:30 P2

**Liquid Interface Scattering Apparatus (LISA) for Petra III: Stability and Characterization** — ●CHRISTIAN KOOPS<sup>1</sup>, BRIDGET MURPHY<sup>1</sup>, MATTHIAS GREVE<sup>1</sup>, ANNIKA ELSSEN<sup>1</sup>, JOCHIM STETTNER<sup>1</sup>, OLIVER SEECK<sup>2</sup>, and OLAF MAGNUSSEN<sup>1</sup> — <sup>1</sup>IEAP, Christian-Albrechts-Universität zu Kiel, D-24098 Kiel, Germany — <sup>2</sup>PETRA III at DESY, Notkestr. 85, D-22603 Hamburg, Germany

The study of liquid - liquid interfaces by x-ray scattering methods requires special diffractometers, capable of tilting the beam at precise angles down onto the interface. We have developed a new, dedicated instrument, the liquid interface scattering apparatus (LISA) for the High Resolution Diffraction Beamline at PETRA III. By means of a non-dispersive tilting double crystal monochromator this diffractometer will allow reflectivity measurements without moving the sample.

The planned instrument will operate in the energy range from 6.4 keV to 30 keV and provide access in momentum space out to  $q_z = 2.5 \text{ \AA}^{-1}$ . For monitoring and calibration the high-precision x-ray optics employed for beam tilting a novel optical position detection system was developed. This alignment aid system consists of small lasers and position sensitive diodes, capable of detecting movements in the submicron range during operation. Results on the diffractometer characterization by this optical system will be described.

The work is supported by BMBF-05-KS7KF3

O 27.33 Tue 18:30 P2

**Liquid Interfaces Scattering Apparatus (LISA) for PETRA III: Design and Modelling** — ●BENJAMIN RUNGE<sup>1</sup>, BRIDGET MURPHY<sup>1</sup>, MATTHIAS GREVE<sup>1</sup>, ANNIKA ELSSEN<sup>1</sup>, JOCHIM STETTNER<sup>1</sup>, OLIVER SEECK<sup>2</sup>, and OLAF MAGNUSSEN<sup>1</sup> — <sup>1</sup>IEAP, Christian-Albrechts-Universität zu Kiel, D-24098 Kiel, Germany — <sup>2</sup>PETRA III at DESY, Notkestr. 85, D-22603 Hamburg, Germany

With the completion of PETRA III at DESY Hamburg a high brilliance synchrotron source will be available. This will create new opportunities for studies of buried interfaces, such as liquid-liquid interfaces.

Our Liquid surface diffractometer, LISA, currently under construction, will operate in the energy range from 6.4keV to 30keV and provide access to a momentum space of up to  $q_z = 2.5 \text{ \AA}^{-1}$ . LISA will take advantage of the low vertical and horizontal divergence available at the high resolution X-ray beamline by employing a double crystal setup instead of a single beam tilt crystal as in current liquid surface diffractometers. As a result the angle of incident can be simply varied through a rotation of the crystal stage eliminating the need to move the sample during reflectivity measurements. Furthermore, the sample stage will be mechanically decoupled from both the beam tilt element and the detector stage. This setup will allow to minimize mechanical vibrations of the liquid interface, a key issue in such studies. We present the design concept for LISA and model calculations for the performance of the x-ray optics.

This work is supported by BMBF-05-KS7KF3.

O 27.34 Tue 18:30 P2

**Coverage dependence of capture numbers in kinetic thin film growth and its impact on island size distributions** — ●MARTIN KÖRNER, MARIO EINAX, and PHILIPP MAASS — Institut für Physik, Technische Universität Ilmenau, Germany

The growth of self-organized structures in thin film metal epitaxy is governed by the nucleation kinetics in the submonolayer regime. In the theoretical description of this nucleation kinetics in terms of mean-field rate equations a long-standing problem is the determination of capture numbers, which describe the ability of clusters on the substrate surface to capture further adatoms. Using extensive Kinetic Monte Carlo simulations we present for the first time a systematic analysis of these capture numbers as functions of coverage and cluster size for both fractal and compact island shapes. This allows us to perform a quantitative check for the validity of the mean-field rate equations and to compare the island size distribution from KMC simulations with numerical results from the corresponding rate equations.

O 27.35 Tue 18:30 P2

**A High-Dimensional Neural Network Potential-Energy Surface for Zinc Oxide** — ●NONGNUCH ARTRITH, MARCUS MASCHKE, and JÖRG BEHLER — Lehrstuhl für Theoretische Chemie, Ruhr-Universität Bochum, D-44780 Bochum, Germany

Zinc oxide is a technologically important material, for example as support in heterogeneous catalysis. In order to study a variety of interesting problems it is necessary to perform long simulations of large systems, which are beyond the capabilities of established methods like density-functional theory. Recently, artificial Neural Networks (NN) trained to first-principles data have shown to provide accurate potential energy surfaces for condensed systems, which are computationally very efficient to evaluate. However, so far these potentials have been applicable only to elemental systems. We show that by including physically derived terms it is possible to extend the NN methodology to multicomponent systems. The capabilities of the method are illustrated by first applications to zinc oxide.

O 27.36 Tue 18:30 P2

**The cross-linked (1×2) surface reconstruction of rutile TiO<sub>2</sub> (110)** — ●HANS HERMANN PIEPER, STEPHAN BAHR, STEFAN TORBRÜGGE, and MICHAEL REICHLING — Institute of Physics, University of Osnabrueck, Germany

Titanium is one of the most investigated metal oxides and its surfaces are frequently taken as model catalysts for the partial oxidation of hydrocarbons. There is a large number of publications dedicated to investigations of the pure unreconstructed rutile (110) surface and its interaction with atoms and molecules. However, the different surface reconstructions found for reduced crystals are still under discussion. We investigate the cross-linked (1 × 2) reconstruction by atomic resolution dynamic scanning force microscopy. We interpret images considering that the atomic tip termination and the tip surface distance have a huge influence on the tip-surface interaction, therefore, strongly influencing the atomic contrast formation. We compare our data to three frequently discussed surface reconstruction models and a perfect agreement with one of them is demonstrated.

O 27.37 Tue 18:30 P2

**Acrolein decomposition on cerium-oxide model-catalysts: Correlation between structure and reactivity** — ●JAN MARKUS ESSEN, CONRAD BECKER, and KLAUS WANDEL — Institute of Physical and Theoretical Chemistry, University of Bonn, Wegelerstrasse 12, D-53115 Bonn, Germany

The mechanism of reversible oxygen transfer by cerium oxide based catalysts is still quite unclear. Depending on order, oxygen vacancies and the presence of noble metals oxygen exchange with the oxide surface respectively oxidation of adsorbed organic molecules takes place in two temperature regimes, at about 600 K and at about 950 K. While on well ordered ceria on Pt(111) acrolein desorbs completely intact, annealing to 1000 K leads to an oxygen vacancy related coupling of acrolein on the surface. Electron bombardment of ceria on Pt(111) at 300 K results in hydroxylated surfaces with adsorbed CO<sub>2</sub> and H<sub>2</sub>O. Acrolein TPD shows no defect formation. Disordered reduced oxides are generated by oxygen adsorption on 2 ML Ce/Pt(111). Acrolein decomposition here proceeds via C<sub>1</sub>-O bond cleavage at 600 K. The remaining propylidene decomposes at 950 K in combination with CO/CO<sub>2</sub> desorption. Finally, Pd deposited on ceria on Pt(111) shows a carbon removal by recombinant CO desorption at about 600 K. The reaction with the surface oxygen at 600 K is suggested to be caused by an enhanced oxygen diffusion starting at this temperature, while the oxidation at 950 K is assumed to result from desorbing oxygen forming O<sub>2</sub> vacancies.

O 27.38 Tue 18:30 P2

**Correlation between structural and optical properties of PTCDA monolayers on NaCl/Ag(100)** — ●MATHIAS MÜLLER, ERIC LE MOAL, OLIVER BAUER, and MORITZ SOKOŁOWSKI — Institut für Physikalische u. Theoretische Chemie, Universität Bonn, Wegelerstraße 12, 53115 Bonn

We have investigated the structural and optical properties of PTCDA-(sub)monolayers adsorbed on NaCl. Using thin epitaxial NaCl films grown on Ag(100) it was possible to characterize the PTCDA layers by spot profile analysis-LEED and in parallel with in-situ photoluminescence spectroscopy. Under optimized evaporation conditions we succeeded to obtain ordered PTCDA films, which can be described as a 3×3 superstructure. This superstructure is similar to the one of PTCDA observed on Ag(100), but the lattice constant and azimuthal broadening prove that PTCDA is adsorbed on NaCl. Presumably due to the commensurability and the high order of the structure we observed sharp peaks in the photoluminescence spectra (similar to [1]) which also show interesting finestructure at low temperature. Furthermore, by cooling the sample at 20 K during evaporation, we prepared a disordered PTCDA phase. By annealing the sample, we could observe a phase transition to the ordered structure by SPA-LEED. This phase transition can also be seen as a redshift in the photoluminescence which we explain by the dipole-dipole-coupling in the PTCDA monolayer. Funding by DFG research unit 557 is gratefully acknowledged. [1] T.Dienel et al., Adv. Mater. 20 (5), 959-963 (2008).

O 27.39 Tue 18:30 P2

**The local adsorption structure of glycine on TiO<sub>2</sub>(110)** — T J LEROTHOLI<sup>1</sup>, W UNTERBERGER<sup>2</sup>, E A KRÖGER<sup>2</sup>, M KNIGHT<sup>1</sup>, D J JACKSON<sup>1</sup>, ●D KREIKEMEYER LORENZO<sup>2</sup>, K HOGAN<sup>3</sup>, C LAMONT<sup>3</sup>, and D P WOODRUFF<sup>1</sup> — <sup>1</sup>University of Warwick, UK — <sup>2</sup>Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, Germany — <sup>3</sup>University of Huddersfield, UK

Scanned-energy mode photoelectron diffraction (PhD) is a well-known technique to determine quantitatively the local structure of adsorbates at surfaces. Here we report the application of this method to study

the adsorption of glycine on TiO<sub>2</sub>(110). The adsorption of such small biologically-related molecules has potential relevance to issues of biocompatibility, and in this context TiO<sub>2</sub> is of particular interest, since many medical implants are fabricated from Ti metal. We know from previous studies on Cu(110) that the deprotonated glycine (glycinate) bonds to the surface through both the carboxylate O atom and the amino N atom in one-fold coordinated sites. However, if the glycinate carboxylate O atoms adopt the same geometry as formate on TiO<sub>2</sub>(110), the spacing of the Ti atoms along [1-10] is much larger than the equivalent Cu-Cu spacing, and has bridging O atoms between, so a similar lying-down geometry seems unlikely. We therefore expect glycine to bond to TiO<sub>2</sub> through either carboxylate O atoms or the amino N atoms. O1s PhD spectra show much stronger modulations than N1s PhD, consistent with bonding only through the carboxylate O atoms which occupy off-atop Ti sites, and a standing-up geometry. Quantitative evaluations of the data confirm this conclusion.

O 27.40 Tue 18:30 P2

**DFT study of TMA on Rutile TiO<sub>2</sub>(110)** — ●ANDREAS GREULING, PHILIPP RAHE, and MICHAEL ROHLFING — Universität Osnabrück, Barbarastr.7,D-49069,Osnabrück

TiO<sub>2</sub> is a semiconductor which is used in many applications. For instance, it is used in biotechnology, cosmetic industry, paint industry, in catalysis or photocatalysis. In addition, it is also an ideal system for studying self-assembly of organic molecules aiming at the construction of nanoscale devices. This results from the combination of moderate molecule-substrate interaction, quasi-one-dimensional behavior, and the possibility of anchoring molecules to surface defects. Motivated by preliminary experimental data for TMA(trimesic acid) on TiO<sub>2</sub>(110)[1] we explore the system within DFT using the SIESTA code to investigate several possible adsorbing orientations. Starting from various initial configurations of TMA molecule we relax the system until mechanical equilibrium is achieved. The adsorption energy of each configuration is corrected for basis-set superposition error. Our results predict that orientations where the TMA lies on the surface are energetically favorable with respect to upright configurations.

[1] P. Rahe will give a talk about TPA (terephthalic acid) on TiO<sub>2</sub> at this conference.

O 27.41 Tue 18:30 P2

**Scanning Tunneling Microscopy and Spectroscopy of Phthalocyanine Molecules on Insulating Films** —

●CHRISTOF UHLMANN<sup>1</sup>, MAURICE ZIOLA<sup>1</sup>, NIKO PAVLIČEK<sup>1</sup>, TOBIAS SONNLEITNER<sup>1</sup>, GERHARD MEYER<sup>2</sup>, and JASCHA REPP<sup>1,2</sup> — <sup>1</sup>Institute of Experimental and Applied Physics, University of Regensburg, 93040 Regensburg, Germany — <sup>2</sup>IBM Research, Zurich Research Laboratory, CH-8803 Rüschlikon, Switzerland

Ultrathin insulating films on metal substrates facilitate the use of the scanning tunneling microscope to study the electronic properties of individual molecules, which are electronically decoupled from the metallic substrate. This geometry represents a double-barrier tunneling junction, in which at the resonances in conductance spectra an electron is temporarily added to or removed from the molecule. To gain a detailed understanding of the spectra, it is desirable to systematically vary the electronic structure of molecules step by step without changing the geometrical structure too strongly. We addressed this issue by studying a series of metal-phthalocyanine molecules. In this series, the lowest unoccupied (LUMO) and the highest occupied molecular orbital (HOMO) can differ greatly in symmetry for the different metal cores [1]. In addition to the variation of the electronic structures of the molecule itself we also varied the level alignment with respect to the Fermi level. The latter was done by varying the substrate system, which is accompanied by a variation in the work-function.

[1] M.-S. Liao and S. Scheiner, J. Chem. Phys. 114, 9780 (2001).

O 27.42 Tue 18:30 P2

**Investigation of the adsorption of CO and simple alcohols on the Rutile(110) surface with He atom scattering and spectroscopic methods** — ●DAVID SILBER<sup>1</sup>, MARTIN KUNAT<sup>1</sup>, FRANZISKA TRAEGER<sup>1</sup>, HENGSHAN QUI<sup>1</sup>, YUEMIN WANG<sup>1</sup>, CHRISTOF WÖLL<sup>1</sup>, PIOTR KOWALSKI<sup>1</sup>, BERND MEYER<sup>2</sup>, and CHRISTOF HÄTTIG<sup>1</sup> — <sup>1</sup>Lehrstuhl für Physikalische Chemie I, Lehrstuhl für Theoretische Chemie an der RUB, Bochum — <sup>2</sup>Interdisziplinäres Zentrum für Molekulare Materialien (ICMM), Erlangen

We have studied the adsorption of CO on the rutile TiO<sub>2</sub>(110) surface. He-atom angular distributions were recorded to characterize the ordering of adsorbed CO and revealed a (1x1) diffraction pattern along both

high-symmetry directions. Surprisingly, the width of the diffraction peaks was strongly different also the two high-symmetry directions. We explain this anomaly by the presence of a structure containing grows of CO-molecules tilted in an alterante fashion, yielding either a (2x1) or a (2x2) superstructure. Both structures exhibit glide planes, leading to peak extinctions along both high symmetry directions. The binding energy of the CO molecule to the surface as determined by using He-TDS and conventional TDS amounts to 8.0 kcal/mol. We also report first results about overlayer structures observed for different alcohols and their binding energies on the same substrates. For methanol and ethanol we provide evidence that the interaction with the surface leads to deprotonation. Data from near edge x-ray absorption spectroscopy supports this conclusion.

O 27.43 Tue 18:30 P2

**Preparation and Investigation of one-dimensional ZnO nanostructures using the CVD process** — ●PATRICIA THOMASEN, YONG LEI, and GERHARD WILDE — Institut für Materialphysik, Westfälische Wilhelms-Universität Münster, Germany

The preparation of one-dimensional (1D) ZnO nanostructures via the CVD process is reported here. The growth follows the VLS process in a self-built CVD system. From the powder source, consisting of equal molar amounts of ZnO and C powders, the reactant vapor is transported to the substrate with the help of constant Argon flow. For the oxidation of the nanowires, only the leakage of oxygen inside the system is used. To obtain a good regularity of the wires, a UTAM (Ultra Thin Alumina Mask) surface nano-patterning process was used to produce regular arrays of catalyst dots on the substrate. The UTAMs were first tested for having a highly ordered arrangement of pores themselves. This was done by AFM measurements and a following Fourier transformation of the data. The so grown nanowires were afterwards characterized by SEM, XRD and PL measurements.

O 27.44 Tue 18:30 P2

**The growth of ultrathin Praseodymia films on passivated highly boron-doped Si(111) surfaces** — ●SEBASTIAN GEVERS<sup>1</sup>, DANIEL BRUNS<sup>1</sup>, FLORIAN BERTRAM<sup>1</sup>, TIMO KUSCHEL<sup>1</sup>, MARTIN SUENDORF<sup>1</sup>, LARS BOEWER<sup>2</sup>, CHRISTIAN STERNEMANN<sup>2</sup>, MICHAEL PAULUS<sup>2</sup>, and JOACHIM WOLLSCHLÄGER<sup>1</sup> — <sup>1</sup>Fachbereich Physik, Universität Osnabrück, Barbarastr. 7, 49069 Osnabrück — <sup>2</sup>DELTA, Universität Dortmund, Maria-Goeppert-Mayer-Str. 2, D-44227 Dortmund, Germany

The Germanium On Insulator (GOI) technology is a cost-effective method to integrate III-V optoelectronic materials like GaAs on the dominating Si material platform. This is due to the negligible thermal and lattice mismatch between Ge and GaAs. Good candidates for the insulating buffer material are lattice matched high quality praseodymia films to grow dielectric heterostructures on Si(111) with low defect density. However, it is essential to use passivated silicon substrates in order to prevent the formation of silicate at the substrate-oxide interface.

In this work hexagonal Pr<sub>2</sub>O<sub>3</sub> films were grown on passivated highly boron-doped Si(111) substrates at different temperatures to realize and characterise high quality praseodymia films on passivated Si(111). During and after the growth process the surface structure and morphology were analysed with Spot Profile Analysis Low Energy Electron Diffraction (SPALED). Additional X-Ray Reflection (XRR) investigations at DELTA were performed to analyse the formation of both oxide film and interfacial silicate.

O 27.45 Tue 18:30 P2

**The growth of ultrathin Praseodymia films on passivated highly boron-doped Si(111) surfaces** — ●SEBASTIAN GEVERS<sup>1</sup>, DANIEL BRUNS<sup>1</sup>, FLORIAN BERTRAM<sup>1</sup>, TIMO KUSCHEL<sup>1</sup>, MARTIN SUENDORF<sup>1</sup>, LARS BOEWER<sup>2</sup>, CHRISTIAN STERNEMANN<sup>2</sup>, MICHAEL PAULUS<sup>2</sup>, and JOACHIM WOLLSCHLÄGER<sup>1</sup> — <sup>1</sup>Fachbereich Physik, Universität Osnabrück, Barbarastr. 7, 49069 Osnabrück — <sup>2</sup>DELTA, Universität Dortmund, Maria-Goeppert-Mayer-Str. 2, D-44227 Dortmund, Germany

The Germanium On Insulator (GOI) technology is a cost-effective method to integrate III-V optoelectronic materials like GaAs on the dominating Si material platform. This is due to the negligible thermal and lattice mismatch between Ge and GaAs. Good candidates for the insulating buffer material are lattice matched high quality praseodymia films to grow dielectric heterostructures on Si(111) with low defect density. However, it is essential to use passivated silicon substrates in order to prevent the formation of silicate at the substrate-oxide interface.

In this work hexagonal Pr<sub>2</sub>O<sub>3</sub> films were grown on passivated highly

boron-doped Si(111) substrates at different temperatures to realize and characterise high quality praseodymia films on passivated Si(111). During and after the growth process the surface structure and morphology were analysed with Spot Profile Analysis Low Energy Electron Diffraction (SPA-LEED). Additional X-Ray Reflection (XRR) investigations at DELTA were performed to analyse the formation of both oxide film and interfacial silicate.

O 27.46 Tue 18:30 P2

**Epitaxial Europiumoxide on Ni(100)** — •DANIEL F. FOERSTER, JÜRGEN KLINKHAMMER, CARSTEN BUSSE, and THOMAS MICHELY — II. Physikalisches Institut, Universität zu Köln, Zùlpicher Str. 77, 50937 Köln, Germany

Stoichiometric EuO is one of the rare ferromagnetic semiconductors. Slightly Eu-rich EuO contains oxygen vacancies which cause an additional semiconductor to metal transition (SMT) with resistivity changes up to 12 orders of magnitude simultaneously with the ferromagnetic transition.

We report on the growth of EuO on Ni(100) using molecular beam epitaxy with film thicknesses ranging from below one atomic layer up to several layers. The growth process is characterised at the atomic scale by in-situ variable temperature scanning tunneling microscopy (STM) and low energy electron diffraction (LEED). Using substrate temperatures of 350°C EuO films grow quasi-pseudomorphically with their [100] direction oriented along the [110] direction of Ni, whereat two Ni nearest neighbour distances fit the EuO lattice constant. In consequence this quasi-pseudomorphic EuO phase is compressed by 3.1%. Based on density functional calculations the compressed EuO must be assumed to possess a significantly higher Curie temperature compared to bulk EuO. Besides the quasi-pseudomorphic phase also EuO islands with a second epitaxial relation are observed as a minority phase of EuO films on Ni(100). This phase grows with the EuO [100] direction oriented along the [100] direction of Ni, thus being rotated 45° compared to the quasi-pseudomorphic phase.

O 27.47 Tue 18:30 P2

**Structure and morphology of epitaxial manganese oxide films on Ag(001)** — •KLAUS MEINEL, MICHAEL HUTH, SEBASTIAN POLZIN, KONRAD GILLMEISTER, and WOLF WIDDRA — Martin-Luther-Universität Halle-Wittenberg, Germany

STM, SPALEED, AES and HREELS have been applied to study the formation and thermal stability of manganese oxide films on Ag(001). The films have been grown by reactive Mn deposition in an O<sub>2</sub> atmosphere. Whereas films deposited at room temperature show a layer-like growth mode, deposition at slightly higher temperatures yields an embedding of film islands in the substrate due to Ag surface diffusion. Film deposition in an O<sub>2</sub> atmosphere of 2x10<sup>-8</sup> mbar and postannealing to 620 K results in a MnO(001)-(1x1) rock salt structure which may display a moiré-like relaxation pattern in SPALEED. For film deposition in 8x10<sup>-8</sup> mbar O<sub>2</sub> and postannealing, a MnO(001)-(2x1) row structure is observed with STM and SPALEED. At a film thickness around 5 ML a new structure develops which is indicated by a brilliant (2x2) diffraction pattern. It is assigned to the formation of a spinel-like Hausmannite Mn<sub>3</sub>O<sub>4</sub>(001) film structure where the lattice vectors are aligned along the [110]-like directions of the Ag(001) substrate. This specific orientation implies an almost vanishing misfit which may explain the high structural perfection of the Mn<sub>3</sub>O<sub>4</sub> films. These results will be compared with recent data for manganese oxide thin films on Pd(001) and Pt(111) [1,2].

[1] Bayer et al., Phys. Rev. B 76, 165428 (2007).

[2] Hagendorf et al., Phys. Rev. B 77, 075406 (2008).

O 27.48 Tue 18:30 P2

**STM study of the structure and morphology of TiO<sub>2</sub> thin films epitaxially grown on Re(10 $\bar{1}$ 0)** — •SEBASTIAN SCHWEDE, SUSANNE SCHUBERT, WILHELMINE KUDERNATSCH, and KLAUS CHRISTMANN — FU-Berlin, Berlin, Germany

We have studied the epitaxy of TiO<sub>2</sub> (rutile) films grown on the oxygen precovered rhenium(10 $\bar{1}$ 0) surface using LEED and STM. These rutile *films* provide, by varying their thickness systematically, an easy method to generate model catalysts with a well-defined roughness.

As a first step, we prepared the well-known (1x3) oxygen superstructure on the Re surface [1], which provides an appropriate template for the subsequent growth of the (2x1) reconstructed rutile(011) phase on the Re(10 $\bar{1}$ 0) surface. STM images taken from the (1x3)-2O structure confirm that it is a reconstructed phase of the 'buckling' type.

Atomically resolved STM images of the rutile films prepared accord-

ing to ref. [2] reveal a clear zig-zag structure of the TiO<sub>2</sub> films and thus confirm their glide mirror symmetry, whereby periodic intensity protrusions in the images provide additional structural information. Larger scale images also support our previous conclusions concerning the growth mechanism and morphology of the (011) rutile films.

[1] J. Lenz et al., Surf. Sci. **269/270** (1992) 410

[2] D. Rosenthal et al., Surf. Sci. **600** (2006) 2830.

O 27.49 Tue 18:30 P2

**Vanadium oxide films on W(110) and on natively oxidized Si: flat and nanostructured model catalysts** — •BENJAMIN BORKENHAGEN<sup>1</sup>, JÖRAN BAUCHROWITZ<sup>2</sup>, GERHARD LILIENKAMP<sup>1</sup>, and WINFRIED DAUM<sup>1</sup> — <sup>1</sup>IPPT TU Clausthal — <sup>2</sup>MPI Hannover

We present results on structural and chemical properties of VO<sub>x</sub> films prepared in two different ways: by V evaporation in an UHV system under O<sub>2</sub> atmospheres on W(110) and by a sol-gel process on Si substrates covered with a native oxide. Under oxidizing or reducing conditions at elevated temperatures the ultrathin VO<sub>x</sub> films on W(110) can be transformed into several superstructures, e.g. (3x1), (2x1) or nearly hexagonal superstructures the latter observed in several orientations relative to the substrate as revealed by LEED. By analysis of AES we are able to relate these superstructures to W-V surface alloys, WO<sub>x</sub> or VO<sub>x</sub> in various oxidation states. We have derived a preliminary diagram of the existence range of surface phases of VO<sub>x</sub> on W(110). We investigated the films with Low Energy Electron Microscopy (LEEM) to determine domain sizes and alignment and to see how transformations between different superstructures occur. Ultrathin VO<sub>x</sub> films with low roughness were prepared by a sol-gel process. Depending on subsequent heating, our AFM studies show the formation of multiple surface topographies such as plateaus, needle-like crystallites and tubs. AES and tunneling AFM (TUNA) were used to determine chemical and physical properties of the structures. LEEM has been applied to distinguish between conducting and insulating crystallites and to study changes in conductivity during annealing of the samples in UHV.

O 27.50 Tue 18:30 P2

**SPA-LEED investigations on highly boron-doped Si(111) Surfaces after annealing in UHV** — •DANIEL BRUNS, SEBASTIAN GEVERS, TIMO KUSCHEL, FLORIAN BERTRAM, MARTIN SUENDORF, THOMAS WEISEMOELLER, GREGOR STEINHOFF, and JOACHIM WOLLSCHLAEGER — Fachbereich Physik, Universitaet Osnabrueck, Barbarastr. 7, 49069 Osnabrück

'Dangling bonds' at the Si(111) surface benefit the formation of thick interface layers between the silicon substrate and oxide films during the deposition process. This is often unwanted for potential electronic applications such as MOSFET or GOI. Therefore it is needful to investigate passivated silicon surfaces which may prevent intermixing of substrate and adsorbate.

Highly boron-doped Si(111) substrates were annealed at 1000°C and cooled down very slowly to achieve complete saturation of the 'dangling bonds' under reconstruction to the Si(111)( $\sqrt{3} \times \sqrt{3}$ )R30° phase. The surface morphology of the prepared substrates was analyzed by SPA-LEED. The diffraction peaks show multiple splittings caused by faceting of the surface. A model with big step-bunches and large terraces was developed to explain our experiments. Afterwards the stability of the ( $\sqrt{3} \times \sqrt{3}$ )R30° phase was tested under UHV conditions at temperatures from 300°C to 700°C.

O 27.51 Tue 18:30 P2

**Decomposition of the Si(111)-2x1 Surface Reconstruction at Room Temperature: an STM Study** — •THOMAS K. A. SPAETH<sup>1</sup>, MARTIN WENDEROTH<sup>1</sup>, KAROLIN LÖSER<sup>1</sup>, JENS K. GARLEFF<sup>2</sup>, and RAINER G. ULBRICH<sup>1</sup> — <sup>1</sup>IV. Phys. Inst., Georg August Univ. Göttingen, Germany — <sup>2</sup>PSN, Eindhoven University of Technologie, the Netherlands

The  $\pi$ -bonded chains of the Si(111)-2x1 reconstructed surface are highly anisotropic with quasi 1-d electronic properties [1, 2]. We prepared the surfaces by cleaving bulk crystals. During STM measurements in UHV (8 · 10<sup>-10</sup> mbar to 6 · 10<sup>-11</sup> mbar) we observed a gradual decomposition of the Si(111)-2x1 surface structure. It starts with small holes which grow gradually. The new surface shows no reconstruction or any periodic structure. Comparing the topographic height with monatomic step as a reference we find that the step height between the original reconstruction and the new surface is only half the height difference of the monolayer. By measurements at diverse UHV pressures we find a variation of the rate of decomposition: with increasing pressure the decomposition takes several days at 6 · 10<sup>-11</sup> mbar, and

only a few hours at  $8 \cdot 10^{-10}$  mbar. Finally the surface ordering vanishes completely. For this type of surface no further degradation is observed. Our findings indicate that the partial and finally even complete removal of the first atomic layer leads to a more stable surface structure which is not long-range ordered.

- [1] M. Roling and S. G. Louie, PRL 83 (4), 856 (1999)  
 [2] J. K. Garleff et al., PRB 76, 125322 (2007)

O 27.52 Tue 18:30 P2

**Direct measurement of surface stress anisotropy on Si(100) surfaces by means of SSIOD and homoepitaxial growth** — •FRIEDRICH KLASING and MICHAEL HORN-VON HOEGEN — University of Duisburg-Essen, Institute for Experimental Physics

Surface stress is one of the most important physical quantities for the formation of structure and morphology of solid surfaces due to its large contribution to the total energy. Unfortunately, the direct measurement of surface stress is not possible, but it can be determined via the elastic response of a thin substrate as utilized in bending sample techniques like surface stress induced optical deflection (SSIOD) [1]. The morphology of bare Si(100) surfaces is strongly influenced by the anisotropic stress of the  $(2 \times 1)$  dimer structure. Theory predicts compressive stress along the dimer bond ( $\sigma_{\parallel} > 0$ ) and tensile stress perpendicular to the dimer bond ( $\sigma_{\perp} < 0$ ). For the technologically most important semiconductor surface - Si(100) - there still is no direct method to measure this important parameter.

Utilizing the formation of a single  $(2 \times 1)$  domain structure during homoepitaxial growth under kinetic limitations at  $400^{\circ} - 500^{\circ}C$  on a slightly vicinal surface it was possible to directly determine the difference of the tensor components  $\Delta\sigma = \sigma_{\perp} - \sigma_{\parallel}$  via SSIOD for the first time. The presented findings are well within predictions.

- [1]: A. Schell-Sorokin et al., Phys. Rev. Lett. 64(9), 1039 (1990)

O 27.53 Tue 18:30 P2

**Surface Characterisation of GaSb-films grown by MOCVD** — •ANDREAS SEEMAYER<sup>1</sup>, ALEXANDER HOMMES<sup>1</sup>, SASCHA HÜMANN<sup>2</sup>, DIRK VOGEL<sup>2</sup>, STEPHAN SCHULZ<sup>3</sup>, and KLAUS WANDEL<sup>1</sup> — <sup>1</sup>Institute for Physical Chemistry, University of Bonn, Germany — <sup>2</sup>Max Planck Institut für Eisenforschung, Düsseldorf, Germany — <sup>3</sup>Department of Chemistry, University of Essen, Germany

III-V semiconductor films used for opto- and microelectronic devices have traditionally been grown by (MO)MBE and LPE processes. An alternative metal-organic CVD-process, which has been established in the last two decades for high-throughput and low-cost fabrication works for nitrides, phosphides and arsenides, but is problematic for antimonides. In particular, for GaSb films an alternative route is a CVD-process using the heterocyclic single source precursor [*t*Bu<sub>2</sub>GaSbEt<sub>2</sub>]<sub>2</sub>.

Subject of the present work is the gas phase behaviour of the used precursor under UHV conditions and the surface characterisation of thin GaSb-films, which were grown in a self-made HV-MOCVD reactor on Si(001), by AES, S-XPS and AFM. The results are discussed in terms of a correlation of the electronic properties with the composition and structure of the films.

O 27.54 Tue 18:30 P2

**The influence of diffusion anisotropy and strain on Ag nanowire formation on flat and vicinal Si(001)** — •DIRK WALL, SIMON SINDERMANN, MICHAEL HORN-VON HOEGEN, and FRANK-JOACHIM MEYER ZU HERINGDORF — Address: Department of Physics and Center for Nanointegration Duisburg-Essen (CeNIDE) Universität Duisburg-Essen, D-47057 Duisburg, Germany

Photoemission Electron Microscopy (PEEM) and Low Energy Electron Microscopy (LEEM) are used to study the self organized growth of Ag nanowires on flat and vicinal Silicon (001) surfaces. The nanowires form along the two dimer row directions on the flat Si substrate. During growth on substrates with higher vicinalities, between  $0^{\circ}$  and  $4^{\circ}$  along the [110] direction, the wires start to form predominantly aligned with the steps. Finally, on a  $4^{\circ}$  vicinal substrate, all wires are aligned with the steps [1]. This increasing alignment of the nanowires along the  $[\bar{1}10]$  direction is attributed to the increase in diffusion anisotropy of Ag adatoms on increasingly vicinal Si substrates [1,2]. For strained islands, calculations predict that the islands will nucleate in a symmetrical shape on the surface until the lattice mismatch forces the islands to become elongated in one direction and shrink in the perpendicular direction [3]. We will show present results as to which of the two mechanisms, strain and/or diffusion anisotropy are affecting wire formation. [1] D. Wall et. al.; J. P.:Cond. Matt. (submitted) [2] D. Wall et. al.; Mater. Res. Soc. Symp. Proc. 1088E; 1088-W05-04(2008) [3]

J. Tersoff, R. M. Tromp; Phys. Rev. Lett. 70 (1993) 2782

O 27.55 Tue 18:30 P2

**Metal induced faceting of Si (112)** — •TOBIAS NABBEFELD, CHRISTIAN WIETHOFF, FRANK-JOACHIM MEYER ZU HERINGDORF, and MICHAEL HORN-VON HOEGEN — Department of Physics and Center for Nanointegration Duisburg-Essen (CeNIDE), University of Duisburg-Essen, 47057 Duisburg

In vapour-liquid-solid growth of Si-nanowires intense faceting of (112)-sidewalls is observed when Au is used as catalyst [1,2]. Other catalyst metals commonly used for the growth of nanowires are Ag and Al. We studied the faceting of Si (112) samples, prepared in ultra-high-vacuum by molecular-beam-epitaxy, in-situ by spot-profile-analysing low-energy-electron-diffraction (SPA-LEED). The SPA-LEED shows facet orientations with high accuracy. Several morphologic phases depending on Ag or Al coverage and temperature were found, and orientations of facets as well as the average step heights, the terrace widths and roughness were identified. The temperature dependence of the faceting process is analysed for temperatures between  $380^{\circ}C$  and  $740^{\circ}C$ . This temperature range covers the temperatures of vapour-liquid-solid-growth mechanism and of vapor-solid-solid-growth mechanism for Al-catalysed Si-nanowires [3]. The results of these experiments will help to optimize the properties of nanowires, which are influenced by surface structures.

- [1] F.M. Ross et al., Phys. Ref. Lett. 95, 146104, 2005  
 [2] C. Wiethoff et al., Nano Lett. 8, 3065, 2008  
 [3] Y. Wang et al., Nature Nanotech. 1, 186, 2006

O 27.56 Tue 18:30 P2

**2D electrical conductivity in the Bi(111) surface state** — •HICHEM HATTAB<sup>1</sup>, GIRIRAJ JNAWALI<sup>1</sup>, THORSTEN WAGNER<sup>2</sup>, ROLF MÖLLER<sup>1</sup>, and MICHAEL HORN-VON HOEGEN<sup>1</sup> — <sup>1</sup>Fachbereich Physik, Universität Duisburg-Essen, Lotharstr. 1, 47048 Duisburg, Germany — <sup>2</sup>Johannes Kepler University Linz, Institute of Experimental Physics, Altenberger Str. 69, A-4040 Linz, Austria.

Bismuth is a semi metal with unique electronic properties. Recent investigations show that for atomically smooth ultra thin Bi(111) films the electronic density of states near the Fermi level is dominated by a highly metallic surface state [1]. Such films are ideally suited to study 2D electronic transport and roughness induced scattering effects.

Epitaxial Bi(111) films are grown on Si(001) at 150 K and annealed at 450 K [2]. The electric contact to the Bi surface is established by 4-point WSi<sub>2</sub> contacts. Since the conductivity of the Bi-films does not depend on the thickness for up to 60 nm, it has to be attributed to the electronic surface state.

Additional Bi deposition  $\Theta_{Bi}$  at 80 K produces a high density of 2D-Bi islands. The island density in the sub-bilayer regime is determined by STM and increases with  $\Theta_{Bi}^{1/3}$ . This short scale roughness significantly decreases the surface state conductivity with  $\Theta_{Bi}^{1/2}$ . This behavior is explained by a simple Boltzmann transport theory for a 2D electron gas.

- [1] Hirahara et al., Appl. Phys. Lett. **91**, 202106 (2007)  
 [2] Jnawali et al., Phys. Rev. B **78**, 035321 (2008)

O 27.57 Tue 18:30 P2

**Angle-resolved inverse photoemission of the H-etched 6H-SiC(0001) surface** — •NABI AGHDASSI, RALF OSTENDORF, and HELMUT ZACHARIAS — Physikalisches Institut, Westfälische Wilhelms-Universität Münster

The etching of 6H-SiC(0001) substrates in molecular hydrogen at elevated temperatures leads to an ordered silicate adlayer as it is confirmed by LEED and AES. LEED patterns clearly feature a  $(\sqrt{3} \times \sqrt{3})R30^{\circ}$  periodicity while AES spectra are evidence for the presence of Si-O bonds. The generated surfaces appear to be fully passivated and therefore stable in ambient air. After cleaning the samples by heating in UHV up to temperatures around  $750^{\circ}C$  angle-resolved inverse photoemission is performed on the SiO<sub>2</sub>/SiC interface. The IPE spectra reveal five features above the Fermi level around 0.5 eV, 1.2 eV, 2.3 eV, 3.5 eV and 5.5 eV, respectively, which show only a weak dispersion along the  $\Gamma - M$  and  $\Gamma - K$  directions of the  $(1 \times 1)$  surface Brillouin zone.

O 27.58 Tue 18:30 P2

**Preparation and Characterization of Gold Micro-Crystals on an artificial SiO<sub>2</sub>-Layer on Silicon** — JAWAD SLIEH, •ANDREAS WINTER, ARMIN BRECHLING, WIEBKE HACHMANN, and ULRICH HEINZ-

MANN — Molecular and Surface Physics, Bielefeld University

We report on the fabrication of gold micro-crystals in the size range between several 100 nm and approximately 3  $\mu\text{m}$ . Gold was deposited on dry oxidized silicon wafer pieces (001) by Ar-sputtering at a deposition rate of 0.11 nm/s and an Ar partial pressure of 13 Pa. The subsequent annealing was made in a nitrogen atmosphere at different temperatures (900°C – 1050°C) as well as at different annealing times (2 h – 10 h). The influence of the deposited gold layer thickness, of the annealing temperature and of the annealing time on the crystal size, on the crystal orientation and on the amount of single crystals were studied systematically. The lateral and vertical sizes of the gold clusters were characterized by means of Scanning Electron Microscopy and Atomic Force Microscopy, respectively. The orientation of the gold crystals relative to the substrate was characterized by X-Ray Diffraction and Laue Diffraction techniques.

O 27.59 Tue 18:30 P2

**FTIR-Spectroscopy of MOCVD-Prepared Silicon (100)** — ●PETER KLEINSCHMIDT, ANJA DOBRICH, HENNING DÖSCHER, SEBASTIAN BRÜCKNER, CHRISTIAN HÖHN, and THOMAS HANNAPPEL — Helmholtz-Zentrum Berlin für Materialien und Energie, Glienicke Str. 100, 14109 Berlin

Using silicon to replace III-V semiconductors or germanium as a substrate material in high-performance devices like high-efficiency multi-junction solar cells is attractive due to cost considerations and better availability. In order to achieve defect-free epitaxy on Si(100), the surface should exhibit double atomic steps. MOCVD-preparation of Si(100) typically results in single atomic steps where Si-Si dimer orientation alternates on adjacent terraces. In the MOCVD reactor, the presence of hydrogen may have a crucial impact on the step formation at the surface.

We have investigated MOCVD-prepared Si(100) using Fourier-transform infrared (FTIR) spectroscopy in an attenuated total reflection (ATR) configuration enabling sensitive measurements of the silicon-hydrogen bonds at the surface. The measurements showed Si-H mono-hydrides, which are characterized by absorption lines due to a symmetric and an antisymmetric stretch mode. This is in agreement with results from low-energy electron diffraction (LEED) and scanning tunneling microscopy (STM), which indicated that the surface unit cell consists of silicon dimers. The FTIR measurements suggest that the dangling bonds of the dimers are saturated with hydrogen.

O 27.60 Tue 18:30 P2

**In-situ RAS analysis of homo- and hetero-epitaxial GaP(100) surfaces grown by MOVPE** — ●HENNING DÖSCHER, SEBASTIAN BRÜCKNER, and THOMAS HANNAPPEL — Helmholtz-Zentrum Berlin für Materialien und Energie, Glienicke Str. 100, 14109 Berlin

Control over the atomic properties of III-V compound semiconductor surfaces is of crucial importance for the preparation of well-defined hetero-interfaces in many thin film devices, e.g. solar cells, lasers, and LEDs. Reflectance anisotropy spectroscopy (RAS) is an extremely surface sensitive optical probe applicable for in-situ measurements in the MOVPE environment. The MOVPE deposition of gallium phosphide on Si(100) is studied here as an exemplary model system for the hetero-epitaxial III-V growth on non-polar substrates since this material combination represents an almost perfect lattice match.

The created hetero-interface gives rise to the formation of anti-phase domains (APDs) according to the step structure of the substrate, which are considered as a crucial defect mechanism in these samples. Recently, RAS was applied for quantitative in-situ measurements for APDs on the surface of GaP/Si(100) thin films. The success of this approach depends on the correct consideration of all influences on the structure and intensity of the characteristic RA spectra. In the case of GaP(100) surfaces, not only the reconstruction, but also the sample temperature and the applied preparation route have to be regarded. In the investigated thin film system additional signal contributions arise due to APD content and interference with the interfacial reflection, which potentially is anisotropic in itself.

O 27.61 Tue 18:30 P2

**Comparison on the local adsorption of cyclopentene and benzene on Si(100)** — ●DANIEL WEIER<sup>1</sup>, TOBIAS LÜHR<sup>1</sup>, AXEL BEIMBORN<sup>1</sup>, ANJA WADEWITZ<sup>1</sup>, and CARSTEN WESTPHAL<sup>1,2</sup> — <sup>1</sup>Fakultät Physik - Technische Universität Dortmund, Otto-Hahn-Str.4, D 44221 Dortmund, Germany — <sup>2</sup>DELTA - Technische Universität Dortmund, Maria-Goepfert-Mayer-Str. 2, D 44227 Dortmund, Germany

There has been considerable interest in the behaviour of the bonding process of unsaturated hydrocarbons with semiconductor surfaces. These systems offer a potential route to optoelectronic and bioanalytical devices if functional groups are added to the base molecules. Examples of these systems are the interaction between cyclopentene and benzene on silicon. In our experiments at beamline 11 (DELTA) these structures were studied using XPS and x-ray photoelectron diffraction. The experimental data were compared to simulation calculations in order to investigate the molecules interaction with the surface. Angle-scanned photoelectron diffraction patterns were recorded within 0-358° and 0-80° for the azimuth and polar angle, respectively. The experimental patterns are compared to simulation calculations of both systems. It will be shown that the adsorption behaviour of cyclopentene and benzene differ from each other. Cyclopentene tends to form only one type of adsorption structure whereas benzene is forming two different structures. Our results showed a combination of the 'standard butterfly' and the 'tilted bridge' structure for benzene, but a upright standing tilted structure for the cyclopentene, respectively.

O 27.62 Tue 18:30 P2

**Band bending via H<sub>2</sub>O adsorption on titanium dichalcogenide surfaces** — ●STEPHAN THÜRMER, ALEXANDER PAULHEIM, LENART DUDY, BEATE MÜLLER, HENDRIK VITA, CHRISTOPH JANOWITZ, and RECARDO MANZKE — Humboldt-Universität zu Berlin, Institut für Physik, Newtonstr. 15, 12489 Berlin

With the method of photoemission it is possible to measure occupied electronic states of a material by detection of the emitted electrons. By means of angle-resolved photoemission (ARPES) the complex electronic structures in reciprocal k-space, such as energy-band dispersion, are accessible. Band bending can be induced by Schottky contacts and therefore normally unoccupied electronic states can be reached. Here, water adsorption onto the van der Waals-like surface of Ti compounds served as contact. Photoemission analysis of the TiSe<sub>2</sub> transition metal dichalcogenide has shown interesting effects of dipole induced band bending [1]. Presuming Schottky contact like effects, the semiconducting behavior of this material was revealed. In accordance, preliminary ARPES measurements of the semimetal TiTe<sub>2</sub> in similar conditions showed no bending of the bands due to charge carrier screening of the dipole field. To further investigate the effects of water physisorption, detailed measurements and comparisons of the isostructural Ti compounds TiSe<sub>2</sub>, TiTe<sub>2</sub>, and TiS<sub>2</sub> with high resolution ARPES will be shown.

[1] J. Rasch et al., Phys. Rev. Lett. 102 (2008)

O 27.63 Tue 18:30 P2

**A spectroscopy study of water adsorption on diamond surfaces** — ●SIMON QUARTUS LUD<sup>1</sup>, DOMINIQUE VERREAULT<sup>2</sup>, PATRICK KOELSCH<sup>2</sup>, MARTIN HUTH<sup>3</sup>, BERT NICKEL<sup>3</sup>, HENDRIK BLUHM<sup>4</sup>, JOHN NEWBERG<sup>4</sup>, MARTIN STUTZMANN<sup>1</sup>, and JOSE ANTONIO GARRIDO<sup>1</sup> — <sup>1</sup>Walter Schottky Institut, Technische Universität München, Am Coulombwall 3, 85748 Garching, Germany — <sup>2</sup>Angewandte Physikalische Chemie, Universität Heidelberg, Im Neuenheimer Feld 253, 69120 Heidelberg, Germany — <sup>3</sup>Department für Physik, Ludwig-Maximilians-Universität München, Geschwister-Scholl-Platz 1, 80539 München, Germany — <sup>4</sup>Chemical Sciences Division, Lawrence Berkeley National Laboratories, Berkeley, CA 94720, USA

We have explored the adsorption of water layers onto different diamond surfaces at the solid-gas interface. X-ray reflectivity (XRR), sum frequency generation (SFG) spectroscopy and X-ray photoelectron spectroscopy (XPS) have been used to investigate the adsorbed water onto the diamond films under controlled humidity. XRR reveals the presence of a water film on the hydrophilic O-terminated surfaces, with a thickness increasing with humidity. Interestingly, even if highly hydrophobic, the hydrogenated surface also shows a humidity-dependent water film. SFG spectroscopy, with its high surface sensitivity, revealed different vibrational modes of interfacial water, including the so-called free OH stretching mode at 3700 cm<sup>-1</sup>. Temperature dependent SFG experiments were performed to investigate the stability of the water films on H-, F- and O-terminated surfaces, unveiling a surprisingly high stability for water even on the hydrophobic surfaces.

O 27.64 Tue 18:30 P2

**HR-EELS and STM study of organic molecules on Si(001)** — ●BOCHRA BOUGHALED ELLAKHMIS and ULRICH KÖHLER — Experimentalphysik IV/AG Oberflächen, Ruhr-Universität Bochum, 44780 Bochum, Germany

The reaction of acrylonitrile with Si(001)-(2x1)-surfaces is studied as a first step in the field of the fabrication of organic/inorganic semiconductor hybrid structures. Layers of nitriles are a possible candidate for a template layer on silicon to enable the anchoring of organic coatings.

A combination of an area averaging spectroscopy, high resolution electron energy loss spectroscopy (HR-EELS) and a local microscopy, scanning tunnelling microscopy (STM) is used to determine the internal structure of the adsorbed molecule and the adsorption geometry on the Si-substrate. A non-dissociative cross dimer row adsorption is present at room temperature and below. HR-EELS is used to study the thermal decomposition of acrylonitrile above room temperature. First results on the reaction of organic molecules with water covered Si(001) surfaces will be shown.

O 27.65 Tue 18:30 P2

**Investigation of antenna resonances for SERS in the near infrared** — ●DANIEL WEBER<sup>1</sup>, FRANK NEUBRECH<sup>1</sup>, CHRISTINA BAUER<sup>2</sup>, ANNEMARIE PUCCI<sup>1</sup>, and HARALD GIESSEN<sup>2</sup> — <sup>1</sup>Kirchhoff-Institut für Physik, Universität Heidelberg, Deutschland — <sup>2</sup>4. Physikalisches Institut, Universität Stuttgart, Deutschland

Gold nanorod arrays were investigated by infrared (IR) microscopy using synchrotron radiation at the Angströmquelle Karlsruhe (ANKA). The regularly shaped gold nanorods (width and height about 100 nm) with lengths between 400 and 1200 nm were prepared by electron beam lithography at the 4th Physics Institute, University of Stuttgart. The nanorods are placed on quartz glass (HeraSil), which is transparent for IR radiation in the near infrared spectral range. Comparable to our results from former IR spectroscopic studies of gold nanowires deposited on zinc sulphide substrates, we observed antenna-like plasmon resonances, which are accompanied by an enhanced electromagnetic field in the vicinity of the nanorods. We intend to exploit this field enhancement for surface-enhanced Raman scattering (SERS) by using an IR laser as exciting light source

O 27.66 Tue 18:30 P2

**attosecond technology towards combining ultrahigh spatiotemporal resolution \* nanoplasmonic optical field microscopy** — ●JINGQUAN LIN<sup>1</sup>, ADRIAN WIRTH<sup>2</sup>, SOO CHEW<sup>1</sup>, NILS WEBER<sup>3</sup>, MICHAEL MERKEL<sup>3</sup>, MATTHIAS KLING<sup>2</sup>, MARK STOCKMAN<sup>4</sup>, FERENC KRAUSZ<sup>1,2</sup>, and ULF KLEINEBERG<sup>1</sup> — <sup>1</sup>Faculty of Physik, LMU, Garching, Germany — <sup>2</sup>Max Plank Institute of Quantenoptics, Garching, Germany — <sup>3</sup>Focus GmbH, Huestetten Kesselbach, Germany — <sup>4</sup>Georgia State University, Atlanta, USA

Nanoplasmonics deals with collective electronic dynamics on the surface of metal nanostructures, which arise as a result of resonant excitations of surface plasmons by light pulse. Because of their broad spectral bandwidth, surface plasmons undergo ultrafast dynamics with timescales as short as a few hundred attoseconds. An approach, which combines photoelectron emission microscopy and attosecond streaking spectroscopy and will provide direct, non-invasive access to the nanoplasmonic collective dynamics with nanometre-scale spatial resolution and temporal resolution on the order of 100 attoseconds, has been proposed. To implement the approach, ToF-PEEM with 25 nm spatial resolution and 50 meV energy resolution has been developed and characterized by use of 400 nm/70ps diode laser. First experimental steps towards time-resolved 2PPE photoemission microscopy as well as vis-pump/XUV-probe attosecond microscopy to measure the temporal evolution of localized optical fields will be described.

O 27.67 Tue 18:30 P2

**Near Field Distribution of Nanostructures with Electromagnetic Coupling** — ●PASCAL MELCHIOR<sup>1</sup>, MARTIN ROHMER<sup>1</sup>, CHRISTIAN SCHNEIDER<sup>1</sup>, DANIELA BAYER<sup>1</sup>, ALEXANDER FISCHER<sup>1</sup>, MIRKO CINCHETTI<sup>1</sup>, DANIEL BENNER<sup>2</sup>, JOHANNES BONEBERG<sup>2</sup>, PAUL LEIDERER<sup>2</sup>, and MARTIN AESCHLIMANN<sup>2</sup> — <sup>1</sup>Department of Physics and Research Center OPTIMAS, University of Kaiserslautern, 67663 Kaiserslautern, Germany — <sup>2</sup>Department of Physics, University of Konstanz, 78457 Konstanz, Germany

Nonlinear photoemission electron microscopy (PEEM) is a powerful tool to directly image the near field distribution of nanostructures. On the other hand, two-photon photoemission (2PPE) spectroscopy allows the investigation of electron dynamics following the excitation with a laser pulse. As follows from Fermi-liquid theory, the electron dynamics strongly depend on the energy.

We combined a PEEM instrument with time-resolved 2PPE and time-of-flight detector (ToF) to simultaneously access space, time and energy. This gives the unique possibility to study the electron dy-

namics at nanostructured surfaces and the influence of near field enhancement on the dynamics not only with highest spatial and temporal resolution but also with the option of spectroscopic analysis of the photoemitted electrons. In particular, we devoted our attention to investigate the influence of coupling effects on the near field distribution of nanostructures with varying dimer distance, the dominant parameter that characterizes the coupling.

O 27.68 Tue 18:30 P2

**Coupling of Single NV-Centres to Surface Plasmons** — ●MERLE BECKER, BERNHARD GROTZ, GOPALAKRISHNAN BALASUBRAMANIAN, ROMAN KOLESOV, FEDOR JELEZKO, and JÖRG WRACHTRUP — <sup>3</sup>Physikalisches Institut, Universität Stuttgart, 70550 Stuttgart, Germany

Subwavelength light localization is the crucial condition to achieve strong coupling between single emitters and nanosystems. Controlling the coupling and therewith controlling light quanta is of great interest in the field of quantum science. Coupling of single emitters to surface plasmons was already shown previously, however when thinking about devices, it is of big importance to gain knowledge about coupling strengths that can be achieved experimentally. As model system, we show the coupling of single NV centres to Ag nanowires at different diameters in comparison to theoretical models. NV centres were chosen as single emitters due to absolute photostability at room temperature and growing importance in quantum optics and MRI [1].

[1] G. Balasubramanian et al. *Nature* 455, 648 - 651 (2008)

O 27.69 Tue 18:30 P2

**Time-Resolved Near-Field Microscopy of Acoustic Vibrations** — ●THORSTEN SCHUMACHER<sup>1,2</sup>, MARKUS LIPPITZ<sup>1,2</sup>, RALF VOGELGESANG<sup>1</sup>, JENS DORFMÜLLER<sup>1</sup>, and KLAUS KERN<sup>1</sup> — <sup>1</sup>Max-Planck-Institute for Solid State Research, Stuttgart - Germany — <sup>2</sup>4th Physics Institute, University of Stuttgart, Stuttgart - Germany

The localized surface plasmon resonance (LSPR) of metal nanoparticles depends directly on the geometry and the dielectric constant of the nanoobject. The resonance is influenced by the electron density which can be modified by acoustic oscillations of the nanostructure. The optical near-field thus contains information on the structure's acoustic oscillation.

The combination of apertureless scanning near-field optical microscopy (aSNOM) and ultrafast pump-probe spectroscopy allows to detect the temporal and spatial dependence of the LSPR. We present our implementation of a pump-probe aSNOM which at the end will allow us to map out nanoscale Chladni figures. We show numerical simulation of the field changes caused by local plasma frequency changes, nanoacoustical modes as well as first experimental results.

O 27.70 Tue 18:30 P2

**Analysis Tools for Time-Resolved Two-Photon Photoelectron Microscopy of Excitations in Metal Nanostructures** — MARTIN AESCHLIMANN<sup>1</sup>, MICHAEL BAUER<sup>2</sup>, DANIELA BAYER<sup>1</sup>, TOBIAS BRIXNER<sup>3</sup>, STEFAN CUNOVIC<sup>4</sup>, FRANK DIMLER<sup>3</sup>, ALEXANDER FISCHER<sup>1</sup>, WALTER PFEIFFER<sup>4</sup>, MARTIN ROHMER<sup>1</sup>, CHRISTIAN SCHNEIDER<sup>1</sup>, FELIX STEEB<sup>1</sup>, ●CHRISTIAN STRÜBER<sup>4</sup>, and DMITRI V. VORONINE<sup>3</sup> — <sup>1</sup>University of Kaiserslautern, Kaiserslautern, Germany — <sup>2</sup>University of Kiel, Kiel, Germany — <sup>3</sup>Ludwigs-Maximilian-Universität, Würzburg, Germany — <sup>4</sup>University of Bielefeld, Bielefeld, Germany

The application of coherent control schemes in nanooptics aims for steering the temporal and spatial evolution of localized excitations. Polarization shaped laser pulses allow tailoring the local excitation of a nanostructure simultaneously with subwavelength spatial resolution and femtosecond timing [1,2]. The investigation of the temporal evolution of the optical near-field is based on time-resolved two-photon photoemission microscopy (TR-2P-PEEM). In such experiments spatial resolution in the nm-scale requires long-term positioning stability of the acquired PEEM patterns. Here, methods are introduced that allow eliminating artefacts because of sample drift. In addition we present the methodology for time-resolved cross correlation measurements using polarization shaped pulses as pump excitation and bandwidth-limited probe pulses.

[1] T. Brixner et al. *Phys. Rev. Lett.* **95** (2005) 093901.

[2] M. Aeschlimann et al. *Nature* **446** (2007) 301

O 27.71 Tue 18:30 P2

**3D-Nanofocusing through the superposition of dipole radiation from second-harmonic emitters** — ●PHILIPP REICHENBACH,

PHILLIP OLK, and LUKAS ENG — Institut für Angewandte Photo-physik, Dresden, Germany

Much research has been carried out on the optical second-harmonic (SH) generation from single metallic nanoparticles (MNP). We theoretically investigate how the second-harmonic radiation from multiple MNP emitters can be superposed to form a nanofocus in 3-dimensional space.

At first we considered the possible SH radiation emitted by single spherical and cone-shaped particles, respectively. Especially nanocones seem to be good dipole SH emitters. Secondly, the SH radiation of multiple particles is then superposed. Arranging MNPs on a circle (for instance) results in a nanofocus of ca.  $\lambda/3$  in diameter, where the focal position can be tuned in space through distinct phase conditioning, such as tilting of the exciting beam.

O 27.72 Tue 18:30 P2

**Evaluation of near-field enhanced Raman spectroscopy on industrial silicon structures** — ●BENJAMIN UHLIG<sup>1</sup>, JENS-HENDRIK ZOLLONDZ<sup>2</sup>, MARTIN HABERJAHN<sup>2</sup>, PETER KÜCHER<sup>3</sup>, and LUKAS M. ENG<sup>4</sup> — <sup>1</sup>Fraunhofer-Institut für Keramische Technologien und Systeme, Winterbergstrasse 28, 01277 Dresden, Germany — <sup>2</sup>Qimonda Dresden GmbH & Co. OHG, Königsbrücker Strasse 180, D-01099 Dresden, Germany — <sup>3</sup>Center of Competence CoC Metrology/Analytic, Fraunhofer-Center Nanoelektronische Technologien CNT, Königsbrücker Straße 180, D-01099 Dresden, Germany — <sup>4</sup>Institut für Angewandte Photophysik, TU Dresden, George-Bähr-Straße 1, D-01069 Dresden, Germany

Following Moore's Law, semiconductor structures become smaller and smaller. The understanding of stress intentionally implemented in devices or stress in multi-layer components due to thermal mismatch is a major challenge for metrology. A promising technique to obtain highly localized stress information is Tip Enhanced Raman Spectroscopy (TERS). This paper discusses under which conditions TERS can be applied to industrial semiconductor structures and which effects can be expected. In order to obtain an idea of the enhancement effects on Silicon, we show several Surface Enhanced Raman Spectroscopy (SERS) experiments using gold and silver nanoparticles. Parameters like particle size, incident laser wavelength and polarization settings are discussed and a first prove of a near-field like, surface sensitive enhancement on a semiconductor sample is shown.

O 27.73 Tue 18:30 P2

**Calculation of optical near and far fields at metal-semiconductor hybrids** — ●PATRICK SCHOLZ, STEPHAN SCHWIEGER, DAVID LEIPOLD, and ERICH RUNGE — Fachgebiet Theoretische Physik I, Technische Universität Ilmenau, 98693 Ilmenau, Germany

We calculate electromagnetic field distributions on nanostructured metal-semiconductor hybrids that are illuminated with photons near the semiconductor exciton resonance. We solve Maxwell's equations in frequency (COMSOL, RF module) and time (Lumerical, inc, FDTD solutions) space. Further, we test an approximative boundary condition (SIBC) to avoid the calculation of the fields inside the metal and speed up the calculations. Surface plasmon polaritons (SPPs) and excitons can coexist in these structures and coupled SPP-exciton modes can be formed. The coupling allows to transfer energy from pumped excitons into SPP modes. This compensates the large SPP losses. We discuss the resulting enhancement of SPP life times and propagation lengths.

O 27.74 Tue 18:30 P2

**Time- and energy resolved photoelectron emission microscopy on micro- and nanostructured samples** — ●CHRISTIAN SCHNEIDER, MARTIN ROHMER, DANIELA BAYER, PASCAL MELCHIOR, and MARTIN AESCHLIMANN — Department of Physics and Research Center OPTIMAS, University of Kaiserslautern, 67663 Kaiserslautern, Germany

The electronic response on optical excitation of nanostructured samples exhibits fascinating effects, such as subwavelength variations of the field strength and local field enhancements. Combining photoelectron emission microscopy (PEEM) with a femtosecond laser pump-probe-setup enables us to investigate these effects with simultaneous subwavelength spatial and femtosecond temporal resolution. A microscopic understanding of the collective electronic oscillations in nanostructures, like localized surface plasmons (LSPs) or surface plasmon polaritons (SPPs) is still missing. The technique of time-resolved PEEM gives us the opportunity to directly measure the transient lo-

cal near field as well as the electron dynamics of metallic nanostructures. The electron dynamic is strongly energy dependent regarding the excited carriers. Therefore, we upgraded our imaging unit with a ToF energy analyser (delayline-detector). This novel setup allows us to simultaneously acquire data with high spatial resolution in the nanometer regime, femtosecond time resolution and energy resolution. We will show first spectra of well prepared surfaces as well as energy resolved lifetime-maps of micro- and nanostructured samples showing LSP- and SPP-resonances.

O 27.75 Tue 18:30 P2

**Tip-Enhanced Optical Microscopy of Single-Walled Carbon Nanotubes** — ●CARSTEN GEORGI<sup>1</sup>, MIRIAM BÖHMLER<sup>1</sup>, HUIHONG QIAN<sup>1</sup>, LUKAS NOVOTNY<sup>2</sup>, and ACHIM HARTSCHUH<sup>1</sup> — <sup>1</sup>Department Chemie und Biochemie & CeNS, Ludwig-Maximilians-Universität München, Germany — <sup>2</sup>The Institute of Optics, University of Rochester, New York 14627, USA

Optical Microscopy with nanoscale spatial resolution is an essential technique for the characterization and investigation of individual nanoobjects. We use the field enhancement in the proximity of a laser-illuminated sharp metal tip to locally probe the optical response of single-walled carbon nanotubes. In particular we image their Raman scattering and photoluminescence properties with a spatial resolution of down to 10nm [1]. We can thereby directly observe the interaction of excitons with localized defects and the local environment of the nanotube, namely DNA-wrapping [2]. Inter-nanotube energy transfer was studied for different pairs of semiconducting nanotubes forming bundles and crossings, related to electromagnetic near-field coupling [3]. We also report on our recent experimental results on electrically contacted nanotubes and the photoluminescence of nanotubes on metal surfaces.

[1] A. Hartschuh, *Angew. Chem. Int. Ed.* 47, 8178 (2008)

[2] H. Qian et al., *Nano Lett.* 8, 2706 (2008)

[3] H. Qian et al., *Nano Lett.* 8, 1363 (2008)

O 27.76 Tue 18:30 P2

**Metamaterial Bragg-Stacks** — ●RALF AMELING and HARALD GIESSEN — 4th Physics Institute, University of Stuttgart, Germany

Double-fishnet metamaterials consist of two layers of crossed metal wires and can show a negative refractive index for visible or infrared light when the unit cell is smaller than the wavelength of light. We demonstrate coupling of the symmetric and anti-symmetric magnetic resonances of the metamaterial with Bragg-modes in the infrared, where the dielectric space between two double-fishnet meshes forms the Bragg-cavity. The meshes with typical periods of several hundred nanometers are fabricated using electron-beam lithography and a layer-by-layer stacking technique. Experiments and simulations of up to four stacked layers of gold meshes with different distances are performed. The behavior of the resonances (anti-crossing) as well as the influence of structure parameter variations is studied. The resonances are measured using FTIR-spectroscopy.

O 27.77 Tue 18:30 P2

**Metamaterial Biosensors** — ●MARTIN MESCH, ZHAOLU DIAO, NA LIU, and HARALD GIESSEN — 4th Physics Institute, University of Stuttgart, Germany

In our work we use the tailored optical properties of metallic metamaterial structures to measure the concentration of biologically relevant molecules in solution.

In metamaterials, the structures consist of a basic element, the well-known split ring resonator (SRR), periodically repeated in two dimensions. Combining two of those SRRs in a symmetry-breaking fashion results in a coupled system which displays a sharp resonance in transmission and reflection of incident light. The structure is very sensitive to its vicinity, and therefore a sensor can be built by observing the shift of the resonance position. To distinguish between different molecules, a sensitive biological element (e.g., antibodies, enzymes, cell receptors) is attached to the structure, which responds positively to the molecules that are supposed to be detected.

Several experimental examples will be demonstrated, and the limits to sensitivity will be discussed.

O 27.78 Tue 18:30 P2

**New designs of scanning nearfield optical microscopy probes for the time resolved investigation of nanostructures** — ●MARC SALOMO, BERNHARD SCHAUF, DANIELA BAYER, MARTIN AESCHLIMANN, and EGBERT OESTERSCHULZE — Technische Universität Kaiser-

slautern, D-67663 Kaiserslautern, Germany

Scanning Nearfield Optical Microscopy (SNOM) is a versatile tool to investigate nanostructured samples. Using a pump-probe setup with a femtosecond laser system as excitation source we have the ability to optically image nanostructures with high spatial and temporal resolution. Another advantage of the probes is the capability to simultaneously perform AFM, thus also gaining topographical information about the sample. This information is essential as local defects on the surface have strong influence on the damping of e.g. localized surface plasmons (LSPs). The nearfield emitted from the SNOM-aperture excites collective electron oscillations. These processes are strongly dependent on the characteristics of the interaction between the sample and the SNOM-tip. Simulations are presented to demonstrate the suitability of the proposed probe designs for time resolved measurements on the subwavelength scale, evaluating transmission capability and pulse dispersion. In the experiment antenna based aperture probes are tailored via focused ion beam milling as well as electron beam lithography of hollow metal coated silicon dioxide pyramids. First measurements on the characterization of the sensors are presented.

O 27.79 Tue 18:30 P2

**Spectroscopy of superconducting  $V_3Si(001)$  in tunneling and contact regime** — NADINE HAUPTMANN, MICHAEL BECKER, JÖRG KRÖGER, and RICHARD BERNDT — Institut für Experimentelle und Angewandte Physik, Christian-Albrechts-Universität zu Kiel, D-24098 Kiel, Germany

The energy gap of the superconductor  $V_3Si$  is monitored on a yet unknown surface reconstruction most likely induced by carbon. Depending on the surface position spectroscopy reveals an asymmetric energy gap. The evolution of the energy gap with decreasing tip-sample distance from the tunneling to the contact regime indicates Andreev reflections in contact spectroscopy. Financial support by the DFG is gratefully acknowledged.

O 27.80 Tue 18:30 P2

**Controlling the Kondo Effect in  $CoCu_n$  Clusters Atom by Atom** — NICOLAS NÉEL<sup>1</sup>, JÖRG KRÖGER<sup>1</sup>, RICHARD BERNDT<sup>1</sup>, TIM WEHLING<sup>2</sup>, ALEXANDER LICHTENSTEIN<sup>2</sup>, and MIKHAIL KATSNELSON<sup>3</sup> — <sup>1</sup>Christian-Albrechts-Universität zu Kiel, D-24098 Kiel, Germany — <sup>2</sup>Universität Hamburg, D-20355 Hamburg, Germany — <sup>3</sup>Radboud University Nijmegen, NL-6525 AJ Nijmegen, The Netherlands

Clusters containing a single magnetic impurity were investigated by scanning tunneling microscopy, spectroscopy, and *ab initio* electronic structure calculations. The Kondo temperature of a Co atom embedded in Cu clusters on Cu(111) exhibits a non-monotonic variation with the cluster size. Calculations model the experimental observations and demonstrate the importance of the local and anisotropic electronic structure for correlation effects in small clusters. Financial support by the DFG through SFB 668 is acknowledged.

O 27.81 Tue 18:30 P2

**Thin epitaxial  $Bi(111)$  films on  $Si(111)$  studied by ARPES** — HOLGER SCHWAB<sup>1</sup>, HENDRIK BENTMANN<sup>1</sup>, FRANK FORSTER<sup>1</sup>, LUCA MORESCHINI<sup>2</sup>, MARCO GRIONI<sup>2</sup>, and FRIEDRICH REINERT<sup>1,3</sup> — <sup>1</sup>Universität Würzburg, Experimentelle Physik II, Am Hubland, D-97074 Würzburg, Germany — <sup>2</sup>Ecole Polytechnique Fédérale de Lausanne (EPFL), Institut de Physique des Nanostructures, CH-1015 Lausanne, Switzerland — <sup>3</sup>Forschungszentrum Karlsruhe, Gemeinschaftslabor für Nanoanalytik, D-76021 Karlsruhe, Germany

Employing angle-resolved photoelectron spectroscopy (ARPES) we have studied thin films of  $Bi(111)$  on a  $Si(111)$  substrate. The film growth was characterized by reflection high energy electron diffraction (RHEED). We present Fermi surfaces and band structures for different film thicknesses. Quantum well states (QWS) as well as the  $Bi(111)$  surface state are observed. Our measurements are in good agreement with previous results. The variation of the line width of the QWS was measured over a broad temperature range from 70K to 300K. This allows for the determination of the electron-phonon coupling constant  $\lambda$  as a function of film thickness.

O 27.82 Tue 18:30 P2

**Spin-resolved inverse photoemission experiments on  $Ni/GaAs(001)$**  — CHRISTIAN EIBL, ANDRÉ BERKEN, MANUEL PRÄTORIUS, ANKE B. SCHMIDT, and MARKUS DONATH — Physikalisches Institut, Westfälische Wilhelms-Universität Münster

To understand the interplay between crystal structure, electronic

states, and magnetism, it is worthwhile to compare the different ferromagnetic elements. Unfortunately, the thermodynamically stable crystal structures of Ni, Fe, and Co are face-centered cubic (fcc), body-centered cubic (bcc), and hexagonal close-packed (hcp), respectively. Thus, a direct comparison is hampered and scientists endeavor to crystallize Fe, Co, and Ni in a non-native structure.

Recently, it was shown by Tian *et al.* that Ni can be stabilized in the bcc structure on a GaAs(001) substrate. In contrast to the fcc structure, it was found that bcc Ni exhibits different magnetic properties, e.g., Curie temperature and magnetic anisotropy. Additionally, a photoemission experiment revealed differences in the electronic structure below the Fermi level [1].

To gain further insight into the electronic structure of bcc Ni also above the Fermi level, we used spin-resolved inverse photoemission to investigate Ni films on GaAs(001) as a function of thickness. Furthermore, we compared our results with measurements on fcc Ni/Cu(001).

[1] C.S. Tian *et al.*, Phys. Rev. Lett. **94**, 137210 (2005)

O 27.83 Tue 18:30 P2

**Comparison of angular resolved photoemission on  $Pt(110)$  with DFT bulk band calculations** — ALEXANDER MENZEL, CHRISTIAN BRAUN, PETER AMANN, and ERMALD BERTEL — Institute for Physical Chemistry, University of Innsbruck, Austria

Angular resolved photoemission (ARPES) experiments of clean and halogenated  $Pt(110)$  are compared with the DFT-derived bulk band structure of Platinum. Numerous dispersion features agree with the calculated one-dimensional density of states (kz-histogram) indicating emission from near surface transitions. In order to distinguish the effects of initial state (surface resonances), matrix element (surface photoemission) and final state (strong photoelectron damping), we varied incident polarization, photon energy, and surface phase symmetry.

O 27.84 Tue 18:30 P2

**Electronic fine structures of perfluoropentacene films by ultraviolet photoelectron spectroscopy** — SHUNSUKE HOSOMI, SHINICHI NAGAMATSU, SATOSHI KERA, and NOBUO UENO — Chiba University, Japan

Pentacene (PEN) and perfluoropentacene (PFP) are currently the most potential conjugated organic molecules as active materials in novel electronic devices[1]. The intramolecular charge reorganization energy ( $\lambda$ ), which is related to the electron-phonon coupling, is important parameter for efficient transport of charges in organic materials and across related interfaces. However,  $\lambda$  has been discussed based on highly-resolved spectra of gas-phase molecules [2]. Recently, we have succeeded to assess  $\lambda$  directly from the fine features in high-resolution UPS of organic solid systems by fabricating a well-ordered monolayer deposited on graphite [3]. In this paper, we compare the electronic structures of the well-ordered monolayer both for PEN/graphite and PFP/graphite. The UPS band derived from the highest occupied molecular orbital (HOMO) for both monolayer systems shows fine structures clearly, indicating the molecular vibrational modes strongly couple to photoelectron (HOMO hole). The  $\lambda$  for PFP is about two times larger than PEN. The take-off angle dependence of the UPS spectra that the Franck-Condon principle is not strictly satisfied in the photoionization process will be discussed.

[1] Y. Inoue *et al.*, Jpn. J. Appl. Phys. **44**, 3663 (2005). [2] J-L. Bredas *et al.*, Chem. Rev. **104**, 4971 (2004). [3] H. Yamane *et al.*, Phys. Rev. B **72**, 153412 (2005).

O 27.85 Tue 18:30 P2

**Tunneling Spectroscopy of nanoporous networks - comparison of experiment and modelization** — WOLFGANG KRENNER<sup>1</sup>, DIRK KÜHNE<sup>1</sup>, FLORIAN KLAPPENBERGER<sup>1</sup>, IÑAKI SILANES<sup>2</sup>, ANDRES ARNAU<sup>2</sup>, JAVIER GARCÍA DE ABAJO<sup>3</sup>, SVETLANA KLYATSKAYA<sup>4</sup>, MARIO RUBEN<sup>4</sup>, and JOHANNES BARTH<sup>1</sup> — <sup>1</sup>Physik Department E20, TU München, Germany — <sup>2</sup>Donostia International Physics Center (DIPC) and Departamento de Física de Materiales and Unidad de Física de Materiales, E-20018 San Sebastian, Spain — <sup>3</sup>Instituto de Óptica CSIC, Serrano 121, 28006 Madrid, Spain — <sup>4</sup>Institute of Nanotechnology, Forschungszentrum Karlsruhe, Karlsruhe, Germany

We present spectroscopic data obtained by Scanning Tunneling Spectroscopy (STS) from self-assembled organic and metal coordinated carbonitrile polyphenyl (CN-Ph<sub>x</sub>-NC) networks deposited on a  $Ag(111)$  surface under ultra high vacuum conditions. The molecules form highly regular organic networks depending on the length of the molecules and coverage. By further evaporating Co onto the sample, metal coordinated honeycomb networks are formed by three CN-Ph<sub>x</sub>-NC molecules

binding to one Co atom.

These networks impose a modulation upon the local density of states (LDOS) of the quasi 2D electron system of the Ag surface state. Different types of networks were investigated by STS. The lateral confinement of the electrons manifested in various standing wave patterns in dI/dV maps at different energies. First results show good agreement with modelling by a boundary element method.

O 27.86 Tue 18:30 P2

**Implementation of the HSE functional in the FLAPW method** — ●MARTIN SCHLIPF, CHRISTOPH FRIEDRICH, and STEFAN BLÜGEL — Institut für Festkörperforschung und Institute for Advanced Simulation, Forschungszentrum Jülich, D-52425 Jülich, Germany

Despite the remarkable success of density-functional theory (DFT) in the local density (LDA) or the generalized-gradient approximation (GGA) for the exchange-correlation functional, these standard functionals do not properly describe the structural and magnetic properties of oxide materials. This failure can in many cases be attributed to the uncompensated self-interaction error in LDA and GGA. In hybrid functionals that incorporate a portion of Hartree-Fock-like exact exchange the self-interaction error is considerably reduced. Among these the HSE [1] functional proved to give exceptionally good agreement with experimental data. In this contribution, we discuss the realization of the HSE functional within the all-electron full-potential linearized augmented planewave (FLAPW) method, where space is partitioned into muffin-tin spheres centered at the atomic nuclei and the interstitial region. Within the muffin-tin spheres the wave functions are expressed by numerical functions on a radial grid time spherical harmonics, while planewaves are used in the interstitial region. The exchange potential is given by an integral over the attenuated Coulomb interaction and four of these basis functions. We discuss the implementation of these integrals.

[1] Heyd, Scuseria, Ernzerhof, J. Chem. Phys. **118**, 9207 (2003)

O 27.87 Tue 18:30 P2

**In situ Epitaxy and Catalysis at the High Resolution Diffraction Beamline at PETRA III** — ●CARSTEN DEITER and OLIVER H. SEECK — Hasylab am DESY, Notkestr. 85, 22607 Hamburg, Germany

In spring 2009 the new synchrotron radiation source PETRA III will become operational. At the High Resolution Diffraction Beamline (P08) the equipment and the beam parameters are highly suited for surface and interface studies. Beside traditional sample environments such as variable temperature (70K-700K) cells with vacuum ( $10^{-6}$ mbar) or inert gas inside, an ultra high vacuum chamber will be available to perform in situ molecular beam epitaxy, sputter cleaning and/or catalysis x-ray experiments. The temperature of the sample can be varied from 100K to 1000K for metals and insulators and from 100K to 1500K for semiconductors, respectively. This chamber will be installed in a six circle diffractometer (Kohzu) for extreme angular resolution and supported by an UHV infrastructure close by.

O 27.88 Tue 18:30 P2

**Improved determination of the IMFP by extracting the optimum loss function from EELS** — ●TINA GRABER<sup>1</sup>, FRANK FORSTER<sup>1</sup>, ACHIM SCHÖLL<sup>1</sup>, and FRIEDRICH REINERT<sup>1,2</sup> — <sup>1</sup>Universität Würzburg, Experimentelle Physik II, Am Hubland, 97074 Würzburg — <sup>2</sup>Gemeinschaftslabor für Nanoanalytik, Forschungszentrum Karlsruhe, 76021 Karlsruhe

A precise knowledge of the inelastic mean free path (IMFP) of electrons in matter is of crucial interest in many respects. If electron spectroscopic techniques are applied in surface and interface science, the attenuation length of the involved electrons has to be established in order to gain information on, e.g., probing depth, adsorbate film thickness, or growth modes. In this work we present a systematic study on the IMFP of electrons in thin films of organic molecules by means of photoelectron spectroscopy (PES) and using the model system PTCDA/Ag(111). This system can be carefully controlled for a precise determination of the IMFP since layer-by-layer growth is necessary. Moreover, an appropriate description of the PES background is needed. For this purpose electron energy loss spectroscopy (EELS) provides valuable information on the relevant loss mechanisms. From the EELS data the optimum loss function can be determined. This loss function was subsequently applied for a Tougaard description of the PES background using the QUASES software[1]. In addition, the dependence of the IMFP on the emission angle has been investigated in order to find evidence for scattering channels or favored emission angles. [1] S. Tougaard, Software Package, Vers. 5.1 (2005)

O 27.89 Tue 18:30 P2

**Soft x-ray standing wave excited photoemission experiments on Si/MoSi<sub>2</sub> multilayer mirrors** — ●FRANK SCHÖNBOHM<sup>1,2</sup>, SVEN DÖRING<sup>1,2</sup>, DANIEL WEIER<sup>1,2</sup>, ULF BERGES<sup>1,2</sup>, FELIX LEHMKÜHLER<sup>1,2</sup>, CHARLES S. FADLEY<sup>3,4</sup>, and CARSTEN WESTPHAL<sup>1,2</sup> — <sup>1</sup>Fakultät Physik - TU Dortmund, Otto-Hahn-Str. 4, 44221 Dortmund, Germany — <sup>2</sup>DELTA - TU Dortmund, Maria-Goeppert-Mayer-Str. 2, 44227 Dortmund, Germany — <sup>3</sup>Materials Sciences Division, LBNL, Berkeley, CA 94720, USA — <sup>4</sup>University of California, Davis, CA 95616, USA

The structure of thin layers and the formation of interfaces is of particular interest in surface science. Element specific sample analysis can be performed by means of photoelectron spectroscopy but the method lacks of a good spatial resolution. On the other hand, reflectivity measurements show a good depth-resolution without chemical sensitivity. Thus x-ray standing wave measurements were conducted in order to combine the advantages of these methods. We used Si/MoSi<sub>2</sub> multilayer mirrors as a sample substrate in order to increase the reflectivity. The measurements were performed at the experimental endstation at Beamline 11 at DELTA at a photon energy of  $h\nu = 650$  eV. The multilayer was handled in ambient air resulting in an oxidized silicon layer at the surface. This Si layer with its SiO<sub>2</sub> cap was used as a first test system for our XSW measurements. Analysis of the received data indicates that the surface oxidation of the upper most Si film results in a SiO<sub>2</sub> layer of 13 Å thickness with a non-oxidized Si-film of 15.5 Å beneath it. In order to check this result we performed hard x-ray reflectivity measurements at  $h\nu = 15.2$  keV for comparison at DELTA.

O 27.90 Tue 18:30 P2

**Prozessoptimierung der Sputterstrategie von fokussierten Ionenstrahlen mit Standard "Focused Ion Beam - FIB" Anlagen** — ●RÜDIGER SCHOTT, PAUL MAZAROV, ROLF WERNHARDT and ANDREAS D. WIECK — Lehrstuhl für Angewandte Festkörperphysik, Ruhr-Universität Bochum, D-44780 Bochum

Fokussierte Ionenstrahlen sind ein vielfältiges und nützliches Werkzeug in Gebieten der Forschung und Industrie. Die Verwendung von Bismutonen zum lokalen, maskenlosen Ionenätzen in Standard FIB-Anlagen ohne Massenseparator besitzt einige Vorteile gegenüber den meist verwendeten Galliumionen. Die Bismut Flüssigmetallionenquelle [1] liefert schwere, monoisotope Ionen (209 u) und deren Cluster, wobei Teilchen mit einfacher Ladung zu 95% dominant sind. Die schweren Ionen und besonders deren Cluster dringen weniger tief in die Oberfläche der Probe ein, wodurch ihr Energieübertrag an die Oberflächenatome erhöht wird. Dies führt zu einer deutlich höheren Sputterrate und einer geringeren Kontaminationstiefe der Oberfläche. Zusätzlich wird der Ionenätzprozess optimiert, indem Parameter wie die Haltezeit pro Punkt variiert und die Ionenätzbedingungen durch das Vorformen der Probenoberfläche verbessert werden.

[1] P.Mazarov, A. Melnikov, R. Wernhardt, and A. D. Wieck, "Long-life bismuth liquid metal ion source for focussed ion beam application", Applied Surface Science **254**, 7401-7404 (2008).

O 27.91 Tue 18:30 P2

**Vielkanal-Spindetektion von niederenergetischen Elektronen** — ●MICHAELA HAHN<sup>1</sup>, PAVEL LUSHCHYK<sup>1</sup>, GERD SCHÖNHENSE<sup>1</sup>, ANDREAS OELSNER<sup>2</sup>, DANIEL PANZER<sup>2</sup>, ALEXANDER KRASYUK<sup>3</sup> und JÜRGEN KIRSCHNER<sup>3</sup> — <sup>1</sup>Institut für Physik, Johannes Gutenberg Universität, Mainz (Germany) — <sup>2</sup>Surface Concept GmbH, Staudingerweg 7, 55128 Mainz (Germany) — <sup>3</sup>Max-Planck-Institut für Mikrostrukturphysik, Halle (Germany)

Die Analyse der Spinpolarisation von Photoelektronen ist für Experimente im Bereich der Atom- und Molekülphysik, der Oberflächen- und Festkörperphysik und vor allem für Untersuchungen von ferromagnetischen Materialien von zentraler Bedeutung. Bisher verwendete Spindetektoren [1] arbeiten 'einkanalig', d.h. monoenergetisch und bei einem Detektionswinkel, was zu einer sehr geringen Messeffizienz führt. Um eine hocheffiziente spinaufgelöste Photoemissionsmessung zu ermöglichen, wird ein Multikanal-Spinpolarimeter in Betrieb genommen. Dieses wird Berechnungen zufolge durch einen Gewinn an Messeffizienz um 2-3 Größenordnungen gekennzeichnet sein. Der neue Spindetektor soll insbesondere in winkelaufgelösten Photoemissionsexperimenten mit Laborlichtquellen bei sehr niedrigen Energien (ARPES) und in Experimenten mit Synchrotronstrahlung im harten Röntgenbereich (HAXPES) zum Einsatz kommen. Ein deutlicher Vorteil ist die Reduzierung der Messzeit hinsichtlich Proben mit reaktiven Oberflächen oder für in-situ präparierte ultradünne Filme.

Gefördert durch DFG (SCHO341/9-1)

[1] J. Kessler, 'Polarized Electrons', Springer 1985

O 27.92 Tue 18:30 P2

**Electrospray Ion Beam Deposition and in-situ Analysis of Functional Molecules** — ●ZHITAO DENG<sup>1</sup>, NICHIA THONTASEN<sup>1</sup>, CHRISTIAN MICHAELIS<sup>1</sup>, NIKOLA MALINOWSKI<sup>1</sup>, STEPHAN RAUSCHENBACH<sup>1</sup>, and KLAUS KERN<sup>1,2</sup> — <sup>1</sup>Max-Planck-Institut für Festkörperforschung, Heisenbergstrasse 1, D-70569 Stuttgart, Germany — <sup>2</sup>Institut de Physique des Nanostructures, Ecole Polytechnique Fédérale de Lausanne, CH-1015 Lausanne, Switzerland

An electrospray ion beam deposition source has been developed for the soft landing deposition in ultra high vacuum of nonvolatile particles such as molecules, clusters and nanoparticles. This enables the surface modification and subsequent in-situ analysis by scanning tunneling microscopy. This poster presents the experimental aspects of ion beam deposition in UHV and gives examples for its application to functional molecules.

O 27.93 Tue 18:30 P2

**High resolution positron annihilation induced Auger spectroscopy on copper** — ●JAKOB MAYER<sup>1</sup>, KLAUS SCHRECKENBACH<sup>1,2</sup>, and CHRISTOPH HUGENSCHMIDT<sup>1,2</sup> — <sup>1</sup>Technische Universität München, Physikdepartment E21, James-Franck-Str., 85748 Garching — <sup>2</sup>ZWE FRM II, Lichtenbergstr.1, 85747 Garching

The high intensity positron source NEPOMUC at the FRM-II in Munich with a stable remoderated positron beam of  $> 10^7$  positrons/s at 20 eV enabled measurement times of 10 hours for one PAES (Positron annihilation induces Auger Electron Spectroscopy) spectrum [1]. Since the intrinsic advantages of PAES over EAES are known and have been shown (e.g. [2]), the reduction of the long measurement times is the main challenge for this non destructive technique for surface studies. For this reason, a new hemispherical electron energy analyzer was installed at the PAES facility of NEPOMUC. Compared to the former analyzer (opening angle  $\pm 3^\circ$ ) it has a much higher solid angle which allows the detection of electrons which are emitted up to an angle of  $\pm 13^\circ$  with respect to the lens system of the analyzer. In addition, the freely selectable pass energy (0-600 eV) guarantees a high transmission. Though a high energy resolution is achievable with the big mean radius of the analyzer (150 mm) and variable slits. The new setup and first spectra obtained for polycrystalline copper surfaces (15 min measurement time) will be presented. [1] C. Hugenschmidt, J. Mayer and K. Schreckenbach, Surf. Sci. 601 (2459-2466) 2007 [2] K. O. Jensen and A. Weiss, Phys. Rev. B 41 (3928-3936) 1990

O 27.94 Tue 18:30 P2

**Reconstruction of surface morphology from coherent scattering of white x-ray radiation** — ●TUSHAR SANT and ULLRICH PIETSCH — Solid State Physics Group, University of Siegen, 57068 Siegen, Germany

Static speckle experiments were performed using coherent white X-ray radiation from a bending magnet at BESSYII. Semiconductor and polymer surfaces were investigated under incidence condition smaller than the critical angle of total external reflection. The scattering pattern of the sample results from the illumination function modified by the surface roughness [1]. The periodic oscillations are caused by the illumination function whereas other irregular features are associated with sample surface. The speckle map of reflection from a laterally periodic structure like GaAs grating is studied [2]. Under coherent illumination the grating peaks split into speckles because of fluctuations on the sample surface. The surface morphology can be reconstructed using phase retrieval algorithms [3]. In case of 1D problem, these algorithms rarely yield a unique and converging solution. The algorithm is modified to contain additional propagator term and the phase of illumination function in the real space constraint. The modified algorithm converges faster than conventional algorithms. A detailed surface profiles from the real measurements of the sample are reconstructed using this algorithm. 1. Pietsch U, et al. Physica B- Condensed Matter, 357 (2005) 45.2. Panzner T, Gleber G, Sant T, Leitenberger W, Pietsch U, Thin Solid Films, 515 (2007) 5563. 3. Vartanyants I A, et al. PRB, 55 (1997) 13193.

O 27.95 Tue 18:30 P2

**Unifit 2009 - Spectrum Processing, Analysis and Presentation Software for Photoelectron Spectra** — ●RONALD HESSE, PETER STREUBEL, RÜDIGER SZARGAN, and REINHARD DENECKE — Wilhelm-

Ostwald-Institut, Universität Leipzig, 04103 Leipzig, Deutschland

The aim of the development of the program UNIFIT is to enable complete qualitative and quantitative analysis of photoelectron spectroscopy data by combining appropriate description of the spectra and their background using adequate models, convenient data handling, and excellent numerical performance for fast calculation with versatile opportunities for data transfer, comfortable handling, extensive graphical design options and fast export of high resolution graphics. To demonstrate the abilities, some major features will be addressed: (i) The three commonly applied models for fitting photoelectron spectra, i.e. product, sum, and convolution of Gaussian and Lorentzian functions, will be discussed. (ii) Improved methods for determination of valence-band edges are implemented. (iii) The determination of the transmission functions  $T(E)$  of any photoelectron spectrometer will be shown. (iv) The batch-processing submenu serves as a fast and comfortable treatment of parameter-dependent experimental series. (v) UNIFIT permits the calculation of fit-parameter errors after peak fitting. (vi) The software offers nine different presentations.

O 27.96 Tue 18:30 P2

**Surface structure of inorganic salt solutions** — ●TOBIAS HAMMER, MANUELA REICHELT, and HARALD MORGNER — Universität Leipzig, Wilhelm Ostwald Institut

The aim of our research is the investigation of the molecular structure and composition of liquid surfaces and surface near range with spectroscopic methods and, furthermore, the correlation of this information with macroscopic properties of solutions (e.g. surface tension, density). One of our most powerful techniques is Neutral Impact Collision Ion Scattering Spectroscopy (NICISS) that makes use of the energy loss of Helium projectiles being backscattered from soft matter targets. With this tool it is possible to determine elemental depth profiles and the surface structure of liquid surfaces. The spectroscopic methods used here are vacuum based techniques. Up until now, this fact has limited the choice of usable solvents to those with low vapor. At present we are about to develop the experimental set up in order to investigate volatile liquids like water. The actual state of our equipment does allow to study aqueous solutions for high salt concentrations at low temperature, while the parts needed for handling low concentrations at ambient temperatures is still under construction. For the time being, we have carried out measurements on the influence of the ion radii of the cation or the anion to the surface structure, with alternative solvents including glycerol.

O 27.97 Tue 18:30 P2

**Surface Structure of Imidazolium Based Ionic Liquids** — ●MANUELA REICHELT, TOBIAS HAMMER, and HARALD MORGNER — Wilhelm-Ostwald Institute for Physical and Theoretical Chemistry, University of Leipzig

The focus of our research interest is the investigation of the composition and molecular structure of liquid surfaces with spectroscopic methods (e.g., XPS, UPS, MIES) and the correlation of these information with macroscopic properties of solutions (e.g., surface tension). One of our most powerful techniques is Neutral Impact Collision Ion Scattering Spectroscopy (NICISS) that uses the energy loss of Helium projectiles being backscattered from soft matter targets.

The last years have seen an increasing research interest in ionic liquids (ILs), salts that are fluid below 100°C and show numberless possible combinations of cations and anions. However, the physico-chemical behavior of ILs is still not completely understood. Additionally, the knowledge of the molecular surface structure and the surface composition of ILs is necessary for understanding chemical reactions at the surface (e.g., the mechanism of catalysis).

In the presented work we combined NICISS and XPS to investigate the elemental surface composition, elemental concentration depth profiles of the near surface area and the molecular surface structure of two homologous series of imidazolium based ILs. While the kind of anion namely hexafluorophosphate and bis(trifluoromethylsulfonyl)imide was fixed, respectively, the alkyl chain length of the cation was varied to analyze their influence on the properties under study.

O 27.98 Tue 18:30 P2

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O 27.99 Tue 18:30 P2

**Graphene-protected iron layer on Ni(111)** — ●YURIY DEDKOV<sup>1</sup>, MIKHAIL FONIN<sup>2</sup>, ULRICH RÜDIGER<sup>2</sup>, and CLEMENS LAUBSCHAT<sup>3</sup> — <sup>1</sup>FHI Berlin — <sup>2</sup>Uni Konstanz — <sup>3</sup>TU Dresden

Magnetic thin films with out-of-plane (or perpendicular) magnetic anisotropy play an important role in nanotechnology. Such systems can be used as perpendicular recording media which are predicted to allow information storage densities of up to 1 Tbit/in.<sup>2</sup> a quadrupling of today's highest areal densities. Along with the widely used materials with out-of-plane magnetic anisotropy such as CoPt or FePt alloys, face-centered cubic (*fcc*) Fe thin films also showing perpendicular magnetic anisotropy have recently attracted considerable interest as possible candidates for applications in novel magnetic data storage devices. Here Fe which originally has body centered cubic (*bcc*) structure can be stabilized in  $\gamma$  phase (*fcc*) at room temperature in thin epitaxial films grown on suitable *fcc* substrates. Here we report a photoemission study of the Fe intercalation underneath a graphene layer on Ni(111). The process of intercalation was monitored by means of x-ray photoemission of corresponding core levels as well as ultraviolet photoemission of the graphene-derived  $\pi$  states in the valence band. Thin *fcc* Fe layers (2-5 ML thickness) at the interface between a graphene capping layer and Ni(111) form epitaxial films passivated from the reactive environment.

O 27.100 Tue 18:30 P2

**STM growth study of epitaxial graphene on SiC(0001)** — ●ANNE MAJERUS, VIKTOR GERINGER, SVEN RUNTE, MARCUS LIEBMANN, and MARKUS MORGENSTERN — II. Physikalisches Institut, RWTH Aachen and JARA-FIT, Otto-Blumenthal-Straße, 52074 Aachen

The easiest way to produce graphene is mechanical exfoliation from graphite crystals [K. S. Novoselov et al., Science 306, 666 (2004)]. However, the preparation of graphene under clean conditions requires the use of ultra high vacuum (UHV) [I. Forbeaux et al., Appl. Surf. Sci. 162, 406 (2000)].

In this work, we present a growth study of graphene on SiC. An untreated SiC(0001) crystal was put through several annealing cycles until we produced a few layers of epitaxial graphene. To determine the changes in the morphology during the different stages of graphitization, low-energy electron diffraction (LEED) and scanning tunneling microscopy (STM) measurements were performed. The surface structures determined by LEED could also be detected directly by STM, exhibiting atomic resolution.

O 27.101 Tue 18:30 P2

**How does graphene grow? Easy access to well-ordered graphene monolayers** — ●FRANK MÜLLER<sup>1</sup>, HERMANN SACHDEV<sup>2</sup>, STEFAN HÜFNER<sup>1</sup>, ANDREW J. POLLARD<sup>3</sup>, EDWARD W. PERKINS<sup>3</sup>, JAMES C. RUSSELL<sup>3</sup>, PETER H. BETON<sup>3</sup>, STEFAN GSELL<sup>4</sup>, MATTHIAS SCHRECK<sup>4</sup>, and BERND STRITZKER<sup>4</sup> — <sup>1</sup>Institut für Experimentalphysik, Universität des Saarlandes, 66041 Saarbrücken, Germany — <sup>2</sup>Institut für Anorganische Chemie, Universität des Saarlandes, 66041 Saarbrücken, Germany — <sup>3</sup>School of Physics and Astronomy, University of Nottingham, NG7 2RD, UK — <sup>4</sup>Institut für Physik, Universität Augsburg, 86135 Augsburg, Germany

In the present study [1], the selective formation of large-scale graphene

layers on a Rh-YSZ-Si(111) multilayer substrate by a surface-induced chemical growth mechanism was investigated using low energy electron diffraction (LEED), x-ray photoelectron spectroscopy (XPS), x-ray photoelectron diffraction (XPD) and scanning tunneling microscopy (STM). It is shown that well-ordered graphene layers can be grown using simple and controllable procedures. In addition, temperature dependent experiments provide insight into the details of the growth mechanisms. A comparison of different precursors shows that a mobile dicarbon species (e.g. C<sub>2</sub>H<sub>2</sub> or C<sub>2</sub>) acts as a common intermediate for graphene formation. These new approaches offer a scalable approach for the large scale production of high-quality graphene layers on silicon based multilayer substrates.

[1] F. Müller, EU-STREP (Specific Targeted Research Project) NanoMesh, Final Meeting, Orscholz, Germany 2008, in submission

O 27.102 Tue 18:30 P2

**Low-temperature elastic and inelastic Scanning Tunneling Spectroscopy on monolayer graphene on SiC** — ●CARSTEN TRÖPPNER<sup>1</sup>, NORBERT MAURER<sup>1</sup>, FLORIAN SPECK<sup>2</sup>, THOMAS SEYLLER<sup>2</sup>, and M. ALEXANDER SCHNEIDER<sup>1</sup> — <sup>1</sup>Lehrstuhl für Festkörperphysik, Universität Erlangen-Nürnberg, Staudtstr. 7, 91058 Erlangen — <sup>2</sup>Lehrstuhl für Technische Physik, Universität Erlangen-Nürnberg, Erwin-Rommel-Str. 1, 91058 Erlangen

We employ Scanning Tunneling Spectroscopy in liquid Helium to investigate the electronic structure of a monolayer graphene grown epitaxially on SiC(0001). Spatially resolved differential conductance maps reveal a richness of features that can partially attributed to the SiC/graphene interface. Area averages of such maps reveal a "standard" spectrum that agrees with spectra obtained in UHV [1]. Furthermore clear evidence for inelastic (phononic) contributions in the differential conductance of the tunnelling junction are found, offering a natural interpretation for the observed "zero bias anomalies" [2]. The spatial dependence of these features is discussed.

[1] P. Lauffer, et al. Phys. Rev. B **77**, 155426 (2008) [2] V.W. Brar et al. Appl. Phys. Lett. **91**, 122102 (2007)

O 27.103 Tue 18:30 P2

**Comparative study of graphene films on two hexagonal SiC surfaces produced in different environments** — ●K.V. EMTSEV<sup>1</sup>, T. OHTA<sup>2</sup>, TH. SEYLLER<sup>1</sup>, L. LEY<sup>1</sup>, A. BOSTWICK<sup>3</sup>, K. HORN<sup>4</sup>, G. KELLOG<sup>2</sup>, J.L. MCCHESENEY<sup>3</sup>, E. ROTENBERG<sup>3</sup>, and A.K. SCHMID<sup>5</sup> — <sup>1</sup>FAU Erlangen-Nürnberg — <sup>2</sup>Sandia National Laboratories, USA — <sup>3</sup>Advances Light Source, USA — <sup>4</sup>FHI, Berlin — <sup>5</sup>National Center for Electron Spectroscopy, USA

In present work we discuss the graphene formation on both hexagonal SiC surfaces carried out in different environments and in dependence of several processing conditions. As was shown recently [1] the domain size of graphene monolayer formed on SiC(0001) surface in an inert atmosphere can extend over several tens of micrometers in contrast to samples prepared in vacuum showing small domains. The graphene layers were characterized by X-ray photoelectron spectroscopy, atomic force microscopy, and low energy electron microscopy. As compared to vacuum annealing, graphitization in inert atmosphere takes place at higher temperature. This has a profound effect on the morphology of the surfaces. The time dependence of graphene film thickness is quite different for two crystal orientations. While the thickness saturates rapidly for graphene on the (0001) surface, the (000-1) surface of SiC shows an unsaturated growth for film thicknesses of up to tens of monolayers. The nucleation of graphene on the (0001) surface is more homogeneous and is initiated at the substrate steps. On the (000-1) surface an inhomogeneous multilayer nucleation is observed. [1] K.V. Emtsev, et al, arXiv:0808.1222v1.

O 27.104 Tue 18:30 P2

**Preparation and investigation of graphene on Rh(111)** — ●OLE ZANDER<sup>1</sup>, MIKHAIL FONIN<sup>1</sup>, SÖNKE VOSS<sup>1</sup>, ULRICH RÜDIGER<sup>1</sup>, and YURI S. DEDKOV<sup>2</sup> — <sup>1</sup>Fachbereich Physik, Universität Konstanz, 78457 Konstanz — <sup>2</sup>Fritz-Haber-Institut der Max-Planck-Gesellschaft, 14195 Berlin, Germany

Graphene, a flat monolayer of carbon atoms packed in a honeycomb-lattice, exhibits exceptional electronic properties characteristic for twodimensional Dirac fermions. There are three major ways of graphene preparation: exfoliation of graphite, thermal decomposition (graphitization) of SiC and low pressure chemical vapor deposition (CVD) on noble metals. The latter method is the most promising route for large-scale graphene preparation yielding excellent film qualities with low defect densities over large length scales. Depending on

the metallic substrate, graphene grows completely flat or corrugated.

By using CVD we succeeded in growing a monolayer of graphite on Rh(111). High resolution scanning tunneling microscopy (STM) imaging revealed a corrugated graphene superstructure of about 30 Å periodicity. Depending on the preparation conditions we observed either a mixture of several superstructures occurring at lower preparation temperatures with periodicities from 11 Å up to 30 Å, or a single phase, the 30 Å moiré-pattern, at higher temperatures. Moreover, we successfully used graphene nanomesh on Rh(111) as a template for the growth of highly-ordered d-metal cluster arrays as suggested in [1].

[1] N'Diaye et al., Phys. Rev. Lett. 97, 215501 (2006).

O 27.105 Tue 18:30 P2

**Atomic Layer Deposition of Aluminum Oxide Films on Graphite and Graphene** — ●FLORIAN SPECK, MARKUS OSTLER, JONAS RÖHRL, KONSTANTIN V. EMTSEV, LOTHAR LEY, and THOMAS SEYLLER — Lehrstuhl für Technische Physik, Universität Erlangen-Nürnberg, Erwin-Rommel-Str. 1, D-91058 Erlangen, Germany

The fabrication of top-gated graphene-based field effect devices requires the deposition of a suitable gate insulator on graphene. Atomic layer deposition (ALD) is a low-temperature process, which could be useful for this purpose. Therefore, we studied the growth of aluminum oxide ( $\text{Al}_2\text{O}_3$ ) from trimethylaluminum (TMA) and water ( $\text{H}_2\text{O}$ ) or ozone ( $\text{O}_3$ ) on highly oriented pyrolytic graphite and graphene. Graphene was prepared by thermal decomposition of SiC. Three different processes were compared: (A) standard ALD growth of  $\text{Al}_2\text{O}_3$  using TMA and  $\text{H}_2\text{O}$ ; (B) ALD growth using TMA and  $\text{O}_3$ ; (C) pre-growth treatment of the substrate using  $\text{O}_3$  pulses followed by standard growth according to (A). The films and interfaces were studied using photoelectron spectroscopy and atomic force microscopy. While process (A) leads to an inhomogeneous nucleation of  $\text{Al}_2\text{O}_3$ , process (B) forms closed films with high nucleation density, but affects the integrity of the graphene layers. Process (C) leads to smooth and conformal  $\text{Al}_2\text{O}_3$  films with little damage to the graphene substrate. The influence of the duration of the initial  $\text{O}_3$  exposure as well as of the growth temperature on the properties of the ALD- $\text{Al}_2\text{O}_3$  films is discussed.

O 27.106 Tue 18:30 P2

**Spin dependent surface barrier resonance studied by spin-polarized electron energy loss spectroscopy** — YU ZHANG<sup>1</sup>, JACEK PROKOP<sup>1</sup>, IOAN TUDOSA<sup>1</sup>, WEN XIN TANG<sup>1</sup>, ●THIAGO R. F. PEIXOTO<sup>1,2</sup>, KHALIL ZAKERI<sup>1</sup>, and JÜRGEN KIRSCHNER<sup>1</sup> — <sup>1</sup>Max-Planck Institut für Mikrostrukturphysik, Weinberg 2, 06120 Halle — <sup>2</sup>Instituto de Física, Universidade de São Paulo, São Paulo, Brazil

It has been shown that the surface barrier resonance can be detected by electron energy loss spectroscopy [1]. In this work, we use the spin-polarized electron energy loss spectroscopy (SPEELS) to investigate the spin dependence of the surface barrier resonance in the oxygen passivated Fe films grown on W(001). The peaks induced by the surface barrier resonance were observed when measuring the intensity of the specularly reflected electrons as a function of the primary energy from 3 to 40 eV. Depending on the spin polarization and the incident angle, the peaks showed different intensities and energies. Large spin asymmetries, up to 80%, were found at about 4 eV. The peaks due to the surface barrier resonance can be also clearly observed in the energy loss spectra measured in the off-specular geometry. The dispersion of the surface barrier resonances obtained from both the peak energies and the momentum transfer clearly shows the spin dependence.

[1] D. Rebenstorff, H. Ibach and J. Kirschner, Solid State Communications, 56, 885 (1985).

O 27.107 Tue 18:30 P2

**Magnetism of Rh nano-structures on inert Xe buffer layers and in contact with Ag(100) surfaces** — ●VIOLETTA SESSI<sup>1</sup>, JIAN ZHANG<sup>1</sup>, KLAUS KUHNKE<sup>1</sup>, CARSTEN TIEG<sup>2</sup>, AXEL ENDERS<sup>3</sup>, JAN HONOLKA<sup>1</sup>, and KLAUS KERN<sup>1</sup> — <sup>1</sup>Max Planck Institut für Festkörperforschung, Stuttgart, Deutschland — <sup>2</sup>European Synchrotron Radiation Facility, Grenoble, France — <sup>3</sup>University of Nebraska, Lincoln, USA

Previous x-ray magnetic circular dichroism measurements have shown that sub-monolayer coverages of Rh directly deposited on Ag(100) at T=5K are not magnetic [1], in contrast to theoretical predictions [2]. We have investigated this discrepancy and studied the magnetism of Rh nano-structures prepared on inert Xe buffer layers (Buffer Layer Assisted Growth [3]) on Ag(100). For Rh nano-structures (monomers, dimers, trimers etc.) situated on the Xe buffer layer we find a cluster

size-dependent magnetic moment similar to the one measured on free clusters in the Stern-Gerlach experiment [4]. During desorption of the Xe layer the Rh nano-structures grow in size and make contact with the substrate, which leads to a full quenching of the magnetic moment. The results are discussed modelling the Rh cluster size distribution and magnetic ordering on Xe and Ag(100).

[1] J. Honolka et al., Phys. Rev. B 76, 144412 (2007) [2] P. Lang, V.S. Stepanyuk, K. Wildberger, R. Zeller, and P.H. Dederichs., Solid State Commun. 92, 755 (1994) [3] J.H. Weaver, G.D. Waddill, Science 251, 1444 (1991) [4] A.J. Cox, J. G. Louderback, and L.A. Bloomfield, Phys. Rev. Lett. 71, 923 (1993)

O 27.108 Tue 18:30 P2

**n-Alkanes in Tubular Nanochannels: Phase Transition Behaviour and Capillary Filling** — ●DANIEL RAU<sup>1</sup>, PATRICK HUBER<sup>1</sup>, and OSKAR PARIS<sup>2</sup> — <sup>1</sup>Faculty of Physics and Mechatronics Engineering, Saarland University, D-66041 Saarbrücken, Germany — <sup>2</sup>Department of Biomaterials, Max Planck Institute of Colloids and Interfaces, Research Campus Golm, D-14424 Potsdam, Germany

We present time-dependent angle-dispersive and energy-dispersive small-angle x-ray diffraction experiments on the capillary filling of tubular nanochannels in a template-grown porous matrix (SBA-15) by a liquid hydrocarbon. These measurements reveal a square root of time, classical Lucas-Washburn law for the channel invasion dynamics. These spontaneous imbibition experiments are complemented by combined x-ray diffraction and specific heat measurements on the filled matrices, which allow us to study the phase transition behaviour of the spatially nanoconfined linear hydrocarbons.

O 27.109 Tue 18:30 P2

**The Limits of Nanomechanical Applications of Shape Memory Alloys: An Optical Approach** — ●ANDREAS KOLLOCH, JOHANNES BONEBERG, and PAUL LEIDERER — Universität Konstanz

Shape Memory Alloys (SMA), with their high strain and stress values for small temperature changes and their excellent durability against environmental influences, may prove to be ideal candidates for the driving force of nanomechanical devices. In spite of this promising potential, however, very little is known about the properties of SMA materials, and in particular thin films, on the nanoscale.

Our work concentrates on the classic SMA, Nitinol, an intermetallic compound consisting of nickel and titanium. While it is completely reversible, the martensite-austenite transition of this material is accompanied by large strain and stress changes of up to 6-8% and 600 MPa, respectively.

The project aims at employing an ultrafast thermo-optical approach to investigating whether there is a lower thickness limit of the martensitic phase transition in NiTi SMAs and what the transition speed for the phase change of these materials is.

O 27.110 Tue 18:30 P2

**Time-resolved spectroscopy beyond optical wavelengths** — ROBERT CARLEY<sup>1</sup>, ●KRISTIAN DÖBRICH<sup>1</sup>, CORNELIUS GAHL<sup>1</sup>, MARTIN TEICHMANN<sup>1</sup>, KAI GODEHUSEN<sup>2</sup>, OLAF SCHWARZKOPF<sup>2</sup>, PHILIPPE WERNET<sup>2</sup>, FRANK NOACK<sup>1</sup>, and MARTIN WEINELT<sup>1,3</sup> — <sup>1</sup>Max-Born-Institut, Max-Born-Straße 2a, 12489 Berlin — <sup>2</sup>Helmholtz-Zentrum für Materialien und Energie, Elektronenspeicherring BESSY II, Albert-Einstein-Str. 15, 12489 Berlin — <sup>3</sup>Fachbereich Physik der Freien Universität Berlin, Arnimallee 14, 14195 Berlin

We are presenting characterization results of our newly developed high-order harmonics XUV source. The beamline will be used to perform time-resolved studies of metal- and semiconductor surfaces.

We use a commercial amplified Ti:Sapphire laser system generating 30 fs pulses at 20 kHz repetition rate. The beam is focused into an argon-filled gas cell to create high-order harmonics. Following separation from the IR with a thin Al filter, the XUV wavelength can be selected using a toroidal grating monochromator. Current efforts are the optimization for an energy resolution of 100 meV and a time resolution below 100 fs.

This beamline is a joint project between MBI and BESSY and will be open as a user facility to external users.

O 27.111 Tue 18:30 P2

**Femtosecond electron dynamics in atomic wires: Si(557)-Au** — ●KERSTIN BIEDERMANN<sup>1</sup>, TILMAN K. RÜGHEIMER<sup>1</sup>, THOMAS FAUSTER<sup>1</sup>, and FRANZ J. HIMPSEL<sup>2</sup> — <sup>1</sup>Lehrstuhl für Festkörperforschung, Universität Erlangen-Nürnberg, Staudtstr. 7, 91058 Erlangen — <sup>2</sup>Department of Physics, University of Wisconsin-Madison, 1150

University Ave, Madison WI 53706, USA

Recent experiments on Si(557)-Au have proven the existence of a spin-split surface state band below  $E_F$  [1] and have provided first information on the unoccupied part of the electronic band structure [2,3]. The dynamics of electrons has not been investigated so far.

We have carried out time-resolved two-photon photoemission experiments using 37 fs infrared (IR,  $E_{IR}=1.55$  eV) and 55 fs ultraviolet (UV,  $E_{UV}=4.65$  eV) laser pulses. High intensity at 0.9 eV kinetic energy (work function  $\Phi=4.88$  eV) and time delay zero corresponds to an image-potential resonance [2,3] and has a lifetime of less than 10 fs. At lower kinetic energies the intensity spreads towards positive as well as negative time delays indicating contributions from several transitions. An intensity pile-up at positive delays (IR before UV) indicates an indirect filling of a state in the bulk band gap of the Si(557) substrate by two long-lived states. We present a detailed analysis of the data by fitting the spectra with optical Bloch equations. Our interpretation involves electron scattering between several surface states.

- [1] I. Barke et al., Phys. Rev. Lett. **97**, 226405 (2006)  
 [2] J. A. Lipton-Duffin et al., Phys. Rev. B **73**, 245418 (2006)  
 [3] T. K. Rügheimer et al., Phys. Rev. B **75**, 121401 (2007)

O 27.112 Tue 18:30 P2

**Themis1000 - A new analyzer for three dimensional measurements** — ●JENS KOPPRASCH<sup>1,2</sup>, MARTIN TEICHMANN<sup>1</sup>, OLIVER SCHAFF<sup>3</sup>, SVEN MÄHL<sup>3</sup>, and MARTIN WEINELT<sup>1,2</sup> — <sup>1</sup>Max-Born-Institut, Max-Born-Straße 2a, 12489 Berlin, Germany — <sup>2</sup>Freie Universität Berlin, Fachbereich Physik, Arnimallee 14, 14195 Berlin, Germany — <sup>3</sup>SPECS GmbH, Voltastraße 5, 13355 Berlin, Germany

We present a newly developed time-of-flight (TOF) spectrometer to measure the energy and two-dimensional angle distribution of emitted electrons. For the development of this wide-angle high-energy resolution electron analyzer a partnership between the company SPECS GmbH and the Max-Born-Institute has been arranged.

The electrostatic lens system of a PHOIBOS electron analyzer is used as a flight tube, with a delay-line detector at the end to detect both flight time and arrival position. Due to the axial symmetry of the lens system the angular distribution is measurable in the two dimensions parallel to the sample surface. We reach the same good angular resolution as for a PHOIBOS analyzer, and the same acceptance angle of about 13°. As opposed to an usual position-sensitive TOF spectrometer, the trajectory of the electrons are not linear. We could show that the mapping from arrival position to emission angle and flight time to energy is unambiguous, and by solving Hamiltons' equations numerically we were able to invert this mapping.

Furthermore, we will show the first measurement of a Cu(111) sample. This is a known system well suited for the characterization of the analyzer.

O 27.113 Tue 18:30 P2

**Time-, energy- and angle-resolved photoelectron spectroscopy of surface dynamics using femtosecond XUV pulses** — ●FREDERIK DEICKE<sup>1</sup>, STEFAN MATHIAS<sup>1</sup>, ANDREAS RUFFING<sup>1</sup>, LUIS MIAJA-AVILA<sup>2</sup>, MARGARET MURNANA<sup>2</sup>, HENRY KAPTEYN<sup>2</sup>, MICHAEL BAUER<sup>3</sup>, and MARTIN AESCHLIMANN<sup>1</sup> — <sup>1</sup>Department of Physics and Research Center OPTIMAS, University of Kaiserslautern, D-67663 Kaiserslautern, Germany — <sup>2</sup>JILA, University of Colorado, Colorado 80309-0440, USA — <sup>3</sup>Institut für Experimentelle und Angewandte Physik, Christian-Albrechts-Universität zu Kiel, D-24908 Kiel, Germany

The angle resolved photoelectron spectroscopy (ARPES) has emerged as a leading technique in identifying static key properties of complex systems such as the electronic band structure of adsorbed molecules, ultrathin quantum-well films or high temperature superconductors. We present an experimental setup combining the ARPES technique with a pump-probe scheme for time-resolved measurements using a 1 kHz femtosecond high-harmonic generation (HHG) XUV source [1]. The performance of the system with respect to time-, energy- and momentum-resolution will be discussed on the basis of ARPES spectra recorded with ultra short photon pulses of  $\tau=7$  fs and  $h\nu=42$  eV [2]. Furthermore, the potential of time-resolved ARPES to study surface dynamics in future experiments, as e.g. photo-induced phase transitions, is considered.

[1] S. Mathias et al., Rev. Sci. Instrum. **78**, 083105 (2007) [2] S. Mathias et al., Journ. of Phys. : conference proc., in print

O 27.114 Tue 18:30 P2

**Space Charge Effects in the Photoemission Electron Micro-**

**scope** — ●JAN GÖHRE, NIEMMA M. BUCKANIE, PING ZHOU, DIETRICH VON DER LINDE, MICHAEL HORN-VON HOEGEN, and FRANK-J. MEYER ZU HERINGDORF — University Duisburg-Essen, Germany

The illumination of samples in a spectroscopic Photoemission Electron Microscope (PEEM) with ultrafast laser pulses combines temporal and spatial resolution. To study the deexcitation of excited electrons, the laser should have sufficiently low pulse energy in order to minimize the space charge. Since most metals have a work function of about 5eV, a high photon energy is needed for a one photon photoemission process (1PPE). We built a regenerative Ti:sapphire amplifier system which generates ultrafast fs-pulses ( $\lambda = 800$ nm, corresponding energy of  $E = 1.55$ eV). The system has a variable repetition rate up to 250kHz. It uses chirped pulse amplification (CPA) to generate laser pulses with a duration of 150fs and variable pulse energies, e.g. 1.2μJ at 250kHz. We studied Ag islands which have been grown (*in-situ*) by self-assembly on Si(111) surfaces. We used the fundamental and the 4th harmonic ( $E = 6.2$ eV) of the amplifier system to study the origin of the space charge effect, i.e., whether the space charge effects are created at the sample surface or in the electron optics of the microscope (Boersch effect). The space charge effect is reflected in an energetic broadening of the electron distribution. Insertion of apertures into the way of the electrons changes the electron density in the electron optics. We report the influence of the laser energy, wavelength, and repetition rate on the energy spectra and the image distortions by space charge effects.

O 27.115 Tue 18:30 P2

**Time resolved core level photoelectron spectroscopy for investigation of femto- and picosecond dynamics of iodophenylphenol monolayers on silicon** — ●MARTIN MICHELWIRTH<sup>1</sup>, HATEM DACHRAOUI<sup>1</sup>, CHRISTIAN SCHÄFER<sup>2</sup>, BJÖRN SCHNATWINKEL<sup>2</sup>, WALTER PFEIFFER<sup>1</sup>, MARKUS DRESCHER<sup>3</sup>, JOCHEN MATTAY<sup>2</sup>, and ULRICH HEINZMANN<sup>1</sup> — <sup>1</sup>Molecular and Surface Physics, Bielefeld University — <sup>2</sup>Organic Chemistry (OC I), Bielefeld University — <sup>3</sup>Ultrafast X-ray Physics, Hamburg University

The photoinduced dynamics of iodophenylphenol adsorbed on silicon were investigated by use of time-resolved UV pump (266 nm)-EUV probe (95 eV) photoemission spectroscopy. The EUV probe pulses were produced by high harmonic generation (HHG). Picosecond and femtosecond dynamic changes of the iodine 4d core level spectra were observed in the pump probe experiment. Because of the localized character of core level spectra the observed dynamics can be directly related to electronic or binding environment changes of the C-I bond. The presented results demonstrate that time-resolved core level spectroscopy provides valuable information about photoinduced intra- and inter molecular dynamics in a complex molecular system environment.

O 27.116 Tue 18:30 P2

**Performance of the XUV split-and-delay line at the free-electron laser in Hamburg** — ●FLORIAN SORGENFREI<sup>1</sup>, TORBEN BEECK<sup>1</sup>, MARTIN BEYE<sup>1</sup>, ALEXANDER FÖHLISCH<sup>1</sup>, MITSURU NAGASONO<sup>2</sup>, BILL SCHLOTTER<sup>1</sup>, and WILFRIED WURTH<sup>1</sup> — <sup>1</sup>Department Physik, Universität Hamburg, Germany — <sup>2</sup>XFEL Project head office, RIKEN, Hyogo, Japan

The high brilliance and short pulse duration of free-electron lasers like FLASH at Hamburg are the basis for novel experiments on ultrafast dynamics in various systems. Combining these properties with X-ray pump/probe techniques enlarges the class of possible experiments even more.

We have permanently implemented a Mach-Zehnder type autocorrelator at the PG2 beamline at FLASH in 2008 which is capable of splitting the XUV pulse from FLASH and introducing a delay between both pulses in the range of about +/- 6ps with a sub-femtosecond resolution. Here, we present the results of test experiments to demonstrate the performance of this device, namely measuring the temporal coherence length of the FLASH radiation and measuring the intensity autocorrelation by He two-photon double-ionization.

We acknowledge financial support from the BMBF priority program FSP301: "FLASH" and the GrK 1355 "Physics with new coherent light sources"

O 27.117 Tue 18:30 P2

**Ultrafast Excitation and Deexcitation Dynamics of Adsorbates on Si-Surfaces: A Time Resolved Electron Diffraction Study** — ●SIMONE MÖLLENBECK, ANJA HANISCH-BLICHARSKI, TOBIAS PELKA, PAUL SCHNEIDER, MARTIN KAMMLER, BORIS KRENZER, and MICHAEL HORN-VON HOEGEN — Department of Physics and Center

for Nanointegration Duisburg-Essen (CeNIDE) Universität Duisburg-Essen, D-47057 Duisburg, Germany

We have set up an experiment for ultra fast electron diffraction. The surface sensitivity in a RHEED (reflection high energy electron diffraction)-geometry was used to analyze the structural dynamics on a ps-timescale upon excitation by fs-laserpulses. In the past we have shown that the nanoscale heat transport in heterolayers can be studied with TR-RHEED utilizing the Debye-Waller Effect. Here we used the unique possibilities of TR-RHEED to study monolayer adsorbate systems on Silicon. As an example we present time resolved measurements of the ( $\sqrt{3} \times \sqrt{3}$ ) Pb/Si(111) adsorbate system. Pb was deposited on Si(111)-(7 × 7) at 100K. By desorption at 500K, the coverage was reduced to a ( $\sqrt{3} \times \sqrt{3}$ ) reconstructed Pb adsorbate system with the coverage of 1 monolayer. We observed the transient surface temperature evolution of the Pb adsorbate system after excitation with a fs-laserpulse. The measured time constant for the cooling process is 150ps. This observation agrees well with a simple theoretical model. We may present further new results to other adsorbate systems.

O 27.118 Tue 18:30 P2

**The cooling process on a picosecond timescale: from bulk to monolayer** — ANJA HANISCH-BLICHARSKI, ●SIMONE MÖLLENBECK, TOBIAS PELKA, PAUL SCHNEIDER, MARTIN KAMMLER, BORIS KRENZER, and MICHAEL HORN-VON HOEGEN — Department of Physics and Center for Nanointegration Duisburg-Essen (CeNIDE), Universität Duisburg-Essen, 47048 Duisburg, Germany

We study the cooling rate of heteroepitaxial thin film systems after fs-laser excitation with ps time resolution by means of ultrafast time resolved electron diffraction in a grazing reflection geometry (RHEED). Diffraction patterns taken at different delays between pumping laser pulse and probing electron pulse are converted to the transient film temperature using the Debye-Waller effect. We present results on ultrathin epitaxial Bi(111)- and Pb(111)-films on Si(001) and Si(111) substrates. For a 6 nm thin Bi-film a rapid increase of the surface temperature from 80 K up to 190 K upon laser excitation is followed by a slow exponential decay with a decay constant of  $\tau = 640$  ps which is determined by the thermal boundary resistance at the hetero interface between film and substrate. The large increase of the surface temperature is caused by the small absorption length of 15 nm for photons with  $\lambda = 800$  nm. For Bi-films the cooling rate varies linearly from  $\tau = 290$  to  $\tau = 3200$  ps with the film thickness which has been varied between 2.5 and 35 nm while a Pb-monolayer within the ( $\sqrt{3} \times \sqrt{3}$ ) reconstruction shows a cooling rate of only 150 ps.

O 27.119 Tue 18:30 P2

**Nanosecond time-resolved measurements of acoustic waves** — ●FABIAN KNEIER, TOBIAS GELDHÄUSER, JOHANNES BONEBERG, and PAUL LEIDERER — Fachbereich Physik, Universität Konstanz, 78457 Konstanz

We have built a Michelson interferometer that is capable of determining surface expansions and accelerations in the sub-nm range with a ns-temporal resolution. For that purpose the interferometer is stabilized by a piezoelectrically driven mirror in the reference arm. This setup is used to study Bulk Acoustic Waves (BAW) and their properties. This is achieved using a Nd:YAG laser to induce BAWs in a silicon wafer irradiating onto the back of the silicon wafer and measuring the surface displacement caused at the front surface. Included in our investigation are, for example, the effect of silicon wafer thickness or the effect of sacrificial layers of different materials on the back side of the wafer where the the BAW is generated. The information gained will be applied to get a deeper understanding of the underlying processes of dry-laser cleaning and particle adhesion on surfaces.

O 27.120 Tue 18:30 P2

**Dynamics of electron transport at the PTCDA/Ag(111)-interface studied with time-resolved 2PPE** — ●CHRISTIAN SCHWALB<sup>1</sup>, SÖNKE SACHS<sup>2</sup>, MANUEL B. MARKS<sup>1</sup>, ACHIM SCHÖLL<sup>2</sup>, EBERHARD UMBACH<sup>2,3</sup>, and ULRICH HÖFER<sup>1</sup> — <sup>1</sup>Fachbereich Physik und Zentrum für Materialwissenschaften, Philipps-Universität Marburg, D-35032 Marburg — <sup>2</sup>Universität Würzburg, Experimentelle Physik II, D-97074 Würzburg — <sup>3</sup>Forschungszentrum Karlsruhe, D-

76021 Karlsruhe

Time-resolved two-photon photoemission (2PPE) is able to provide very detailed information about the electronic structure and the dynamics of electron transfer processes of well-ordered interfaces between organic semiconductors and metals. As a model system we have investigated thin epitaxial PTCDA films on Ag(111). A dispersing unoccupied state with an effective electron mass of  $0.39 m_e$  at the  $\bar{\Gamma}$ -point emerges 0.6 eV above the metallic Fermi level  $E_F$ . Its short lifetime of 55 fs is a clear indication that this state has a strong overlap with the metal and essentially originates from an upshift of the Shockley surface state of the Ag substrate [1]. In order to investigate the role of the interface state for charge carrier injection, we populate the LUMO of PTCDA in films of varying thickness and simultaneously record fluorescence and photoemission spectra. A long lived component observed in the 2PPE signal close to  $E_F$  clearly correlates with film thickness and fluorescence lifetime.

[1] C.H. Schwalb *et al.*, Phys. Rev. Lett. **101**, 146801 (2008)

O 27.121 Tue 18:30 P2

**Momentum-Resolved Dynamics of Electrons in Image-Potential States on Ag(111) and Cu(111)** — ●A. DAMM<sup>1</sup>, K. SCHUBERT<sup>1</sup>, S.V. EREMEEV<sup>2</sup>, A.G. BORISOV<sup>3</sup>, E.V. CHULKOV<sup>4</sup>, P.M. ECHENIQUE<sup>4</sup>, J. GÜDDE<sup>1</sup>, and U. HÖFER<sup>1</sup> — <sup>1</sup>Fachbereich Physik und Zentrum für Materialwissenschaften, Philipps-Universität, D-35032 Marburg, Germany — <sup>2</sup>Institute of Strength Physics and Material Science, 634021 Tomsk, Russia — <sup>3</sup>Laboratoire des Collisions Atomiques et Moléculaires, Université Paris-Sud, 91405 Orsay Cedex, France — <sup>4</sup>Donostia International Physics Center, 20018 San Sebastián, Basque Country, Spain

We report on the momentum-dependence of the decay rate of electrons in image-potential states on Ag(111) and Cu(111) investigated by time- and angle-resolved two-photon photoemission (2PPE). On these surfaces, the  $n = 1$  image-potential state is located within the projected bulk band gap only close to the  $\bar{\Gamma}$ -point, whereas it becomes degenerated with a projected bulk band at  $k_{\parallel} \approx 0.2 \text{ \AA}^{-1}$ . This offers the opportunity to investigate differences in the electron dynamics of surface gap states and resonances within one model system. While the lifetime of gap states is dominated by inelastic decay due to electron-hole-pair excitations, an additional decay channel due to elastic charge transfer into the bulk exists for resonances. We observe a continuous increase of the decay rate with  $k_{\parallel}$  on both surfaces without a sudden change at the band edge. We compare these results with a theoretical description based on many-body calculations for the inelastic decay and a wave-packet propagation method for the elastic charge transfer.

O 27.122 Tue 18:30 P2

**Non-perturbative approach to photoemission by direct simulation of photo-currents** — ●HENNING HUSSER, JAN VAN HEYS, and ECKHARD PEHLKE — Institut für Theoretische Physik und Astrophysik, Universität Kiel, Germany

We present a non-perturbative ab initio approach for the calculation of photo-currents by direct simulation of the photoemission process. The electronic structure of the solid surface, which is initially in its electronic ground state, is calculated within density functional theory using a slab geometry. In a first approach, we integrate the time-dependent single-particle Kohn-Sham equations only for a frozen-in effective potential. The excitation by a fs laser-pulse is accounted for within the dipole approximation. Decoupling of the slabs is achieved by an optimized absorbing potential in the vacuum region. Inelastic scattering of the photo-excited electrons in the solid is roughly accounted for by an absorptive gauge-invariant (constructed in analogy to [1]) optical potential, which is acting only on the excited-state admixtures to the time-dependent wave-functions. The spectra are derived from the Fourier transform of the time-dependent wave-functions. The integration of the time-dependent single-particle equations is carried through with an extended [2] version of the *fhimd* code from the Fritz-Haber-Institut in Berlin. We present photoemission spectra for the Si(001) surface. We argue how the method can be extended to highly excited systems.

[1] S. Ismail-Beigi *et al.*, Phys. Rev. Lett. **87**, 087402 (2001).

[2] J. van Heys *et al.*, Phase Transitions **78**, 773 (2005).

## O 28: Invited Talk (Lanny Schmidt)

Time: Wednesday 9:30–10:15

Location: HSZ 02

**Invited Talk** O 28.1 Wed 9:30 HSZ 02  
**Catalytic Autothermal Reforming of Renewable Fuels at Millisecond Times** — ●LANNY SCHMIDT — Dept of Chem Eng and Mat Sci, U of Minnesota, Minneapolis MN 55455

Autothermal reactors have great promise for hydrogen and chemicals production because they have reactor residence times of 10-3 seconds and require very simple reactors. We describe the production of hydrogen and olefins from fossil fuels from methane to diesel and from renewable fuels such as ethanol, biodiesel, soy oil, cellulose, and lignocellulose in millisecond reactors.

Biofuels generally have higher conversions than fossil fuels because the hydroxyl and ester linkages in these fuels produce higher sticking coefficients than for saturated alkanes. Consequently, conversions of all

biofuels in these processes are nearly 100%. Highly oxygenated feedstocks tend to produce mostly syngas with little olefins or oxygenated products because surface reactions dominate, and these larger products are formed predominantly by homogeneous reaction processes after all oxygen is consumed.

Recent results on production of syngas by reactive flash volatilization of nonvolatile liquids and solids will also be described. We show that, by impinging cold liquid drops or small solid particles onto the hot catalyst surface, the process can be operated in steady state with no carbon formation for many hours. This occurs because, while pyrolysis of vegetable oils and carbohydrates at low temperatures produces carbon, above ~600°C the equilibrium shifts to produce syngas rather than solid carbon.

## O 29: Nanostructures at surfaces: preparation

Time: Wednesday 10:30–12:45

Location: SCH A01

O 29.1 Wed 10:30 SCH A01  
**Formation of Nanostructures by Bimodal Growth of a Low Symmetry Magnetic Molecule on a Weakly Interacting Substrate** — SWEETLANA FREMY<sup>1</sup>, ●ALEXANDER SCHWARZ<sup>1</sup>, KNUD LÄMMLE<sup>1</sup>, ROLAND WIESENDANGER<sup>1</sup>, and MARC PROSENC<sup>2</sup> — <sup>1</sup>Universität Hamburg, Department Physik, IAP, Jungiusstr. 11, 20355 Hamburg — <sup>2</sup>Universität Hamburg, Department Chemie, IAAC, Martin-Luther-King Platz 6, 20146 Hamburg

We are interested in the properties of nanostructures formed by magnetic molecules. In this non-contact atomic force microscopy (NC-AFM) investigation we study the growth of Co-Salen, a planar Schiff-Base complex with Co as magnetic center, on NaCl(001). On this large band gap insulator we expect a rather weak coupling between molecule and surface. Apart from step decoration, we find nanowires, which form networks at higher coverages, and compact nanocrystallites. Molecular resolution on nanowires and nanocrystallites indicate that in both cases the molecules are arranged in the monoclinic bulk unit cell, which consists of 8 Co-Salen dimers. For the nanowires (nanocrystallites) the c-axis is oriented parallel (perpendicular) to the surface normal. From NC-AFM images recorded at 8 K after evaporating small quantities of molecules onto a cold substrate ( $T < 30$  K), we know that the molecules initially adsorb as monomers. Hence, a transition from monomers to dimers must take place before the nanowires and nanocrystallites start to grow. In this presentation, the origin of the bimodal growth, the stability of nanowires and nanocrystallites as well as a model how and where the monomer-to-dimer transition takes place will be discussed.

O 29.2 Wed 10:45 SCH A01  
**Fabrication of a full-coverage polymer nanobrush on electron beam activated template** — NIRMALYA BALLAV, SÖREN SCHILP, and ●MICHAEL ZHARNIKOV — Angewandte Physikalische Chemie, Universität Heidelberg, D-69120 Heidelberg, Germany

Along with chemistry, morphology is an important tool to adjust properties of surfaces and interfaces. One of the most promising approaches to control over surface morphology down to the nanometer scale is the fabrication of 3D polymer brush patterns by surface-initiated polymerization (SIP) combined with electron beam lithography (EBL). However, polymer brush patterns made by EBL-SIP are chemically inhomogeneous. Whereas the polymer brush itself is comprised of a polymer, the areas between the 3D features have a different chemical identity determined by the original template. As a result, the effects of morphology on one side and chemistry and surface energy on the other side can be entangled when using such patterns as model surfaces for, e.g., biology-inspired research. Here, we show that this drawback can be overcome by using a sophisticated primary template comprised of monolayer film with mostly deactivated amino tail groups suitable for SIP. Whereas SIP on such a template gives a thin but homogeneous background brush, the regeneration of these groups by electron beam activation lithography promotes the controlled growth of 3D polymer features on this background, resulting in the formation of chemically

homogeneous morphology pattern exclusively comprised of the polymer material. The technique relies upon commercially available compounds and requires a low patterning dose (less than 1 mC/cm<sup>2</sup>).

O 29.3 Wed 11:00 SCH A01  
**Selective adsorption of C<sub>60</sub> on Si/Ge nanostructures** — KONSTANTIN ROMANYUK, ●VASILY CHEREPANOV, and BERT VOIGTLÄNDER — Institute of Bio- und Nanosystems (IBN) and JARA-Fundamentals of Future Information Technology, Forschungszentrum Jülich, D-52425 Jülich, Germany

The similar nature of Si and Ge allows to grow epitaxial Si/Ge nanostructures using a surfactant like Bi to suppress Si-Ge intermixing. Those Si/Ge structures with an atomically sharp interface are suited to be used as templates for a next step of self-organized growth of a different material which selectively bonds to Si or Ge. For instance adsorption of organic molecules only on Si or Ge areas of the surface may lead to a desired fictionalization of the surface. We have explored a chemical selectivity for C<sub>60</sub> deposition on Bi covered surface containing Si and Ge areas. It is found that molecules of C<sub>60</sub> selectively adsorb on the Ge area substituting Bi atoms of the termination layer. Interestingly, this process is fully reversible. The C<sub>60</sub> molecules desorb from the surface under Bi flux thereby restoring initial structure of the template surface. The obtained selectivity for adsorption of C<sub>60</sub> gives new challenging opportunities for a successive fabrication of Si/Ge based nanostructures.

O 29.4 Wed 11:15 SCH A01  
**Heat transfer in swift heavy ion irradiated Insulators** — ●ORKHAN OSMANI<sup>1,2</sup>, MARIKA SCHLEBERGER<sup>1</sup>, and BÄRBEL RETHFELD<sup>2</sup> — <sup>1</sup>Universität Duisburg-Essen, Fachbereich Physik, 47057 Duisburg — <sup>2</sup>Technische Universität Kaiserslautern, Fachbereich Physik, 67653 Kaiserslautern

After irradiation of insulators of the perovskite type with an MeV ion beam under glancing incidents periodic nano patterns on the surface can be observed [1]. To interpret the experimental data ab initio assisted calculations for the model system 100 MeV Xe → SrTiO<sub>3</sub> have been performed [2]. For this system the electronic energy loss is calculated and used to compute the electronic excitation induced by the primary ion. The heat transport into the lattice away from the track core is performed in terms a two temperature model (TTM), a coupled system of diffusion equations. The heat transport is governed by a diffusivity parameter which is usually treated as a constant. However in the case of an insulator this is not appropriate. Therefore, a temperature dependent diffusivity is introduced, resulting in locally molten areas which agree well with the experimentally observed nano patterns. It will be shown that with a temperature dependent diffusivity, the TTM solution is no longer unique and is strongly depending on the spatial discretization chosen for the modeling [3].

[1] Nature Nanotechnology 2, 290-294 (2007)

[2] Journal of Physics: Condensed Matter 20, 315001 (2008)

[3] Laser and Particle Beams (Submitted)

O 29.5 Wed 11:30 SCH A01

**Lithographic Fabrication of Clean Iron Nanostructures via Electron-Beam Induced Deposition in UHV** — ●THOMAS LUKASCZYK<sup>1,2</sup>, MICHAEL SCHIRMER<sup>1,2</sup>, MARIE-MADELEINE WALZ<sup>1,2</sup>, FLORIAN VOLLNHALS<sup>1,2</sup>, HANS-PETER STEINRÜCK<sup>1,2</sup>, and HUBERTUS MARBACH<sup>1,2</sup> — <sup>1</sup>Lehrstuhl für Physikalische Chemie II — <sup>2</sup>Interdisciplinary Center for Molecular Materials (ICMM), Universität Erlangen-Nürnberg, Egerlandstr. 3, D-91058 Erlangen

The generation of nanostructures with arbitrary shapes and well defined chemical composition is still a challenge. One approach is the technique of electron-beam induced deposition (EBID) in which a highly focused electron-beam is used to locally crack, e.g. metal containing, precursor molecules, resulting in the deposition of the non-volatile fragments. Up to now, virtually all experiments were performed in high vacuum environments, resulting in a typical metal content of the EBID deposits of 15% to 60%. By utilizing an ultra-high vacuum system, we achieved an iron purity of at least up to 95% with the precursor iron pentacarbonyl ( $Fe(CO)_5$ ) [1]. The purity and morphology of the deposits is strongly influenced by the surface quality and by the sample temperature. The findings discussed in the work at hand represent a route towards the lithographic fabrication of metallic nanostructures (< 20 nm) with arbitrary shapes and high purity as well as the large scale generation of iron clusters (< 10 nm) with controlled cluster density and an extremely narrow size distribution. This work was supported by the DFG under grant MA 4246/1-1.

[1] T. Lukaszcyk, et al., Small 4(6) (2008) 841.

O 29.6 Wed 11:45 SCH A01

**Surface vacancy channels through ion channeling** — ●ALEX REDINGER<sup>1</sup>, SEBASTIAN STANDOP<sup>1</sup>, YUDI ROSANDI<sup>2</sup>, HERBERT M. URBASSEK<sup>2</sup>, and THOMAS MICHELY<sup>1</sup> — <sup>1</sup>II. Physikalisches Institut, Universität zu Köln, Zùlpicher Strasse 77, 50937 Köln, Germany — <sup>2</sup>Fachbereich Physik, Technische Universität Kaiserslautern, Erwin-Schrödinger-Straße, D-67663 Kaiserslautern, Germany

Damage patterns of single ion impacts on Pt(111) have been studied by scanning tunneling microscopy (STM) and molecular dynamics simulations (MD). Low temperature experiments, where surface diffusion is absent, have been performed for Argon and Xenon ions with energies between 1 keV and 15 keV at an angle of incidence of 86° measured with respect to the surface normal. Ions hitting preexisting illuminated step edges penetrate into the crystal and are guided in open crystallographic directions, one or more layers underneath the surface (subsurface channeling). In the case of Argon channeling the resulting surface damage consists of adatom and vacancy pairs aligned in ion beam direction. After Xenon channeling thin surface vacancy trenches along the ion trajectories - surface vacancy channels - are observed. They result from very efficient sputtering and adatom production along the ion trajectory. This phenomena is well reproduced in molecular dynamics simulations of single ion impacts at 0 K. The damage patterns of Argon and Xenon impacts can be traced back to the different energy losses of the particles in the channel. Channeling distances exceeding 1000 Å for 15 keV Xenon impacts are observed.

O 29.7 Wed 12:00 SCH A01

**Simulation of nanostructuring on sputtered surfaces by multi/rotating ion beams** — ●TAHA YASSERI<sup>1</sup>, REINER KREE<sup>1</sup>, and ALEXANDER K. HARTMANN<sup>2</sup> — <sup>1</sup>Institute for Theoretical Physics, University of Göttingen, Friedrich-Hund Platz 1, D-37075 Göttingen,

Germany. — <sup>2</sup>Institute for Physics, University Oldenburg, Carl-von-Ossietzky Strasse 9-11, D-26111 Oldenburg, Germany

Pattern formation on solid surfaces by ion beam sputtering (IBS) is intensively studied. Recent studies use continuously rotating samples or rotation with only a discrete number of directions. We have used our previously developed Monte Carlo model of IBS to systematically study these situations. For discrete directions we found: (1) either a superposition of single ion-beam patterns or a dominant pattern, depending upon the directions may be observed. (2) In the special case of two beams aligned in opposite directions, roughness of the surface decreases and movement of patterns is suppressed. A sudden change in azimuthal angle ( $\Delta\phi$ ) of ion beam leads to a relaxation of existing ripples into a new direction. We have determined this relaxation time ( $\tau_0$ ), which defines a characteristic angular frequency  $\omega_0 = \Delta\phi/\tau_0$ . For rotating sample with frequency  $\omega \approx \omega_0$  we found an oscillatory behavior of patterns and roughness of the surface.

O 29.8 Wed 12:15 SCH A01

**Ion beam noise may support pattern formation by sputtering** — REINER KREE<sup>1</sup>, ●TAHA YASSERI<sup>1</sup>, and ALEXANDER K. HARTMANN<sup>2</sup> — <sup>1</sup>Institute for Theoretical Physics, University of Göttingen, Friedrich-Hund Platz 1, D-37075 Göttingen, Germany. — <sup>2</sup>Institute for Physics, University Oldenburg, Carl-von-Ossietzky Strasse 9-11, D-26111 Oldenburg, Germany

It is discussed in the literature that, beam divergence may produce new scenarios of pattern formation on surfaces by ion beams sputtering (IBS). We have extended the continuum theory and the Monte Carlo simulation of IBS. Pattern formation to include noisy beam which is following a *Kent distribution*, which is a reasonable approximation of the experimentally observed beam divergence.

We found several pattern forming scenarios differing from the Bradley-Harper scenario, which are discussed mainly using Monte Carlo data and a linear mode analysis of the continuum theory.

O 29.9 Wed 12:30 SCH A01

**Metastable wetting on structured surfaces** — ●ROSA POETES, KATHRIN HOLTZMANN, and ULLRICH STEINER — Cavendish Laboratory, University of Cambridge, Cambridge, UK

Wetting on surfaces has traditionally been divided into hydrophobic and hydrophilic wetting. More complex behaviour on structured surfaces has been explained using the differences between Cassie-Baxter and Wenzel wetting. Recently, it has been shown that other metastable wetting states, which cannot be explained fully by either Wenzel or Cassie-Baxter wetting, can exist on rough or structured surfaces.

We are exploring metastable wetting states on hydrophilic and hydrophobic surfaces. In order to find the parameters influencing the existence and lifetime of metastable wetting states, we use both highly rough non-regular and highly structured regular surfaces with hydrophilic and hydrophobic material properties.

We are exploring the pressure dependence of the metastable states using a water tank for immersion of the samples and also studying how the wetting changes with time. Further, we are exploring the influence of different structural parameters upon the metastable state stability by using highly structured samples with different height, width and overhang ratios.

Understanding the lifetime and stability of metastable wetting states will allow for further research into strong superhydrophobic materials with predictable surface properties.

## O 30: Metal substrates: Adsorption of organic / bio molecules IV

Time: Wednesday 10:30–13:00

Location: SCH A118

O 30.1 Wed 10:30 SCH A118

**Evidence of Charge Transfer in UHV-Deposited Coronene-hexaone and Hexamethoxycoronene Sandwich Layers** — K. MEDJANIK<sup>1</sup>, S. NAGHAVI<sup>2</sup>, R. RIEGER<sup>3</sup>, D. KUTNYAKHOV<sup>1</sup>, S.A. NEPLJKO<sup>1</sup>, ●G. SCHÖNHENSE<sup>1</sup>, V. ALIJANI<sup>2</sup>, C. FELSER<sup>2</sup>, M. BAUMGARTEN<sup>3</sup>, and K. MÜLLEN<sup>3</sup> — <sup>1</sup>Institut für Physik, Universität Mainz — <sup>2</sup>Institute for Analytic and Anorganic Chemistry Univ. Mainz — <sup>3</sup>Max-Planck-Institute for Polymer Research, Mainz

The electronic structure of UHV-deposited sandwich layers of the donor hexamethoxycoronene and the acceptor coronene-hexaone on Au has been studied by UPS. In a donor-acceptor multilayer super-

structure a new signal close to the Fermi energy arises that is absent in films of the pure species. The electron injection barrier of the acceptor is lowered such that charge transfer occurs into its LUMO. The charge depletion in the donor molecules leads to a shift of their HOMO position to higher binding energies by 0.26eV. A significant band bending occurs due to the polar interface between the metal and the organic film as discussed by Koch [1]. In turn, the UPS signal of the charge transfer complex rises significantly above that of the Au substrate (by 0.35eV in the as-deposited multilayer film and by 0.55eV upon annealing of the film at 80°C). In AFM and optical microscopy we observe triangular-shaped nanocrystals with dendritic growth mode.

Funded by DFG through Transregio SFB TRR 49 (B8)

[1] N. Koch, *J. Phys. Cond. Matt.* 20 (2008) 184008

O 30.2 Wed 10:45 SCH A118

**Reactions on surfaces for the creation of template structures**

— ●MEIKE STÖHR<sup>1</sup>, MANFRED MATENA<sup>1</sup>, MARKUS WAHL<sup>1</sup>, THOMAS A. JUNG<sup>2</sup>, JÖRG ZEGENHAGEN<sup>3</sup>, and LUTZ H. GADE<sup>4</sup> — <sup>1</sup>University of Basel, Switzerland — <sup>2</sup>Paul-Scherrer-Institute, Switzerland — <sup>3</sup>ESRF Grenoble, France — <sup>4</sup>University of Heidelberg, Germany

Molecular assemblies on surfaces can be used as templates that allow the study of host guest interactions and provide in a further step an ideal starting point for the generation of more complex hierarchic structures. An important prerequisite besides the regularity of such structures is their stability. We reported the formation of a molecular honeycomb network generated by thermal dehydrogenation of a perylene derivative (DPDI) on a Cu(111) surface [1]. By thermal activation, these molecules become H-bond donors/acceptors and form a highly regular honeycomb structure which is commensurate to the Cu substrate. This network can be used as a template for the incorporation of guest molecules in its hexagonal 'holes' [2]. In addition, XSW (x-ray standing wave) experiments were carried out to determine the height of the DPDI molecules above the Cu surface before and after annealing the sample. It turned out that for the not annealed sample the DPDI molecules mainly interact through their amine end groups with the substrate while the molecule is in a bridge-like configuration. After annealing, the height difference between the end groups and the perylene core is lowered what is required to enable H-bonding between the molecules. [1] M. Stöhr et al., *Angew. Chem. Int. Ed.* 44 (2005) 7394 [2] M. Stöhr et al., *Small* 3 (2007) 1336

O 30.3 Wed 11:00 SCH A118

**Covalent interlinking on the surface by condensation polymerization of *p*-phenylenediamine and terephthaloyl chloride** — ●CHRISTOPH H. SCHMITZ, JULIAN IKONOMOV, and MORITZ SOKOLOWSKI — Inst. f. Physikal. u. Theoret. Chemie, Universität Bonn

Long-range ordered structures of organic adsorbates on metal surfaces are mainly based on weak adsorbate-adsorbate interactions, such as van der Waals-forces, dipole interactions and hydrogen bonds. Technical applications require more robust and durable layers, that may be realized by covalent networks. Examples of the direct covalent interlinking of small organic molecules on the surface are scarce [1-3] and the reactions are mainly induced by heating, which limits the range of possible substances. We herein report on the formation of covalently interlinked structures of a polyamide via condensation polymerization directly on the surface. The vapour-deposition polymerization (VDP) technique was combined with ultra-high vacuum preparations methods to obtain polymer monolayers. We demonstrate this concept by the reaction of *p*-phenylenediamine (PPD) and terephthaloyl chloride (TPC) to form poly(*p*-phenylene terephthalamide) (PPTA) on the Ag(111) surface at room-temperature. After removal of the excess monomer, the polyamide chains arrange in long-range ordered islands on the surface. The structures have been characterized by variable temperature scanning tunneling microscopy (VT-STM). (Funded by DFG through SFB 624) [1] L. Grill et al., *Nature Nanotech.* 2007, 2, 687. [2] N. A. A. Zwaneveld et al., *J. Am. Chem. Soc.* 2008, 130, 6678. [3] S. Weigelt et al., *Angew. Chem.* 2008, 120, 4478.

O 30.4 Wed 11:15 SCH A118

**Controlling the organization and heat induced coupling of biphenyl derivatives on metal surfaces** — ●SERPIL BOZ<sup>1</sup>, MEIKE STÖHR<sup>1</sup>, UMUT SOYDANER<sup>2</sup>, and MARCEL MAYOR<sup>2</sup> — <sup>1</sup>University of Basel, Department of Physics, Klingelbergstrasse, CH-4056 Basel, Switzerland. — <sup>2</sup>University of Basel, Department of Chemistry, St. Johannsring 19, CH-4056 Basel, Switzerland.

The development of scanning probe methods enabled the investigation of molecules on surfaces with impressive resolutions. A delicate balance between molecule - substrate and intermolecular interactions such as van der Waals interactions, H-bonding or dipolar coupling guides the arrangement of the molecules in well ordered patterns.

A very appealing concept is to profit from the order of these pre-organized structures and to interlink the molecular building blocks to macromolecules.

Previously, we presented our new concept to control both, the molecular self-assembly and the subsequent intermolecular coupling reactivity by protection group chemistry and described the heat induced formation of individual polymeric structures from a biphenyl derivative

on single crystal Cu (111) and Ag(111) substrates. Here we would like to present how to control the arrangement and the size of the resulting polymeric structures by modification of the end groups of the previously presented biphenyl unit.

O 30.5 Wed 11:30 SCH A118

**Molecules with "wheels" on a metal surface** — ●CARLOS VILLAGOMEZ<sup>1</sup>, TAKASHI SASAKI<sup>2</sup>, JAMES M. TOUR<sup>2</sup>, and LEONHARD GRILL<sup>1</sup> — <sup>1</sup>Institut für Experimentalphysik, Freie Universität Berlin, 14195 Berlin — <sup>2</sup>Chemistry Department, Rice University, Houston Texas, USA

The design and creation of molecular nanostructures with specific mechanical functions is one of the fundamental issues in nanotechnology. In this context, wheels are an interesting component for the molecular motion, because they are expected to alter the diffusion properties on surfaces, for instance by allowing only directed motion. In the presented work, we show the absorption of functional molecules studied by scanning tunneling microscopy under ultrahigh vacuum at low temperatures of about 7 K. The molecules consist of a phenyl chain, equipped with carborane side groups that represent the molecular "wheels". Additionally, bromine atoms are attached to the terminal groups of the molecules, which should allow the covalent connection of individual molecules, according to our recently presented "on-surface-synthesis" method. The high mobility of the molecules during deposition, at room temperature, enables them to form molecular nanostructures. Characteristic appearances of the molecules, due to different molecular configurations, are found. Furthermore, lateral manipulation was used to displace molecules and to probe their intermolecular interactions.

O 30.6 Wed 11:45 SCH A118

**Tuning surface reactivity by alloying - Acrolein adsorption on well ordered Pt<sub>x</sub>Ce/Pt(111) alloys** — ●JAN MARKUS ESSEN, CONRAD BECKER, and KLAUS WANDEL — Institute of Physical and Theoretical Chemistry, University of Bonn, Wegelerstrasse 12, D-53115 Bonn, Germany

The reactivity of Pt(111) surfaces towards acrolein is mainly determined by the d-band molecule interaction at the Fermi edge. Depending on the initial coverage a  $\eta_4$ -trans, a  $\eta_3$ -cis and a  $\eta_2$ -cis and -trans conformation of adsorbed acrolein is stable. A Pt-O interaction is not favored. Acrolein decomposition proceeds via C<sub>1</sub>-C<sub>2</sub> bond cleavage by a Pt addition into the C-C bond which leads mainly to CO and ethene. In contrast to that, the reactivity of acrolein on pure polycrystalline cerium films is mainly caused by the stability of simultaneously generated cerium oxides. A Ce-O interaction is favored which leads to a strongly distorted adsorption geometry. The decomposition proceeds via C<sub>1</sub>-O bond cleavage by a reductive coupling forming benzene and 1,3,5-hexatriene. Alloying of cerium with Pt results in the formation of several well ordered alloy phases. In general these phases have the same adsorption properties in common. Acrolein adsorbs on the top-most Pt-layer in the same conformation as on Pt(111). Only the  $\eta_4$  conformation is not stable caused by ensemble effects. In contrast to pure Pt(111) however no decomposition takes place. Acrolein desorbs completely intact from these alloy phases at about 230 K.

O 30.7 Wed 12:00 SCH A118

**A quantitative model for the monolayer growth of hydrocarbons on noble metals: HBC on Ag(111) and Au(111)** — ●CHRISTIAN WAGNER, DANIEL KASEMANN, MORITZ ESSLINGER, ROMAN FORCKER, CHRISTIAN GOLNIK, and TORSTEN FRITZ — Institut für Angewandte Photophysik, TU-Dresden, George-Bähr-Str. 1, 01069 Dresden

In our contribution we compare the growth of hexa-perihexabenzocoronene (HBC) on Ag(111) and Au(111) for monolayer (ML) and sub-ML coverage[1,2]. Despite the always present *attractive* van der Waals force we observe a net *repulsive* interaction between individual HBC molecules on the Au(111) surface, resulting in a complex growth behavior: Unlike the situation on Ag(111) no lattice epitaxy is observed for HBC MLs on Au(111) in the predominant phase. Instead, we find a coverage dependent lattice constant (between 13.6 Å and 14.7 Å). Including coulomb and van der Waals forces as well as Pauli repulsion (by the respective OPLS force fields) between the molecules on one hand, and the influence of the metal substrates, namely attractive binding, mirror charges and even a screening of the van der Waals attraction on the other hand, we propose a quantitative model of the interaction potential of HBC on both metals that can be fitted to the experimental results and is indeed able to explain all findings

with reasonable values for the parameters used. Furthermore, we can assign the orientation of HBC domains on Au(111) to the interaction with the surface reconstruction pattern.

- [1] H. Proehl et al. *Phys. Rev. B* **63**, 205409 (2001)  
 [2] P. Ruffieux et al. *J. Am. Chem. Soc.* **129**, 5007 (2007)

O 30.8 Wed 12:15 SCH A118

**Covalently bound molecular chains on an ultrathin insulating film** — ●CHRISTIAN BOMBIS<sup>1</sup>, LEIF LAFFERENTZ<sup>1</sup>, HAO YU<sup>2</sup>, STEFAN HECHT<sup>2</sup>, FRANCISCO AMPLÉ<sup>3</sup>, CHRISTIAN JOACHIM<sup>3</sup>, and LEONHARD GRILL<sup>1</sup> — <sup>1</sup>Institut für Experimentalphysik, Freie Universität Berlin, Arnimallee 14, 14195 Berlin, Germany — <sup>2</sup>Institut für Chemie, Humboldt Universität zu Berlin, Brook-Taylor-Str. 2, 12489 Berlin, Germany — <sup>3</sup>CEMES-CNRS, 29 rue J. Marvig, PO Box 4347, 31055 Toulouse Cedex, France

The adsorption of single covalently bound molecular chains on an ultrathin insulating film of NaCl on a metallic substrate is presented for the first time. In the emerging field of molecular electronics, ultrathin films of NaCl are attracting increasing attention since it was successfully demonstrated that they provide mandatory electronic decoupling of single organic molecules from an underlying metallic substrate while still allowing a sufficient flow of current for the investigation by scanning tunneling microscopy (STM). Conjugated polymers are promising candidates as organic nano-wires. The studied covalently bound molecular chains are formed by organic on-surface-synthesis of dibromoterefluorene (DBTF) molecules on a Au(111)-surface. The adsorption of these polymeric chains, which form molecular interconnects from the metallic substrate on top of an insulating NaCl film, is investigated at the single-molecule level with an STM working at low temperatures (13 K). To further illuminate the adsorption properties of DBTF on top of the ultrathin film of NaCl, electron scattering quantum chemistry (ESQC) calculations are performed.

O 30.9 Wed 12:30 SCH A118

**Nanostructuring of an ultrathin insulating film of NaCl on Cu(111)** — ●CHRISTIAN BOMBIS<sup>1</sup>, JOHANNES MIELKE<sup>1</sup>, MICHAEL MANNSBERGER<sup>1</sup>, FRANCISCO AMPLÉ<sup>2</sup>, CHRISTIAN JOACHIM<sup>2</sup>, and LEONHARD GRILL<sup>1</sup> — <sup>1</sup>Institut für Experimentalphysik, Freie Universität Berlin, Arnimallee 14, 14195 Berlin, Germany — <sup>2</sup>CEMES-CNRS, 29 rue J. Marvig, PO Box 4347, 31055 Toulouse Cedex, France  
 By using the atomic scale scanning tunnelling microscope (STM) ma-

nipulation ability, the nano-mechanical properties and the nanostructuring of NaCl crystalline nanoplates adsorbed on Cu(111) were investigated. Thin films of NaCl as spacer layers are attracting increasing attention, because they retain many of the insulator characteristics while still allowing sufficient current flow to enable STM probing. The thus enabled electronic decoupling of organic molecules from an underlying metal substrate was recently demonstrated and is of particular interest in the emerging field of molecular electronics. Here, we present the nanostructuring of an insulating film of NaCl, which covers cutting of different atomic layers, breaking of nano-islands as well as island manipulation on the metallic substrate. The achieved manipulation abilities are highly relevant with respect to the controlled formation of desired planar molecular interconnects. To further illuminate our current understanding of the nano-mechanical behaviour of the ultrathin film of crystalline NaCl on Cu(111), molecular mechanics calculations will be presented.

O 30.10 Wed 12:45 SCH A118

**Vibrational Kondo effect in a metal-free organic self-assembled molecular layer** — ●ISABEL FERNANDEZ-TORRENTE, KATHARINA JENNIFER FRANKE, and JOSE IGNACIO PASCUAL — Institut für Experimentalphysik, Freie Universität Berlin, Germany

Molecular magnetism is achieved by localising unpaired electrons within molecules. The traditional approach entails the synthesis of metal-organic coordination compounds, where the unpaired spin is provided by paramagnetic transition metal atoms. Here we show that localization of a spin also occurs in a molecular layer of a pure organic charge transfer compound, TTF-TCNQ, self-assembled on a metal surface. The structure adopted by this salt on Au(111) leads to localization of an unpaired electron in a pi-molecular orbital (LUMO) of the acceptor molecule. This free radical state can be demonstrated by the observation of the Kondo effect, obtained in transport experiments carried out in a low temperature scanning tunneling microscope. The unpaired electron is also coupled with molecular vibrations. This phonon-assisted spin flip induces splitting of the Kondo resonance in vibrational sidebands that exhibit different intensities across the TCNQ molecule. These variations arise from intramolecular alterations of the electron-phonon coupling. The analysis of STS curves taken along individual TCNQ molecules allows us to identify the atomic motion involved in the vibrations.

## O 31: Nano-optics of metallic and semiconducting nanostructures (theory)

Time: Wednesday 10:30–12:30

Location: SCH A216

O 31.1 Wed 10:30 SCH A216

**Coherent control in hybrid metal-semiconductor nanostructures** — MATTHIAS REICHELT and ●TORSTEN MEIER — Department Physik, Fakultät für Naturwissenschaften, Universität Paderborn, Warburger Str. 100, D-33098 Paderborn, Germany

Recently it has been shown experimentally that it is possible to coherently control nano-optical excitations by using sophisticated shaped laser pulses. [1] In this work a similar technique is used to theoretically investigate a hybrid nanostructure which consists of a metal aperture and a quantum wire. It is shown that one can concentrate the optically excited electron density at an arbitrary position due to wave packet dynamics [2] by choosing particular frequency components and phases of the chirped laser pulse. The optimization process is performed with a genetic algorithm [3] which is linked to a 3D-FDTD solver.

- [1] M. Aeschlimann *et al.*, *Nature* **446**, 301 (2007)  
 [2] T. Meier, P. Thomas, and S.W. Koch *Coherent Semiconductor Optics*, Springer (2007)  
 [3] A.E. Eiben and J.E. Smith, *Introduction to Evolutionary Computing*, Springer (2003)

O 31.2 Wed 10:45 SCH A216

**Impedance matching and emission properties of optical antennas in a nanophotonic circuit** — JER-SHING HUANG, ●THORSTEN FEICHTNER, PAOLO BIAGIONI, and BERT HECHT — Nano-Optics & Biophotonics group, Department of Experimental Physics 5, University of Würzburg, Germany

An experimentally realizable prototype nanophotonic circuit, consist-

ing of a receiving and an emitting nano antenna connected by a two-wire optical transmission line is studied using finite-difference time-and frequency-domain simulations. It is pointed out, that nanoantennas can efficiently convert propagating photons into plasmonic excitations of a transmission line, whose effective wavelength is determined with both a mode solver and a reflection coefficient analysis. The coupling between the nanophotonic circuit elements is optimized applying impedance matching concepts in analogy to radio frequency technology. It will be shown that the degree of impedance matching, and in particular the impedance of the transmitting nano antenna, can be inferred from the standing wave pattern on the transmission line. We demonstrate the possibility of matching the nano antenna impedance to the transmission line characteristic impedance by variations of the antenna length and width realizable by modern microfabrication techniques. The radiation efficiency of the transmitting antenna also depends on its geometry but is independent of the degree of impedance matching. Our systems approach to nanophotonics provides the basis for realizing general nanophotonic circuits and a large variety of derived novel devices.

O 31.3 Wed 11:00 SCH A216

**Plasmonic Optical Enhancement in an Au-Ag Hybrid Device for Bio Sensors** — ●CHRISTIN DAVID<sup>1</sup>, INEZ WEIDINGER<sup>2</sup>, PETER HILDEBRANDT<sup>2</sup>, MARTEN RICHTER<sup>1</sup>, and ANDREAS KNORR<sup>1</sup> — <sup>1</sup>Technische Universität Berlin, Institut für Theoretische Physik — <sup>2</sup>Technische Universität Berlin, Institut für Chemie

We present a model for plasmonic excitations in Au coated metal bio sensors. Our goal is to illustrate the interplay of surface plasmon po-

laritons (SPP) in metal layers with localized surface plasmon states (LSP) in the roughened electrode. We find a dielectric gap between electrode and metal layers to be crucial to produce a significant field enhancement.

O 31.4 Wed 11:15 SCH A216

**From curved space to optical cloaking** — ●TOLGA ERGIN<sup>1</sup>, NICOLAS STENGER<sup>1</sup>, JONATHAN MUELLER<sup>1</sup>, JAD HALIMEH<sup>1</sup>, and MARTIN WEGENER<sup>1,2</sup> — <sup>1</sup>Institut für Angewandte Physik, Universität Karlsruhe, 76131 Karlsruhe, Germany — <sup>2</sup>Institut für Nanotechnologie, Forschungszentrum Karlsruhe in der Helmholtz-Gemeinschaft, 76021 Karlsruhe, Germany

Transformation optics is a powerful approach to manipulate the propagation of electromagnetic waves [1]. Here, the curvature of space is mimicked by an anisotropic metamaterial, which is described by effective medium theory [2,3]. An interesting application of such composite metal-dielectric metamaterials is a non-resonant optical cloak. We present full-wave finite element simulations of feasible cloak designs in homogeneous medium approximation as well as in full geometry. Real world losses as well as microscopic phenomena are discussed and possible ways for the realization of such cloaking structures are shown.

- [1] U. Leonhardt, *Science* 312, 1777 (2006)
- [2] J.B. Pendry, et al., *Science* 312, 1780 (2006)
- [3] W. Cai, et al., *Nature Photonics* 1, 224 (2007)

O 31.5 Wed 11:30 SCH A216

**Poisson's Spot and Focusing of Surface Plasmon Polaritons** — ●DOMINIC ZERULLA, BRIAN ASHALL, and BRIAN VOHNSEN — University College Dublin, School of Physics, Dublin 4, Ireland.

Surface plasmon polaritons (SPPs) are surface waves bound to the interface between a metal and a dielectric. Their wave characteristics make them ideal candidates for the study of 2d-wave propagation on the nanoscale. This was recently demonstrated in a study of Young's classical interference experiment realized with SPPs. Here we examine another classic of wave optics, namely Poisson's bright spot that appears in the shadow region behind an obstacle. Constructive interference produced by SPPs from opposing sides of a linear obstacle is expected to be less apparent than in the optical case where the field across the entire rim of a circular obstacle contributes. The finite propagation length of the SPPs limits the total propagation length and the outcome will therefore be an elongated spot in the shadow region. This can be considered as a first step towards realizing Fresnel lenses for SPPs. Focusing is required to fully explore the potential of SPPs in integrated optical components and sensors. Typically, mirror-like arrangements have been used to accomplish this. An alternative option, however, is dielectric loading to modify the phase of the SPP. Ultimately, a high numerical aperture is required and in such a case their vectorial nature must be taken into account. Here we examine the potential use of Poisson's spot for SPP confinement and the focusing of SPPs in more general terms. Our numerical predictions are compared with the outcome of preliminary experimental studies.

O 31.6 Wed 11:45 SCH A216

**Collective Surface Plasmons in Metallic Nanorod Arrays** — ●RENÉ KULLOCK<sup>1</sup>, WILLIAM R. HENDREN<sup>2</sup>, ANDREAS HILLE<sup>1</sup>, STEFAN GRAFSTRÖM<sup>1</sup>, PAUL R. EVANS<sup>2</sup>, ROBERT J. POLLARD<sup>2</sup>, RON ATKINSON<sup>2</sup>, and LUKAS M. ENG<sup>1</sup> — <sup>1</sup>Institut für Angewandte Physik, TU Dresden, 01062 Dresden, Germany — <sup>2</sup>Centre for Nanostructured Media, IRCEP, The Queens University of Belfast, Belfast BT7 1NN, UK

Metallic nanorod arrays exhibit several surface plasmon resonances: a short-axis resonance that occurs always [1], and several long-axis resonances appearing for p-polarized light under specific incident angles [2]. Until today, time-consuming numerical calculations were needed to fully describe these properties theoretically. Here we use propagating surface plasmons for an easier description.

Starting with single nanowires exhibiting surface plasmon polaritons (SPPs) we show how the SPPs on nanowires arranged in parallel couple to form collective surface plasmons (CSPs), which have a drastically changed dispersion. For nanorod arrays, such CSPs can be excited by illumination with p-polarized light. Since these arrays act as resonators, CSPs oscillate inside the structures and obey a standing wave condition [3]. Hence, with our model a fast prediction of the optical properties is possible which allows for an easy optimization of these structures for specific purposes and applications.

- [1] R. Atkinson et al., *Phys. Rev. B* 73, 235402 (2006)
- [2] P. Evans et al., *Adv. Func. Mater.* 18, 1075 (2008)
- [3] R. Kulloock et al., *Opt. Express* (2008) submitted

O 31.7 Wed 12:00 SCH A216

**The Discontinuous Galerkin Time-Domain Method for Nanophotonics** — KAI STANNIGEL<sup>1</sup>, ●MICHAEL KÖNIG<sup>1,2</sup>, JENS NIEGEMANN<sup>1,2,3</sup>, and KURT BUSCH<sup>1,2,3</sup> — <sup>1</sup>Institut für Theoretische Festkörperphysik, Universität Karlsruhe — <sup>2</sup>Karlsruhe School of Optics & Photonics (KSOP), Universität Karlsruhe — <sup>3</sup>DFG Centrum für Funktionelle Nanostrukturen (CFN), Universität Karlsruhe

Numerical methods have become invaluable tools for research in the field of photonics and plasmonics. The Discontinuous Galerkin Time-Domain (DGTD) method, complemented by numerous extensions, allows us to solve Maxwell's equations on unstructured grids while maintaining an efficient, explicit time-stepping scheme. Using adaptive meshes we can accurately resolve complex geometric features without staircasing, thereby overcoming one of the key limitations of the widely used Finite-Difference Time-Domain algorithm.

As an example, we apply the DGTD method in three dimensions to the analysis of V-shaped silver nanostructures. In particular, we discuss local field enhancement effects, the onset of the quasi-static limit, and we investigate the possibility of coherent control.

O 31.8 Wed 12:15 SCH A216

**Investigation of the dispersion relation of nanometer meander structures** — ●HEINZ SCHWEIZER, LIWEI FU, THOMAS WEISS, and HARALD GIESSEN — Universität Stuttgart, 4.Phys.Inst., Pfaffenwaldring 57

On the basis of a Fourier modal method we analyze the dispersion relation of nanometer meander structures. Meander structures are of special interest for designing metamaterials with respect to efficient coupling of the magnetic field into the meander loop at all angles of incidence [1] and for designing plasmonic lasers [2]. To understand in detail the behaviour of the meander structures we analyzed the dispersion relation of propagating electromagnetic fields with respect to the transversal component of the propagation vector. Varied coupling strength between the long range and short range plasmonic modes are observed. By tuning the local meander geometry and parameters such as width, depth, and metal layer thickness we are able to engineer the bandgap of the dispersion relation in a large range and in a simple way, which provides a large application potential for plasmonic lasers [2] and other plasmonic devices.

- [1] H. Schweizer et al., *phys. stat. sol. (a)* 204, 3886 (2007). [2] T. Okamoto et al, *Phys. Rev. B* 77, 115425 (2008).

## O 32: Surface or interface magnetism

Time: Wednesday 10:30–12:30

Location: SCH A315

O 32.1 Wed 10:30 SCH A315

**Surface Plasmon Excitation on Magnetoactive Materials** — LUCA SAPIENZA and ●DOMINIC ZERULLA — University College Dublin, School of Physics, Dublin 4, Ireland.

The interaction of surface plasmons - fluctuations in the electron density at the interface between media with dielectric constants of opposite sign - with magnetically ordered systems has attracted a lot of interest in the last ten years, as a result of the possibility of enhancing magneto-optical properties, like the Faraday and Kerr ef-

fect. More recently, research has been focused on the merging of the areas of spintronics and plasmonics, developing of a new field, called spin-plasmonics.

Here, we will present a systematic study of the excitation of surface plasmons on ferromagnetic materials in multilayered structures composed of thin films of nickel, iron, cobalt, capped by a silver layer [1]. The electromagnetic properties of the systems are theoretically and experimentally investigated as a function of the metal layers' thickness and the critical parameters in this study of the interaction between

surface plasmon waves and the magneto-active material are discussed. Finally, an optimized structure for the investigations of spin-plasmonic effects in thin films is proposed.

[1] L. Sapienza, D. Zerulla, "Surface Plasmon Excitation on Magneto-active Materials", Phys. Rev. B (accepted Nov. 2008)

O 32.2 Wed 10:45 SCH A315

**Electric field control of the magnetic anisotropy of ultra-thin Fe films** — •DANIEL WORTMANN, GUSTAV BIHLMAYER, and STEFAN BLÜGEL — Institut für Festkörperforschung and Institute for Advanced Simulation, Forschungszentrum Jülich, 52425 Jülich, Germany

With the advancement of spintronics, magnetoelectric coupling phenomena move into the focus of research. They offer the possibility to manipulate the magnetic state by means of an electric field. In particular, such effects are useful in magnetic multilayers in which an applied bias voltage and its resulting field might assist in switching magnetic layers. While different magnetoelectric effects can be considered we will focus here on a change of the magnetic anisotropy due to an applied electric field.

We present DFT-type *ab initio* calculations performed with the FLEUR code (www.flapw.de) utilizing the full-potential linearized augmented planewave method (FLAPW). The magnetic systems we studied are 1-2 monolayers of Fe on a Au(100) substrate. To simulate a tunneljunction setup we compared the effect of an electric field acting on a surface, i.e. a Fe/vacuum interface to a MgO covered system, i.e. a Fe/MgO interface. We observe a significant enhancement of the field-dependence by covering the Fe film with the insulator.

O 32.3 Wed 11:00 SCH A315

**Depth-resolved photoemission studies on the system MgO/Fe** — •SVEN DÖRING<sup>1,2</sup>, FRANK SCHÖNBOHM<sup>1,2</sup>, ULF BERGES<sup>1,2</sup>, SEEHUN YANG<sup>3</sup>, CHRISTIAN PAPP<sup>3,4</sup>, BENJAMIN BALKE<sup>3,4</sup>, REINERT SCHREIBER<sup>5</sup>, DANIEL E. BÜRGLER<sup>5</sup>, CLAUD M. SCHNEIDER<sup>5</sup>, CHARLES S. FADLEY<sup>3,4</sup>, and CARSTEN WESTPHAL<sup>1,2</sup> — <sup>1</sup>DELTA, TU Dortmund — Maria-Goeppert-Mayer-Str. 2, 44221 Dortmund, Germany — <sup>2</sup>Experimentelle Physik 1, TU Dortmund, Otto-Hahn-Str. 4, 44221 Dortmund, Germany — <sup>3</sup>Materials and Sciences Division, Lawrence Berkeley National Laboratory, Berkeley, CA 94720, USA — <sup>4</sup>University of California, Davis, CA 95616, USA — <sup>5</sup>Jülich Forschungszentrum, IFF-9, 52425 Jülich, Germany

A high depth-resolution in photoemission experiments can be obtained by exciting the photoemission process with nm-scale x-ray standing waves above a multilayer mirror (e.g. Yang et al., J. Appl. Phys. 103, 07C519 (2008)). With this technique, we investigated a model MgO/Fe magnetic tunnel junction, in particular exploring the degree of Fe oxidation at the interface between the two layers, which is thought to critically affect the tunnel magnetoresistance. With the Fe in a wedge profile, the MgO-Fe interface can be moved through the standing wave field by moving the sample relative to the beam. The experiments were performed at DELTA (Dortmund), the ALS (Berkeley), and BESSY II (Berlin). Such standing wave/wedge scans, as well as rocking curves, allow us to develop a depth-profile of our sample. As one preliminary conclusion, we find no evidence for the presence of iron oxide at the interface.

O 32.4 Wed 11:15 SCH A315

**Non-collinear magnetic phases in the electron gas: Results from Hartree-Fock and RDMFT** — •FLORIAN EICH<sup>1,2</sup>, STEFAN KURTH<sup>2,3</sup>, CÉSAR R. PROETTO<sup>2,4</sup>, SANGEETA SHARMA<sup>1,2</sup>, and E. K. U. GROSS<sup>2</sup> — <sup>1</sup>Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin — <sup>2</sup>Institut für Theoretische Physik, Freie Universität Berlin, Arnimallee 14, D-14195 Berlin — <sup>3</sup>Nano-Bio Spectroscopy Group and European Theoretical Spectroscopy Facility (ETSF), Dpto. de Física de Materiales, Universidad del País Vasco UPV/EHU, Centro Mixto CSIC-UPV/EHU, Av. Tolosa 72, E-20018 San Sebastián, Spain — <sup>4</sup>Centro Atómico Bariloche and Instituto Balseiro, 8400 S. C. de Bariloche, Río Negro, Argentina

In 1962 Overhauser [1] demonstrated that the Homogeneous Electron Gas exhibits an instability w.r.t. a Spin Density Wave (SDW) within the Hartree-Fock approximation. Overhauser showed that it is possible to construct a spin-spiral state that is lower in energy than the collinear paramagnetic state at any density. We investigated the properties of this broken symmetry groundstate using the framework of Reduced Density Matrix Functional Theory (RDMFT). Specifically we determined the dependence of the spin-spiral wavelength on the density. Furthermore it was possible to determine a critical density for which

a transition to the ferromagnetic configuration takes place.

[1] A.W. Overhauser, Phys. Rev. 128, 1437 (1962)

O 32.5 Wed 11:30 SCH A315

**Single electron capture versus double electron capture by slow He-ions above transition metal surfaces** — •CHRISTIAN TUSCHE and JÜRGEN KIRSCHNER — MPI für Mikrostrukturphysik, D-06120 Halle, Germany

We studied the electron-capture by slow Helium ions (kinetic energy  $\leq 30\text{eV}$ ) scattered at epitaxial films of the transition metals Mn, Fe, and Ni, grown on a W(110) substrate. At a distance of 2-5Å above the surface, metastable He\*\* is formed by resonant transfer of electrons from the metal to the 2s or 2p shells of the projectile. The decay of He\*\* proceeds via the emission of a He-KLL Auger electron with an energy of  $\approx 34.5\text{eV}$  or  $36.0\text{eV}$  for a *triplet* or *singlet* term, respectively. In the experiment, either a beam of metastable He\*\* (2s), or doubly charged He<sup>++</sup> is used. In the former case, only one electron is transferred to the He ion, while He<sup>++</sup> captures two electrons.

Based on the assumption of two subsequent, but independent one-electron transitions Unipan et al. [1] related the population of *singlet* and *triplet* terms simply to the spin-polarization of the surface. In contrast, we observe largely different *triplet* contributions using He\*\* (2s) and He<sup>++</sup>, that cannot be explained by a two-step process. Instead, we propose the simultaneous capture of two correlated electrons. Moreover, the *triplet* population, using double-capture, is particularly sensitive to minute modifications of the surface electronic structure, e.g., by adsorption of sub-monolayers of C and O.

[1] M. Unipan, A. Robin, R. Morgenstern and R. Hoekstra: Phys. Rev. Lett. **96**, 177601 (2006)

O 32.6 Wed 11:45 SCH A315

**Time-Of-Flight and Spin Filtering in Low Energy Electron Microscopy** — •LUSHCHYK P.<sup>1</sup>, HAHN M.<sup>1</sup>, SCHÖNHENSE G.<sup>1</sup>, OELSNER A.<sup>2</sup>, PANZER D.<sup>2</sup>, KRASYUK A.<sup>3</sup>, and KIRSCHNER J.<sup>3</sup> — <sup>1</sup>Institut für Physik, Johannes Gutenberg Universität Mainz — <sup>2</sup>Surface Concept GmbH, Staudingerweg 7, 55128 Mainz — <sup>3</sup>Max-Planck-Institut für Mikrostrukturphysik, Halle

The spin degree of freedom in microscopy is exploited in SEMPA [1] and SP-LEEM [2] using diffraction of polarised electrons from magnetic surfaces for generating high magnetic contrast. We are developing two alternative approaches by implementing an imaging spin-filter into the column of a low-energy microscope. In the first set-up, spin-polarised electron diffraction from a single crystal surface is used for spin filtering. The method makes use of the Bragg condition for the electron rays in combination with spatial separation of the rays analogous to an optical mirror. An alternative method uses spin dependent transmission through an ultra thin ferromagnetic foil at low electron energies. From spectroscopy experiments it is known that the optimum analysing power of such a transparent foil can be very high due to the differences in inelastic mean free path for low-energy electrons in ferromagnets [3].

Funded by DFG (Scho 341/9)

[1] H.P. Oepen, J. Kirschner, Scanning Microsc. 5 (1991) 1 [2] Th. Duden, E. Bauer, Surf. Rev. Lett. 5 (1998) 1213 [3] G. Schönhense, H. C. Siegmann, Ann. Phys. 2 (1993) 465

O 32.7 Wed 12:00 SCH A315

**Spin polarized STM on an artificially engineered atomic structure** — •DAVID SERRATE<sup>1</sup>, YASUO YOSHIDA<sup>1</sup>, PAOLO FERRIANI<sup>1</sup>, SAW-WAI HLA<sup>1,2</sup>, MATTHIAS MENZEL<sup>1</sup>, OLIVER FERDINAND<sup>1</sup>, KIRSTEN VON BERGMANN<sup>1</sup>, STEFAN HEINZE<sup>1</sup>, ANDRÉ KUBETZKA<sup>1</sup>, and ROLAND WIESENDANGER<sup>1</sup> — <sup>1</sup>Institute of Applied Physics, University of Hamburg, Germany — <sup>2</sup>Department of Physics & Astronomy, Ohio University, USA

Manipulation of single atoms using a scanning tunneling microscope (STM) tip offers the possibility to build functional structures with precision down to the atomic scale. On the other hand, atomically resolved magnetic contrast can be achieved by means of spin polarized STM (SP-STM). In this work we demonstrate the combination of both techniques, which constitutes a major breakthrough in the field of low dimensional magnetism. We used an iron coated tungsten tip to precisely position individual magnetic atoms on a magnetic substrate having well defined local magnetization directions. Here, the substrate plays the role of a magnetic template for the adatoms. SP-STM performed with the same tip on the atomically engineered magnetic nanostructure reveals clear spin contrast, which can be explained on the basis of density functional theory calculations. Thus, this work

opens up a novel research direction for engineering spin structures at the atomic scale with simultaneous magnetic imaging capability.

O 32.8 Wed 12:15 SCH A315

**Correlation between morphology and magnetism of Ni films on adsorbate modified Cu(110)** — ●MARIELLA DENK, RICHARD DENK, MICHAEL HOHAGE, LIDONG SUN, and PETER ZEPPEFELD — Institut für Experimentalphysik, Johannes Kepler Universität Linz, A-4040 Linz, Austria

We have investigated the growth and magnetism of thin Ni films evaporated on adsorbate modified Cu(110) in situ and under UHV conditions. In particular, we used Cu(110)-(2×1)O, Cu(110)-c(6×2)O, and Cu(110)-(2×3)N as substrates. In all cases the adsorbates (O, N) were found to float on top of the Ni film, acting as surfactants. Combining complementary methods like STM and Reflectance Difference

Spectroscopy (RDS), as well as utilizing the sensitivity of RDS to the polar Magneto-Optic Kerr Effect (RD-MOKE), structural and magnetic properties have been probed simultaneously. For nickel grown on Cu(110)-(2×1)O we find an extremely sharp reversal of the magnetic easy axis from in-plane to out-of plane at 9 ML, while for the growth on Cu(110)-c(6×2)O the transition takes place at slightly higher coverages (10 ML), apparently due to a rougher Ni film. However, for growth on Cu(110)-(2×3)N no switching of the easy axis to out-of plane has been observed, even though the film roughness and morphology is similar as in the Cu(110)-c(6×2)O case. Thus, the termination by O or N of the Ni film is crucial for the magnetic properties. Indeed, oxygen exposure during the growth of Ni on Cu(110)-(2×3)N leads to a partially O-terminated Ni film and to the appearance of out-of plane ferromagnetism.

## O 33: Methods: Electronic structure theory II

Time: Wednesday 10:30–12:00

Location: SCH A316

O 33.1 Wed 10:30 SCH A316

**Exploring the Interaction between Graphene Sheets: a Local xc Correction Study** — ●ANDREA SANFILIPPO<sup>1</sup>, XINGUO REN<sup>1</sup>, PATRICK RINKE<sup>1,2</sup>, ALEXANDER TKATCHENKO<sup>1</sup>, VOLKER BLUM<sup>1</sup>, MATTHIAS SCHEFFLER<sup>1,2</sup>, and KARSTEN REUTER<sup>1</sup> — <sup>1</sup>Fritz-Haber-Institut, D-14195 Berlin (Germany) — <sup>2</sup>UC Santa Barbara, CA 93106 (USA)

The interaction between two graphene sheets has become an important test case when assessing the performance of approximate treatments of electronic exchange and correlation (xc) in the context of van der Waals interactions. Of interest is not only the interaction strength at equilibrium separation, but also the long-range asymptotic behavior, which is expected to be influenced by the half-metallic nature of the graphene band structure. Practical work in this direction is hitherto hampered by existing limitations in applying more sophisticated xc approaches, like correlated wave function techniques, to extended systems. We demonstrate how this can be overcome using a local xc correction formalism [1], which enables an accurate extrapolation of energetics and forces obtained from small cluster calculations. We illustrate this using hybrid functionals, MP2 and the random phase approximation, and compare the obtained ab initio results [2] to analytical predictions for the asymptotic behavior of the electrostatic and dispersive interactions. [1] Q.M. Hu, K. Reuter, and M. Scheffler, Phys. Rev. Lett. **98**, 176103 (2007). [2] V. Blum *et al.*, Comp. Phys. Commun. (in press).

O 33.2 Wed 10:45 SCH A316

**Density functional study of the adsorption of Aspirin on (001) surface of  $\alpha$ -quartz** — ●AFSHIN ABBASI<sup>1,2</sup>, EBRAHIM NADIMI<sup>1,2</sup>, PHILIPP PLÄNITZ<sup>2</sup>, and CHRISTIAN RADEHAUS<sup>2,3</sup> — <sup>1</sup>Institut für Physik, Technische Universität Chemnitz, D-09107 Chemnitz, Germany — <sup>2</sup>GWT-TUD GmbH - Geschäftsstelle Chemnitz, Annaberger Str. 240, 09125 Chemnitz, Germany — <sup>3</sup>Fakultät für Elektrotechnik und Informationstechnik, Technische Universität Chemnitz, D-09107 Chemnitz, Germany

In this study the adsorption geometry of aspirin molecule on the hydroxylated (001)  $\alpha$ -quartz surface has been investigated using DFT calculation. The optimized adsorption geometry indicates that both adsorbed molecule and substrate are strongly deformed. Strong hydrogen bonding between aspirin and surface hydroxyls, leads to the breaking of original hydroxyl-hydroxyl Hydrogen bonds on the surface as well as the covalent bond between aspirin acidic oxygen and hydrogen (O-H). In this case new hydrogen bonds on the hydroxylated (001)  $\alpha$ -quartz surface are resulted which significantly differ from ones on the clean surface. The 1.11 eV adsorption energy reveals that the interaction of aspirin with  $\alpha$ -quartz is an exothermic chemical interaction. These observations have been used to explain previous experimental results, which had studied the stability of aspirin in the aspirin-silica solid mixtures.

O 33.3 Wed 11:00 SCH A316

**Tailoring the electronic properties of LaAlO<sub>3</sub> films on SrTiO<sub>3</sub>(001) via a SrTiO<sub>3</sub>-capping layer** — ●KATRIN OTTE<sup>1</sup>, ROSSITZA PENTCHEVA<sup>1</sup>, and WARREN E. PICKETT<sup>2</sup> — <sup>1</sup>Section Cryst-

tallography, Dept. of Earth and Environmental Sciences, University of Munich — <sup>2</sup>Department of Physics, UC Davis

The two-dimensional electron gas emerging at the LaAlO<sub>3</sub>(LAO)/SrTiO<sub>3</sub>(STO) interface [1] is an example of the novel electronic states that can be realized in heterostructures of a polar and a nonpolar band insulator. Recently, Thiel *et al.* [2] reported a critical thickness of four monolayers (MLs) beyond which the interface of LAO-films on a STO(001) substrate becomes conducting. Using density functional theory (DFT) calculations we demonstrate here that an STO-capping layer can trigger the insulator-to-metal transition already at two MLs of LAO. We have varied both the number of LAO and STO-capping layers and find that already the first STO-capping layer reduces the band gap by 1.2 eV, while additional layers only have a small impact. We identify O2p surface states of alternating  $p_x$ ,  $p_y$ -character as the origin for the band gap collapse. Structural optimization indicates that the lattice polarization in the STO-capping layer has opposite sign to the LAO film.

Altogether, an STO-capping layer represents an alternative pathway to tune the electronic properties of the system with potential for future device applications.

[1] A.Ohtomo and H.Y.Hwang, Nature **427**, 423 (2004)

[2] S.Thiel *et al.*, Science **313**, 1942 (2006)

O 33.4 Wed 11:15 SCH A316

**On the accuracy of DFT exchange-correlation functionals for hydrogen bonds in small water clusters** — ●B. SANTRA<sup>1</sup>, A. MICHAELIDES<sup>1,2</sup>, and M. SCHEFFLER<sup>1</sup> — <sup>1</sup>Fritz-Haber-Institut der MPG, Berlin, Germany. — <sup>2</sup>University College London, London, UK.

Recent studies have raised concerns over the ability of DFT exchange-correlation (xc) functionals to reliably describe the structure and properties of liquid water. Hoping to shed light on this issue, we have performed systematic studies of the true ability of several DFT xc functionals to describe hydrogen bonds in small water clusters, making reference to 2<sup>nd</sup> order Møller-Plesset perturbation theory and diffusion quantum Monte Carlo<sup>[1,2]</sup>. Errors from basis set incompleteness have been minimized in both the reference data and the DFT calculations. For the total binding energies, the hybrid X3LYP and PBE0 functionals offer the best performance - with absolute errors <10 meV/H<sub>2</sub>O - and among the pure generalized gradient approximation functionals, mPWLYP and PBE1W perform best. But when the relative energies of different low energy isomers become important, problems with the xc functionals are encountered. Specifically, for the water hexamer, none of the xc functionals tested predict the correct low total energy isomer. Many-body decompositions of the total interaction energies of the clusters indicates that van der Waals forces need to be accounted for in order to correctly discriminate between different isomers with similar energies. The relevance of these results to DFT simulations of liquid water is also briefly discussed. [1] B. Santra *et al.* J. Chem. Phys. **127**, 184104 (2007). [2] B. Santra *et al.*, J. Chem. Phys. (in press).

O 33.5 Wed 11:30 SCH A316

**Subsurface Confinement of Oxygen Vacancies in Anatase TiO<sub>2</sub>** — ●ANNABELLA SELLONI and HONGZHI CHEN — Department

of Chemistry, Princeton University, Princeton, NJ-08540, USA.

First principles Density Functional Theory calculations are carried out to study the relative stabilities of oxygen vacancies at surface and subsurface sites of anatase TiO<sub>2</sub>(101) and TiO<sub>2</sub>(001) and, for comparison, of the prototypical rutile TiO<sub>2</sub>(110) surface. Our results show that these defects are substantially more stable at subsurface than at surface sites in the case of anatase surfaces, whereas bridging oxygen sites are favored for O-vacancies at rutile TiO<sub>2</sub>(110). Also, calculations of vacancy diffusion pathways for anatase (101) show that the energy barrier to diffuse from surface to subsurface sites is sufficiently low to ensure a rapid equilibration of the vacancy distribution at typical surface annealing temperatures. These results can explain why experimentally anatase surfaces are found to have a significantly lower defect concentration and/or to be more difficult to reduce than those of rutile.

O 33.6 Wed 11:45 SCH A316

**Trapping of electrons on ice surfaces: an ab initio study** — ●M. BOCKSTEDTE<sup>1,2</sup>, F. BALETTO<sup>3</sup>, S. SCANDOLO<sup>4</sup>, and A. RUBIO<sup>2,5</sup> — <sup>1</sup>Lst. Theoretische Festkörperphysik, Universität Erlangen-Nürnberg, Erlangen, Germany — <sup>2</sup>ETSF, Universidad del País Vasco, San Sebas-

tian, Spain — <sup>3</sup>Physics Department, King's College, London, UK. — <sup>4</sup>The Abdus Salam International Center of Theoretical Physics (ICTP) and INFN/Democritos National Simulation Center, Trieste, Italy. — <sup>5</sup>Centro Mixto CSIC-UPV/EHU, San Sebastian, Spain.

Water, water clusters and ice possess the fascinating ability to bind and solvate excess electrons. On crystalline ice films on Ru(0001) a long-living excess electron state was found.<sup>1</sup> The electron resides in pre-existing traps at the surface and shows a continuous energy relaxation on a time scales from femtoseconds to minutes. The nature of the initial trap site and its evolution is an open question. Within the frame work of density functional theory we address prototypical trapping sites for the excess electron on (0001) surface of hexagonal ice (*I<sub>h</sub>*). As the primary traps we identify admolecules, orientational defects and reconstructed orientational defects that have sufficiently low formation energy to explain the experimentally deduced abundance of trapping sites. The electron binds to the dipole moment resulting from H-O groups oriented towards the vacuum and is entirely localized in front of the surface. Its tunneling into the metal is thus sufficiently suppressed to allow for an enhancement of the screening by thermally activated reconstruction of the ice network around the trap.

[1] Bovensiepen *et al* J. Phys. Chem. in print.

## O 34: Focused Session: Epitaxial Graphene IV

Time: Wednesday 10:30–13:00

Location: SCH 251

### Topical Talk

O 34.1 Wed 10:30 SCH 251

**Looking through the Dirac window: Graphene on Ir(111)** — ●CARSTEN BUSSE — II. Physikalisches Institut, Universität zu Köln, 50937 Köln, Germany

Epitaxial graphene can be grown by catalytic decomposition of hydrocarbons on Ir(111). Scanning tunneling microscopy reveals that C/Ir(111) has a high degree of structural quality ( $\mu\text{m}$ -sized domains, coherent overgrowth of surface defects). The system is characterized by weak metal-graphene bonding and shows a pronounced moiré superstructure. The growth process can be tuned to yield different morphologies ranging from compact, nm-sized flakes to uniform sample coverage on the mm-scale.

The Dirac cone in the electronic structure of free graphene (i. e. the linear dispersion relation for electrons close to the Fermi energy) is preserved in this system. The substrate induces slight p-doping and the superstructure leads to the opening of additional mini-gaps. The localized, possibly spin-polarized electronic edge state predicted for zigzag edges in free graphene can be observed for nanoflakes on Ir(111).

C/Ir(111) is a template for the growth of metal cluster lattices showing a narrow size distribution and exceptional thermal stability. The clusters bind strongly via a rehybridization of C from  $sp^2$  to  $sp^3$  leading to the formation of covalent carbon-metal bonds. This effect is rather general and has been observed for a range of cluster materials.

Contributions to this work by R. Brako, J. Coraux, R. Djemour, T. Gerber, P. J. Feibelman, M. Kralj, P. Pervan, I. Pleticosić, T. Michely, and A. T. N'Diaye are acknowledged.

### Topical Talk

O 34.2 Wed 11:00 SCH 251

**Exotic properties of graphene at interfaces: spin filtering and mass generation** — ●JEROEN VAN DEN BRINK — Universiteit Leiden, The Netherlands — Stanford University, USA

We investigate a number of exotic electronic properties of graphene at interfaces by means of ab initio density functional calculations.

First we show that it is possible to generate a mass for the Dirac fermions in graphene by putting it on a hexagonal boron nitride substrate. The breaking of the two-sublattice symmetry causes the opening of band gap of about 53 meV [1]. This gap can greatly improve room temperature pinch-off characteristics of graphene-based field effect transistors [2].

Second we investigate the spin filtering properties of graphite and graphene. Based upon the observations (i) that their in-plane lattice constants match almost perfectly and (ii) that their electronic structures overlap in reciprocal space for one spin direction only, we predict perfect spin filtering for interfaces between graphite and (111) fcc or (0001) hcp Ni or Co [3,4]. The spin filtering is quite insensitive to roughness and disorder.

[1] Giovannetti *et al.*, Phys. Rev. B. 76, 073103 (2007).

[2] Van den Brink, Nature Nanotechnology 2, 199 (2007).

[3] Karpan *et al.*, Phys. Rev. Lett. 99, 176602 (2007).

[4] Karpan *et al.*, Phys. Rev. B. 78, 195419 (2008).

O 34.3 Wed 11:30 SCH 251

**Compressive strain relaxation through wrinkle formation in epitaxial graphene on Ir(111)** — ●ALPHA T. N'DIAYE<sup>1</sup>, RAOUL VAN GASTEL<sup>2</sup>, JOHANN CORAUX<sup>1</sup>, RABIA DJEMOUR<sup>1</sup>, DIRK WALL<sup>3</sup>, NIEMMA BUCKANIE<sup>3</sup>, FRANK-J. MEYER ZU HERINGDORF<sup>3</sup>, BENE POELSEMA<sup>2</sup>, THOMAS MICHELY<sup>1</sup>, and CARSTEN BUSSE<sup>1</sup> — <sup>1</sup>II. Phys. Inst., Universität zu Köln — <sup>2</sup>MESA+ Institute for Nanotechnology, University of Twente, The Netherlands — <sup>3</sup>Institut für Exp. Physik, Universität Duisburg-Essen, Germany

The growth of epitaxial graphene is often accompanied by the growth of protruded elongated structures (e.g. on Pt(111)[1], 6H-SiC [2], Ir(111) ) which are sometimes interpreted as nanotubes or scrolls.

With scanning tunneling microscopy and low energy electron microscopy we have observed the growth of such structures during the growth of epitaxial graphene by chemical vapour deposition of ethene on Ir(111) . We suggest an alternative mechanism for the formation of such structures: Graphene is grown at elevated temperatures ( $\approx 1200\text{K}$ ). During cooldown compressive strain is induced due to the different thermal expansion coefficients of graphene and the iridium substrate. This strain can be partly relaxed through the formation of wrinkles in the graphene sheet. The remaining compressive strain at 300 K ( $\approx 0.4\%$ ) corresponds to a lock-in temperature between 700 K and 800 K. The length of wrinkles per surface area can be used to deduce the amount of compressive strain which they compensate for.

[1] D.E. Starr *et al.* Surface Science, 600 (2006) 2688-2695

[2] V. Derycke *et al.* Nano Letters, Vol. 2, No. 10 (2002) 1043-1046

O 34.4 Wed 11:45 SCH 251

**Manipulation of the electronic structure of graphene on Ir(111)** — ●MARKO KRALJ<sup>1</sup>, IVO PLETIKOSIĆ<sup>1</sup>, PETAR PERVAN<sup>1</sup>, MILORAD MILUN<sup>1</sup>, ALPHA N'DIAYE<sup>2</sup>, CARSTEN BUSSE<sup>2</sup>, and THOMAS MICHELY<sup>2</sup> — <sup>1</sup>Institut za fiziku, Zagreb, Croatia — <sup>2</sup>II. Physikalisches Institut, Köln, Germany

Epitaxial graphene on Ir(111) exhibits effects of the 2.5 nm moiré superperiodicity which is due to the mismatch of graphene and iridium lattices. Angle resolved photoelectron spectroscopy (ARPES) reveals intact Dirac cone, slight p-doping (0.1 eV) and opening of minigaps in the band structure of graphene due to the superperiodic potential of the order of 100 mV [1].

In this work, electronic doping of graphene by alkalis (Na, Cs, K) at varying concentrations shifted the position of the Dirac point up to 1.4 eV below the Fermi energy. Moreover, upon the intercalation of alkalis the effects of the superperiodicity vanished and the minigaps disappeared. In the (maximum doping) regime where graphene Fermi surface becomes pronouncedly trigonal, an anisotropic effect of the pi-

band dispersion renormalization was clearly observed. We interpret this as a signature of an enhanced electron-phonon coupling in doped graphene.

[1] I. Pletikosić et al., arXiv:0807.2770.

O 34.5 Wed 12:00 SCH 251

**Pt and other transition metal cluster lattices on graphene** — ●TIMM GERBER, ALPHA T. N'DIAYE, RABIA DJEMOUR, JOHANN CORAUX, CARSTEN BUSSSE, and THOMAS MICHELY — II. Physikalisches Institut, Universität zu Köln

Highly ordered arrays of Ir Clusters had been obtained by depositing Ir on a Ir(111) surface covered with a graphene monolayer. The periodicity of these arrays is determined by the moiré pattern of graphene on Ir(111). [1]

In order to show that other materials form clusters on the same substrate we deposited Pt, W and Re instead of Ir. Pt is of great interest due to its catalytic properties. The optimum deposition temperature varies for each deposit: At room temperature, we obtained highly ordered cluster lattices of Pt as well as of W. Pt clusters are stable up to 500K. By evaporating Re at 200K we obtained as well highly ordered lattices which were stable at room temperature.

Based on the binding mechanism of the clusters to graphene – local diamond formation between the cluster and the substrate – we propose criteria for the ability of a material to form a cluster lattice. These involve the cohesive strength, the lattice parameter and the valence orbital radius of the deposit.

[1] A. T. N'Diaye et al. PRL 97, 215501 (2006)

O 34.6 Wed 12:15 SCH 251

**Imaging atomic structure of graphene on metallic substrates** — ●MIKHAIL FONIN<sup>1</sup>, OLE ZANDER<sup>1</sup>, SÖNKE VOSS<sup>1</sup>, ULRICH RÜDIGER<sup>1</sup>, and YURY S. DEDKOV<sup>2</sup> — <sup>1</sup>Fachbereich Physik, Universität Konstanz, 78457 Konstanz — <sup>2</sup>Fritz-Haber-Institut der Max-Planck-Gesellschaft, 14195 Berlin, Germany

Unusual transport properties of graphene, a single monolayer of graphite, have stimulated an intense activity for developing graphene-based nanoelectronics. From the technological point of view the observation of large carrier mobilities and ballistic transport up to room temperature are the most intriguing features. However, the potential for applicable graphene-based electronics rests not only on device performance but also on the ability to fabricate uniform graphene layers on large length scales. Unlike exfoliation techniques, epitaxially grown graphene layers offer a realistic solution for large-scale fabrication and patterning of graphene structures.

In this study, growth and structure of graphene on Ni(111) and Rh(111) has been investigated by means of scanning tunneling microscopy. We show that graphene prepared on Ni(111) forms a flat monolayer exhibiting remarkably large-scale continuity of carbon lattice over terraces and containing only a very low density of defects. Whereas prepared on Rh(111), graphene forms a nanomesh. Depending on the preparation conditions graphene layer on Rh(111) shows either a single phase and very good rotational alignment or a multi-phase with coexisting different superstructures.

## O 35: Invited Talk (Gaede Prize) (Jürgen Fassbender)

Time: Wednesday 14:00–14:45

Location: HSZ 02

### Invited Talk

O 35.1 Wed 14:00 HSZ 02

**Engineering surfaces, interfaces and structural phases to tailor magnetic properties** — ●JÜRGEN FASSBENDER — Institute of Ion Beam Physics and Materials Research, Forschungszentrum Dresden-Rossendorf e. V., P. O. Box 51 01 19, D-01314 Dresden — Träger des Gaede-Preises

Surfaces and interfaces play an important role in order to determine the overall properties of ultrathin magnetic films and multilayers. In particular, the morphology and roughness of the surface and the sharpness of mutual interfaces between magnetic and non-magnetic thin films are crucial. All these parameters are easily accessible by means of ion irradiation [1,2], ion implantation [2,3] and ion erosion approaches

O 34.7 Wed 12:30 SCH 251

**Rashba-type effect in the graphene/Ni(111) system (interchanged with O 34.8)** — ●YURIY DEDKOV<sup>1</sup>, MIKHAIL FONIN<sup>2</sup>, ULRICH RÜDIGER<sup>2</sup>, and CLEMENS LAUBSCHAT<sup>3</sup> — <sup>1</sup>FHI Berlin — <sup>2</sup>Uni Konstanz — <sup>3</sup>TU Dresden

A high efficiency spin-FET device requires a long spin relaxation time compared to the mean time of transport through the channel combined with a sufficient difference of the spin rotation angles between two states ("0" and "1") as well as an insensitivity of spin rotation to the carrier energy. Long electronic mean free paths and negligible spin-orbit coupling in the carbon-based systems, i.e., large spin relaxation times, make graphene an ideal material for the observation of nearly ballistic spin transport and thus realization of the spin-FET. Here we report on angle-resolved photoemission studies of the electronic  $\pi$  states of high-quality epitaxial graphene layers on a Ni(111) surface. In this system the electron binding energy of the  $\pi$  states shows a strong dependence on the magnetization reversal of the Ni film. The observed extraordinarily large energy shift up to 225 meV of the graphene-derived  $\pi$  band peak position for opposite magnetization directions is attributed to a manifestation of the Rashba-type interaction between spin-polarized electrons in the  $\pi$  band and the large gradient of the effective electric field at the graphene/Ni interface. Our findings show that an electron spin in the graphene layer can be manipulated in a controlled way and have important implications for graphene based spintronic devices.

O 34.8 Wed 12:45 SCH 251

**Quasifreestanding graphene on metallic substrates: preparation, structure, properties (interchanged with O 34.7)** — ●A. VARYKHALOV<sup>1</sup>, A. SHIKIN<sup>2</sup>, J. SANCHEZ-BARRIGA<sup>1</sup>, E. VESCOVO<sup>3</sup>, D. MARCHENKO<sup>2</sup>, A. RYBKIN<sup>2</sup>, D. USACHOV<sup>2</sup>, C. BISWAS<sup>1</sup>, and O. RADER<sup>1</sup> — <sup>1</sup>HZB, BESSY-II, Berlin, Germany — <sup>2</sup>St.-Petersburg State University, Russia — <sup>3</sup>NLSL, USA

Quasifreestanding graphene was prepared by cracking of propylene on metallic Ni(111) and Co(0001) followed by intercalation of Au monolayer into the interface between graphene and its substrate. Structural properties of such graphene as well as intercalation kinetics were monitored by means of scanning tunneling microscopy and angle-resolved photoelectron spectroscopy. Our high-resolution photoemission study reveal quasiparticles in the vicinity of the Fermi level due to interaction between graphene and Au. We demonstrate that in quasifreestanding graphene on Au, that Dirac crossing energy and Fermi energy coincide meaning charge neutrality and electronic properties are identical to those of ideal graphene. Using spin-resolved photoemission we show that the  $\pi$ -band of graphene on Au is spin-split and spin-polarized according to the Rashba model. Photoemission measurements allow us to conclude that *hybridization* between graphene band and spin-orbit split electronic states in high- $Z$  material Au is responsible for the observed spin-polarization. Results are compared to the case of graphene on light material Cu where no spin-polarization and no interfacial hybridization were evidenced. Additionally we emphasize the protective role of graphene showing the band structure of graphene/Au/Ni(111) sampled before and after exposure to atmosphere.

[4]. Also structural phase transitions can be accompanied by magnetic ones [5] which allow the creation of nanomagnets in the sub-100 nm regime [6]. In this talk I am going to present a survey of ion beam modifications of magnetic materials with special emphasis on the basic phenomena including some technological applications. Supported by DFG FA 314/3-1, FA 314/6-1 and FA 314/7-1.

[1] J. Fassbender, D. Ravelosona, Y. Samson, J. Phys. D 37, R179 (2004). [2] J. Fassbender, J. McCord, J. Magn. Mat. 320, 579 (2008). [3] J. McCord, L. Schultz, J. Fassbender, Adv. Mater. 20, 2090 (2008). [4] M. O. Liedke et al., Phys. Rev. B 75, 220407(R) (2007). [5] J. Fassbender et al., Phys. Rev. B 77, 174413 (2008). [6] E. Menendez et al., Small, in press.

## O 36: Particles and clusters

Time: Wednesday 15:00–16:45

Location: SCH A01

O 36.1 Wed 15:00 SCH A01

**Nature of Ar bonding to small  $\text{Co}_N^+$  clusters and its implications for the structure determination by far-infrared absorption spectroscopy** — ●RALF GEHRKE, PHILIPP GRUENE, ANDRÉ FIELICKE, GERARD MEIJER, and KARSTEN REUTER — Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, Germany

Far-infrared vibrational spectroscopy by multiple photon dissociation has proven to be a very useful technique for the structural fingerprinting of small metal clusters [1]. Whereas previous work on cationic vanadium clusters assumed a negligible influence of the adsorbed Ar probe atoms, measured vibrational spectra of small cationic cobalt clusters show an intriguing dependence on the number of adsorbed Ar atoms, which becomes stronger with decreasing cluster size. Focusing on  $\text{Co}_4^+$  to  $\text{Co}_8^+$  we therefore use density-functional theory to analyze the Ar- $\text{Co}_N^+$  bond and its role for the IR spectra. First, low-lying isomers are identified through first-principles basin-hopping runs. A comparison of their computed spectra with the experimental data then enables in some cases a unique assignment of the cluster structure. Independent of the specific isomer, we obtain a pronounced increase of the Ar binding energy for the smallest cluster sizes, which correlates with the observed increased influence of the Ar atoms on the IR spectra. Further analysis of the electronic structure motivates an electrostatic picture that not only explains this binding energy trend, but also why the influence of the rare-gas atom is much stronger than in the previously studied systems. [1] A. Fielicke, A. Kirilyuk, C. Ratsch, J. Behler, M. Scheffler, G. von Helden, G. Meijer, *Phys. Rev. Lett.* **93** (2), 023401 (2004)

O 36.2 Wed 15:15 SCH A01

**Aqueous Suspensions of Detonation Nanodiamond Particles, Investigations of Deaggregation and Deagglomeration with Mechanical Disintegration Methods** — ●MARTIN RUDOLPH<sup>1,2</sup>, JÖRG OPITZ<sup>2</sup>, INGA HANNSTEIN<sup>2</sup>, URS ALEXANDER PEUKER<sup>1</sup>, and JÜRGEN SCHREIBER<sup>2</sup> — <sup>1</sup>TU Bergakademie Freiberg, Institut für Mechanische Verfahrenstechnik und Aufbereitungstechnik, Freiberg, Germany — <sup>2</sup>Fraunhofer Institut für zerstörungsfreie Prüfverfahren, Dresden, Germany

Detonation synthesized Nanodiamonds (DND) have been of great interest since their discovery in the mid 1960s. They were first published in 1988. First applications in the fields of Material and Life Sciences are already being established.

This study deals with aqueous suspensions of DND and the possibilities of producing stable colloidal dispersions only by mechanical disintegration methods and electrostatic stabilization. Three methods of disintegration were utilized including a planetary ball mill, a 200 W Ultrasound device with sonotrode as well as the new method of bead assisted sonic deaggregation (BASD) first published by Ozawa et al. A new model of the aggregates before and after mechanical treatment is established showing a difference between the methods of hard and soft disintegration, referring to milling as well as BASD and simple ultrasound, respectively. To the knowledge of the author it was the first time reagglomeration effects have been found to take place while mechanically disintegrating DND particles. A theoretical model for this effect has been developed therefore.

O 36.3 Wed 15:30 SCH A01

**Metal-Nanoparticle-Induced Fluorescence Enhancement from a Single Layer of Dye Molecules** — ●RENÉ SCHNEIDER, THOMAS HÄRTLING, PHILIPP REICHENBACH, and LUKAS M. ENG — Institute of Applied Photophysics, TU Dresden, Germany

We investigate the applicability of metal nanoparticles (MNPs) to enhance the fluorescence signal of a monolayer of dye molecules. The dependence of the signal strength on the distance between the molecules in the layer and a single MNP is examined by means of a scanning near-field optical microscope (SNOM), the scanning probe of which is equipped with a single gold nanoparticle [1]. This setup allows to change the separation between the particle and the illuminated sample and monitor the optical response of the system under various illumination conditions.

We show that single 80 nm gold particles embedded in immersion oil enhance the fluorescence signal from a layer of molecules when illuminated with a Gaussian focus. By changing the separation between

MNP and sample we observed a modulated fluorescence signal. This modulation is induced by the interference of incoming and scattered light of the particle. The results of analogous investigations using radially polarized light will be presented and compared with the previous measurements.

[1] M. T. Wenzel, T. Härtling, P. Olk, S. C. Kehr, S. Grafström, S. Winnerl, M. Helm, and L. M. Eng, *Opt. Express*, **16**, 12302 (2008).

O 36.4 Wed 15:45 SCH A01

**Initial-state effects in X-ray absorption spectra of size-selected transition metal clusters** — ●MATTHIAS GRAMZOW, RALF GEHRKE, and KARSTEN REUTER — Fritz-Haber-Institut der Max-Planck-Gesellschaft, Faradayweg 4-6, 14195 Berlin, Germany

X-ray absorption spectra (XAS) at the  $L_{2,3}$  edge of 3d transition metal solids are known to be sensitively affected by the created core hole. The recently reported experimental access to XAS of size-selected cationic transition metal clusters provides therefore a unique possibility to study the evolution of core hole screening from the atomic to the bulk-like limit [1]. While the measured data for the  $L_{2,3}$  branching ratio and the  $L_3$  absorption onset for cationic Ti, V and Co clusters containing up to 10 atoms shows indeed pronounced variations, it is unclear how much of this is simply due to the varying atomic coordination in the different isomer geometries (initial-state effects). As a first step towards a detailed interpretation of the experimental spectra we therefore use density-functional theory in conjunction with a basin-hopping sampling algorithm to identify the energetically lowest-lying isomers. On the basis of the obtained structures we disentangle the initial-state effects from the experimental data, and further quantify the amount of core hole screening using a Slater-Janak transition-state approach. [1] J.T. Lau *et al.*, *Phys. Rev. Lett.* **101**, 153401 (2008).

O 36.5 Wed 16:00 SCH A01

**Non-IPR isomers of  $\text{C}_{60}$  on HOPG** — ●DANIEL LÖFFLER<sup>1</sup>, NOELIA BAJALES<sup>1</sup>, PATRICK WEIS<sup>1</sup>, SERGEI LEBEDKIN<sup>1</sup>, ANGELA BIHLMEIER<sup>2</sup>, WIM KLOPPER<sup>2</sup>, ARTUR BÖTTCHER<sup>1</sup>, and MANFRED KAPPES<sup>1</sup> — <sup>1</sup>Institut für physikalische Chemie, Universität Karlsruhe — <sup>2</sup>Institut für theoretische Chemie, Universität Karlsruhe

Thin monodisperse films consisting of exclusively non-IPR  $\text{C}_{60}$  molecules have been generated by depositing vibronically excited  $\text{C}_{60}$  cations onto HOPG followed by sublimation of the more volatile  $\text{C}_{60}(\text{I}_h)$  isomers. A beam of  $\text{C}_{60}$  cations was generated by the electron-impact mediated heating and ionization of  $\text{C}_{70}$ . The associated excitation and fragmentation leads to the formation of  $\text{C}_{60}^+$  cages with non-IPR sites (in addition to the dominant  $\text{C}_{60}(\text{I}_h)$  derived cation). The fabrication of pure  $\text{C}_{60}$  (non-IPR) films has been achieved simply by heating the film grown up to 600 K which results in the thermal removal of all IPR cages,  $\text{C}_{60}(\text{I}_h)$ . The topography of the resulting films, is governed by the aggregation of the  $\text{C}_{60}$  (non-IPR) cages, which is in turn driven by intercage bonds constituted by non-IPR sites (e.g. pairs of adjacent pentagonal rings). These covalent intercage bonds are responsible for the high stability of the  $\text{C}_{60}$  (non-IPR) films as mirrored by a sublimation temperature of 1100 K - significantly higher than for pure  $\text{C}_{60}(\text{I}_h)$ . The valence band of the  $\text{C}_{60}$  (non-IPR) films exhibits a triplet with a well distinguishable additional peak at a binding energy of 2.6 eV. The  $\text{C}_{60}$  (non-IPR) films exhibit a narrower HOMO-LUMO gap than that found for  $\text{C}_{60}(\text{I}_h)$  films.

O 36.6 Wed 16:15 SCH A01

**Optical properties of single alkali-earth particles on MgO films** — ●PHILIPP MYRACH, NIKLAS NILIUS, and HANS-JOACHIM FREUND — Fritz-Haber-Institut der MPG, D14195 Berlin, Germany

Light emission spectroscopy with an STM is employed to study the optical properties of single Mg and Ca particles deposited on 8 ML thick MgO/Mo(001) films. The particles grow with distinct rectangular shapes due to the strong affinity of the alkali-earth atoms to the O ions in the oxide surface. The overall emission properties are governed by material-dependent plasmon excitations, giving rise to photon peaks at 2.3 and 2.1 eV for Mg and Ca particles, respectively. However, a characteristic fine-structure is superimposed on the optical response that originates from the plasmon excitation mechanism via inelastic electron transport in a double barrier STM junction. High excitation cross sections are observed at photon energies that correspond to the

separation of quantized electron levels in the MgO conduction band, so called Gundlach resonances.

O 36.7 Wed 16:30 SCH A01

**Reaction of Cu and Au clusters with single crystalline ZnO surfaces** — ●MARTIN KROLL, THOMAS LÖBER, and ULRICH KÖHLER — Experimentalphysik IV / AG Oberflächenphysik, Ruhr-Universität Bochum, 44780 Bochum, Germany

As model systems in heterogeneous catalysis metal clusters on single ZnO-crystals grown in UHV are used as a first step to understand the complex reactions under real catalytical conditions. STM and SEM were used to examine nucleation and thermal behaviour of the sys-

tems Cu/ZnO(0001)-Zn, Au/ZnO(0001)-Zn and Cu/ZnO(10 $\bar{1}$ 0) up to 500°C. Cu and Au were deposited using MBE. Additionally a CVD-source was used for Cu-deposition. On the polar ZnO(0001) surface and on the mixed terminated ZnO(10 $\bar{1}$ 0) surface separated clusters are formed at room-temperature and a partial entrenching of Cu into the ZnO substrate at elevated temperatures of  $T \geq 400^\circ\text{C}$  was found[1]. In contrast, Au on ZnO initially forms a closed layer at room-temperature and annealing to comparable temperatures shows a pile-up of Au-material into a network of connected island without any reaction with the ZnO-support.

[1] M.Kroll, U. Köhler; Surf. Sci 601 (2007) 2182

## O 37: Metal substrates: Adsorption of organic / bio molecules V

Time: Wednesday 15:00–17:30

Location: SCH A118

O 37.1 Wed 15:00 SCH A118

**A new approach to probe molecular orientation in aromatic self-assembled monolayers** — NIRMALYA BALLAV<sup>1</sup>, BJÖRN SCHÜPBACH<sup>2</sup>, OLE DETHLOFF<sup>2</sup>, PETER FEULNER<sup>3</sup>, ANDREAS TERFORT<sup>2,4</sup>, and ●MICHAEL ZHARNIKOV<sup>1</sup> — <sup>1</sup>Angewandte Physikalische Chemie, Universität Heidelberg, 69120 Heidelberg, Germany — <sup>2</sup>Department Chemie, Philipps-Universität Marburg, 35032 Marburg, Germany — <sup>3</sup>Physikdepartment E20, Technische Universität München, 85747 Garching, Germany — <sup>4</sup>Institut für Anorganische u. Analytische Chemie, Goethe-Universität Frankfurt, 60438 Frankfurt, Germany

The emergence of new technologies has triggered significant interest in aromatic self-assembled monolayers (SAMs). Applications of these systems rely on a precise knowledge of their structure, which can be in particular studied by near-edge X-ray absorption fine structure (NEXAFS) spectroscopy. There are, however, principal constraints, which makes it impossible to get complete information on the molecular orientation in aromatic SAMs on the basis of the NEXAFS data. To avoid these constraints, we apply a new approach, attaching to the oligophenyl backbone a specific group (nitrile) with two mutually perpendicular molecular orbitals, which, due to the hybridization with the orbitals of the phenyl rings comprising the backbone, are oriented either perpendicular or parallel to the backbone plane. Analysis of the data suggests that that aromatic molecules in the respective SAMs on Au(111) substrate are not only tilted, but also noticeably twisted, with the exact twist angle depending on molecular architecture.

O 37.2 Wed 15:15 SCH A118

**Adatom driven self-assembly of TAPP molecules on Cu(111) surface** — ●JONAS BJÖRK<sup>1</sup>, MATTHEW DYER<sup>1</sup>, MANFRED MATENA<sup>2</sup>, MEIKE STÖHR<sup>2</sup>, THOMAS JUNG<sup>3</sup>, and MATS PERSSON<sup>1</sup> — <sup>1</sup>Surface Science Research Centre, University of Liverpool, Liverpool, United Kingdom — <sup>2</sup>NCCR Nanoscale Science and Institute of Physics, University of Basel, Basel, Switzerland — <sup>3</sup>Paul Scherrer Institute, Villigen, Switzerland

A combined density-functional theory (DFT) and scanning tunneling microscopy (STM) study of a self-assembled network of 1,3,8,10-tetraazaperopyrene (TAPP) molecules on Cu(111) is presented. The TAPP molecule, deposited on a Cu(111) surface at a temperature of 150°C, self-assembles in a porous network, commensurate with the underlying Cu substrate. Structural optimization with DFT shows that the system is stabilized by the presence of Cu adatoms in the network. STM experiments show a bright protrusion in the crossing between four molecules, dominating the images at a sample voltage of 3 V. Simulated STM images show that the bright protrusion is a signature of the presence of Cu adatoms. The electronic feature responsible for the bright protrusion is shown to come from the interaction between TAPP molecules and Cu adatoms, and does not depend upon the underlying Cu substrate.

O 37.3 Wed 15:30 SCH A118

**Di-4-mercaptopyridine on Au(111): A Tunneling Microscopy and Spectroscopy Study** — ●BERNDT KOSLOWSKI, ANNA TSCHETSCHETKIN, and PAUL ZIEMANN — Universität Ulm, Institut für Festkörperphysik, Albert-Einstein-Allee 11, D-89069 Ulm

We report on STM and STS measurements at low temperature of di-4-mercaptopyridine (di-4MPy) molecules adsorbed on Au(111). The

di-4MPy is typically used as precursor for SAM deposition of 4MPy in an electrochemical cell. Here, the molecules were sublimated from a crucible onto the Au sample held at a temperature slightly below 0 °C. By STM, we find two distinct kinds of molecules at the Au surface: the first is small and similar to the appearance of 4MPy monomers, and the second appears much larger in topography and is attributed to a catalytic activity of steps dissociating dimers. Within terraces, the di-4MPy form islands expelling the herringbone reconstruction of the Au substrate. The structure within islands is complicated and is most probably a  $c(12 \times 8\sqrt{3})$  built from two enantiomeric unit meshes having a windmill structure composed of 5 or sometimes 6 molecules. We analyze the LUMO of di-4MPy by  $z$ - $V$  spectroscopy, and we discuss the absorption geometry of the molecules.

O 37.4 Wed 15:45 SCH A118

**Understanding Pd island formation on self assembled 4-mercaptopyridine monolayers on Au(111)** — ●JOHN KEITH and TIMO JACOB — Institut für Elektrochemie, Universität Ulm, 89081 Ulm

Self-assembled monolayers (SAMs) on metallic substrates show great potential for applications such as molecular sensors or biological nanodevices. Efforts have been made to metallize small, aromatic SAMs such as 4-mercaptopyridine (4MP) on Au(111) through electrochemical deposition methods with Pd. However, these methods have not yet been successful due to formation of 2-dimensional islands exhibiting non-metallic character [1]. Motivated by this study, we investigated Pd adsorption and diffusion on a 4MP-SAM using periodic density functional theory [2]. For different Pd coverages, we calculated potential energy surfaces for adsorption and diffusion across the 4MP-SAM, allowing investigation of diffusion processes that explain how Pd islands form. Our studies clearly show Pd cannot diffuse on the clean 4MP-SAM surface. Rather, Pd atoms aggregate into regions above the Au surface and between 4MP monomers. When Pd diffuses across a surface where Pd is already pre-adsorbed, diffusion barriers are greatly reduced from the presence of small particles of Pd. This suggests diffusion and island formation require pre-deposited Pd on the SAM and that these islands are not strictly 2-dimensional.

[1] H.-G. Boyden, *et al.*, *Nature Mater.*, **5**, 394 (2006). [2] J. A. Keith, T. Jacob, *Nano Lett.*, submitted.

O 37.5 Wed 16:00 SCH A118

**Magnetic adatoms confined in L-methionine biomolecular nanogratings: from atomic diffusion to adatom self-alignment** — ●AGUSTIN SCHIFFRIN<sup>1,2</sup>, JOACHIM REICHERT<sup>2</sup>, WILLI AUWÄRTER<sup>2</sup>, GESINE JAHNZ<sup>1</sup>, YAN PENNEC<sup>1</sup>, ALEXANDER WEBER-BARGIONI<sup>1</sup>, VALERI S. STEPANYUK<sup>3</sup>, LARISSA NIEBERGALL<sup>3</sup>, PATRICK BRUNO<sup>3,4</sup>, and JOHANNES V. BARTH<sup>2</sup> — <sup>1</sup>Chemistry Department, University of British Columbia, Vancouver, Canada — <sup>2</sup>Physik Department, TU München, Germany — <sup>3</sup>MPI für Mikrostrukturphysik, Halle, Germany — <sup>4</sup>ESRF, Grenoble, France

We exploit the self-assembly properties of the L-methionine amino acid on Ag(111) to steer the one-dimensional ordering of cobalt and iron adatoms. Our low-temperature scanning tunneling microscopy observations reveal how the individual adatoms spontaneously self-align with a preferred  $\sim 25$  Å next-neighbor spacing in the self-assembled biomolecular nanogratings. For Co strings the pertaining equilibrium

statistics and dynamics were monitored to assess the underlying long-range interactions with their anisotropic energy landscape. The effect of the surface-state electron quantum confinement on the atomic self-alignment is revealed by scanning tunneling spectroscopy (STS) mapping and ab initio calculations. Also, the influence of this electronic quantum confinement on the LDOS Kondo signature of the magnetic Co adatoms is assessed with STS measurements.

[1] A. Schiffrin et al., Phys. Rev. B 78, 035424 (2008).

O 37.6 Wed 16:15 SCH A118

**Formation of azobenzene containing self-assembled monolayers on gold monitored by optical second harmonic generation** — ●FLORIAN VOGEL<sup>1</sup>, MARIO MEIER<sup>2</sup>, ULRICH SIEMELING<sup>2</sup>, and FRANK TRÄGER<sup>1</sup> — <sup>1</sup>Institut für Physik and Center for Interdisciplinary Nanostructure Science and Technology – CINSaT, Universität Kassel, Kassel, Germany — <sup>2</sup>Institut für Chemie and Center for Interdisciplinary Nanostructure Science and Technology – CINSaT, Universität Kassel, Kassel, Germany

The azobenzene derivative Bis[4-(phenylazo)phenyl]disulfide was synthesized and used for the preparation of self-assembled monolayers (SAM) on gold substrates. Azobenzene derivatives can be switched between their “cis” and “trans” isomers by irradiation with light. This molecular system, which is an ideal candidate for photoswitchable devices, represents the most widely studied system for SAMs bearing photoactive functional units.

The adsorption dynamics of the molecules have been investigated in situ and in real time by optical second harmonic generation (SHG). It has been shown that the adsorption of the molecules on the gold substrate can be well described by second order Langmuir kinetics.

Additional ellipsometric measurements have confirmed that, in fact, a monolayer of the molecules has been formed. The thickness was determined to be  $(12 \pm 1)$  Å. This is in good agreement with the theoretical value.

O 37.7 Wed 16:30 SCH A118

**Structure and excitonic coupling in self-assembled monolayers of azobenzene-alkanethiols on gold** — ●CORNELIUS GAHL<sup>1</sup>, ROLAND SCHMIDT<sup>1,2</sup>, DANIEL BRETE<sup>1,2</sup>, ERIK MCNELLIS<sup>3</sup>, WOLFGANG FREYER<sup>1</sup>, ROBERT CARLEY<sup>1</sup>, KARSTEN REUTER<sup>3</sup>, and MARTIN WEINELT<sup>1,2</sup> — <sup>1</sup>Max-Born-Institut, Max-Born-Str. 2a, 12489 Berlin, Germany — <sup>2</sup>Fachbereich Physik, Freie Universität Berlin, Arnimallee 14, 14195 Berlin, Germany — <sup>3</sup>Fritz-Haber-Institut der MPG, Faradayweg 4-6, 14195 Berlin, Germany

Self-assembled monolayers of azobenzene-functionalized alkanethiols have been investigated with respect to their geometric structure and optical properties by UV/Visible and near-edge X-ray absorption fine structure spectroscopy in combination with density-functional theory. By attaching a trifluoro-methyl endgroup to the chromophore both the molecular tilt and twist angle of the azobenzene moiety are determined. Based on this detailed structure analysis the energetic shifts observed in optical reflection spectroscopy can be qualitatively described within an extended dipole model. This substantiates sizeable excitonic coupling among the chromophores and elucidates why *trans* to *cis* isomerization of the azobenzene photoswitch is strongly suppressed in densely-packed self-assembled monolayers.

O 37.8 Wed 16:45 SCH A118

**Theoretical investigation of the adsorption of dithiolates on Au surfaces** — ●KATRIN TONIGOLD and AXEL GROSS — Institute for Theoretical Chemistry, Ulm University, D-89069 Ulm, Germany

Thiolates are one of the most commonly used anchor groups of molecules that form self assembled monolayers (SAMs), as they yield stable monolayers because of the strong Au-S-interaction. An even higher stability should be expected if disulfide-containing anchor groups are used. Such groups are bigger than single thiolates and might lead to different structures on the surface that could be used as a new type of template for surface reactions.

In cooperation with experimentalists from the chair of Physical Chemistry I at the Ruhr-University Bochum, the adsorption of 1,2-dithiolan species and related  $\alpha,\gamma$ -dithiolates has been investigated by means of DFT-GGA-calculations. In order to understand the molecule-surface interaction, the electronic structure of the most stable adsorption configurations at different coverages has been analyzed. Furthermore, the effect of different rest groups attached to disulfide-containing anchor groups has been examined. Weak van der Waals forces between these rests were taken into account via post-Hartree-Fock calculations of molecular pairs in the gas phase.

Additionally, as there are both experimental and calculational hints [1] that thiolate adsorption on Au can induce surface rearrangements, the influence of defects on the molecule-surface interaction has been considered.

[1] P. Maksymovych et al., Phys. Rev. Lett. 97, 146103 (2006).

O 37.9 Wed 17:00 SCH A118

**Influence of water on the structure of SAMs formed by mercaptopyridine and aminothiophenol on Au(111): a DFT study** — ●JAN KUČERA and AXEL GROSS — Institut für Theoretische Chemie, Universität Ulm, D-89069 Ulm, Germany

Self-assembled monolayers (SAMs) of nitrogen containing aromatic thiolates on gold have been proposed as a fundamental element for nanoelectronic devices. The formation of aromatic SAMs as well as the preparation of metal-SAM-metal contacts [1] usually occur in an aqueous environment. However, theoretical studies addressing the structure and stability of SAMs typically neglect the influence of the solvent. Hence the detailed influence of the aqueous environment on the geometric and electronic structure of SAMs remains unclear.

We have studied the effects of water on the structural and electronic properties of Au(111)/mercaptopyridine (MPy) and Au(111)/aminothiophenol (ATP) complexes by means of density functional theory calculations. The interaction of water with both the nitrogen- as well as with the sulfur-tail of MPy and ATP on Au(111) were examined. Water binds to the N-tails of SAM/Au complexes via the formation of hydrogen bonds [2], but its interaction with the S-tail is rather weak. The overall effect of water on the binding of the SAMs to the Au substrate is negligible, however, this is significantly changed when ions bound to the SAMs are considered.

[1] Mila Manolova et al., Adv. Mater., doi:10.1002/adma.200801634, in press.

[2] J. Kučera, A. Groß, Langmuir, doi:10.1021/la802368j, in press.

O 37.10 Wed 17:15 SCH A118

**Scanning tunnelling microscopy study of 4'-nitro-1,1'-biphenyl-4-thiol self-assembled monolayers on Au(111)** — ●HEIKO MUZIK, LAXMAN KANKATE, ANDREY TURCHANIN, and ARMIN GÖLZHÄUSER — Fakultät für Physik, Universität Bielefeld, 33615 Bielefeld

Self-assembled monolayers (SAMs) of 4'-nitro-1,1'-biphenyl-4-thiol (NBPT) on gold is a useful system for applications in chemical nanolithography<sup>1</sup>. Nanopatterning of NBPT SAMs by electrons or extreme UV radiation results in the formation of amino terminated cross-linked areas<sup>1,2</sup>. This transformation can flexibly be utilized for the engineering of complex molecular assemblies on gold surfaces, as for instance protein chips<sup>3</sup>. Despite of many promising applications, the structure of NBPT SAMs has not been characterized in detail. Here we present the first scanning tunnelling microscope study of NBPT SAMs on the technologically relevant Au(111) surfaces. The samples were prepared in solution and by vapour deposition in vacuum. We show that the structure of NBPT SAMs exhibits a complex polymorphic behaviour which strongly depends on the temperature and preparation details. We also discuss the observed reconstruction of the gold substrate.

[1] A. Gölzhäuser et al, Adv. Mater. 13 (2001) 806.

[2] A. Turchanin et al, Small 3 (2007) 2114.

[3] A. Turchanin et al, Adv. Mater. 20 (2008) 471.

**O 38: Nano-optics of metallic and semiconducting nanostructures (experiments I)**

Time: Wednesday 15:00–17:30

Location: SCH A216

O 38.1 Wed 15:00 SCH A216

**Nanometer scale imaging and spectroscopy of an organic semiconductor film** — ●ALFRED J. MEIXNER<sup>1</sup>, DAI ZHANG<sup>1</sup>, UTE HEINEMEYER<sup>2</sup>, FRANK SCHREIBER<sup>2</sup>, and REINHARD SCHOLZ<sup>3</sup> — <sup>1</sup>Institute of Physical and Theoretical Chemistry, University of Tübingen — <sup>2</sup>Institute of Applied Physics, University of Tübingen — <sup>3</sup>Walter Schottky Institute, TU-München

The local electronic and optical properties of molecular semiconductors depend sensitively on the local film morphology such as grain boundaries and localized defects. However, quantitative spectroscopic measurements with a resolution matching the molecular morphology of organic semiconductor films has been plagued either by a lack of resolution, contrast or sensitivity. We have investigated an organic molecular semiconductor film (diindenoperylene, DIP) grown by molecular beam deposition on a Si (100) substrate covered with a native oxide layer by tip-enhanced nanometer scale spectroscopic imaging by the use of a novel parabolic-mirror assisted near-field optical microscope. We could for the first time resolve grain boundaries and defects both in the topography and in the near-field optical image and relate them to local PL- and Raman spectra with a spatial resolution on the order of 10 nm.

O 38.2 Wed 15:15 SCH A216

**Investigation of Geometry-dependent Dipole Coupling using Near-field Optical Microscopy of Au-nanoantennas** — ●KAI BRAUN<sup>1</sup>, DAI ZHANG<sup>1</sup>, MONIKA FLEISCHER<sup>2</sup>, DIETER P. KERN<sup>2</sup>, and ALFRED J. MEIXNER<sup>1</sup> — <sup>1</sup>Institut fuer Physikalische und Theoretische Chemie, Auf der Morgenstelle 8, 72076 Tuebingen — <sup>2</sup>Institut fuer Angewandte Physik, Auf der Morgenstelle 10, 72076 Tuebingen

The plasmon coupling between two dipoles is strongly dependent on their relative positions. Theoretical simulations predicted a red shift of the localized plasmon resonance (LPR) for a dipole top-on-top geometry while a blue shift for a dipole side-by-side geometry[1]. However the corresponding experiments are hard to be realized due to the difficulties of aligning two dipoles into desired configurations. We will use a newly developed parabolic mirror assisted near-field optical microscope (SNOM) to precisely position a gold tip at different positions with respect to a gold cone. By replacing the objective lens with a parabolic mirror, this setup provides the unique possibility of obtaining a 14 times stronger electric field distribution in the longitudinal direction than that of the transversal direction[2]. Since both the gold tip and cone have strong oscillating dipoles in the longitudinal direction, this microscope allows us to study the geometry-dependent dipole coupling more accurately and flexibly. [1] Prashant K. Jain et al (2006), J. Phys. Chem. B, 110 18243-18253 [2] Fleischer M. et al (2008), Applied Physical Letters, 93 1

O 38.3 Wed 15:30 SCH A216

**Antenna enhanced Pump-Probe Spectroscopy of Single Metal Nanoparticles** — ●DAVID MOLNAR<sup>1,2</sup> and MARKUS LIPPITZ<sup>1,2</sup> — <sup>1</sup>Max-Planck-Institut für Festkörperforschung, Stuttgart — <sup>2</sup>4. Physikalisches Institut, Universität Stuttgart

Tailoring a nanoparticle's properties for technological applications requires a profound understanding of its different characteristics compared to those of its bulk material. One arising question is: Down to which lengths can a material be expected to show bulk behaviour?

Acoustical eigenfrequencies of a single gold nanoparticle give insight to its mechanical properties such as density or Young's modulus. A laser induced mechanical oscillation yields a periodical change of the electron density, i.e., a periodically changing plasmon resonance. This change is optically detectable using a pump-probe technique and reveals the dynamics of the particle's oscillation.

As absorption is proportional to the third power of the particle's radius the optical detection of mechanical oscillations of a single metal particle with a diameter of 40nm or less is almost impossible. However using an adequate antenna enhancing the signal oscillations of a single particle, 10nm in size or less, become detectable.

We will show calculations of the signal enhancement by an antenna as well as first experimental results in this field.

O 38.4 Wed 15:45 SCH A216

**A Simple Fabrication of Nanoantennae over Large Areas** —

●RETO GIANNINI<sup>1</sup>, ARDA KRISTOPURYAN<sup>1</sup>, YASIN EKINCI<sup>1</sup>, PRATAP K. SAHOO<sup>2</sup>, and JÖRG F. LÖFFLER<sup>1</sup> — <sup>1</sup>Laboratory of Metal Physics and Technology, Department of Materials, ETH Zurich, 8093 Zurich, Switzerland — <sup>2</sup>Laboratory of Micro- and Nanotechnology, Paul Scherrer Institute, 5232 Villigen, Switzerland

Metallic nanoparticles are very promising candidates for the creation of nanoantennae. Such nanoantennae can be used to excite fluorophores more efficiently or to increase the emission of molecules and quantum dots leading to applications in biosensing, nanophotonics and Raman-/fluorescence spectroscopy. The basis of using metallic nanoparticles as nanoantennae is their capability to create a huge electromagnetic enhancement. This enhancement is a consequence of the resonant excitation of charge density oscillations, known as surface plasmons. A further significant increase of the enhancement can be achieved by coupling of two closely-spaced nanoparticles (dimers). Reproducible and cost-effective methods, applicable to large areas, are readily available for single nanoparticles, whereas well-defined dimers are difficult to obtain with comparable simple methods. We have fabricated gold and silver nanoantennae using colloidal lithography and thermal evaporation providing nanoparticle dimers with small gaps over large areas. We measured the plasmon resonances of individual gold and silver dimers with different structural parameters and performed surface-enhanced Raman spectroscopy to determine the relative near-field enhancement factors of the fabricated nanoantennae.

O 38.5 Wed 16:00 SCH A216

**Three-dimensional metal photonic nanostructures using direct laser writing and electrodeposition** — ●JUSTYNA KINGA GANSEL<sup>1</sup>, MICHAEL THIEL<sup>1</sup>, KLAUS BADE<sup>2</sup>, VOLKER SAILE<sup>2</sup>, GEORG VON FREYMAN<sup>1</sup>, STEFAN LINDEN<sup>1</sup>, and MARTIN WEGENER<sup>1</sup> — <sup>1</sup>Institut für Nanotechnologie, Forschungszentrum Karlsruhe; DFG-Center for Functional Nanostructures (CFN) and Institut für Angewandte Physik, Universität Karlsruhe (TH) — <sup>2</sup>Institut für Mikrostrukturtechnik, Forschungszentrum Karlsruhe

An interesting part of the field of photonic nanostructures are metamaterials. Particularly, three-dimensional (3D) structures like 3D negative index metamaterials [1] or optical cloaking devices [2] attract increasing attention. Yet, few techniques for the fabrication of true 3D metamaterials exist [3, 4]. Here we present a method for the fabrication of 3D metal nanostructures. A positive or negative photoresist layer can be structured by direct laser writing, facilitating a wide amount of structure designs. The template is backfilled with gold using electrodeposition, where an ITO-layer below the photoresist acts as a cathode. After removal of the resist, free-standing gold nanostructures emerge. A structure design that can be realized using this method are 3D gold spirals. Corresponding simulations have shown that these structures possess interesting chiral properties.

[1] J. Valentine et al., Nature **455**, 376 (2008)[2] J. B. Pendry et al., Science **312**, 1780 (2006)[3] M. S. Rill et al., Nature Mater. **7**, 543 (2008)[4] N. Liu et al., Nature Mater. **7**, 31 (2008)

O 38.6 Wed 16:15 SCH A216

**Fabrication and optoelectronic properties of individual gold nanostructures** — ●MONIKA FLEISCHER<sup>1</sup>, SEBASTIAN JÄGER<sup>2</sup>, MARCUS SACKROW<sup>2</sup>, DAI ZHANG<sup>2</sup>, RUDOLF EHLICH<sup>3</sup>, CATRINEL STANCIU<sup>2</sup>, J.K. HEINRICH HÖRBER<sup>3</sup>, ALFRED J. MEIXNER<sup>2</sup>, and DIETER P. KERN<sup>1</sup> — <sup>1</sup>Institut für Angewandte Physik, Eberhard Karls Universität Tübingen, Deutschland — <sup>2</sup>Institut für Physikalische und Theoretische Chemie, Eberhard Karls Universität Tübingen, Deutschland — <sup>3</sup>H.H. Wills Laboratory, University of Bristol, England

When interacting with the electromagnetic field of a focused laser beam, individual gold nanostructures can act as optical antennas. For efficient excitation, the shape and size of the nanostructures need to be adjusted to the applied laser mode and wavelength. Cone structures e.g. are particularly well suited for excitation with a radially polarized beam [1]. In a process based on electron beam lithography and ion milling, individual gold nanostructures are fabricated in a range of different shapes, whose critical dimensions are varied systematically. The structures are characterized by means of confocal microscopy, NSOM, SEM, AFM and STM. Results of these studies are presented together with spectra indicating the shape and size dependent resonance fre-

quencies of the gold structures.

[1] M. Fleischer et al., Appl. Phys. Lett. 93, 111114 (2008).

O 38.7 Wed 16:30 SCH A216

**20 nm Optical Resolution Using Gold Nanospheres as Near-Field Probes** — HADI EGHLEDI, KWANG GEOL LEE, XUEWEN CHEN, MARIO AGIO, ●STEPHAN GÖTZINGER, and VAHID SANDOGHDAR — Laboratory of Physical Chemistry and optETH, ETH Zürich, CH-8093 Zürich, Switzerland

Apertureless Scanning Near-Field Optical Microscopy (SNOM) has reported spatial resolution below 20 nm in isolated cases. However, researchers have confronted considerable difficulties in reproducing tips that deliver this performance. Several years ago, we developed reliable and reproducible near-field probes consisting of single gold nanospheres attached to the end of glass tips. It has been also shown that such probes can act as resonant dipole nanoantennas to enhance the fluorescence of single molecules by more than 25 times [1, 2]. We report on experimental images of single molecules obtained using different gold nanoparticle probes with diameters between 40 nm and 100 nm. Resolutions as high as 20 nm were demonstrated at a high yield and with different particle sizes. Furthermore, fluorescence enhancements greater than 30 times were observed. For very small gold particles, the competition between quenching and enhancement of the molecular fluorescence becomes important because the ratio of the absorption to the scattering cross section inverses. We discuss this paradigm shift and its implications for ultrahigh resolution SNOM.

[1] S. Kühn et al., Phys. Rev. Lett. 97, 017402 (2006).

[2] S. Kühn et al., Mol. Phys. 106, 893 (2008).

O 38.8 Wed 16:45 SCH A216

**Near-Field Investigation of Plasmonic Nano-Wire Eigenmodes** — ●JENS DORFMÜLLER<sup>1</sup>, RALF VOGELGESANG<sup>1</sup>, and KLAUS KERN<sup>1,2</sup> — <sup>1</sup>Max Planck Institute for Solid State Research, 70569 Stuttgart, Germany — <sup>2</sup>Ecole Polytechnique Fédérale de Lausanne, 1015 Lausanne, Switzerland

We use apertureless Scanning Near-Field Optical Microscopy (aSNOM) with cross-polarization of the excitation and scattered radiation, which allows us to map nearly unperturbed eigenmodes of plasmonic nanostructures. We study optical wire antennas produced by electron beam lithography. In contrast to far-field measurements, aSNOM allows us to compare plasmon resonances of many individual single wires simultaneously on a relatively small substrate area. We show measured amplitude and phase maps of the z-component of electromagnetic near-fields around these nano-structures.

Our amplitude images show lobes which indicate a strong z-component of the electromagnetic field and neighbouring lobes show a phase difference of 180° in the phase image. Depending on their size, the wires show multipolar resonances. The dipolar resonance is observed at a wire length  $\approx \lambda_{\text{vac}}/5.6$  and higher order resonances at odd multiples of the dipolar resonance length. Higher multipole orders, show less near-field intensity but a broader resonance in the wire-length domain.

We show that it is possible to break the symmetry of the exciting

electromagnetic field by turning the sample and excite the otherwise symmetry forbidden even modes.

O 38.9 Wed 17:00 SCH A216

**Nanostructure Symmetry Induced Surface Plasmon Propagation Guiding and Polarisation Twisting** — ●BRIAN ASHALL and DOMINIC ZERULLA — UCD Dublin, School of Physics, Dublin 4, Ireland

In a recent letter [1], we have demonstrated that symmetry properties of tailor designed nanostructures have a well defined impact on propagation characteristics of Surface Plasmon Polaritons (SPPs) excited on the nanostructured arrayed surfaces. Highlighted, were the SPP excitation, propagation and wave-guiding processes on the nanostructured arrays.

Building on these findings, more recent experiments have focused on the ability of 120° symmetric nanostructures to predictably twist the polarisation of the reemitted light with respect to the illumination polarisation.

This effect has been both, directly observed through polariser - analyser experiments, and indirectly observed as a shift in the polarisation at which the most efficient SPP confinement on the nanostructured surface occurs. The degree by which the polarisation can be twisted is a function of the geometry of the nanostructures, and as such is an initial free design parameter. The only apparent restriction for the efficiency of the polarisation twisting effect for a given nanostructured array are the SPP excitation conditions.

[1] B. Ashall, M. Berndt, D. Zerulla, Appl. Phys. Lett. 91, 203109 (2007).

O 38.10 Wed 17:15 SCH A216

**Observations of selective near-field focusing on three-fold symmetric, mesoscopic surface patterns - measured with PEEM** — ●MICHAEL BERNDT<sup>1,2</sup>, BRIAN ASHALL<sup>1</sup>, MARTIN ROHMER<sup>3</sup>, CHRISTIAN SCHNEIDER<sup>3</sup>, MARTIN AESCHLIMANN<sup>3</sup>, and DOMINIC ZERULLA<sup>1</sup> — <sup>1</sup>University College Dublin, School of Physics, Belfield, Dublin 4, Ireland — <sup>2</sup>MPI of Molecular Cell Biology and Genetics, 01307 Dresden, Germany — <sup>3</sup>Technische Universität Kaiserslautern, Fachbereich Physik, 67663 Kaiserslautern, Germany

Optically active, structured surfaces, which provide strong localisation of excitation energies in certain “hot-spots” on their surface are required for many applications.

We examine the modification and polarisation dependence of optical near-fields on the surface of an array of three-fold symmetric, mesoscopic, silver-coated structures produced by e-beam lithography. For mapping the spatially resolved near-fields and examining the influence of polarisation of the excitation light, we use a photoelectron emission microscope (PEEM). We find that the presented structures show strong increase of the near-field intensity in certain “hot-spots” in a polarisation dependent manner. Hence we demonstrate that breaking of symmetry can provide additional centres of “hot-spots”, which will be employed as the basis of an improved structure design to gain highly efficient near-fields focusing.

## O 39: Metal substrates: Solid-liquid interfaces

Time: Wednesday 15:00–17:30

Location: SCH A315

O 39.1 Wed 15:00 SCH A315

**First-principles characterization of water structures at the metal-water interface** — ●SEBASTIAN SCHNUR and AXEL GROSS — Institute für Theoretische Chemie, Universität Ulm, D-89069 Ulm, Germany

A molecular level understanding of the structural arrangement of water molecules at a metal-water interface is one of the most important issues in electrochemistry. Despite numerous studies, the exact microscopic structure of water at a metal-water interface is not fully understood and is still subject of debate between state-of-the-art theory and in-situ surface science techniques. On a number of metal surfaces, deposition of water usually leads to well-ordered structures. In particular, ice-like water bilayers with a  $\sqrt{3} \times \sqrt{3}$  hexagonal pattern have been investigated most intensively. The crucial question is whether such an ice-like water pattern remains intact even at room temperature or whether it transforms to a liquid-like structure.

We used ab initio molecular dynamics simulations based on density functional theory to study the water bilayer on different closed packed metal surfaces. Vibrational spectra were obtained from the velocity autocorrelation function recorded in the MD simulation to characterize the water structure. Furthermore, we examined details of the metal-water interaction by considering charge density and work function changes to elucidate the nature of the metal-water interaction. Our results contribute to bridge the gap between theory and experiment by giving a direct molecular level explanation for results obtained in finite-temperature in-situ spectroscopy experiments.

O 39.2 Wed 15:15 SCH A315

**Role of anharmonic contributions for the elasticity of ice** — ●MIRA TODOROVA, LARS ISMER, and JÖRG NEUGEBAUER — Max-Planck Insitut für Eisenforschung GmbH, Düsseldorf

Water, one of the simplest molecules in chemistry, forms a liquid and

solid phase with features essential to life and environment. Many of these can be attributed to hydrogen bonding, but that does not mean that they are fully understood. Ice should be an easier material to understand, because its molecules are arranged on a regular lattice. Yet even the determination of such basic properties as the bulk modulus and the elastic constants proves to be a challenge.

Using first principles calculations we investigate the bulk properties of hexagonal ice. Our initial density-functional theory calculations (GGA-PBE level) yield values, which are much too high when compared to experiment. Even though the consideration of thermal effects within the quasi-harmonic approximation leads to a qualitative agreement between measured and calculated quantities, such as the linear expansion coefficient, ice remains much too hard. The large overestimation of the ice' softness demonstrates the importance of anharmonic contributions, which will be shown to be crucial and lead to a dramatic reduction of the bulk modulus and the elastic constants.

O 39.3 Wed 15:30 SCH A315

**Theoretical Studies on the Inner Potential Drop in Pt/Electrolyte-Interfaces** — ●JOCHEN BANDLOW, JOSEF ANTON, and TIMO JACOB — Institut für Elektrochemie, Universität Ulm, 89081 Ulm

Understanding the processes occurring at solid/liquid interfaces is of great importance not only for basic electrochemistry, but also for various applications such as fuel cells. However, these interfaces (i.e., the so-called electric double-layers) are rather complex involving different aspects as surface dipoles, a potential drop, specific and non-specific adsorption, or modified surface structures. Since many experimental techniques that are well-established in surface science are not applicable for systems under "wet" conditions, theoretical modeling might help understanding the double-layer on the microscopic level.

In order to evaluate the drop of the electrostatic potential within the electric double-layer first we performed molecular dynamics studies on pure water under different pressure and temperature conditions. We found that many commonly used interaction potentials reported in literature are only valid for a rather limited part of the phase-space. Afterwards, we studied the molecular structure of charged platinum electrodes in contact with an aqueous solution containing various concentrations of NaCl. This allowed us to evaluate the peak and also the averaged potential distribution.

O 39.4 Wed 15:45 SCH A315

**Optimizing a bimetallic surface - electrochemical oxygen reduction at  $Pt_xRu_{1-x}/Ru(0001)$  surface alloys** — ●OTAVIO ALVES, HARRY E. HOSTER, and R. JÜRGEN BEHM — Institute of Surface Chemistry and Catalysis, Ulm University, 89069 Ulm, Germany

We report on the activity of  $Pt_xRu_{1-x}/Ru(0001)$  surface alloys [1] prepared in ultrahigh vacuum (UHV) towards the electrochemical oxygen reduction reaction (ORR). The potential-dependent reaction currents are measured in a wall-jet type flow cell sited in an electrochemical pre-chamber attached to the main UHV system. The kinetically controlled currents depend on the Pt:Ru ratio and exhibit an optimum close to a Pt content of 100%. The high activity of the  $Pt_xRu_{1-x}/Ru(0001)$  surface alloys can be rationalized by the versatility of mixed adsorption sites whose reactivity is between that of Ru(0001) on the one hand, which binds reactive intermediates too strongly, and Pt monolayer islands ( $Pt_{xML}/Ru(0001)$ ,  $x = 0..1$ ) on the other hand, whose lower activities are attributed to the sluggish  $O_2$  dissociation as predicted from strain and vertical ligand effects [2,3]. We discuss in how far the high optimum Pt content can be rationalized in an atomic-scale picture of the reaction process.

[1] H. E. Hoster *et al.*; Phys. Chem. Chem. Phys. 2008, 10, 3812.

[2] M. Mavrikakis *et al.*; Phys. Rev. Lett. 1998, 81, 2819.

[3] M. Lischka *et al.*; Electrochim. Acta 2007, 52, 2219.

O 39.5 Wed 16:00 SCH A315

**CO electrooxidation at  $Pt_xRu_{1-x}/Ru(0001)$  surface alloys and Pt modified Ru(0001)** — ●HARRY E. HOSTER, OTAVIO ALVES, ANDREAS BERGBREITER, and R. JÜRGEN BEHM — Institute of Surface Chemistry and Catalysis, Ulm University, D-89069 Ulm, Germany

We report on the activity of  $Pt_xRu_{1-x}/Ru(0001)$  surface alloys [1] and Ru(0001) with and without Pt islands [2] towards continuous electrochemical oxidation of CO. The samples were prepared in ultrahigh vacuum (UHV) but the potential dependent CO oxidation currents were recorded under enhanced mass transport conditions in a flow cell attached to the UHV system. On bare Ru(0001), measurable CO ox-

idation only takes place at  $E > 0.55$  V. Whereas modification by Pt islands does not change this threshold, the attainable oxidation currents become much higher, which we explain by a catalytic effect where Pt helps maintaining high local coverage of CO+O(H) adlayer at the Ru areas. Atomically dispersed  $Pt_xRu_{1-x}/Ru(0001)$  surface alloys show an even higher activity, which results from the higher versatility of mixed or electronically varied adsorption sites with intermediate bonding power. The role of the lateral atom distribution of PtRu surfaces for their local adsorption properties and the reactivity of mixed adlayers under reaction conditions are discussed and compared to previous experimental and theoretical findings.

[1] H.E. Hoster *et al.*, Phys.Chem.Chem.Phys. 10 (2008) 3812.

[2] H.E. Hoster *et al.*, J. Phys. Chem. B 108 (2004) 14780.

O 39.6 Wed 16:15 SCH A315

**Anomalous Helmholtz-Capacitance on Stepped Surfaces of Silver and Gold** — ●GUILLERMO BELTRAMO, HARALD IBACH, and MARGRET GIESEN — Institute for Bio- und Nano-Systems (IBN), Jülich Forschungszentrum, D-52425 Jülich, Germany

Interest in generation and functionalization of nanoscale structures on solid templates has grown tremendously because of their eminent role in many areas of technology. In vicinal surfaces, the presence of arrays of atomic steps separated by flat terraces creates regions of varying local atomic coordination, which renders unique properties to these surfaces, quite distinct from those of flat surfaces. [1]. We have studied the capacitance of the solid/electrolyte interface on Ag(11n) and Au(11n) surfaces in KClO<sub>4</sub> and HClO<sub>4</sub> as function of the electrolyte concentration and the step density. We find that the inner layer capacitance (Helmholtz-capacitance) is dramatically reduced on stepped surfaces [2]. Standard theories which describe the Helmholtz-capacitance by properties of the liquid, a hard wall boundary condition and the polarizability of the electron gas at the metal surface fail to describe this behavior. We propose that the different polarizability of water bonded to the surface need be taken into account and attribute the reduced capacitance at steps to the lower polarizability of water molecules bonded to step edges. The results will be discussed. [1] H. Ibach, M. Giesen *ann W. Schmickler*, J. Electroanal. Chem. 544 (2003) 13. [2] G.L. Beltramo, H. Ibach and M. Giesen, Surf. Sci. 601 (2007) 1876.

O 39.7 Wed 16:30 SCH A315

**Dependency of the Vibrational Stark-Effect on the pre-adsorbed Anion-Species on a Cu(100) Electrode Surface** — ●MELANIE RÖEFZAAD, DUC THAN PHAM, PETER BROEKMANN, and KLAUS WANDEL — Institute for Physical and Theoretical Chemistry, University of Bonn

Fourier transform infrared reflection absorption spectroscopy (FT IR-RAS), combined with electrochemical STM, has been used to monitor the vibrational frequency shifting as a function of the electrode potential and the pre-adsorbed anion-species. As probe-molecule served the redoxactive 1,1'-diphenyl-4,4'-bipyridinium (DPV). Halogenide anions are pre-covering the electrode surface by specific adsorption in a wide potential range.<sup>[1]</sup> These highly ordered anion-layers are able to serve as a template for the adsorption of DPV. EC-STM studies revealed no structural changes in the adsorbed monolayer while changing the anion or the potential. Excluding changes in IRRA-spectra through reorientation, shifts induced by changing the applied potential are nicely visible. The expected effect was missing in the case of pre-adsorbed Cl<sup>-</sup> and Br<sup>-</sup>. Only with I<sup>-</sup> significant changes in the IRRA-spectra could be observed. Specific bands show a clear shift to higher frequencies. Those shifts indicate a strengthening of the bonds between the adsorbed molecules formed through charge-transfer-complexation. This gives a clue to a higher electrostatic effect on the organic adlayer with pre-adsorbed iodide due to its reduced partial charge and as a consequence, a more covalent bonding to the copper surface.

<sup>[1]</sup> Broekmann *et al.*, Surf. Sci. 517 (2002) 123

O 39.8 Wed 16:45 SCH A315

**The influence of additives on the Cu(001)/electrolyte interface** — YVONNE GRÜNDER, ●ARNE DRÜNKLER, FREDERIK GOLKS, DANIEL KAMINSKI, KLAUS KRUG, JOCHIM STETTNER, and OLAF M. MAGNUSSEN — Christian-Albrechts-Universität Kiel, Germany

Copper electrodeposition from multicomponent electrolytes containing organic additives is an important process for the defect-free filling of trenches on ultra large scale integrated (ULSI) microchips [1]. In these electrolytes, polyethers, usually polyethylene glycol (PEG), in combination with chloride ions form an overlayer on Cu that inhibits

the electrodeposition reaction [2]. Despite the numerous studies on Cu superconformal electrodeposition the precise influence of the additive on the elementary steps of this deposition reaction is largely not understood, mostly due to the difficulty in making direct experimental observations of the growth mechanisms on the atomic scale. In-situ Surface X-Ray Diffraction (SXRD) offers unique possibilities to study the electrochemical processes under the film and could provide first direct data on the atomic-scale growth mechanism under these conditions. SXRD experiments revealed on Cu(001) in PEG containing electrolyte the existence of an ordered Cl- adlayer underneath the inhibiting film. Moreover we found evidence for a pronounced kinetic limitation for the formation of this adlayer structure.

References: [1] P.C. Andricacos, et al., *Electroch. Microf.* 42, 567 (1998) [2] P.M. Vereecken, R.A. Binstead, H Deligianni, P.C. Andricacos, *IBM J. Res. Develop.* 49, 3 (2005)

O 39.9 Wed 17:00 SCH A315

**Variation of the electrode potential with elastic strain** — ●MAXIM SMETANIN<sup>1</sup>, DOMINIK KRAMER<sup>1</sup>, SENTHILNATHAN MOHANAN<sup>2</sup>, ULRICH HERR<sup>2</sup>, and JOERG WEISSMUELLER<sup>1,3</sup> — <sup>1</sup>Forschungszentrum Karlsruhe, Institut für Nanotechnologie, Karlsruhe — <sup>2</sup>Universität Ulm, Institut für Mikro- und Nanomaterialien, Ulm — <sup>3</sup>Universität des Saarlandes, Technische Physik, Saarbrücken

A fundamental parameter in electrochemistry, the electrode potential,  $E$ , is intricately related to the solids Fermi energy and to its work function in vacuum. How does  $E$  at the metal-electrolyte interface vary when the electrode is subjected to an elastic tangential deformation with strain  $\epsilon$ ? This is of interest in relation to strain effects on the metals band structure, which can affect catalytic processes, to corrosion science, and to recent attempts to understand the response of the surface stress,  $f$ , of metals to changes in the superficial charge density,  $q$ . The connection to surface stress rests on a Maxwell re-

lation,  $df/dq=dE/de$ . While the left-hand-side has been studied in several experiments, we know of no quantitative experiment exploring the right-hand side. Our approach is to use a small cyclic strain of a thin-film gold electrode along with sensitive potential monitoring. We found that the potential varies linearly with the strain; the response parameter is negative. In 10 mM HClO<sub>4</sub>, for quasi-static straining  $dE/de=-1$  V, whereas the value converges to -1.8 V at frequencies around 100Hz. The sign agrees with early predictions, the magnitude is in good agreement with recent results from density functional theory for Au(111) in vacuum and with experimental results for  $df/dq$  in electrolyte.

O 39.10 Wed 17:15 SCH A315

**Influence of anions on dealloying of Cu<sub>3</sub>Au (111): An in-situ x-ray study** — ●APARNA PAREEK, GENESIS ANKAH, SASCHA HÜMANN, MICHAEL ROHWERDER, and FRANK RENNER — Max-Planck Institut für Eisenforschung, Max-Planck Strasse 1, 40237 Düsseldorf

Dealloying is a well-known process occurring at the alloy surfaces, which are composed of elements with widely different Nernst potentials. The dealloying behaviour of Cu<sub>3</sub>Au in 0.1M H<sub>2</sub>SO<sub>4</sub> was previously investigated using electrochemical measurements combined with in-situ X-ray diffraction. We reported the formation of an ultra-thin epitaxial passive Au layer at lower overpotentials with a reversed stacking sequence, which transforms to thicker Au islands at higher overpotentials. Here we investigated the influence of various anionic species (Br, I) dissolved in 0.1M H<sub>2</sub>SO<sub>4</sub> on the above electrochemical corrosion process. Presence of these anionic additives influences the potential where the ultra-thin passive layer transforms to the thicker Au islands. To corroborate the results obtained from X-ray measurements, ex-situ AFM measurements were performed, where the topographical changes with the potential change were recorded. In addition, we present first results of high resolution TEM studies.

## O 40: Methods: Scanning probe techniques I

Time: Wednesday 15:00–17:30

Location: SCH A316

O 40.1 Wed 15:00 SCH A316

**Detection of charges using scanning force microscopy in contact mode\*** — ●FLORIAN JOHANN, AKOS HOFFMANN, and ELISABETH SOERTEL — Institute of Physics, University of Bonn, Wegelerstr. 8, 53115 Bonn, Germany

Electrostatic force microscopy is the standard technique to detect surface charges using a scanning force microscope (SFM). Therefore the SFM is operated in non-contact mode with an alternating voltage applied to the tip. The electrostatic interaction between the tip and the charges to be measured lead to oscillations of the cantilever that can be read-out using a lock-in amplifier. Now, operating the SFM in contact-mode results in the same electrostatic interaction between tip and surface charges. However, in this case, the tip can not move freely due to its being in contact with the sample surface. To still allow for charge detection in contact-mode, e.g. a deformation of the sample surface underneath the tip caused by the electrostatic forces must occur. To reveal the limits of charge detection in contact-mode SFM we performed a detailed analysis of the relevant parameters such as cantilever stiffness, tip load, and elastic properties of the sample.

\*Financial support from the Deutsche Telekom AG is gratefully acknowledged.

O 40.2 Wed 15:15 SCH A316

**Investigation of isolated single molecules on an insulating substrate** — ●KNUD LÄMMLE<sup>1</sup>, ALEXANDER SCHWARZ<sup>1</sup>, MARC PROSENC<sup>2</sup>, and ROLAND WIESENDANGER<sup>1</sup> — <sup>1</sup>Universität Hamburg - Institut für Angewandte Physik, Jungiusstrasse 11a, 20355 Hamburg — <sup>2</sup>Universität Hamburg - Department Chemie, Martin-Luther-King Platz 6, 20146 Hamburg

To tailor new molecular based devices, it is important to understand the characteristic features of their building blocks, i.e., the properties of individual molecules. Here, we utilized non-contact atomic force microscopy (NC-AFM) to study isolated Co-Salen molecules on NaCl(001). On this large band-gap insulator hybridization effects, which strongly alter the properties of molecules if adsorbed on metallic surfaces, are eliminated.

Immobilization of the rather small molecule is achieved by evaporat-

ing them *in situ* onto a 20 K cold substrate and by performing subsequent measurements at 8.2 K. NC-AFM images acquired on wide terraces reveal randomly distributed isolated banana-shaped objects with long and short axis of about 1.5 and 0.6 nm, respectively. By comparison with the known structure of the molecule, they can be identified as individual molecules adsorbed in a planar configuration. Surprisingly, the bananas appear asymmetric, i.e., the 60 pm high maximum is considerably shifted away from the center. Details of the orientation with respect to the underlying substrate as well as the exact adsorption site will be discussed by evaluating images, were isolated molecules and atomic resolution on the substrate are visible simultaneously.

O 40.3 Wed 15:30 SCH A316

**High Resolution 3D-Force-Field-Spectroscopy on Fe/W(001)** — ●RENE SCHMIDT, CESAR LAZO, UWE KAISER, ALEXANDER SCHWARZ, STEFAN HEINZE, and ROLAND WIESENDANGER — Institut für Angewandte Physik, Universität Hamburg

Three-dimensional force fields with atomic resolution have been measured by atomic force microscopy in the non-contact regime (NC-AFM) in ultrahigh vacuum and at low temperatures. Force spectroscopy allows a site specific determination of the distance dependence of tip and sample interaction potential and force on the investigated system. Here, we study a purely metallic system, i.e., the iron monolayer epitaxially grown on a W(001) substrate with a metallic tip.

The high resolution data consists of 128×128 curves on a 2 nm×2 nm surface area. The curves were recorded in a distance range of 270 pm close to the surface with  $\Delta z$ -steps of 10 pm. Additionally, one single curve was recorded up to a distance of 20 nm to determine the long-range tip-sample forces. The resulting total force at each lattice site can be separated into long- and short-range contributions. The experimentally obtained short-range forces are compared quantitatively with first principles calculations based on density functional theory.

O 40.4 Wed 15:45 SCH A316

**3D-Force-Spectroscopy and -Dissipation Data of an Organic-Inorganic Interface: PTCDA on Ag(111)** — ●DANIEL-ALEXANDER BRAUN, GERNOT LANGEWISCH, HARALD FUCHS, and ANDRE SCHIRMEISEN — CeNTech (Center for Nanotechnology) & Institute

of Physics, University of Münster, Germany

Organic semiconductors have attracted intensive research over the last years. Especially the adsorption of  $\pi$ -conjugated organic molecules on metal substrates in view of potential applications in organic and molecular electronics gained a lot of interest. One of the most studied molecules is 3,4,9,10-perylene-tetracarboxylic-dianhydride (PTCDA) and it has been investigated on a wide range of substrates.

Noncontact atomic force microscopy (ncAFM) experiments with PTCDA adsorbed on Cu(111) revealed, that the intramolecular contrast of PTCDA-molecules depends strongly on the local adsorption environment [1]. Here we present experimental ncAFM results of 3-dimensional force and dissipation spectroscopy experiments of PTCDA adsorbed on Ag(111) with submolecular resolution. The dissipation is understood as a hysteresis of forces between approach and retraction of the tip and is caused by bistabilities in the potential energy surface of the tip-sample system. Therefore the dissipation signal can reveal information about the mechanical properties of individual molecules.

[1] B. Such, D. Weiner, A. Schirmeisen and H. Fuchs Applied Physics Letters 89 (2006), 093104

O 40.5 Wed 16:00 SCH A316

**Static and Sliding Friction of Nanoparticles** — ●DIRK DIETZEL, MICHAEL FELDMANN, and ANDRÉ SCHIRMEISEN — Institute of Physics and Center for Nanotechnology, University of Münster, Germany

We present a new approach for identifying static and sliding friction during atomic force microscopy (AFM) manipulation of nanoparticles [1]. In this approach the AFM-tip is centered on top of an antimony nanoparticle, which is weakly bound to a graphite surface. Depending on the normal load of the cantilever two scan modes are then possible: At low normal forces the tip will scan on top of the particle, whereas higher normal forces can lead to a movement of the particle simultaneously with the tip. We measure the lateral force during this transition, which allows us to extract values for static as well as sliding friction. We find that the static friction is reproducible during several subsequent manipulation events of the same nanoparticle. Once the particle is moving, further increase of the normal force might also make load dependent friction measurements possible.

O 40.6 Wed 16:15 SCH A316

**A low-temperature high resolution scanning tunneling microscope with a three-dimensional magnetic vector field operating in ultra-high vacuum** — ●MARCO PRATZER, TORGE MASHOFF, and MARKUS MORGENSTERN — II. Institute of Physics B, Otto-Blumenthal-Straße, RWTH Aachen and JARA-FIT, 52074 Aachen

Scanning tunneling microscopy and spectroscopy at low temperatures lead to a detailed microscopic understanding of electronic interactions. The combination of a low-temperature spin-polarized STM with a rotatable magnetic vector field, in addition, allows to determine the full map of magnetic anisotropies for individual nano-entities. Moreover, complex noncollinear spin structures of nanoclusters could be mapped by appropriately aligning the relative magnetization axis of probe and sample with the help of the external fields.

We present a low-temperature ultra-high vacuum scanning tunneling microscope setup with a combination of a superconducting solenoid coil and two split-pair magnets, providing a rotatable magnetic field of 500 mT applicable in all spatial directions. An absolute field maximum of  $B=7$  T (3 T) can be applied perpendicular (parallel) to the sample surface. The instrument is operated at a temperature of 5 K. Topographic and spectroscopic measurements on tungsten carbide and indium antimonide revealed a  $z$ -noise of  $600 \text{ fm}_{pp}$  even in magnetic field. The energy resolution is, at least, below  $6.5 \text{ meV}$ . In addition the microscope is equipped with a tip exchange mechanism and a lateral sample positioning stage.

O 40.7 Wed 16:30 SCH A316

**Intrinsic and extrinsic corrugation of monolayer graphene deposited on SiO<sub>2</sub>** — ●VIKTOR GERINGER<sup>1</sup>, MARCUS LIEBMANN<sup>1</sup>, TIM ECHTERMAYER<sup>2</sup>, SVEN RUNTE<sup>1</sup>, MATTHIAS SCHMIDT<sup>1</sup>, REINHARD RÜCKAMP<sup>1</sup>, MAX LEMME<sup>2</sup>, and MARKUS MORGENSTERN<sup>1</sup> — <sup>1</sup>II. Physikalisches Institut, RWTH Aachen and JARA-FIT, Otto-Blumenthal-Straße, 52074 Aachen — <sup>2</sup>Advanced Microelectronic Center Aachen (AMICA), Otto-Blumenthal-Straße 25, 52074 Aachen

Using scanning tunneling microscopy (STM) in ultra high vacuum and atomic force microscopy, we investigate the corrugation of graphene flakes deposited by exfoliation on a Si/SiO<sub>2</sub> surface. While the corrugation on SiO<sub>2</sub> is long-range with a correlation length of about 25 nm,

some of the graphene monolayers exhibit an additional corrugation with a preferential wave length of about 15 nm. A detailed analysis shows that the long range corrugation of the substrate is also visible on graphene, but with a reduced amplitude, leading to the conclusion that the graphene is partly freely suspended between hills of the substrate. Thus, the intrinsic rippling observed previously on artificially suspended graphene can exist as well, if graphene is deposited on SiO<sub>2</sub> [1].

[1] J. C. Meyer, A. K. Geim, M. I. Katsnelson, K. S. Novoselov, T. J. Booth, and S. Roth, Nature 446, 60 (2007).

O 40.8 Wed 16:45 SCH A316

**Cross-sectional Scanning Tunneling Microscopy across a Metal-Semiconductor Interface - Structural and Electronic Properties on the Atomic Scale** — LARS WINKING, MARTIN WEN-DEROTH, ●TIM IFFLÄNDER, THOMAS DRUGA, and RAINER G. ULBRICH — IV. Physikalisches Institut, Georg-August-Universität Göttingen

Understanding the formation of Schottky barriers has been a major theme of surface science for more than half a century. However, the various mechanisms that determine the barrier height are still subject to discussion. To a large part this is due to the lack of appropriate experimental techniques with atomic resolution and the difficulties associated with preparing well-defined epitaxial interfaces.

We report scanning tunnelling spectroscopy (STS) across a cleaved epitaxial GaAs(110)/Fe interface. It provides information on the structural as well as the electronic properties of the heterointerface on the atomic scale. Furthermore, in combination with 3D simulations of the tip induced band bending we are able to quantify both the local Schottky barrier height and the influence of single dopant atoms on the electrostatic potential landscape representing the space charge layer in the semiconductor. Our experimental data are discussed in the context of existing theoretical models for Schottky barrier formation, like the advanced unified defect model or the metal-induced gap states model.

This work was supported by the SFB 602 TP A7.

O 40.9 Wed 17:00 SCH A316

**Plasmon enhanced luminescence from fullerene molecules using a scanning tunneling microscope** — ●FRÉDÉRIC ROSSEL, MARINA PIVETTA, FRANÇOIS PATTHEY, and WOLF-DIETER SCHNEIDER — Ecole Polytechnique Fédérale de Lausanne (EPFL), Institut de Physique des Nanostructures, CH-1015 Lausanne, Switzerland

Luminescence from supported C<sub>60</sub> and C<sub>70</sub> molecules induced by tunneling electrons in a scanning tunneling microscope (STM) has been observed. The fullerene nanocrystals were electronically decoupled from the Au(111) substrate by an ultrathin NaCl film. Intramolecular fluorescence and phosphorescence associated with the transitions between the lowest electronic excited state and the ground state of C<sub>70</sub> molecules were identified, demonstrating the capability of this technique for chemical recognition on the nanometre scale. Moreover we show that the molecular luminescence is selectively enhanced in the STM tip-sample gap by localized surface plasmons excited in an inelastic electron tunneling process.

We acknowledge financial support of the Swiss National Science Foundation.

O 40.10 Wed 17:15 SCH A316

**Manipulating surface diffusion ability of single molecules by scanning tunneling microscopy** — DINGYONG ZHONG<sup>1,2</sup>, JÖRN-HOLGER FRANK<sup>1</sup>, ●TOBIAS BLÖMKER<sup>3</sup>, GERHARD ERKER<sup>3</sup>, HARALD FUCHS<sup>1,2</sup>, and LIFENG CHI<sup>1</sup> — <sup>1</sup>Physikalisches Institut, Universität Münster, Wilhelm-Klemm-Str. 10, 48149 Münster, Germany & Center for Nanotechnology (CeNTech), Universität Münster, Heisenbergstr. 11, 48149 Münster, Germany — <sup>2</sup>Institut für Nanotechnologie, Forschungszentrum Karlsruhe, 76021 Karlsruhe, Germany — <sup>3</sup>Organisch-Chemisches Institut, Universität Münster, Corresstr. 40, 48149 Münster, Germany

The bonding of single diferrocene [Fc(CH<sub>2</sub>)<sub>14</sub>Fc, Fc = ferrocenyl] molecules on a metal surface can be enhanced by partial decomposition of Fc groups induced by the tunneling current in scanning tunneling microscopy. Although the isolated intact molecule is mobile on the terrace of Cu(110) at 78 K, the modified molecule is immobilized on the terrace. Calculations based on density functional theory indicate that the hollow site of the Cu(110) surface is the energetically favorable adsorption site for both ferrocene and the Fe-cyclopentadienyl complex, but the latter one possesses a much higher binding energy with the substrate.

## O 41: Ab-initio approaches to excitations in condensed matter I

Time: Wednesday 15:00–17:30

Location: SCH 251

O 41.1 Wed 15:00 SCH 251

**Accurate van-der-Waals interactions from (semi)-local density functional theory** — ●ALEXANDRE TKATCHENKO and MATTHIAS SCHEFFLER — Fritz-Haber-Institut der MPG, Berlin, Germany

Non-covalent forces, such as hydrogen bonding and van der Waals (vdW) interactions, are crucial for the formation, stability and function of molecules and materials. At present, vdW interactions can only be satisfactorily accounted for by high-level quantum-chemical wave function or by the Quantum Monte Carlo (QMC) method. In contrast, (semi)-local DFT and Hartree-Fock approximation fail for the description of vdW forces. We present a parameter-free method for describing the long-range vdW interaction in (semi)-local DFT. The leading  $C_6$  coefficients are derived from the electron density of a molecule/solid and accurate reference values for the free atoms. The mean absolute error in the  $C_6$  coefficients is 5.5% when compared to accurate experimental values for 1225 intermolecular pairs. We show that the  $C_6$  coefficients depend strongly on the bonding type and geometry of molecules/solids. Finally, we analyze the vdW radii and the damping function in the  $C_6R^{-6}$  correction method for DFT calculations.

O 41.2 Wed 15:15 SCH 251

**Proton momentum distribution in hydrogen bonded systems** — JOSEPH A. MORRONE, LIN LIN, and ●ROBERTO CAR — Princeton University, Princeton, USA

Recently the momentum distribution of the protons has been measured in neutron Compton scattering experiments: this property gives access to the local potential energy surface experienced by the protons in hydrogen bonded environments. Theoretically, the momentum distribution can be simulated using path integral Car-Parrinello molecular dynamics. In this talk recent results obtained with this approach for the proton momentum distribution in water and ice under standard thermodynamic conditions will be reviewed. Then, ice under very high pressure will be used to illustrate how the momentum distribution of the protons changes when the latter undergo quantum tunneling.

This work was partially supported by the DOE under grant DE-FG02-05ER46201.

O 41.3 Wed 15:30 SCH 251

**Static Correlation in the Description of the Oxygen-Metal Interaction** — ●CHRISTIAN CARBOGNO and AXEL GROSS — Institut für Theoretische Chemie, Universität Ulm,

The correct treatment of *static correlation*, i.e. the necessity to include multiple determinants to describe a wave function of a certain symmetry, is critical for the correct simulation of molecules, particularly if excited open-shell singlet states are addressed. Whereas these effects can be tackled unambiguously with CI, only an approximate description in terms of fractional occupation numbers is possible when solving the Kohn-Sham equations. For extended systems, where DFT methods are widely applied due to their numerical efficiency, such effects are typically negligible, especially if the interaction of a molecule with a metal surface is addressed. The thereby occurring *adiabatic* charge transfer, as described within the Born-Oppenheimer approximation, generally breaks the symmetry of the molecule: Thus one basic requirement for the manifestation of static correlation gets lost. For the oxygen chemistry on metal substrates, however, the Born-Oppenheimer approximation may fail under certain circumstances, as experimental [1] and theoretical [2] studies suggest. In such cases, the correct description of the molecule's excited states becomes of vital importance for the comprehension of the ongoing chemical processes. Accordingly, we will discuss the role of static correlation for this model system by comparing state-of-the-art MRCI and GGA-DFT calculations.

[1] R. Burgert *et al.*, Science **319**, 438 (2008).

[2] C. Carbogno *et al.*, Phys. Rev. Lett. **101**, 096104 (2008).

O 41.4 Wed 15:45 SCH 251

**Implementation of the exact-exchange Kohn-Sham functional within the all-electron FLAPW method** — ●MARKUS BETZINGER<sup>1</sup>, CHRISTOPH FRIEDRICH<sup>1</sup>, STEFAN BLÜGEL<sup>1</sup>, and ANDREAS GÖRLING<sup>2</sup> — <sup>1</sup>Institut für Festkörperforschung and Institute for Advanced Simulation, Forschungszentrum Jülich, 52425 Jülich, Germany

— <sup>2</sup>Lehrstuhl für Theoretische Chemie, Universität Erlangen-Nürnberg, Egerlandstr. 3, 91058 Erlangen, Germany

The success of density-functional theory (DFT) relies on the availability of accurate approximations for the exchange-correlation (xc) functional. Standard xc functionals, such as the local-density and the generalized-gradient approximation, suffer from several shortcomings: an unphysical electronic self-interaction, no discontinuity of the xc potential at integral particle numbers, wrong asymptotic behavior etc. Orbital-dependent functionals are a promising new generation of xc functionals. The simplest variant consistent with the Kohn-Sham theory requiring a local xc-potential is the exact-exchange (EXX) functional. It does not exhibit the above mentioned deficiencies. We implemented the EXX functional within the full-potential augmented-planewave (FLAPW) method using a specifically designed auxiliary basis set for the optimized effective potential (OEP) equation. We demonstrate that the auxiliary and FLAPW basis must be properly balanced to avoid spurious oscillations in the exact exchange potential and show first results for prototype semiconductors and insulators.

O 41.5 Wed 16:00 SCH 251

**Towards a low-dimensional Lieb-Oxford bound** — ●CÉSAR R. PROETTO<sup>1,2</sup>, KLAUS CAPELLE<sup>3</sup>, STEFANO PITTALIS<sup>1</sup>, and ESA RÄSÄNEN<sup>4</sup> — <sup>1</sup>Institut für Theoretische Physik, Freie Universität Berlin, Arnimallee 14, D-14195 Berlin, Germany and European Theoretical Spectroscopy Facility (ETSF) — <sup>2</sup>Centro Atómico Bariloche and Instituto Balseiro, 8400 S. C. de Bariloche, Río Negro, Argentina — <sup>3</sup>Departamento de Física e Informática, Instituto de Física de São Carlos, Universidade de São Paulo, São Paulo, 13560-970, Brazil — <sup>4</sup>Nanoscience Center, Department of Physics, P. O. Box 35 FIN-40014 University of Jyväskylä, Finland

Exact constraints on the unknown exchange-correlation (xc) energy functional are of fundamental importance in density-functional theory (DFT): One main and successful strategy in the never-ending challenge for the building of more accurate xc functionals consist of satisfying as many exact constraints as possible. The Lieb-Oxford bound (LOB) for three-dimensional (3D) systems is one of such exact constraints, and in its more useful version within the context of DFT is given as a lower bound on the correlation energy, in terms of a power of the particle density. For the bound to be useful, it should be as tight as possible. In this talk, we will provide the construction of the equivalent of the 3D LOB, but for the low-dimensional cases. In particular, by using scaling analysis and exploiting the fact that for some low-dimensional systems we know the ground-state xc energy and density, we have computed the expression for the bound in the 1D and 2D cases, and analyzed in detail the dimensionality crossover in between.

O 41.6 Wed 16:15 SCH 251

**Exploring the random phase approximation: application to CO adsorption, bulk metals, and weakly bonded molecules** — ●XINGUO REN<sup>1</sup>, PATRICK RINKE<sup>1,2</sup>, and MATTHIAS SCHEFFLER<sup>1,2</sup> — <sup>1</sup>Fritz-Haber-Institut der MPG, D-14195 Berlin, Germany — <sup>2</sup>Materials Dept., UC Santa Barbara, CA 93106, USA

Density-functional theory (DFT) within the generalized gradient approximation (GGA) has been immensely successful in describing the ground state properties of a diverse range of materials. However, inherent strong self-interaction effects and the absence of van der Waals (vdW) interactions are two prominent examples of GGA's failures. These severely affect the description of (bio)molecules and in certain cases (e.g. CO) their adsorption on (transition)metal surfaces. Many-body perturbation theory in the random phase approximation (RPA) presents a promising way to go beyond GGA since it is expected to perform well for molecular, metallic and vdW systems alike. However, despite the recent interest the RPA has generated, a comprehensive assessment of its performance is not available. Using CO@Cu(111), a selection of bulk metals, and the benzene dimer, a prototypical  $\pi$ -conjugated system, as examples, we demonstrate the performance of the RPA for different types of systems. We show that the potential-energy surface of CO adsorbed on Cu(111) can be correctly described within RPA at a quantitative level. The binding energy of the benzene dimer, on the other hand, is considerably underestimated. We further show that these RPA results are not sensitive to the DFT functional chosen for the description of the unperturbed system.

O 41.7 Wed 16:30 SCH 251

**Exact Kohn-Sham potential of strongly correlated finite systems** — ●NICOLE HELBIG, ILYA TOKATLY, and ANGEL RUBIO — Nano-Bio Spectroscopy group and ETSF, Dpto. de Física de Materiales, Universidad del País Vasco and Centro Mixto CSIC-UPV/EHU, San Sebastián, Spain

The description of strongly correlated systems within density functional theory has proven very difficult in the past. The dissociation of molecules, even the most simple hydrogen molecule, cannot be described accurately with any of the presently available density functionals. These problems have led to a discussion of what properties the local Kohn-Sham potential has to satisfy in order to correctly describe strongly correlated systems. We use a one-dimensional, two electron model system to investigate the behavior of the exact Kohn-Sham potential, which can be calculated easily for this system. We present an analytic expression for the potential at the dissociation limit and show that the numerical calculations indeed approach and reach this limit as we dissociate the system. It is shown that the functional form of the Kohn-Sham potential is independent of the details of the system under consideration making the results easily transferable to other systems. We use this knowledge to calculate the exact Kohn-Sham potential of the hydrogen molecule in the dissociation limit.

O 41.8 Wed 16:45 SCH 251

**Discontinuity of chemical potential in reduced density matrix functional theory: open shell formulation** — ●N.N. LATHIOTAKIS<sup>1,2,4</sup>, N. HELBIG<sup>2,3,4</sup>, and E.K.U. GROSS<sup>2,4</sup> — <sup>1</sup>TPCI, NHRF, Vass. Constantinou 48, Athens, Greece — <sup>2</sup>Institut für Theoretische Physik, FU Berlin, Arnimallee 14, D14195 Berlin, Germany — <sup>3</sup>Nano-Bio Spectroscopy group, Dpto. de Física de Materiales, Universidad del País Vasco UPV/EHU and Centro Mixto CSIC-UPV/EHU, San Sebastián, Spain — <sup>4</sup>European Theoretical Spectroscopy Facility

In reduced-density-matrix-functional theory, approximations of the total energy as a functional of the one-body-reduced-density matrix are minimized. In an open-shell treatment, this minimization involves two Lagrange multipliers that ensure the conservation of the number of particles separately for each spin. We prove that these Lagrange multipliers are the chemical potentials, i.e. the derivatives of the total energy with respect to the numbers of spin up and spin down electrons. For the exact functional, these Lagrange multipliers show a discontinuity at integer values of the spin-resolved particle numbers which equals the fundamental gap. We test present-day RDMFT functionals for this property and find that many of them reproduce a step-like behavior, in resemblance to the exact theory. This behavior is improved in the

open-shell treatment i.e. when all fractional electrons are added to the same spin. The obtained discontinuities are in very good agreement with the gaps of the studied finite systems. These promising results are a motivation for the application of RDMFT to problems like the band gaps of solids where DFT results deviate from experiments.

O 41.9 Wed 17:00 SCH 251

**Reduced Density Matrix Functional for Many-Electron Systems** — SANGEETA SHARMA<sup>1,2,3</sup>, ●KAY DEWHURST<sup>1,2,3</sup>, NEKTARIOS LATHIOTAKIS<sup>4,3</sup>, and E. K. U. GROSS<sup>2,3</sup> — <sup>1</sup>Fritz Haber Institute of the Max Planck Society, Faradayweg 4-6, D-14195 Berlin, Germany. — <sup>2</sup>Institut für Theoretische Physik, Freie Universität Berlin, Arnimallee 14, D-14195 Berlin, Germany — <sup>3</sup>European Theoretical Spectroscopy Facility (ETSF) — <sup>4</sup>Theoretical and Physical Chemistry Institute, The National Hellenic Research Foundation, Vass. Constantinou 48, 11635 Athens, Greece

We explore the performance of reduced-density-matrix-functional theory (RDMFT) for solids, in particular, for strongly correlated solids. To this end, we introduce a novel exchange-correlation functional of RDMFT based on a fractional power of the one-body density matrix. We show that, compared to other functionals, this new functional produces more accurate total energies as a function of particle number. Moreover, it captures the correct band gap behavior for conventional semiconductors as well as strongly correlated Mott insulators, where a gap is obtained in absence of any magnetic ordering.

O 41.10 Wed 17:15 SCH 251

**Stroboscopic wavepacket description of non-equilibrium many-electron problems** — ●PETER BOKES — Dept. of Physics, Slovak University of Technology FEI STU, Bratislava, Slovakia

We introduce the construction of a orthogonal wavepacket basis set, using the concept of stroboscopic time propagation, tailored to the efficient description of non-equilibrium extended electronic systems. Thanks to three desirable properties of this basis, significant insight is provided into non-equilibrium processes (both time-dependent and steady-state), and reliable physical estimates of various many-electron quantities such as density, current and spin polarization can be obtained. The use of this novel tool is demonstrated for time-dependent switching-on of the bias in quantum transport, and new results are obtained for current-induced spin accumulation at the edge of a 2D doped semiconductor caused by edge-induced spin-orbit interaction.

[1] P. Bokes, F. Corsetti, and R. W. Godby, *Phys. Rev. Lett.* 101, 046402 (2008)

**O 42: Poster Session II (Nanostructures at surfaces: arrays; Nanostructures at surfaces: Dots, particles, clusters; Nanostructures at surfaces: Other; Nanostructures at surfaces: Wires, tubes; Metal substrates: Adsorption of O and/or H; Metal substrates: Clean surfaces; Metal substrates: Adsorption of organic/bio molecules; Metal substrates: Solid-liquid interfaces; Metal substrates: Adsorption of inorganic molecules; Metal substrates: Epitaxy and growth; Heterogeneous catalysis; Surface chemical reactions; Ab-initio approaches to excitations in condensed matter; Organic, polymeric, biomolecular films— also with adsorbates; Particles and clusters)**

Time: Wednesday 17:45–20:30

Location: P2

O 42.1 Wed 17:45 P2

**Realization of Large-Scale Nano-Patterned Surfaces by the UTAM-Technique** — ●STEFAN OSTENDORP, YONG LEI, and GERHARD WILDE — Institut für Materialphysik, Westfälische Wilhelms-Universität Münster, Wilhelm-Klemm-Str. 10, 48149 Münster, Germany

Using an UTAM (ultra-thin alumina membrane) surface nano-patterning technique, large-scale arrays of highly regular metallic and semiconductor nano-particles were fabricated on silicon and sapphire substrates. The structural parameters of the synthesized nano-particles are controllable, including the diameter, spacing, and shape. Different metallic nano-particles have been oxidized using a well-controlled oxidation process in a modified CVD-system. The aim of the experiment is to obtain a core-shell nanostructure with a metallic core and an oxide shell. During the oxidation of some metallic nano-particles (chromium and nickel) on a silicon substrate, an interesting

nano-porous silicon oxide surface structure with embedded metallic oxide nano-particles evolved. These surface nano-porous structures are under investigation now by AFM, EFM, SEM and TEM to determine the details of their growth mechanism.

O 42.2 Wed 17:45 P2

**Terephthalic acid (TPA) on Si(111)- $\alpha$  and  $\beta$ -( $\sqrt{3} \times \sqrt{3}$ )-Bi surfaces** — ●TAKAYUKI SUZUKI<sup>1</sup>, THERESA LUTZ<sup>1</sup>, GIOVANNI COSTANTINI<sup>1,2</sup>, and KLAUS KERN<sup>1,3</sup> — <sup>1</sup>Max Planck Institute for Solid State Research, Heisenbergstrasse 1, 70569 Stuttgart, Germany — <sup>2</sup>Department of Chemistry, University of Warwick, Coventry, CV4 7AL, United Kingdom — <sup>3</sup>Institute de Physiques des Nanostructures, Ecole Polytechnique Fédérale de Lausanne, CH-1015 Lausanne, Switzerland

We have carried out scanning tunneling microscopy (STM) experiments of terephthalic acid (TPA) adsorption on Si(111)- $\alpha$  and  $\beta$ -

$(\sqrt{3}\times\sqrt{3})$ -Bi surfaces in order to study supramolecular self-assembly on passivated semiconductor surfaces. Both Si(111)- $\alpha$  and  $\beta$ - $(\sqrt{3}\times\sqrt{3})$ -Bi are passivated semiconductor surfaces without highly reactive Si dangling bonds, and have Bi coverages of 1/3 and 1 monolayer, respectively. The TPA molecules adsorb randomly on  $\alpha$ - $(\sqrt{3}\times\sqrt{3})$ -Bi and do not form any ordered supramolecular layer. On the other hand, they form ordered supramolecular layers on  $\beta$ - $(\sqrt{3}\times\sqrt{3})$ -Bi with at least four different types of coexisting structures. This completely different supramolecular self-assembly behavior on the  $\alpha$  and  $\beta$ - $(\sqrt{3}\times\sqrt{3})$ -Bi surfaces is quite striking since the two substrates are composed by the same atomic species and are characterized by the same unit cell. The different behavior is related to the differences in the electronic structure of these surfaces. Similar to the Si dangling bond states on Si(111)- $7\times 7$ , localized surface states exist on Bi adatoms on  $\alpha$ - $(\sqrt{3}\times\sqrt{3})$ -Bi, but not on Bi trimers on  $\beta$ - $(\sqrt{3}\times\sqrt{3})$ -Bi.

O 42.3 Wed 17:45 P2

**Faceted Lead Clusters on Nano Structured HOPG** — ●NIKLAS GRÖNHAGEN, FARHAD GHALEH, and HEINZ HÖVEL — Technische Universität Dortmund, Experimentelle Physik I, 44221 Dortmund

Lead as a cluster material shows an interesting behavior which distinguishes it from other metals. Lead starts diffusing at quite low temperatures and tends to form facets very easily. This is because Pb atoms can reorganize within or between clusters, consequently lowering their surface energy and thus transform into clusters with improved stability.

In the present study we produced faceted lead clusters by deposition of lead atoms on graphite (HOPG) samples, prestructured with nanometer sized pits [1]. The nano-pits were either distributed randomly on the sample or produced in an array using focussed ion beam lithography (ionLiNE system, Raith GmbH) [2].

Subsequently the clusters were investigated by scanning tunneling microscopy. We observed a fine structure in the height distribution given by Pb monolayer steps and an odd-even-oscillation. By measurements with scanning tunneling spectroscopy we were able to show that "Quantum Well States" are responsible for this growth behavior.

[1] H. Hövel, Appl. Phys. A 72, 295 (2001) [2] F. Ghaleh, R. Köster, H. Hövel, L. Bruchhaus, S. Bauerdick, J. Thiel, R. Jede: J. Appl. Phys. 101, 044301 (2007)

O 42.4 Wed 17:45 P2

**Selective and Hierarchical Bonding Interactions in 2D Multi-Component Supramolecular Networks at Surfaces** — ●ALEXANDER LANGNER<sup>1</sup>, STEVEN L. TAIT<sup>1</sup>, CHANDRASEKAR RAJADURAI<sup>2</sup>, NIAN LIN<sup>1</sup>, MARIO RUBEN<sup>2</sup>, and KLAUS KERN<sup>1,3</sup> — <sup>1</sup>Max-Planck-Institut für Festkörperforschung, Stuttgart — <sup>2</sup>Institut für Nanotechnologie, Forschungszentrum Karlsruhe — <sup>3</sup>Ecole Polytechnique Fédérale de Lausanne, Switzerland

Self-assembly of organic molecules is an efficient bottom-up approach to pattern surfaces with unique two-dimensional (2D) architectures at the nanometer scale. In order to achieve extended and highly ordered supramolecular networks, the spontaneous self-organization process has to be steered by selective, directional and strong, but non-covalent bonding interactions, such as hydrogen bonding or metal-organic complex formation. Here we concentrate on the surface supported self-assembly of aromatic ligand mixtures studied by scanning tunneling microscopy (STM) under ultra high vacuum (UHV) conditions. The various molecular building blocks are provided with either carboxylic acid or pyridyl moieties. In these ligand mixtures, selectivity of the functional groups towards different co-evaporated metal coordination centers is observed, which can lead to ligand separation or the formation of complex multi-component networks, stabilized by hierarchical bonding (i.e. hydrogen bonding as well as metal-ligand coordination). We will demonstrate that the selective and hierarchical character of the bonding interactions allow the controlled manipulation of structural network parameters.

O 42.5 Wed 17:45 P2

**In-situ scanning tunneling microscope growth studies of InAs and InN quantum dots during MOVPE growth** — ●MATTHIAS SCHMIES, RAIMUND KREMZOW, MARKUS PRISTOVSEK and MICHAEL KNEISSL — TU Berlin, Institut für Festkörperphysik, EW 6-1, Hardenbergstr. 36, D-10623 Berlin, Germany

Novel optoelectronic devices, like single-photon emitters and semiconductor lasers demand a better understanding of the growth process and control of quantum dots (QD). Most optoelectronic devices are grown

by metal organic vapour phase epitaxy (MOVPE) systems which allows mass fabrication for industrial applications. While QD growth has been studied intensively for InGaAs, the understanding of the mechanisms responsible for the formation of the QDs and especially of the ripening process during annealing and cooling down after growth is still relatively poor. The InGaN material system is even less understood. In order to investigate the growth dynamics and to clarify the theory of QD ripening we employed a in-situ scanning tunnelling microscope (STM) which allows measurements during MOVPE growth. In this paper we will discuss the ripening process of InAs QDs on GaAs(001):Si at 475°C. For the InAs/GaAs system the development of the structure density agrees to the mean field theory of Lifshitz, Slyozov and Wagner (LSW-theory) of the Ostwald ripening process for three dimensional island on a two dimensional substrate. Additionally, we will present first experiments of InN QDs grown on GaN/templates sapphire using tertiarybutylhydrazine (tBHy) as nitrogen precursor.

O 42.6 Wed 17:45 P2

**Monodisperse micro-island formation on Ni/Ru(0001) monolayers** — ●PETER JAKOB<sup>1</sup>, KAI ANHUT<sup>1</sup>, SEBASTIAN SCHNUR<sup>2</sup>, and AXEL GROSS<sup>2</sup> — <sup>1</sup>Fachbereich Physik, Philipps-Universität Marburg, D-35032 Marburg, Germany — <sup>2</sup>Institut für Theoretische Chemie, Universität Ulm, D-89069 Ulm, Germany

The formation of virtually identical and thermally stable Ni micro-islands (trimers) is presented. In our combined experimental and theoretical investigation we define the conditions for their unusual creation (expulsion of Ni atoms or trimers from the underlying substrate by means of adsorbate induced compressive stress) and give a detailed characterization of the micro-islands' structural properties, chemical composition and electronic/magnetic properties [1]. Specifically, we show that their exceptional structural and thermal stability can be ascribed to oxygen attached to the islands, thereby forming (metallic) Ni-oxygen composites. Our observation of a high density of identical clusters represents a major contribution to overcome a common challenge in materials science related to establishing a correlation between structural and catalytic/electronic properties of nanoscale objects. Usually, the various approaches lead to a dazzling array of sizes and shapes rather than monodisperse particles in a well-defined environment.

[1] P. Jakob, K. Anhut, S. Schnur, and A. Groß, Phys. Rev. Lett. 101, 206101 (2008).

O 42.7 Wed 17:45 P2

**Theoretical study of nucleation processes on patterned surfaces** — ●STEFAN FRIEDER HOPP and ANDREAS HEUER — Institut für Physikalische Chemie, Universität Münster, 48149 Münster, Germany

The properties of template-directed nucleation are studied in the transition region where full nucleation control is lost and additional nucleation beyond the pre-patterned structure is observed. To get deeper insight into the microscopic mechanisms, Monte Carlo simulations are performed. In this context, the previously used continuous algorithm [1] is replaced by a discrete one to reduce simulation time and to allow more detailed calculations. The applied method is based on the assumption that the molecules on the surface occupy the sites of a simple fcc lattice. It is shown that the simulation results presented in [1],[2] can be reproduced quite well by the discrete algorithm. Furthermore, the new method facilitates the calculation of the distribution of nuclei on the surface by using the radial distribution function  $g(r)$  which provides another possibility of comparison with experimental data.

[1] F. Kalischewski, J. Zhu, A. Heuer. Loss of control in pattern-directed nucleation: a theoretical study. Phys. Rev. B 77, 155401, (2008).

[2] F. Kalischewski, A. Heuer. Dynamic effects on the loss of control in template-directed nucleation, preprint (2008)

O 42.8 Wed 17:45 P2

**Nanopartikel - eine Perspektive für die tribologische Anwendung in der Industrie?** — ●SVEN MARTIN PROPPERT, KATJA TÖNSING und DARIO ANSELMETTI — Universität Bielefeld, Experimentelle Biophysik und angewandte Nanowissenschaften, Deutschland

Angestoßen durch wiederholte Medienberichte über nanopartikuläre Festschmierstoffe für Verbrennungsmotoren[1] wird in dieser Arbeit in einem kombinierten mikroskopischen (AFM) und makroskopischen (Pin on Disk Tribometer) Ansatz untersucht, inwieweit sich Schmier- und Verschleißschutzwirkung bei der Verwendung unterschiedlicher Nanopartikel nachweisen lassen.

Wir untersuchten mittels AFM in Modellversuchen das Adsorptionsverhalten auf glatten Oberflächen wie Glas oder Glimmer und quantifizierten sowohl mikro- als auch makroskopisch die Reibwerte der gebildeten Oberfläche. Darüber hinaus wurden die Oberflächen auch auf mechanische- sowie Temperaturstabilitätseigenschaften geprüft.

[1] Wirtschaftswoche Nr.047, Seite 106, 2008-11-17

O 42.9 Wed 17:45 P2

**Local spectroscopy of metallic thin layers and clusters on semiconducting surfaces** — ●JEDRZEJ SCHMEIDEL, MATHIAS MENDE, CHRISTOPH TEGENKAMP, and HERBERT PFNÜR — Institut für Festkörperphysik, Leibniz Universität Hannover, Abteilung Oberflächen, Appelstrasse 2, 30167 Hannover, Germany

Many physical and chemical properties of metallic nanostructures depend strongly on their size and the coupling to their supports. Although transport concepts, like Schottky barriers and Coulomb blockade effects, are understood on a mesoscopic scale, the knowledge of influence of atomic sized defect structures (islands, steps, grains) is still lacking. Using Ag wetting layers on Si(111), we have investigated the adsorption sites and I(V) characteristics of silver clusters adsorbed at different lattice sites by means of STM and STS. Using Ag  $\sqrt{3} \times \sqrt{3}$  reconstruction on Si(111), strong band bending leads to charge depletion in Si close to the hybrid interface, i.e. the 2d template is electrically isolated. It was noticed in the I(V) curves, that the Debye length is around 100nm (10G $\Omega$ ) for properly n-doped samples.

Additional evaporation of Ag followed by annealing to 300K results in the formation of nm-sized Ag clusters on top. Using the STM tip as a second tunneling junction, Coulomb blockade effects at 100K have been found in form of dI/dV resonance structures within the Si band gap range. The separation of these peaks is inversely proportional to the dot size as classically expected.

O 42.10 Wed 17:45 P2

**One-dimensional Structure of Boron Nitride on Chromium (110): A Study of the Growth of Boron Nitride by Chemical Vapour Deposition of Borazine** — ●FRANK MÜLLER<sup>1</sup>, HERMANN SACHDEV<sup>2</sup>, and STEFAN HÜFNER<sup>1</sup> — <sup>1</sup>Institut für Experimentalphysik, Universität des Saarlandes, 66041 Saarbrücken — <sup>2</sup>Institut für Anorganische Chemie, Universität des Saarlandes, 66041 Saarbrücken

In a recent study [1], the nucleation and growth of boron nitride films on a Chromium (110) surface by thermal decomposition of borazine, (HBNH)<sub>3</sub>, was investigated by low energy electron diffraction (LEED), X-ray photoelectron spectroscopy (XPS) and X-ray photoelectron diffraction (XPD). The boron nitride film forms a chemically non-uniform one-dimensional superstructure with short range order along the [1-10] direction and long range order along [001]. Also the thermal stability of the resulting BN film was investigated and a chemical reaction with the substrate was observed leading to the formation of Cr-B- and Cr-N- bonds at the interface, indicating the onset of the formation of hard boride and nitride phases in the system Cr-B-N.

[1] F. Müller, S. Hüfner, H. Sachdev, Surf. Sci. 602 (2008) 3467

O 42.11 Wed 17:45 P2

**Epitaxial Growth of Boron Nitride on a Rh-YSZ-Si(111) Multilayer System: Formation and Fine Tuning of a BN NanoMesh by Substrate Effects** — ●FRANK MÜLLER<sup>1</sup>, HERMANN SACHDEV<sup>2</sup>, and STEFAN HÜFNER<sup>1</sup> — <sup>1</sup>Institut für Experimentalphysik, Universität des Saarlandes, 66041 Saarbrücken — <sup>2</sup>Institut für Anorganische Chemie, Universität des Saarlandes, 66041 Saarbrücken

The epitaxial growth of boron nitride on the surface of a Rh-YSZ-Si(111) multilayer system by CVD of borazine (HBNH)<sub>3</sub> was investigated by low energy electron diffraction (LEED). The formation of a (14x14) h-BN on (13x13) Rh superstructure was observed, which is different in size from an already reported (13x13) h-BN on (12x12) Rh(111) superstructure grown on a Rh(111) single crystal substrate ("h-BN nanomesh"). We found hints that differences between the thermal expansion behaviour of the multilayer substrates and the single crystal substrate can be the reason for the formation of different sized superstructures [1].

[1] F. Müller, S. Hüfner, H. Sachdev, Surf. Sci. in press (doi:10.1016/j.susc.2008.10.033)

O 42.12 Wed 17:45 P2

**A liquid phase injection method for the deposition of molecules and clusters on atomically defined Si/Ag surfaces** — ●MATHIAS MENDE, JEDRZEJ SCHMEIDEL, HERBERT PFNÜR, and CHRISTOPH TEGENKAMP — Institut für Festkörperphysik, Universität

Hannover, Abteilung Oberflächen, Appelstrasse 2, 30167 Hannover, Germany

Techniques for the deposition of nano-sized objects with limited thermal stability like organic molecules, metallic clusters and functionalized CNT's are highly needed and therefore in the focus of current research. Besides electrospray ion beam deposition [1] also pulse valve injection is used [2].

We developed a technique for the soft deposition of neutral molecules and clusters out of a solvent in a controlled Argon atmosphere. Using a microdispenser system, droplets of different solvents with a diameter of 55  $\mu\text{m}$  were reliably injected onto any surface, which can be prepared under UHV conditions. In order to correlate the concentration of Au clusters (3-5nm) on the surface with the concentration in the solvent, the droplets have been investigated by SEM and XPS. The distribution of height and size of the clusters was determined by STM on clean Si(111) 7x7 and Si(111) Ag  $\sqrt{3} \times \sqrt{3}$  surfaces. To test the functionality of the Au clusters and to demonstrate the preservation of the atomic structure in the vicinity of the nano-sized objects, STS measurements have been performed.

[1] S. Rauschenbach et al., Small 2, 540 (2006)

[2] Y. Terada et al., e-J. Surf. Sci. Nanotech. 2, 28 (2004)

O 42.13 Wed 17:45 P2

**Winkel- und Impulsverteilungen von Photoelektronen aus Metallclustern** — ●BERNHARD FABER, PHILIPP WOPPERER und PAUL-GERHARD REINHARD — Institut für Theoretische Physik II, Uni Erlangen, Staudtstr. 7, 91058 Erlangen, Deutschland

Die Winkel- und Impulsverteilung der Photoelektronen aus kleinen Na<sub>N</sub>-Clustern werden untersucht. Die Anregung durch einen linear polarisierten fs-Laser und die nachfolgende Clusterdynamik werden mit zeitabhängiger Dichtefunktionaltheorie simuliert. Für freie Cluster wird über ein Ensemble von Orientierungen gemittelt. Es bleibt eine reine Polarwinkelabhängigkeit, die im Detail vom emittierenden Einzelchenzustand bestimmt ist.

Es werden auch Cluster betrachtet, die auf einer Ar(001) oder MgO(001) Oberfläche deponiert sind. (Dabei kann, als weitere Variante, unter der Isolatorschicht noch eine Metallunterlage folgen.) Hier ist die Orientierung wohldefiniert und die Winkelverteilungen zeigen wesentlich reichere Strukturen in Polar- und Azimutwinkel. Die Emission wird von Oberflächenabstoßung und anziehender Bildladungskraft stark beeinflusst.

O 42.14 Wed 17:45 P2

**STM/STS Investigations of early stage of the growth of silicides** — ●MACIEJ CEGIEL, MACIEJ BAZARNIK, JAN RÖNSPIES, and HERBERT PFNÜR — Leibniz Universität Hannover, Institut für Festkörperphysik, Appelstr. 2, 30167 Hannover, Germany

Investigations of transition metals and their silicides are extremely interesting as for certain transition metals stable, lattice matched and metallic structures can be grown. In general this process is compatible with silicon technology, i.e. these silicides can be used as contacts and interconnects in electric circuits. Furthermore, using lattice anisotropies can be used skilfully to grow either quantum dots or atomic wires with extraordinary high aspect ratios and one-dimensional band structures simply by self-organization. This fact facilitates silicides even for applications in nanoelectronics devices. In particular, the shape and the electronic properties of these objects depend not only on the annealing temperature but also on the initial amount of the deposited material. In this contribution we report on Co, Ti and Dy silicide formation on Si(111) and vicinal Si(111) surfaces. For the former the the diffusion dependent formation of silicide islands have been investigated for both (7x7) and Ni ( $\sqrt{19} \times \sqrt{19}$ ) substrates. For submonolayer coverage of Ti the early state of growth on Si(111) 7x7 has been studied by STM. Using STS resonant states with maxima at -1,19eV (HOMO), +0,49eV and +1,51eV (LUMO) were found in between Ti clusters and discussed as quantum well states. On the contrary, this states were not found in between Ti clusters grown Si(111)-( $\sqrt{19} \times \sqrt{19}$ )

O 42.15 Wed 17:45 P2

**Topography dependent distribution of Ag on Si surfaces during surfactant sputtering** — ●TAHA YASSERI<sup>1</sup>, KUN ZHANG<sup>2</sup>, HANS HOFSSÄSS<sup>2</sup>, and REINER KREE<sup>1</sup> — <sup>1</sup>Institute for Theoretical Physics, University of Göttingen, Friedrich-Hund Platz 1, D-37077 Göttingen, Germany. — <sup>2</sup>2nd Institute of Physics, University of Göttingen, Friedrich-Hund-Platz 1, D-37077 Göttingen, Germany.

Surface pattern formation by ion beam sputtering (IBS) can be modified by a mono layer steady-state coverage of surfactant atoms during the erosion (Surfactant Sputtering). An experimental set-up which allows a systematic study of this effect for various substrates and surfactants has been recently realized by us. Meanwhile we also extended a continuum theory and a Monte Carlo model to include surfactant effects, which makes it possible to compare experimental and theoretical findings.

Here, we present the case study of a Si substrate irradiated by 5keV Xe ions and Ag surfactants. We discuss the distribution of Ag atoms on the structured (rippled) Si surface using SEM and AFM imaging, MC data and numerical solutions of the continuum theory. We find that Ag is clustering preferentially on the crests of ripples, in accordance with a simple physical picture.

O 42.16 Wed 17:45 P2

**Optical spectroscopy of single laser-trapped gold nanoparticles** — ●NINET BABAJANI, STEPHAN EIFEL, MAXIMILIAN REISMANN, and GERO VON PLESSEN — Inst. of Physics (IA), RWTH Aachen University, 52056 Aachen, Germany

The plasmon lines of chemically synthesized noble-metal nanoparticles of nearly spherical shape and approximately equal size exhibit surprisingly large particle-to-particle variations of their resonance peak positions and line widths [1].

The reasons for these spectral variations are still unknown. Possible explanations include faceting of the nominally spherical particles, charges and chemical effects within the suspension, and interactions with the substrate.

In this work, a method is presented in which a single gold nanoparticle suspended in an aqueous environment is trapped by an optical tweezer and its light-scattering spectrum, which is free of substrate effects, is measured. Subsequently the trapped nanoparticle is deposited onto a substrate using the optical tweezer and its spectrum is measured again. A comparison of the single-particle spectra allows us to draw conclusions about the origin of the spectral differences between the particles.

[1] C. Sönnichsen et al., New J. Phys. (2002) vol. 4 pp. 93

O 42.17 Wed 17:45 P2

**Localized plasmons in defined silver microdisks investigated by PEEM** — ●FLORIAN SCHERTZ<sup>1</sup>, JOCHEN MAUL<sup>1</sup>, NOELIA BOCCHIO<sup>2</sup>, ANDREAS UNGER<sup>2</sup>, GERD SCHÖNHENSE<sup>1</sup>, and MAX KREITER<sup>2</sup> — <sup>1</sup>Institut für Physik, Johannes Gutenberg-Universität, D-55099 Mainz — <sup>2</sup>Max-Planck-Institut für Polymerforschung, D-55128 Mainz

Well-defined silver-disks with a diameter of 1micrometer and a height of 40nm deposited on a Si substrate are illuminated by Ti-sapphire femtosecond-laser pulses with a wavelength of 400nm corresponding to a photon energy of 3.1 eV. The emitted electrons are detected by means of a photoelectron emission microscope (PEEM).

As the electric field vector of the photons changes from p- to s-polarization, a bimodal electron emission pattern emerges, indicating the excitation of nanoplasmonic fields in the Ag particles. In addition, we observe a correlation between elliptical deformation of the area of the Ag disks with distinct photoelectron emission and the fraction of the s-polarization of the impinging photons.

Furthermore, the photoemission yield was investigated as a function of laser power revealing different power exponent dependencies for s- and p-polarized light.

O 42.18 Wed 17:45 P2

**Klusterexperimente an dünnen Co-PLD-Schichten und Schichtsystemen** — MARKUS TRAUTMANN, ROBER HÄHLE, JANINE FISCHER, INGO SILL, ANDRE BIKOWSKI, THOMAS SCHMIDT, VEIT GROSSE, ●FRANK SCHMIDL und PAUL SEIDEL — FSU Jena, Institut für Festkörperphysik, Helmholtzweg 5, 07743 Jena, Germany

Für das gezielte Wachstum von Kohlenstoffnanoröhren (CNT's) spielen ferromagnetische Kluster (Co,Fe,Cr) eine entscheidende Rolle. Wir stellen Untersuchungen zur strukturierten Abscheidung von dünnen Co-Schichten mittels lasergestützter Abscheidung (PLD) vor. Es wurden Klusterexperimente auf Si-Substraten mit und ohne SiO<sub>2</sub>-Einzelschichten bzw. Schichtsystemen durchgeführt. Wir diskutieren die Messungen zur Klustergröße in Abhängigkeit von Ausgangsschichtdicke, Klustertemperatur und Substratmaterial im Hinblick auf eine mögliche in-situ Abscheidung von CNT's mittels PLD.

O 42.19 Wed 17:45 P2

**Electron beam induced deposition: How to use an electron beam as a pen and precursor molecules as ink to write nanopatterns** — MICHAEL SCHIRMER<sup>1,2</sup>, MARIE-MADELEINE WALZ<sup>1,2</sup>, THOMAS LUKASCZYK<sup>1,2</sup>, FLORIAN VOLLNHALS<sup>1,2</sup>, HANS-PETER STEINRÜCK<sup>1,2</sup>, and ●HUBERTUS MARBACH<sup>1,2</sup> — <sup>1</sup>Lehrstuhl für Physikalische Chemie II — <sup>2</sup>Interdisciplinary Center for Molecular Materials (ICMM), Universität Erlangen-Nürnberg, Egerlandstr. 3, D-91058 Erlangen

The fabrication of chemically and structurally well-defined nanostructures is still a challenge and important for a large number of envisioned technological applications. We explore the technique of electron-beam induced deposition (EBID) to realize the engineering of such nanostructures: By exploiting a highly focused electron-beam of a scanning electron microscope (SEM) we directly write nanostructures by locally dissociating adsorbed precursor molecules. In contrast to previous studies our novel approach is to work in an ultra high vacuum (UHV) environment. This allows us to overcome the hitherto existing limitation concerning the rather poor cleanliness of the deposits [1]. In this work, we present the successful generation of clean metallic (Fe) and oxidic nanostructures (TiOx, FeOx) with lithographically controlled shapes and lateral dimensions partially smaller than 10 nm on different substrates. The concept of EBID, basic physical principles and the promising perspectives and applications of this nanostructuring tool will be presented. This work was supported by the DFG under grant MA 4246/1-1.[1] T. Lukaszcyk, et al., Small 4(6) (2008) 841.

O 42.20 Wed 17:45 P2

**Surface energy gradient produced by collision cascades: effects on pattern formation by ion beam sputtering** — REINER KREE<sup>1</sup>, ●TAHA YASSER<sup>1</sup>, and ALEXANDER K. HARTMANN<sup>2</sup> — <sup>1</sup>Institute for Theoretical Physics, University of Göttingen, Friedrich-Hund Platz 1, D-37075 Göttingen, Germany. — <sup>2</sup>Institute for Physics, University Oldenburg, Carl-von-Ossietzky Strasse 9-11, D-26111 Oldenburg, Germany

In the existing theories of pattern formation due to ion beam sputtering, the energy of collision cascades leads to sputtering of atoms. But the lateral displacements at the surface due to the excess energy are not taken into account. We provide a continuum and a Monte Carlo model, which include this effect. Both models are based on standard transport theory.

We discuss the importance of the additional lateral transport on ripple formation using results of MC simulations and numerical (finite element) solutions of the continuum model.

O 42.21 Wed 17:45 P2

**Nanostructuring of thin V2O3 films on Au(111) by sputtering** — ●LIZ MICHAELA RÖSKEN, FLORIAN LOVIS, ARMIN FELDHOFF, and RONALD IMBIHL — Institut für Physikalische Chemie und Elektrochemie, Leibniz-Universität Hannover, Callinstr. 3-3a, D-30167 Hannover, Germany

Thin V2O3 films of approximately 1 - 100 ML thickness on Au(111) were prepared by evaporation of vanadium in an O2 atmosphere (p(O2) = 10-7 mbar). The films were characterized by LEED, Auger electron spectroscopy and photoelectron emission microscopy (PEEM). With annealing at T = 350° C epitaxial V2O3 films were found exhibiting (sqrt(3) x sqrt(3))R30° and (2x2) structures. Only after longer exposure to hydrogen (1-3 h) some reduction of the V2O3 film could be seen as evidenced by an increase of the PEEM brightness corresponding to a work function decrease. Upon sputtering the film displayed some unexpected optical effects: depending on the angle of observation the films appeared red or green. Secondary electron microscopy (SEM) revealed that the sputtering has led to island formation on the surface. The islands exhibit an average diameter of 20 nm and an average separation from each other of 20 nm. As possible mechanisms causing the island formation selective sputtering and the transformation of the 2D layer V-oxide into a 3D layer are discussed.

O 42.22 Wed 17:45 P2

**Laser induced backside wet etching of transparent materials with ultrashort laser pulses** — ●MARTIN EHRHARDT and KLAUS ZIMMER — Leibnitz-Institut für Oberflächenmodifizierung, Leipzig

The surface micro structuring of transparent dielectric materials with lasers can be achieved by direct laser ablation using VUV - wavelength or ultrashort pulses. Another approach to structuring these materials are indirect laser processing methods. Such methods use an enhanced absorption at interface of the material which can be achieved by an addi-

tional liquid, temporary plasma or absorption layer. At LIBWE (Laser induced backside wet etching) the backside of the transparent material is immersed to an absorbing liquid. That results in an intense energy deposition near the interface. For LIBWE with ns laser pulse the influence of several process parameter on e.g. etch rate, surface morphology were investigated detailed by Zimmer et al for a number of materials. However, for an improve understanding of the involved time processes an investigation of the influence of the pulse length for e.g. etch rate and surface morphology is important. In this presentation we will show recent results of the investigation of fused silica etched by LIBWE with ultrashort pulses. In particular the influence of the laser fluence and pulse number of the etch characteristic were investigate detailed und discussed. Furthermore morphological investigations were performed on the etched surfaced by different analytic techniques to characterize the surface quality. The results will by discussed with respect to the etch model for LIBWE with ns Pulse to figure out the influence of the ultrashort pulse effects of the etching process.

O 42.23 Wed 17:45 P2

**Laser-induced mechanical excitation of nanostructures (and their measurement by means of SXM)** — ●MARKUS SCHMOTZ<sup>1</sup>, TOBIAS GELDDHAUSER<sup>1</sup>, PATRICK BOOKJANS<sup>2</sup>, and PAUL LEIDERER<sup>1</sup> — <sup>1</sup>Universität Konstanz, Deutschland — <sup>2</sup>James Madison University, USA

Information about deformations of nanostructures in the Gigahertz regime is rather sparse until now. Especially irradiation with short laser pulses is hardly studied. Our work aims at creating Surface Acoustic Waves (SAW) in the Gigahertz range based on short laser pulse techniques and using them to excite nanostructures. Generation and optically based detection of SAWs by single shot experiments showed first results. A new approach to the GHz regime is to utilize raster-probe techniques. Therefore we are developing a new detection method based on a homebuilt, variable temperature Scanning Tunneling Microscope (STM). Exploiting the highly non-linear  $I(z)$ -characteristic of the tunnelling-gap allows us to determine elongation in the sub-Å regime with high lateral resolution. Since the STM lacks a suitable temporal resolution for GHz-waves, we started to investigate vibrational modes in thin, free standing silicon membranes (thickness some hundred nm) in the kHz to MHz regime. In this range our STM electronics are fast enough to resolve the vibrations almost one-to-one. Comparison between optically gained information and corresponding STM data show excellent agreement. Measurements with the STM and according optical techniques at frequencies up to the GHz regime are currently under investigation.

O 42.24 Wed 17:45 P2

**Investigations on Focused Electron and Focused Ion Beam Induced Deposition of WC, PdC and PtC** — ●HOLGER MOTZKAU<sup>1,2</sup> and DETLEF SPODDIG<sup>2</sup> — <sup>1</sup>Experimental Condensed Matter Physics, Department of Physics, Stockholm University, Roslagstullsbacken 21, SE-104 06 Stockholm, Sweden — <sup>2</sup>Abteilung für Supraleitung und Magnetismus, Institut für Experimentelle Physik II, Universität Leipzig, Linnéstr. 5, D-04103 Leipzig, Germany

Metallic nanostructures were grown by means of Focused Electron and Focused Ion Beam Induced Deposition (FEIBID/FIBID) in a Dual Beam Microscope (DBM). The used precursors were tungsten hexacarbonyl, palladium(II) bis-(hexafluoroacetylacetonate) and methylcyclopentadienyl(trimethyl)platinum(IV). This investigation will present an optimization of the growth rates and homogeneities on an insulating SiN-surface. The chemical composition of the nanostructures were discussed by means of Energy Dispersive X-Ray Spectroscopy (EDX). Detailed AFM-scans reveal strong inhomogeneities for the W and Pd deposits as well as a small nonlinear growth at small thicknesses below 50 nm for all used precursors.

O 42.25 Wed 17:45 P2

**Coverage-Dependent Faceting of Au Chains on Si(557)** — ●I. BARKE<sup>1</sup>, F. ZHENG<sup>2</sup>, S. BOCKENHAUER<sup>2</sup>, K. SELL<sup>1</sup>, V. v. OEYNHAUSEN<sup>1</sup>, K. H. MEIWES-BROER<sup>1</sup>, and F. J. HIMPEL<sup>2</sup> — <sup>1</sup>Universität Rostock, Institut für Physik, 18051 Rostock — <sup>2</sup>Dept. of Physics, University of Wisconsin Madison, 1150 University Ave, Madison, WI 53706

The structural and electronic phase diagram of Au on Si(557) is established using scanning tunneling microscopy (STM) and angle-resolved photoemission (ARPES). Five phases consisting of altogether seven facets are observed in the sub-monolayer regime. Four of them consist of two coexisting structures. In order of increasing Au coverage the

five phases are: Si(111)7×7 + Si(112), Si(557)1×2-Au, Si(111)5×2-Au + Si(335)-Au, Si(111)√3×√3-Au + Si(335)-Au, and Si(111)√3×√3-Au + Si(5 5 11)-Au. The relative surface areas of the five phases and seven facets are determined accurately by depositing a Au wedge ranging from 0 to 0.8 monolayer and performing automatic pattern recognition on large-scale STM images. Angle-resolved photoemission spectra are decomposed into contributions from the five phases. The Fermi wave vectors of various facets are identified. Using Si(557)1×2-Au as reference we find a coverage of 3 Au chains per unit cell for the frequently-studied Si(111)5×2-Au surface (instead of the widely-used value of 2 Au chains). The impact of this finding on structural models is discussed.

O 42.26 Wed 17:45 P2

**Temperature- and adatom-induced conductance modification of In/Si(111)-(4x1) nanowires** — ●NADJA KOCH, SIMONE SANNA, STEFAN WIPPERMANN, and WOLF GERO SCHMIDT — Lehrstuhl für theoretische Physik, Universität Paderborn, Warburger Str. 100, 33098 Paderborn

Quasi one-dimensional structures, such as artificial atomic-scale wires, attract considerable attention due to their fascinating physical properties and large technological potential [1]. Highly anisotropic surface superstructures such as the In/Si(111)-(4x1) nanowire array are suitable model systems to explore atomic-scale wires both experimentally and computationally [2,3]. As a contribution to the understanding of the controversially discussed low-temperature phase transition of the In nanowires, we present ab-initio calculations of their temperature-dependent Landauer conductance. Additionally, we calculate the influence of adatoms (In, Pb, H, O) on the nanowire cond. [4]. Our results for In deposition, where exp. data are available, agree very well with the measurements [5]. The cond. drop due to adatoms is explained in terms of potential-well scatt. and/or structural deform. of the nanowires.

[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] A A Stekolnikov, K Seino, F Bechstedt, S Wippermann, W G Schmidt, A Calzolari, M B Nardelli, Phys Rev Lett 98, 026105 (2007)

[4] S Wippermann, N Koch and W G Schmidt, Phys Rev Lett 100, 106802 (2008).

[5] T Tanikawa et al., Phys Rev Lett 93, 016801 (2004).

O 42.27 Wed 17:45 P2

**Electron beam stimulated thermal desorption of oxygen: a lithographic method** — ●JAN RÖNSPIES, TAMMO BLOCK, and HERBERT PFNÜR — Leibniz Universität Hannover, Institut für Festkörperphysik, Appelstr. 2, 30167 Hannover, Germany

We explored the structural limits of unconventional electron beam lithography by directly writing with an electron beam into ultra-thin SiO<sub>2</sub> films. These bare silicon window structures are suitable for growing contiguous metallic nanowires with thickness of a few monolayers. These uncovered structures with lateral dimensions down to 10nm were analyzed further by tunneling microscopy. The Auger excitation process (Knotek-Feibelman mechanism) necessary for electron-beam stimulated thermal desorption of oxygen (EBSTD) allows generation of ultra-small structures. The subsequent processing step combines thermal desorption of the remaining monoxide and simultaneous etching promoted by thermally activated silicon atoms, which turns out to be a strongly anisotropic process close to step edges [1]. Applying this combination of processes to a regularly stepped Si(557) sample which consists of a periodic array of small (111) and (112) oriented mini-facets with an average periodicity of 5.7nm normal to the steps, line widths close to the resolution of the electron microscope of 5nm were obtained. Thus exploitation of the quantized nature of ultrasmall structures far above liquid He temperatures becomes feasible as well as contacting of single molecules.

[1] *J.Appl.Phys.* **103**, 064303(2008)

O 42.28 Wed 17:45 P2

**The formation of Au nanowires on Ge(001): an ab-initio study** — ●SIMEON SAUER<sup>1</sup>, FRANK FUCHS<sup>1</sup>, JÜRGEN FURTHMÜLLER<sup>1</sup>, FRIEDHELM BECHSTEDT<sup>1</sup>, CHRISTIAN BLUMENSTEIN<sup>2</sup>, SEBASTIAN MEYER<sup>2</sup>, JÖRG SCHÄFER<sup>2</sup>, and RALPH CLAESSEN<sup>2</sup> — <sup>1</sup>Institut für Festkörpertheorie und -optik, Universität Jena, D-07743 Jena — <sup>2</sup>Physikalisches Institut, Universität Würzburg, D-97074 Würzburg

Deposition of approximately 0.5 ML of Au on the Ge(001) surface leads to self-organized formation of chains along the [110] direction [1]. These chains are characterized by some unprecedented features:

low-defect growth, high aspect ratio and rather high spacing between adjacent chains. This system seems to be a possible candidate for the formation of a Luttinger liquid.

Assuming a  $c(8 \times 2)$  translational symmetry we propose several models of Au chain structures. They are investigated in the framework of a density functional theory approach. For each model, different features including surface energy, STM images, band structure, etc. are calculated. The computed properties are compared to experimental data and used to evaluate the different models.

[1] J. Schäfer, C. Blumenstein, S. Meyer, M. Wisniewski, and R. Claessen, Phys. Rev. Lett. 101, in press (Dec. 2008).

O 42.29 Wed 17:45 P2

**Large Area Growth of Pt-induced Atomic Nanowires on Ge(001)** — ●SEBASTIAN MEYER<sup>1</sup>, KATHRIN ROENSCH<sup>1</sup>, MARC WISNIEWSKI<sup>1</sup>, CHRISTIAN BLUMENSTEIN<sup>1</sup>, JÖRG SCHÄFER<sup>1</sup>, ANDREJ STEKOLNIKOV<sup>2</sup>, FIEDHELM BECHSTEDT<sup>2</sup>, and RALPH CLAESSEN<sup>1</sup> — <sup>1</sup>Physikal. Institut, Universität Würzburg, 97074 Würzburg — <sup>2</sup>Inst. f. Festkörpertheorie u. -optik, Universität Jena, 07743 Jena

The structural properties of atomic nanowires are closely affecting both self-organized growth and resulting conduction behavior. A fascinating case are Pt nanowires on the Ge(001) surface. A dimerization along the chains observed in scanning tunneling microscopy (STM) is reminiscent of a charge density wave. However, sideways dimer elements also exist, which indicate dimerized back-bonds. Near the Fermi level, dimerization is not observed, and a spatially rather uniform charge density exists. It is consistent with metallic character at room temperature, as is confirmed by tunneling spectroscopy. Concerning the bonds involved, rather high substrate temperatures ( $\sim 700$  °C) are needed to initiate large-area growth. The experimental findings can be understood within a structural model obtained from ab-initio simulation [1]. It turns out that Pt-Ge bonds are favored. Moreover, the prominent dimerization along the chain is explained by Ge dimers rather than Pt ones. Instead, the metal atoms are incorporated as chain of alternating Pt and Ge atoms adjacent to the top ridge. Such complex bond rearrangement makes it plausible that high activation energies are needed for a structural reorganization.

[1] A. A. Stekolnikov et al., Phys. Rev. Lett. 100, 196101 (2008).

O 42.30 Wed 17:45 P2

**Suppression of phase transition by doping: atomic Pb chains on Si(557)** — MARCIN CZUBANOWSKI, ●MELANI GAUCH, CHRISTOPH TEGENKAMP, and HERBERT PFNÜR — Leibniz Universität Hannover, Festkörperphysik, Abteilung Oberflächen

The adsorption of Pb on Si(557) substrate leads to the formation of anisotropic metallic structures as reveal by conductivity measurements, SPA-LEED and ARPES. The annealing of at least 1.3ML Pb at 640K forms atomic chain structure within a (223) facet, which shows below  $T_c = 78K$  a metallic conductance along the wires, whereas the perpendicular direction is insulating. As revealed by ARPES and LEED, the interplay between the filling of the surface bands, determined by the Pb coverage, and the reciprocal lattice vector, defined by the inter-chain spacing, results below  $T_c$  in a perfect nesting condition. Due to a temperature driven refaceting transition, the system switches into a 2d regime, where conductivity is seen in both direction. In our recent experiments, the influence of additional Pb atoms on the phase transition at  $T_c$  has been investigated by means of SPA-LEED. The electronically stabilized system at 1.3ML has been doped by a small amount of addition Pb (in steps of 0.01ML). The structural phase transition is gradually suppressed as the coverage reaches 1.5ML. As judged from SPA-LEED the excess coverage starts to decorate the steps, obviously changing the filling factors of the surface states.

O 42.31 Wed 17:45 P2

**Surface Photo Voltage and Local Work Function Variations of Nanostructures on Si(111) measured by STM** — ●KRISTIAN SELL, INGO BARKE, STEFAN POLEI, VIOLA VON OEYNHAUSEN, and KARL-HEINZ MEIWES-BROER — Universität Rostock, Institut für Physik, 18051 Rostock, Germany

We present surface photo voltage (SPV) and local work function (LWF) measurements of Si(111)5x2-Au atomic chains and deposited clusters on a Si(111)7x7 surface. Quantitative results are obtained from spatially resolved I(V) spectra. On a Si(111) surface partially covered by the quasi one-dimensional Si(111)5x2-Au structure we determine the SPV as a function of laser power at different locations. Based on these results we establish and discuss a simple model for the band bending which leads to LWF variations on a sub-nanometer

scale. This model is confirmed by spatially resolved LWF measurements using I(Z) spectroscopy. In addition we present preliminary SPV measurements on clusters produced in an arc cluster ion source (ACIS) and deposited on Si(111)7x7.

O 42.32 Wed 17:45 P2

**Field Emission Resonances on Junctions between Si(111)7x7 and Si(111)5x2-Au** — ●STEFAN POLEI, INGO BARKE, KRISTIAN SELL, VIOLA V. OEYNHAUSEN, and KARL-HEINZ MEIWES-BROER — Institut für Physik, Universität Rostock, Universitätsplatz 3, D-18051 Rostock

The image state derived field emission resonances (FER) are investigated on a Si(111)7x7 substrat which is partially covered by the quasi one-dimensional Si(111)5x2-Au structure. These states can be observed by dI/dV measurements of the unoccupied energy range if the STM is operated in a field emission mode. A shift of the FER peak positions on Si(111)7x7 patches vs. Si(111)5x2-Au patches is found which happens on a scale of one nanometer. The origin of that shift is attributed to work function differences [1] caused by the different Fermi level pinning. The results are discussed in view of local work function changes determined by I(Z) spectroscopy across a (7x7)-(5x2-Au) junction.

[1] H. C. Ploigt, C. Brun, M. Pivetta, F. Patthey, and W. D. Schneider, Phys. Rev. B 76, 195404 (2007).

O 42.33 Wed 17:45 P2

**Investigation of self-sustained molecular wires by STM** — ●KERRIN DÖSSEL<sup>1</sup>, MAYA LUKAS<sup>1</sup>, ALEXANDRINA STUPARU<sup>1</sup>, CHRISTOPHE STROH<sup>1</sup>, MARCEL MAYOR<sup>1,2</sup>, and HILBERT V. LÖHNESEN<sup>3,4</sup> — <sup>1</sup>Forschungszentrum Karlsruhe, Institut für Nanotechnologie, D-76021 Karlsruhe — <sup>2</sup>Universität Basel, Department of Chemistry, CH-4056 Basel — <sup>3</sup>Universität Karlsruhe, Physikalisches Institut, D-76128 Karlsruhe — <sup>4</sup>Forschungszentrum Karlsruhe, Institut für Festkörperphysik, D-76021 Karlsruhe

In recent years the electronic structure and in particular the conductance of organic molecules have been investigated in a growing number of experiments. A method frequently used to measure molecular conductance is the mechanically controlled break junction (MCBJ) technique. However, in MCBJs the nature of the contact of the molecule to the electrodes is not known. Theory is thus lacking important information to exactly model and thus understand molecular conductance. It is therefore desirable to fully characterize molecular wires which are binding stably to the electrodes. We investigate self-sustained molecules, that are designed to stand upright on a conducting substrate, which serves as one electrode, while the head-group is sticking out freely from the surface, accessible by the tip of our UHV STM. We used STM and STS to investigate the molecules' position and surrounding on the surface, the bond to the surface and the electronic properties of our tripod molecules on several metallic surfaces at low temperature (30K).

O 42.34 Wed 17:45 P2

**Growth of horizontally aligned carbon nanotubes on single crystalline surfaces** — ●FLORIAN SZILLAT, HANS KLEEMANN, PHILIPP ZEIGERMANN, MICHAEL BLECH, MATHIAS STEGLICH, and BERND SCHROETER — Universität Jena, Institut fuer Festkoerperphysik, Max-Wien-Platz 1, 07743 Jena, Deutschland

A controlled growth of aligned carbon nanotubes with particular structural and electronic properties at predefined positions is a prerequisite to utilize them in electronic or nanooptical devices. Alignment could be reached by applying electric fields during growth via chemical vapor deposition or by using single crystalline substrates. In the latter case the anisotropic arrangement of the surface atoms create an intrinsic electric field. An easy and fast way to analyze the crystallographic orientation of the substrate is the use of electron channeling pattern. The metal catalyst is deposited and prestructured at the substrate surface to support the aligned growth of CNTs. The carbon nanotubes are produced by catalytic chemical vapor deposition using ethanol or methane as precursor gas. The quality of these nanotubes is tested by raman and x-ray spectroscopy. Morphology and orientation of the nanotubes are characterized by scanning electron and atomic force microscopy.

O 42.35 Wed 17:45 P2

**Oxide formation on reconstructed Au(110) surfaces** — ●MARC LANDMANN, EVA RAULS, and WOLF GERO SCHMIDT — Lehrstuhl für Theoretische Physik, Universität Paderborn

The stability of oxygen adstructures on the unreconstructed (1x1) and the "missing row" type reconstructed (1x2) and (1x3) Au(110) surfaces [1,2] has been investigated by density-functional theory calculations, considering experimentally typical ultra high vacuum conditions. Three Au-O chain like structures have been identified to be especially stable under specific (T,p) conditions. These chain structures, oriented along the atomic ridges of the reconstructed surfaces, are clearly favored over oxygen conglomerates on (1xr) surfaces and represent the most stable form of chemisorbed atomic oxygen on Au(110) surfaces.

Our investigation of surface oxidation directly connects the adsorption of atomic oxygen on Au(110) single-crystal surfaces to experimental [3] and theoretical [4] results that have recently shown that oxygen incorporation in freely suspended atomic gold chains results in a stabilization of these structures.

[1] A. G. Sault, R. J. Madix and C. T. Campbell, Surf. Sci. 169, 347, (1986)

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O 42.36 Wed 17:45 P2

**Entropy changes stability of Au(110) surface reconstructions** — EVA RAULS, ●MARC LANDMANN, and WOLF GERO SCHMIDT — Lehrstuhl für Theoretische Physik, Universität Paderborn

In contrast to the unreconstructed single-crystal surfaces of Cu and Ag, the Au(110) surface is subject to short range reconstructions of a missing row type. Even the lowest energy surface in (111) direction shows a long range surface reconstruction. Experimentally, Au(110) reconstructions with (1x2) and (1x3) periodicity are observed [1,2], while in theoretical works, the stability order is discussed controversially [3].

We have carried out density-functional theory calculations to resolve this controversy. If we consider the contributions of vibrational entropy, we find different stabilizations for the different reconstructions. This leads to a temperature dependent stability order, with the (1x3) reconstruction being the most stable structure at zero temperature, while, at room temperature, the most often observed (1x2) reconstruction is most stable, demonstrating the crucial role of entropy.

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O 42.37 Wed 17:45 P2

**STM/CITS Characterization of 1D and 2D Superstructures Evolving on Pure Highly Ordered Pyrolytic Graphite** — ●AARON GRYZIA, MARC D. SACHER, ARMIN BRECHLING, and ULRICH HEINZMANN — Molecular and Surface Physics, Bielefeld University

The last decades have shown highly ordered pyrolytic graphite (HOPG) as one of the most important substrates for studying adsorbates such as metal atoms, organic molecules, polymers and many others by Scanning Tunneling Microscopy (STM) and Scanning Tunneling Spectroscopy (STS) techniques. Although HOPG is in use for many years, known effects such as 1D[1] and 2D[2] superstructures have been studied very sparsely. These native HOPG superstructures are often very similar to the investigated adsorbates. Therefore the understanding of the properties of the substrate and its special features is of vital importance. In reverse the effects themselves may lead to new applications e.g. in using these 2D-superstructures as templates for adsorbing molecules in array like structures[3]. We focus our research on chain like structures and arrays on HOPG measured by STM and Current Image Tunneling Spectroscopy (CITS) under UHV conditions in order to understand the origin of these effects. First results of these measurements will be presented.

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O 42.38 Wed 17:45 P2

**STM study of the adsorption of phthalocyanine molecules on anisotropic surfaces** — ●TOBIAS PERTRAM<sup>1</sup>, QIHUI WU<sup>2</sup>, CONRAD BECKER<sup>1</sup>, and KLAUS WANDELT<sup>1</sup> — <sup>1</sup>Institute of Physical and Theoretical Chemistry, University of Bonn, Wegelerstr. 12, 53115 Bonn,

Germany — <sup>2</sup>Department of Physics, La Trobe University, Victoria 3086, Australia

The {110} surfaces of fcc metals show an intrinsic anisotropy due to the rectangular surface unit cell. This anisotropy can be even more pronounced in the case of the (1x2) missing row reconstruction, which has been found for metals such as Pt and Au. In contrast, on Pd(110) this reconstruction is only stable after the adsorption of hydrogen [1]. The clean Pd(110) does not show the tendency to reconstruct. After deposition of small amounts of Au (< 1 ML) on the unreconstructed Pd(110) surface pseudomorphic Au islands are observed, whereas in the case of higher Au amounts (> 2 ML) the resulting Au layer shows the characteristic (1x2) reconstruction, which however is still remains pseudomorphic to Pd(110) [2]. We used both reconstructed surfaces, the hydrogen induced Pd(110)-(1x2) surface and the Au modified one as a substrate for the deposition of phthalocyanine molecules. STM investigations under UHV conditions reveal a specific adsorption behaviour of the phthalocyanine molecules, which are oriented along rows of the reconstructed surfaces ("template effect").

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O 42.39 Wed 17:45 P2

**Puzzling effects of side chains on self-assembled molecular nanostructures** — ●STEPHAN BLANKENBURG, EVA RAULS, and WOLF GERO SCHMIDT — Theoretische Physik, Universität Paderborn, Germany

Molecular self-assembly and self-organization is presently seen as a promising alternative to the top-down design for future electronic devices. The experimental and theoretical study of well-defined model systems is an essential step for understanding the basic mechanisms responsible for the formation of complex supramolecular structures [1-4]. In this context, the influence of alkyl side chains on hydrogen bonded molecular surface networks were analyzed with scanning tunneling microscopy [5]: the adsorption of cyanuric (CYA), diethylbarbituric (DEB) and butyrcyanuric acid (BuCYA) at Au(111) show large differences in their ordering at the surface. Here we use density-functional theory calculations within the generalized-gradient approximation to rationalize these differences in terms of hydrogen bonds as well as intermolecular H-H interactions.

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O 42.40 Wed 17:45 P2

**Charge transfer in the TCNQ-sexithiophene complex** — ●KAI-FELIX BRAUN and SAW-WAI HLA — Nanoscale & Quantum Phenomena Institute and the Department of Physics & Astronomy, Ohio University, Athens, Ohio 45701, USA.

Molecular crystals from thiophene molecules can be doped with TCNQ-F4 molecules for use in all-organic opto-electronic and semiconductor devices. The charge transfer and the molecular orbital energy level formation in between these two organic molecules is investigated here by density functional theory calculations (DFT). The isolated molecules are calculated non-bonded and bonded together forming a charge transfer complex (CTC). The relaxed structure of the complex shows essentially coplanar and centered molecules with the  $\alpha$ -sexithiophene rings tilted alternately by 4.8°. The bond formation of these molecules results in a charge transfers of ~0.4 e- from the  $\alpha$ -sexithiophene to the TCNQ-F4 molecule. The HOMO-LUMO gap width is reduced as compared to the isolated molecules due to the newly formed orbitals in the CTC complex. Upon adsorption on a Au(111) surface electrons are transferred onto the molecule complex thereby causing the molecular levels to align asymmetric with respect to the charge neutrality level. The theoretical results for the single molecule and CTC layer are compared to experimental photoemission and scanning tunneling spectroscopy results. Journal of Chemical Physics 129 (2008), 064707.

O 42.41 Wed 17:45 P2

**Two dimensional structure formation controlled by metal-ligand interactions** — ●ACHIM BREITRUCK, HARRY E. HOSTER, and R. JÜRGEN BEHM — Institute of Surface Chemistry and Catalysis, Ulm University, D-89069 Ulm

Using highly oriented pyrolytic graphite (HOPG) as substrate, two di-

mensional structure formation of bisterpyridine (BTP) molecules in the presence of metal atoms was studied by scanning tunnelling microscopy (STM) under ultrahigh vacuum (UHV) conditions. BTP molecules form highly ordered networks stabilized by C-H...N type hydrogen bonds. [1,2] Upon metal deposition (Ag, Cu), these hydrogen bonds are partially lifted in favour of metal...N-pyridine interactions. This results in new network structures that strongly depend on the metal-to-molecule ratio. Surprisingly, we find the same sequence of metal coverage dependent structures for Ag and Cu addition, while theory predicts the Cu...N-pyridine interaction to be about 3 times stronger than the Ag...N-pyridine interaction.[3] Possible reasons for this will be discussed.

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O 42.42 Wed 17:45 P2

**Spatial modulation of molecular adsorption energies due indirect interactions** — ●STEPHAN BLANKENBURG and WOLF GERO SCHMIDT — Theoretische Physik, Universität Paderborn, Germany

The autonomous ordering and assembly of atoms and molecules on atomically well-defined surfaces appears as a very promising alternative route to even smaller functional systems with nanometre dimensions. However, the mechanisms controlling the self-ordering phenomena need to be thoroughly understood in order to use them for nanofabrication processes. In this context we investigate computationally the origin of long-range order observed experimentally for the adsorption of (i) (s)-glutamic acid on Ag(110) [1] and (ii) phenylglycine and adenine on Cu(110) [2,3]. In both cases we find long-wave oscillations of the substrate charge density to be decisive for the adsorption configuration. In case of glutamic acid adsorbed on Ag(110), long-range strain field are very important as well, while they are nearly negligible for phenylglycine and adenine adsorbed on Cu(110).

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O 42.43 Wed 17:45 P2

**2D chemistry on Au(111) surfaces** — ●EVA RAULS, STEPHAN BLANKENBURG, and WOLF GERO SCHMIDT — Theoretische Physik, Universität Paderborn, Germany

The design of functional two-dimensional molecular networks has become an area of intense research [1,2]. The constraint to 2 in contrast to the availability of 3 dimensions has a large impact on many chemical reactions. Chemical reactions between surface adsorbed molecules may lead to products very different from those obtained in solutions or the gas phase. The imide formation between a diaminoterphenyl (DATP) and a PTCDA molecule [3] is one very interesting example in this respect. In scanning tunneling microscopy (STM) experiments, it has been observed that the Au surface changes both the reaction path and the reaction product compared to 3D. In order to understand these experimental observations, we have studied the chemical reactions both in solution and on the Au(111) surface by density-functional theory calculations in the generalized-gradient approximation.

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O 42.44 Wed 17:45 P2

**Adsorption geometry and self assembly of corrole molecules on different copper facets** — ●LEONID LICHTENSTEIN, STEFAN KUCK, GERMAR HOFFMANN, and ROLAND WIESENDANGER — Institute of Applied Physics, University of Hamburg

A new member of the metalloporphyrinoid class is the one-carbon short corrole which is a very accessible, easily tunable compound with many potential applications in material science and catalysis. These molecules differ from the parent porphyrin molecules [1] mainly by their lower inherent symmetry and the smaller cavity. In this study using STM we address the conformation (orientation and chirality) and self assembly of iron-triphenylcorrole (FeTPC) molecules on Cu(100) and Cu(111). At low coverage FeTPC molecules show restricted symmetry and can be controllably switched among different conformations [2]. At higher coverage formation of regular aggregates can be observed. We will present the results of the growth study in dependence

of surface geometry and coverage and discuss results of scanning tunneling spectroscopy investigations of these systems.

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O 42.45 Wed 17:45 P2

**Adsorption of metal phthalocyanines on Cu(111) and Cu(100): A STM study** — ●SHIH-HSIN CHANG, JENS BREDE, JÖRG SCHWÖBEL, STEFAN KUCK, GERMAR HOFFMANN, and ROLAND WIESENDANGER — Institute of Applied Physics, University of Hamburg, Jungiusstrasse 11 D-20355 Hamburg, Germany

The temperature dependent adsorption behavior of 4-fold symmetric metal phthalocyanines (MPcs) on metals with commensurate and incommensurate symmetries was investigated by means of scanning tunneling microscopy. On the 4-fold symmetric Cu(100) surface, planar and 4-fold molecular structures in two equivalent orientations were found for MPcs when prepared at room temperature. In addition, two metastable orientations were identified when prepared at low temperature which can be depopulated upon annealing. MPcs adsorbed on the 6-fold symmetric Cu(111) surface showed a disturbed molecular appearance. The symmetry of molecular structures changed from 4-fold to 2-fold which is discussed in terms of molecule-substrate interaction.

O 42.46 Wed 17:45 P2

**Coverage-dependence adsorbed structure of tetracene on Ag(110)** — ●HAN HUANG<sup>1,2</sup>, FEI SONG<sup>1,3</sup>, QIAO CHEN<sup>4</sup>, WUZONG ZHOU<sup>5</sup>, and SHING BAO<sup>1</sup> — <sup>1</sup>Department of Physics, Zhejiang University, Hangzhou 310027, P. R. China — <sup>2</sup>Department of Physics, National University of Singapore, 117542, Singapore — <sup>3</sup>ISA and iNANO, University of Aarhus, 8000C, Denmark — <sup>4</sup>Department of chemistry, University of Sussex, Sch Life Sci, Brighton BN1 9QJ, E Sussex England — <sup>5</sup>School of Chemistry, University of St Andrews, St Andrews KY16 9ST, Fife Scotland

The ordered adsorption structures of tetracene on Ag(110) have been studied by low energy electron diffraction (LEED), scanning tunneling microscopy (STM) and density functional theory (DFT) calculations. At a low coverage, as calibrated with LEED, both p(4 x 4) and c(8 x 4) ordered structures are simultaneously formed on an Ag(110) surface at room temperature. STM images suggest the molecular plane is parallel to the Ag surface with its long molecular axis aligned along the [001] azimuth. DFT optimization reveals a separation of 0.3 nm between the molecular plane and substrate surface while the center of the tetracene molecule is on the long bridge site. Increasing coverage slightly, a (6,2;2,5) structure is formed while the adsorbed molecules maintain the flat-lying geometry with adjacent molecules alternating their height relative to the surface.

O 42.47 Wed 17:45 P2

**Photoemission studies of ex-situ prepared butanethiol and azobenzene derivative SAMs on Au(111): heat- and light-induced modifications of electron spectra** — ●TILL LEISSNER, NILS HEINEMANN, TIMM ROHWER, OLEKSIY ANDREYEV, and MICHAEL BAUER — Institut für Experimentelle und Angewandte Physik, Uni Kiel

Molecular switches and their intriguing properties attract much interest in the field of molecular electronics. Wet chemical deposition is a generally used method for coating of metallic surfaces with azobenzene-based switching molecules. In fact, the obtained SAMs are often imperfect and very inhomogeneous.

In this contribution we will present an improved technology of the ex-situ SAMs preparation. For our studies we choose butanethiol molecules as a model system for the molecular switch 3-(4-(4-Hexylphenylazo)phenoxy)propan-1-thiol adsorbed on a Au(111) surface. The quality of the obtained butanethiol and molecular switch SAMs was checked by means of two photon photoemission (2PPE) and LEED.

Furthermore, we will present data showing the impact of annealing and laser illumination (80 MHz fs-laser system) on butanethiol/Au(111) samples. In contrast to butanethiol, the molecular switch revealed strong irreversible modifications of the electronic structure under laser irradiation. This result will be discussed particularly in the context of a potential switching mechanism.

O 42.48 Wed 17:45 P2

**Scanning tunneling microscopy of polyoxometaltes on Au(111)** — ●LEONID KLIUIENKO<sup>1</sup>, PAUL KÖGERLER<sup>2</sup>, and BERT VOIGTLÄNDER<sup>1</sup> — <sup>1</sup>Institute of Bio- und Nanosystems (IBN)

and JARA-Fundamentals of Future Information Technology, Forschungszentrum Jülich, D-52425 Jülich, Germany — <sup>2</sup>Institute of Solid State Research (IFF) and JARA-Fundamentals of Future Information Technology, Forschungszentrum Jülich, D-52425 Jülich, Germany

Single and aggregated  $\{Mo_7Fe_{30}\} \cdot H_2O$  polyoxometalate (POM) clusters have been studied by low-temperature ultra high vacuum (UHV) scanning tunneling microscope (STM). Several methods were tried to deposit polyoxometalates on the Au(111) surface. "Drop casting" from a water solution in N<sub>2</sub> atmosphere and pulse injection techniques were used for POM cluster deposition onto a previously cleaned Au(111) surface. After subsequent annealing in UHV samples were studied in the STM. STM images shows that POM clusters were adsorbed on clean Au (111) surface and reveal a strong affinity towards cluster agglomeration. Nevertheless it was possible to image single POM clusters.

O 42.49 Wed 17:45 P2

**STM study of growth, structure, and stability of DMDS on Au(111)** — ●PATRICK MEHRING, AXEL BEIMBORN, DANIEL WEIER, FRANK SCHÖNBOHM, TOBIAS LÜHR, and CARSTEN WESTPHAL — Fakultät Physik - Technische Universität Dortmund, Otto-Hahn-Str. 4, D 44221 Dortmund, Germany

Systems of self-assembled monolayers (SAM) are in the focus of present research activities due to their potential applications in fields like molecular electronics, bio-sensing, and the manipulation of metallic surface characteristics. Therefore, monolayers of linear alkanethiols are considered as ideal model systems. In this study the growth, structure, and stability of Dimethyldisulfide (DMDS) layers on Au(111) was investigated by scanning tunneling microscopy. SAMs were formed by solution deposition methods at room temperature. We varied the deposition time from 6h to 24h. Subsequently, several thermal annealing steps with increasing temperatures were performed in vacuum. After each step, the monolayer was investigated by STM. A stripe phase with increasing coverage as a function of the deposition time was observed. After annealing at 80°C molecular islands were observed at the surface. After island formation the stripe phase is removed completely due to the rearrangement of molecules at the surface. Between the islands an amorphous phase was found. Increasing the temperature to 150°C leads to a disappearance of the islands. The herringbone reconstruction of the gold surface reappeared.

O 42.50 Wed 17:45 P2

**Comparison of Different Porphyrin Derivatives in Scanning Tunneling Microscopy** — ●FLORIAN VOLLNHALS, FLORIAN BUCHNER, INA KELLNER, YUN BAI, MARTIN SCHMID, J. MICHAEL GOTTFRIED, HANS-PETER STEINRÜCK, and HUBERTUS MARBACH — Lehrstuhl für Physikalische Chemie II, Interdisciplinary Center of Molecular Materials (ICMM), Universität Erlangen-Nürnberg, Egerlandstr. 3, D-91058 Erlangen

Porphyrin derivatives are considered as ideal building blocks for the self-assembly of molecular devices due to their rigid structure triggering long range order and versatile functionalities. Here we explore the appearance of different porphyrin derivatives, namely octaethylporphyrins (OEP) and tetraphenylporphyrins (TTP), on Ag(111) in scanning tunneling microscopy (STM). Additional information concerning the electronic structure, in particular the density of states close to the Fermi level, was acquired by means of ultraviolet photoelectron spectroscopy (UPS) and scanning tunneling spectroscopy (STS). It will be shown that the contrast in a layer of intermixed CoTPP and 2HTPP [1] and the appearance of individual CoTPP molecules in STM depends on the applied bias voltage. The comparison in particular of CoTPP and CoOEP reveals similar signatures in UPS but different bias dependent appearance in STM. These findings will be discussed in terms of intramolecular conformation, molecule substrate interaction and the corresponding electronic structure. Supported by the DFG through SFB 583. [1] K. Comanici et al., *Langmuir*, 24(2008), 1897.

O 42.51 Wed 17:45 P2

**Organic-Metal Interface: Cysteine on Au(110)** — ●BENJAMIN HÖFFLING, FRANK ORTMANN, KARSTEN HANNEWALD, and FRIEDHELM BECHSTEDT — Institut für Festkörpertheorie und -optik, Friedrich-Schiller-Universität, Jena, Germany

The interaction of thiol groups with gold surfaces is of particular importance in the research of transport properties of organic materials (organic electronics) since the sulfur-gold interaction is strong and es-

tablishes a link between electrode and organic semiconductor. Additional functional groups, however, might have an influence on this bond and deserve attention in adsorption studies. By means of density functional calculations, we study such an interplay of different functional groups upon adsorption for the model system of the amino acid cysteine on the Au(110) surface. The interaction of the functional groups with the surface is investigated in detail. We present results on the electrostatic potential, the charge redistribution upon adsorption, and induced changes in the density of states. Finally, we predict four qualitatively different adsorption configurations for cysteine on Au(110) and compare their characteristics.

O 42.52 Wed 17:45 P2

**Room temperature STM investigation of organic molecules deposited by pulse injection** — ●CARMEN PÉREZ LEÓN<sup>1</sup>, CHRISTOPH SÜRGER<sup>1</sup>, MARCEL MAYOR<sup>2,3</sup>, and HILBERT V. LÖHNEISEN<sup>1,4</sup> — <sup>1</sup>Physikalisches Institut und DFG-Center for Functional Nanostructures (CFN), Universität Karlsruhe, D-76128 Karlsruhe, Germany — <sup>2</sup>Forschungszentrum Karlsruhe, Institut für Nanotechnologie, D-76021 Karlsruhe, Germany — <sup>3</sup>Department of Chemistry, University of Basel, CH-4056 Basel, Switzerland — <sup>4</sup>Forschungszentrum Karlsruhe, Institut für Festkörperphysik, D-76021 Karlsruhe, Germany

$\pi$ -conjugated oligomers C<sub>114</sub>H<sub>158</sub>O<sub>8</sub>S<sub>2</sub>Si<sub>2</sub> (CHOSSi) have been deposited on clean Cu(111) at room temperature using the pulse-injection method with tetrahydrofuran (THF) as solvent. Scanning tunneling microscopy measurements in ultra-high vacuum at room temperature demonstrate that the CHOSSi and THF molecules coadsorb on the copper surface. The solvent molecules form ordered structures with distinct orientations and domain boundaries suggesting a strong interaction of THF with the substrate. Individual and small clusters of CHOSSi molecules appear randomly distributed on the surface with no apparent correlation with the solvent. A detailed study of the self-organized adsorption of the THF molecules on Cu(111) will be presented.

O 42.53 Wed 17:45 P2

**Self-assembly of amino acids on noble metal surfaces: universality of the amino acid bonding scheme** — ●JOACHIM REICHERT<sup>1</sup>, AGUSTIN SCHIFFRIN<sup>1,2</sup>, YAN PENNEC<sup>2</sup>, WILLI AUWÄRTER<sup>1</sup>, ALEXANDER WEBER-BARGIONI<sup>2</sup>, MATTHIAS MARSCHALL<sup>1</sup>, DEAN CVETKO<sup>3</sup>, ALBANO COSSARO<sup>3</sup>, ALBERTO MORGANTE<sup>3</sup>, and JOHANNES V. BARTH<sup>1</sup> — <sup>1</sup>Physik Department, TU München, Germany — <sup>2</sup>Chemistry Department, University of British Columbia, Vancouver, Canada — <sup>3</sup>INFN/TASC, Trieste, Italy

We investigated the molecular self-assemblies of L-methionine on Cu(111) and L-tyrosine on Ag(111) by means of STM, HAS, XPS and NEXAFS in UHV. The self-assembly of L-methionine on Cu(111) is strongly influenced by the substrate reactivity and reveals a temperature dependent structural transformation involving a chiral orientational switch and the emergence of an ordered 1D high temperature phase. XPS data show that this transformation is triggered by a thermally activated deprotonation of the NH<sub>3</sub><sup>+</sup> group. The ordered phase shows noncovalent molecular dimerization and alignment into chains which are commensurate with the underlying substrate. L-tyrosine on Ag(111) self-assembles into linear nanoribbons primarily following the substrate crystalline symmetry. A zwitterionic noncovalent molecular dimerization is observed, and NEXAFS data provide evidence of a non-flat adsorption of the phenol ring. This dimerization scheme is reminiscent of methionine on Cu(111) and Ag(111), and supports a universal self-assembling trend for amino acids on close-packed noble metal surfaces.

O 42.54 Wed 17:45 P2

**Substrate Effect in the structure of ordered Bis-terpyridine monolayer networks** — ●THOMAS WALDMANN<sup>1</sup>, DANIELA KÜNZEL<sup>2</sup>, HARRY E. HOSTER<sup>1</sup>, AXEL GROSS<sup>2</sup>, and R. JÜRGEN BEHM<sup>1</sup> — <sup>1</sup>Institute of Surface Chemistry and Catalysis, Ulm University, D-89069 Ulm, Germany — <sup>2</sup>Institute of Theoretical Chemistry, Ulm University, D-89069 Ulm, Germany

We present different supramolecular networks formed by monolayers of a Bis-terpyridine derivative (2,4'-BTP)[1,2] on the (100) and (111) surfaces of Ag and Au. On all four substrates, ordered and disordered structures are observed by STM and LEED under UHV conditions at T = 300 K and at 90 K. On Ag(111) and Au(111) surfaces, single 2,4'-BTP molecules are observed in 12 different orientations with 30° difference. This is explained by a best fit of the molecules to the sub-

strate, maximizing the number of N atoms being adsorbed a-top of substrate atoms [3,4]. This simple model fully explains the resulting molecular networks on Ag(111) and Au(111). Its suitability for rationalizing monolayer networks on the (100) surfaces of Ag and Au is tested.

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O 42.55 Wed 17:45 P2

**Substrate-induced molecular orientation of ClGa-phthalocyanine studied by MAES and UPS** — •T. HOSOKAI<sup>1</sup>, A. GERLACH<sup>1</sup>, H. MACHIDA<sup>2</sup>, Y. SUZUKI<sup>2</sup>, S. DUHM<sup>2</sup>, N. KOCH<sup>3</sup>, S. KERA<sup>2</sup>, U. NOBUO<sup>2</sup>, and F. SCHREIBER<sup>1</sup> — <sup>1</sup>Institut für Angewandte Physik, Universität Tübingen, Germany — <sup>2</sup>Graduate School of Advanced Integration Science, Chiba university, Japan — <sup>3</sup>Institut für Physik, Humboldt-Universität zu Berlin, Germany

Understanding the substrate-molecule interactions is a prerequisite for the control of organic film growth. Here we report the substrate-induced molecular orientation of the non-planar chlorogallium phthalocyanine (ClGaPc) molecules on Cu(111) and graphite by means of UPS and metastable atom electron spectroscopy (MAES). In the monolayer MAES shows distinctively different features on Cu(111) and graphite: On the Cu(111) surface bands corresponding to non-bonding orbitals of the Cl-atom, i.e. those largely distributed parallel and perpendicular to the molecular plane, are not observed, whereas on the graphite both bands can be found. Because of the high surface sensitivity of the MAES technique these results indicate a different orientation of ClGaPc on Cu(111) and graphite. On Cu(111) ClGaPc molecules orient with the Cl-atom directed towards the Cu surface, whereas on the graphite ClGaPc molecules orient with the Cl-atom directed towards the vacuum. Although it is often found that Pc molecules orient to maximize the overlap with the substrate electrons, we show that the central atoms also play a role for the orientation of polar Pc molecules on different substrates.

O 42.56 Wed 17:45 P2

**Organic and Metal-Organic Networks Based on NC - Ph - CN** — •MATTHIAS MARSCHALL<sup>1</sup>, JOACHIM REICHERT<sup>1</sup>, WILLI AUWÄRTER<sup>1</sup>, KNUD SEUFERT<sup>1</sup>, FLORIAN KLAPPENBERGER<sup>1</sup>, SVETLANA KLYATSAKYA<sup>2</sup>, MARIO RUBEN<sup>2</sup>, ALEXANDER WEBER-BARGIONI<sup>3</sup>, and JOHANNES V. BARTH<sup>1</sup> — <sup>1</sup>Physik Department, TU München, Germany — <sup>2</sup>Institut für Nanotechnologie, Karlsruhe, Germany — <sup>3</sup>Department of Physics and Astronomy, University of British Columbia, Vancouver, Canada

The assembly of metal-organic networks is a promising method to fabricate well defined, highly stable supramolecular nanostructures. We investigated the molecular structures by means of Scanning Tunneling Microscopy (STM) and Near Edge X-ray Adsorption Fine Structure (NEXAFS). A systematic investigation of such a metal organic network on Ag(111) and Cu(111) revealed several highly ordered and complex networks. The complexity and the variety of the observed molecular networks is presumably caused by the numerous degrees of freedom of the investigated molecules. Upon absorption the molecules obtain a surface induced chirality and their supramolecular assemblies were studied in dependence of the coverage and preparation parameters. At certain conditions even highly stable macromolecules were formed.

O 42.57 Wed 17:45 P2

**Conformation-controlled networking of H-bonded assemblies on surfaces** — MANFRED MATENA<sup>1</sup>, MIHAELA ENACHE<sup>1</sup>, ANNA LLANES-PALLAS<sup>2</sup>, DAVIDE BONIFAZI<sup>2</sup>, THOMAS A. JUNG<sup>3</sup>, and •MEIKE STÖHR<sup>1</sup> — <sup>1</sup>University of Basel, Switzerland — <sup>2</sup>University of Trieste, Italy — <sup>3</sup>Paul-Scherrer-Institute, Switzerland

In order to prepare networks that could undergo phase transitions through a thermally-induced inversion of the molecular conformation leading to a variation of the intermolecular interactions, directional intermolecular forces can be regarded as promising candidates. In particular, H-bonding interactions will be exploited since their intermolecular interaction strength and geometry can be controlled by the number and arrangement of available H-bonding donor or acceptor moieties. We studied the 2D self-organization of a conjugated molecule bearing terminal 2,6-di(acylamino)pyridine moieties [1], which are well-known to form H-bonds, on a Ag(111) surface by STM. The hexagonal porous network, which is formed for room temperature deposition, is transformed into a close-packed rhombic pattern by a thermally induced

trans-cis inversion of the terminal groups. This transformation can be explained by the fact that the system wants to minimize its energy: at the same time the free surface energy is minimized while the number of H-bonds per terminal group is doubled from two to four. [1] A. Llanes-Pallas et al., Angew. Chem. Int. Ed. 2008, 47, 7726

O 42.58 Wed 17:45 P2

**Porphine on Copper (110) - Adatoms make the difference** — •ABEL ROBIN, MATTHEW STEPHEN DYER, SAM HAQ, MATS PERSSON, and RASMITA RAVAL — University of Liverpool, Liverpool, U.K.

We have studied the adsorption of free-base (H<sub>2</sub>-P) and copper porphine (Cu-P) molecules on a Cu(110) surface.

Using scanning tunnelling microscopy (STM), reflection absorption infrared spectroscopy (RAIRS) and density functional theory (DFT) calculations we gain insight into the details driving the adsorption and organization of porphine molecules on metal surfaces. Interestingly, we find Cu-P molecules organizing upon adsorption in regular 2D assemblies whereas H<sub>2</sub>-P only exhibits local ordering - even after annealing.

Experiments and calculations reveal another major difference between the two investigated systems, that is Cu-adatoms are attracted by H<sub>2</sub>-P molecules; a process not observed for Cu-P adsorption. The adatom-attachment to H<sub>2</sub>-P has - next to a number of interesting features - an influence on the ability of the porphine molecule to self-assemble into a regular structure. Metallization experiments of H<sub>2</sub>-P do not lead to a significant improvement in molecular ordering, suggesting that the molecules do remember the original adsorption environment, therefore, the adatom attachment to H<sub>2</sub>-P induces irreversible adsorption features.

Finally, we will present experimental and theoretical details of the highly organized Cu-P assembly. This structure is promising for technological applications since it does not require complicated functional groups attached to the porphyrin molecule for self-assembly.

O 42.59 Wed 17:45 P2

**Self-assembly of highly ordered ferrocenyl nanostructures monitored by second harmonic generation** — •ROBERT OSSIG<sup>1</sup>, FLORIAN VOGEL<sup>1</sup>, JENS HOSSBACH<sup>2</sup>, ULRICH SIEMELING<sup>2</sup>, and FRANK TRÄGER<sup>1</sup> — <sup>1</sup>Institut für Physik and Center for Interdisciplinary Nanostructure Science and Technology - CINSaT, Universität Kassel — <sup>2</sup>Institut für Chemie and Center for Interdisciplinary Nanostructure Science and Technology - CINSaT, Universität Kassel

Custom-made molecules are ideal candidates to prepare stable self-assembled monolayers (SAM), which yield a wide range of applications, for example, as electronic or sensoric devices. In this contribution we present two recently synthesized ferrocene-functionalized tripod ligands with ferrocene as a reactive head group. The anchor groups of the ligands consist of three thioether-chains, each with 8 or 12 carbon atoms, respectively. Due to their structure, these molecules show a very high rigidity, which is an important pre-condition to form stable SAMs. To monitor the SAM formation, second harmonic generation (SHG) has been applied. The in situ SHG measurements show an initial fast decrease of the signal followed by a slower decrease as a function of immersion time. For a deeper insight of the involved processes, concentration dependent measurements have been performed. From these measurements we conclude that the SAM formation of both molecules occurs in a two-step process, a fast adsorption and a subsequent slow ordering. Further ex situ measurements (ellipsometry and scanning-tunneling-microscopy) confirm the formation of highly ordered monolayers.

O 42.60 Wed 17:45 P2

**Diffusion of 1,4-butanedithiol on unreconstructed Au(111)** — ANDREAS FRANKE and •ECKHARD PEHLKE — Institut für Theoretische Physik und Astrophysik, Christian-Albrechts-Universität zu Kiel

Extending our previous density-functional studies on the diffusion of alkanethiols on gold surfaces, we now focus on more complex sulfur anchored molecules diffusing on the unreconstructed Au(111) surface. As a benchmark system we choose 1,4-butanedithiol radicals (BDT: S-(CH<sub>2</sub>)<sub>4</sub>-S) which bind to the gold surface via two sulfur atoms. Molecules that bind to the surface via more than one site are expected to show diffusion properties beyond isotropic diffusion of single adsorbate atoms (e.g. [1]). Unreconstructed Au(111) exists under certain electrochemical conditions [2]. Density functional calculations are carried out using the VASP code by Hafner, Kresse *et al.* [3]. We compare various adsorption geometries of one BDT per (4x3) unit cell. For the most favourable geometry both S-atoms bind close to fcc-hollow sites with d<sub>S-S</sub>=4.9Å. Taking the free, spinpolarized radical as reference, the

adsorption energy was calculated to be  $-3.3$  eV. Due to lateral interactions, the adsorption energy changes to  $-3.8$  eV in a (6x6) surface unit cell. We found a diffusion path with a small maximum energy barrier of  $0.3$  eV which results in a translation perpendicular to the S-S-axis of the molecule. Notably, the energy barrier increases to approx.  $0.5$  eV in case of the larger (4x6) surface unit cell.

[1] K.-Y. Kwon, et al., *Phys. Rev. Lett.* **95**, 166101 (2005).

[2] M. A. Schneeweiss, et al., *Appl. Phys. A* **69**, 537 (1999).

[3] <http://cms.mpi.univie.ac.at/vasip/>

O 42.61 Wed 17:45 P2

**Surface mobility and its impact on the stability of oligopyridine mono- and multilayer phases on HOPG - a thermal desorption study** — ●MICHAEL ROOS, HARRY E. HOSTER, and R. JÜRGEN BEHM — Institute of Surface Chemistry and Catalysis, Ulm University, D-89069 Ulm, Germany

We report on the temperature and coverage dependent desorption rates from layers of two types of Bis(terpyridine)derivatives (BTP) on HOPG [1-4]. These rates are much higher for thicker films than for monolayers. These variations do not predominantly arise from changes in the energetic desorption barriers but are dominated by the frequency factors. Due to the large mass (618 amu) and the correspondingly large moments of inertia of the BTP molecules, the frequency factor approaches  $10^{26}$  Hz for desorption from an immobile initial state (multilayer), whereas it is changed by a factor of  $10^{-9}$  for desorption out of a mobile state (monolayer). This fits to STM observations at 300 K, which revealed that the most stable phase for both molecules is not a close packed hydrogen bonded one, but a dilute 2D gas, where translation and planar rotation are active. We compare the frequency factors and activation energies for desorption of the two types of BTP, which differ in the position of the peripheral N atoms, and discuss possible reasons for the differences.

[1] C. Meier et al., *J Phys. Chem. B* **109**, 21015 (2005).

[2] C. Meier et al., *Angew. Chem. Int. Ed.* **47**, 3821 (2008).

[3] H. E. Hoster et al., *Langmuir* **23**, 11570 (2007).

[4] A. Breittrück et al., *Surf. Sci.* **601**, 4200 (2007).

O 42.62 Wed 17:45 P2

**Co-porphyrin molecules on metal surfaces: from single molecules to molecular arrays and bilayer islands** — ●WILLI AUWÄRTER, KNUD SEUFERT, FLORIAN KLAPPENBERGER, JOACHIM REICHERT, and JOHANNES V. BARTH — Physik Department, TU München, Germany

We report on scanning tunneling microscopy (STM) and spectroscopy (STS) experiments on Co-tetraphenylporphyrin (CoTPP) molecules adsorbed on Ag(111) and Cu(111) surfaces. Starting by a characterization of the electronic and geometric structure of individual CoTPP's, we proceed to CoTPP arranged in highly organized arrays, where we discuss subtle modifications of the electronic structure induced by the packing of CoTPP. The inequivalent adsorption sites of CoTPP assembled in islands on Ag(111) results in a moire-type modulation of the lowest unoccupied molecular orbital. In a next step we address the imaging of CoTPP molecules immobilized on a CoTPP monolayer. The modification of the electronic structure clearly indicates that these 2nd layer molecules are electronically decoupled from the metal substrate. In addition, we compare the morphology of CoTPP on Cu(111) and Ag(111) with free-base porphyrins, which allows us to discuss the influence of specific molecule-substrate interactions on the molecular conformation and the mobility.

O 42.63 Wed 17:45 P2

**Formation of metal-organic networks of azobenzene molecular switches on a Au(111) surface** — ●CHRISTOPH LIMBACH, NILS HENNINGSEN, KATHARINA J. FRANKE, and JOSE IGNACIO PASCUAL — Freie Universität Berlin, Berlin, Germany

Azobenzene is a model molecular system for conformational switches, whose adsorption on metal surfaces has lately attracted a lot of interest due to its possible application to switchable molecular electronic devices. Using low temperature scanning tunnelling microscopy and spectroscopy (STM/STS) we investigate the coadsorption of di-metacyano azobenzene (DMC) molecules and cobalt atoms on a Au(111) surface. Room temperature co-deposition of both species results in the formation of metal-organic chains as well as small clusters.  $dI/dV$  spectroscopy and conductance maps plotting the distribution of unoccupied resonances are used to localize the coordination bonds between Co atoms and DMC. We find that coordination bonds can be formed indistinguishably at two intramolecular sites: the cyano termination

and the di-azo bridge (N=N). This leads us to conclude that the metal organic bond is probably mediated by the lone-pair electrons of nitrogen atoms, as found recently [1]. We envision a controlled modification of the transition metal properties by switching the molecular ligands.

[1] U. Schlickum et. al. *Nano Lett.* **7**, 3813, 12007

O 42.64 Wed 17:45 P2

**Structure-function relation in the photoswitch tetra-tert-butyl-azobenzene (TBA) on Au(111)** — ●ROLAND SCHMIDT<sup>1,2</sup>, DANIEL BRETE<sup>1,2</sup>, SEBASTIAN HAGEN<sup>2</sup>, ROBERT CARLEY<sup>1</sup>, CORNELIUS GAHL<sup>1</sup>, PETRA TEGEDER<sup>2</sup>, and MARTIN WEINELT<sup>1,2</sup> — <sup>1</sup>Max-Born-Institut, Berlin — <sup>2</sup>Freie Universität-Berlin, Berlin

We have investigated tetra-tert-butyl-azobenzene (TBA) adsorbed on Au(111) by X-ray absorption (XAS) and autoionization spectroscopy at the Berlin synchrotron facility BESSY. In TBA the azobenzene photoswitch is decoupled from the substrate by four tert-butyl legs. XAS reveals a slight bending of the azo group of the trans isomer towards the Au(111) surface. The interaction of the N=N bond with the gold substrate is also reflected by an interchange of HOMO and HOMO-1, as identified from participator decay in Resonant-Raman-Auger. Autoionization of the  $Cl1s^{-1}\pi^{+1}$  excited state mainly occurs via spectator and participator decay, while the  $N1s^{-1}\pi^{+1}$  state shows an additional non-resonant Auger contribution of comparable strength. This demonstrates that charge transfer from the LUMO to the substrate is faster when exciting at the nitrogen edge and can explain the quite exceptional dependence of the TBA photoisomerization yield on photon energy [1].

[1] S. Hagen, P. Kate, F. Leyssner, D. Nandi, M. Wolf, and P. Tegeder *J. Chem. Phys.* (2008), **129**, 164102

O 42.65 Wed 17:45 P2

**In situ STM study of Cu modified Au(100) electrodes in alkaline solution** — ●CHRISTIAN SCHLAUP and KLAUS WANDEL — Institute for Physical und Theoretical Chemistry, University of Bonn, Wegelerstr. 12, D-53115 Bonn

Ultrathin Cu layers were prepared on Au(100) electrodes using the well-known Cu underpotential deposition. After a two step electrolyte exchange process these Cu modified Au(100) electrodes were exposed to a 0.01 M NaOH electrolyte. In dependence on the electrochemical potential different surface structures were found and characterized. Starting at low potentials where the adsorbate free pseudomorphic Cu adlayer remains stable, two barely ordered structures were formed during potential increase. In a first step  $OH^{-}$  ions are adsorbed, forming an largely disordered overlayer with a next neighbor distance of about 0.6 nm. During further potential increase the Cu layer is oxidized yielding a CuO film, which shows a characteristic stripe structure. In contrast to bulk Cu(100) electrodes, where a two step oxidation process via an intermediate  $Cu_2O$  species was found, the CuO film is formed directly under these conditions. However, an additional structure was found in the transition regime between the uncovered and  $OH^{-}$  covered Cu layer. After keeping the potential constant for at least 20 minutes, islands with a hexagonal lattice and a next neighbor distance of about 0.3 nm appear. Both, the small lattice constant and the slow kinetic may point to the formation of a Au/Cu surface alloy.

O 42.66 Wed 17:45 P2

**Structural transitions of Heptyl Viologen adlayers on a Cu(100) electrode: In situ STM study** — ●MIN JIANG, KNUD GENTZ, and KLAUS WANDEL — Institute for Physical and Theoretical Chemistry, University of Bonn, Wegelerstr.12, D-53115 Bonn

Surface redox processes and structural transitions of heptyl viologen (1,1'-Diheptyl-4,4'-bipyridinium dichloride,  $DHV^{2+}$ ) was studied on a Cu(100) electrode by cyclic voltammetry (CV) and in situ scanning tunneling microscopy (STM). Typical for a redox-active molecule,  $DHV$  in KCl electrolyte solution exhibited two pairs of spike-like current waves and two-step one-electron redox processes. The  $DHV^{2+}$  species spontaneously formed four kinds of highly ordered phases on the preadsorbed chloride  $c(2 \times 2)$  adlayer under non-reactive condition, which were composed of two mirror domains and two rotational domains. One-electron reduction of the dication  $DHV^{2+}$  caused a phase transition to a stripe pattern which arises from a  $\pi - \pi$  stacking of the corresponding monocation radical  $DHV^{+}$  species. This phase transition involved not only reduction of the pre-adsorbed  $DHV^{2+}$  species but also a further adsorption and reduction of  $DHV^{2+}$  species from the solution phase. During the cathodic sweep, the stripe pattern of the cation radicals changed from a loose array to a more compact structure. At more negative potential, the ordered stripe pattern disap-

peared gradually and a reversible order-disorder transition happened. This is caused by chloride desorption-adsorption through the viologen film.

O 42.67 Wed 17:45 P2

**Water clusters and thin films on clean and oxygen-adsorbed Ni(111) surfaces** — ●STEFAN WIPPERMANN und WOLF GERO SCHMIDT — Lehrstuhl für theoretische Physik, Universität Paderborn, Warburger Str. 100, 33098 Paderborn

Despite the importance of water-surface interaction for many technological applications and surface science, it is only poorly understood in many instances. Inspired by recent experimental [1] and theoretical work [2], we explore the adsorption of water on clean and oxygen-adsorbed Ni(111) surfaces using density functional theory. Calculations on the water adsorption geometries and vibrational frequencies were performed for a wide range of monomer, dimer, trimer and hexamer structures adsorbed on the p(2x2)-Ni(111)-O and clean Ni(111) surfaces [3]. While our results agree well with the experimental findings of Nakamura and Ito [1], they suggest a different interpretation in terms of mainly two candidate structures: (i) Formation of an ice Ih-like bilayer structure with the free OH-bonds pointing upwards along the surface normal, and (ii) Formation of cyclic buckled hexamers similar to the ones discussed in Ref. [4]. In the latter case, each water molecule forms an OH-O<sub>ad</sub>(2x2) hydrogen bond with two different hydrogen bond types depending on the water molecule's normal position in the buckled hexamer.

[1] M Nakamura and M Ito, Phys Rev Lett 94, 035501, 2005.

[2] D Sebastiani et al., J Chem Theory Comput 1, 78, 2005.

[3] S Wippermann and W G Schmidt, Phys Rev B (submitted)

[4] A Michaelides and K Morgenstern, Nature Materials 6, 597, 2007.

O 42.68 Wed 17:45 P2

**SXPS Studies of Porphyrin Adsorption on Copper/Electrolyte Interfaces** — ●STEPHAN BREUER<sup>1</sup>, DUC THANH PHAM<sup>1</sup>, GENNADY CHERKASHIN<sup>2</sup>, THOMAS MAYER<sup>2</sup>, and KLAUS WANDEL<sup>1</sup> — <sup>1</sup>Universität Bonn, Institut für Physikalische und Theoretische Chemie, Wegelerstraße 12, 53115 Bonn — <sup>2</sup>Technische Universität Darmstadt, FB Materialwissenschaft, Petersenstraße 23, 64284 Darmstadt

We have studied electrochemically prepared Tetra-(methylpyridinium)-porphyrin (TMPyP) adsorbates on anion precovered copper surfaces by Synchrotron X-ray Photoelectron Spectroscopy (SXPS) at the synchrotron light source BESSY II. In order to correlate existing structural data with the chemical composition of the adsorbate layer we have systematically changed the underlying anion coverage (sulphate, chloride), the substrate symmetry (Cu(100), Cu(111)) and the applied potential. In contrast to vapour deposition, electrochemistry offers a pathway to deposit also thermolabile organic molecules. Our studies have revealed that the N1s signal, that indicates the presence of TMPyP on the surface, can be deconvoluted in several signals which are very sensitive to changes of the chemical environment and the redox state. As TMPyP counterion we have used tosylate which stabilizes the adsorbate layer.

O 42.69 Wed 17:45 P2

**A new in-situ X-ray diffraction setup: Electrodeposition of Zn from ionic liquids** — APARNA PAREEK, DIMITAR BORISOV, MICHAEL ROHWERDER, DIRK VOGEL, and ●FRANK RENNER — Max-Planck Institut für Eisenforschung, Max-Planck Strasse 1, 40237 Düsseldorf

To facilitate the investigation of the UHV prepared electrochemical interfaces by in situ x-ray diffraction using synchrotron radiation, an electrochemical cell setup combined with a portable UHV chamber was reported earlier. In the current work, we re-engineered the above electrochemical setup to investigate the Zn electrodeposition on the Au (111) surface from ionic liquids. Ionic liquids have very low vapor pressure, which means they can be handled in UHV environments. A smart addition of heating stage was used to overcome the problems like high viscosity and less conductivity, which are usually associated with ionic electrolytes. Furthermore, with this setup, the electrolyte contact with the sample surface can be attained in the controlled gas atmosphere. Here we report the first results of Zn electrodeposition and re-dissolution obtained using this new setup. In-situ x-ray diffraction enabled to track the initial steps of Zn deposition on the Au (111) surface, where the growth of an epitaxially ordered Zn film was observed.

O 42.70 Wed 17:45 P2

**Surface-enhanced resonators for microfluidic and nanofluidic applications** — ●BEYNOR ANTONIO PAEZ-SIERRA<sup>1</sup> and VIKTORIIA KOLOTOVSKA<sup>2</sup> — <sup>1</sup>QUBITON Laboratories KG, 4040 Linz, Austria — <sup>2</sup>Zentrum für Biomedizinische Nanotechnologie, Upper Austrian Research, Austria, 4020 Linz, Austria

Revealing and understanding phenomena at interfaces is an important issue concerning biology, chemistry, engineering, physics, and many other disciplines. Science and technology at the nano- and micro-scale have myriads of proven examples where surface-to-volume ratio becomes dominant for process performance. Thereby, it is of great interest to pursue surface chemistry, tuning of energetic surface levels, control of trap states, or engineering of interface barriers among others, in order to overcome into stable and high efficient optoelectronic processes. We report simulations on surface-enhanced Raman resonators (SERRs) for microfluidic and nanofluidic applications. The process has its origins on the surface-enhanced Raman spectroscopy (SERS) phenomenon, where one main feature consists on the coupling between external electric fields with surface plasmons at structured metallic surfaces or colloids, resulting in strong local electric fields. The implementation of surface-enhanced reservoirs or enhanced walls at the fluidic chip, allow to acquire more intense signals of various spectroscopic probes, and hence to reduce the acquisition time.

O 42.71 Wed 17:45 P2

**Homeopitaxial electrodeposition on Cu(001) in different electrolytes** — ●ARNE DRÜNKLER, FREDERIK GOLKS, YVONNE GRÜNDER, DANIEL KAMINSKI, KLAUS KRUG, JOCHIM STETTNER, and OLAF M. MAGNUSSEN — Christian-Albrechts Universität Kiel, Germany

Cu electrodeposition is used for the defect-free filling of trenches with dimensions <100nm on ultra large scale integrated (ULSI) microchips [1]. Multicomponent electrolytes containing organic additives are used cause a faster growth at the bottom of the trench than at the upper walls resulting in void free filling of the trench. Even though the influence of the additives combination on the shape evolution of the Cu deposit was subject of numerous studies [2,3], their precise role during the elementary steps of the deposition is largely not understood. Surface X-Ray diffraction (SXRD) is ideal for the investigation of electrochemical metal deposition on atomic scale, as buried interfaces and structural information of the interface are accessible. In a first step the potential dependent interface structure of Cu(001) was investigated in copper free electrolyte. Furthermore, kinetic growth investigations in HCl and H<sub>2</sub>SO<sub>4</sub> solution are presented. Electrodeposition studies of Cu(001) in CuSO<sub>4</sub> containing HCl indicated step flow growth over a wide potential regime. In a Cu containing electrolyte mixture of H<sub>2</sub>SO<sub>4</sub> and HCl evidence for a transition from 2D- to 3D-growth is found.

References: [1] P.C. Andricacos, et al., Electroch. Microf. 42, 567 (1998), [2] T.P. Moffat, D. Wheeler, M.D. Edelstein, D. Josell, IBM J. Res. Develop. 49, 19 (2005), [3] D. Josell, D. Wheeler, W.H. Huber, T.P. Moffat, Phys. Rev. Lett. 87, 016102-1 (2001)

O 42.72 Wed 17:45 P2

**(111)-Textured Platinum Thin-Layer Electrodes on  $\alpha$ -Al<sub>2</sub>O<sub>3</sub>(0001) for Spectro-Electrochemistry** — ●BJÖRN BRAUNSCHWEIG, ALEXEJ MITIN, and WINFRIED DAUM — Institut für Physik und Physikalische Technologien, TU Clausthal, Leibnizstrasse 4, D-38678 Clausthal-Zellerfeld

The use of infrared vibrational spectroscopy to study electrochemical reactions on surfaces of bulk metal electrodes in aqueous electrolytes is often impaired by diffusion limitations as thin-layer electrolytes are required to minimize IR absorption in the liquid. Alternatively, thin-layer electrodes on IR-transparent substrates may be used to access the metal-electrolyte interface by IR transmission through the solids. While the latter strategy does not suffer from diffusion limitations of the electrolyte, it usually lacks the advantages of well-defined, single-crystalline electrode surfaces desired for model studies. We report the preparation of well-characterized Pt thin-film electrodes suitable for spectro-electrochemistry. Thin Pt layers with a thickness of 3 to 15 nm were grown by vapor deposition on atomically smooth  $\alpha$ -Al<sub>2</sub>O<sub>3</sub>(0001) single crystal surfaces and characterized by AES, cyclic voltammetry, AFM and STM. We used iodine adsorption to characterize the crystallographic surface orientation of our Pt films. Atomically resolved STM images of the iodine adlayer on the thin films reveal the same superstructures as found on Pt(111) bulk single crystals and demonstrate high structural order and (111) texture of our films. The effects

of growth temperature and film thickness on the surface morphology of the thin-film electrodes are discussed.

O 42.73 Wed 17:45 P2

**The adsorption of CO<sub>2</sub> and CO on Ca and CaO films studied with MIES, UPS and XPS** — ●SEBASTIAN DAHLE<sup>1</sup>, FLORIAN VOIGTS<sup>1</sup>, KAI VOLGMANN<sup>1</sup>, FABIAN BEBENSEE<sup>2</sup>, and WOLFGANG MAUS-FRIEDRICH<sup>1</sup> — <sup>1</sup>Institut für Physik und Physikalische Technologien, TU Clausthal, Leibnizstrasse 4, 38678 Clausthal-Zellerfeld, Germany — <sup>2</sup>Lehrstuhl für Physikalische Chemie II, Universität Erlangen-Nürnberg, Egerlandstrasse 3, 91058 Erlangen, Germany

The adsorption of different atmospheric molecules on metals is both of fundamental and of technological interest that arises from several applications. Ca especially is used to enhance the performance of high temperature oxygen sensors based on SrTiO<sub>3</sub>, as a promoter in many catalytic reactions and as a metal electrode in different organic or polymeric semiconductor components. A lot of studies of the effect of Ca on different catalysts neglect the interaction of Ca itself with different gases, although this might contribute considerably to the role of Ca as a promoter in catalysis.

Our results for the interaction of Ca and CaO films with CO<sub>2</sub> and CO are presented in this poster. For our studies, we employed Metastable Induced Electron Spectroscopy (MIES), Ultraviolet Photoelectron Spectroscopy (UPS), and X-ray Photoelectron Spectroscopy (XPS). Both CO<sub>2</sub> and CO lead to the formation of CO<sub>3</sub><sup>2-</sup> complexes on top of the surface while being exposed to Ca or CaO.

O 42.74 Wed 17:45 P2

**Interaction of Fe and Fe<sub>2</sub>O<sub>3</sub> with reactive gases** — ●KAI TRISTAN VOLGMANN, FLORIAN VOIGTS, and WOLFGANG MAUS-FRIEDRICH — Institut für Physik und Physikalische Technologien, TU Clausthal, Leibnizstr. 4, 38678 Clausthal-Zellerfeld

Mars' atmosphere contains a rather high portion of methane and formaldehyde with 10 ppb respectively 100 ppb. Different sources including extraterrestrial life have been proposed, but the origin of these gases is still unknown. It has been found earlier that methane and formaldehyde can be produced through a photocatalytical process on a hematite surface with adsorbed water in a CO<sub>2</sub> atmosphere.

The scope of this work is to examine the underlying processes which happen on granular powders of hematite. As a first step thin films of iron and Fe<sub>2</sub>O<sub>3</sub> are examined.

These thin films are investigated by means of their interaction with reactive gases like O<sub>2</sub>, CO<sub>2</sub> and H<sub>2</sub>O. These reactions have been studied with photoelectron spectroscopy. X-ray photoelectron spectroscopy is used to determine stoichiometry of the samples, while Ultraviolet photoelectron spectroscopy and Metastable Induced Electron Spectroscopy are used to analyse the valence band region and to gain information about changes in workfunction due to reactions on the surfaces.

O 42.75 Wed 17:45 P2

**Characterization and catalytic properties of bimetallic Au-Pd(111) surfaces** — ●MARCO MOORS<sup>1</sup>, TOMASZ KOBIELA<sup>2</sup>, CONRAD BECKER<sup>1</sup>, and KLAUS WANDEL<sup>1</sup> — <sup>1</sup>Institute of Physical and Theoretical Chemistry, University of Bonn, Wegelerstr. 12, D-53115 Bonn, Germany — <sup>2</sup>Faculty of Chemistry, Warsaw University of Technology, Noakowskiego 3, 00 664, Warsaw, Poland

Investigations of bimetallic systems with regard to their surface composition and morphology are of great importance for the development of new catalysts. In this work the compositional, electronic and structural properties of thin Au films deposited on a Pd(111) single crystal have been studied by ultraviolet photoelectron spectroscopy (UPS), photoemission of adsorbed xenon (PAX) and CO titration as a function of film thickness (ranging from submonolayer amounts up to multilayers) and temperature. The surface morphology of the system Au on Pd(111) exhibits a strong temperature dependence. Depositing Au at 150 K results in closed films, which undergo a smoothening of the topmost atomic layer by annealing the sample up to 250 K. At a surface temperature of 450 K the Au-Pd intermixing begins at the interface between substrate and overlayer eventually reaching the outermost surface at annealing temperatures of 650 K. Annealing to 850 K and above results in a fast Au depletion in the surface region, which is completed at 1050 K. Additionally performed reaction studies of the partial hydrogenation of butadiene to 1-butene using temperature programmed desorption (TPD) have shown a significant improvement of the catalytic properties of the alloyed Au-Pd surface compared to pure Pd(111).

O 42.76 Wed 17:45 P2

**Growth of ultrathin well-ordered Ni-Al alloyed layers on Ni(111) : a Grazing Incidence X-ray Diffraction study** — ●SÉVERINE LE MOAL<sup>1</sup>, GEOFFROY PRÉVOT<sup>2</sup>, DIDIER SCHMAUS<sup>2</sup>, RÉMI LAZZARI<sup>2</sup>, and BERNARD CROSET<sup>2</sup> — <sup>1</sup>Institute of Physical and Theoretical Chemistry, University of Bonn, Wegelerstr. 12, D-53115 Bonn, Germany — <sup>2</sup>Institut des NanoSciences de Paris, Universités Paris 6 et Paris 7, CNRS, 140 rue de Lourmel, F-75015 Paris, France

Ni-Al alloys are of great technological interest because of their remarkable mechanical and thermal properties. They are also resistant to corrosion due to the formation at their surface of a passive ultrathin film of aluminum oxide that acts as a diffusion barrier. Previously, we reported the epitaxial growth of NiAl and Ni<sub>3</sub>Al films on a Ni(111) single crystal [Le Pévédic et al, Surf. Sci. 600 (2006) 565 and Surf. Sci. 601 (2007) 395]. We recently studied their structure and the kinetics of formation by Grazing Incidence X-ray Diffraction (ESRF, ID03). Starting from an initial Al deposit, the growth and the structural and chemical ordering of the Ni<sub>3</sub>Al and NiAl layers are followed upon annealing. Disordered NiAl already forms at room temperature. In the 573-673 K temperature range the thickness of the NiAl layer increases and chemical ordering takes place. Once NiAl has grown up to the surface, ordered Ni<sub>3</sub>Al starts to form. Simultaneously, the diffraction signal of NiAl decreases and characteristic diffraction spots of Ni<sub>3</sub>Al appear and get sharper. The Ni<sub>3</sub>Al layer is stable up to 773 K. The lattice constants of the films were measured throughout growth and annealing time.

O 42.77 Wed 17:45 P2

**Vibrational spectroscopy of the rough Cu(111) surface** — ●DIANA VOGEL, OLAF SKIBBE, and ANNEMARIE PUCCI — Kirchhoff-Institut für Physik, Universität Heidelberg, Im Neuenheimer Feld 227, D-69120 Heidelberg

It is known that defect sites on a surface have a strong influence on adsorbates due to the changed electronic structure compared to the clean surface. In this work we characterize the rough Cu(111) surface by using High-Resolution Electron Energy Loss Spectroscopy (HREELS). The roughness has been produced by evaporating small amounts of copper onto the cooled surface so small islands are assumed to be grown. In our spectroscopic study, a vibrational state has been found at a quite high loss energy compared to the bulk phonon band. After annealing of the surface another vibrational state at an even higher energy has been detected. In analogy to known investigations on stepped copper surfaces the observed vibrational modes can be attributed to low coordinated step atoms of the islands [1]. The observed change of the vibrational spectra with increasing annealing temperature can be related to a morphology change of the islands. Measurements of the work function change of the surface after evaporating and annealing confirmed this result.

[1] A. Kara, P. Staikov and T. S. Rahman, Phys. Rev. B 61, 5714 (2000).

O 42.78 Wed 17:45 P2

**Surface phases and structure determination of thin silver films grown on the Re(10 $\bar{1}$ 0) surface** — ●VIKTOR SCHERF, LYRIA MESSAHEL, CHRISTIAN PAULS, and KLAUS CHRISTMANN — Institut für Chemie und Biochemie der FU Berlin, Takustr.3, D-14195 Berlin

We have examined the growth of silver films on the Re(10 $\bar{1}$ 0) surface under UHV conditions by means of electron diffraction techniques (MEED and LEED), and carried out a quantitative structure determination of the (1×1)-Ag phase by LEED. In the submonolayer range, the following LEED phases were observed with increasing silver coverage: c(2×2), p(1×4), p(1×5) and p(1×1), their I,V curves will be presented here. The in situ measured MEED curves of the (0,0) beam at 700 K show with increasing Ag coverage permanently two local maxima and minima; both maxima correlate with the formation of c(2×2) structure at different surface coverages. Once the p(1×1) phase is formed, the MEED intensity decreases almost linearly with the deposited amount of Ag indicating the formation of rough silver multilayers which grow according to a Stranski-Krastanov mechanism. We will also present the first dynamic LEED calculation for the Ag p(1×1) structure which clearly suggests the formation of a silver bilayer. The results will be discussed and compared with previous work on the same system as well as on the Au/Re(10 $\bar{1}$ 0) system [1].

[1] C. Pauls and K. Christmann, J. Physics Condensed matter, submitted

O 42.79 Wed 17:45 P2

**Kinetic Monte Carlo study of growth of Co on Cu(110) at room temperature** — OLEG V. STEPANYUK<sup>1</sup>, ●NIKOLAY N. NEGULYAEV<sup>2</sup>, ALEXANDER M. SALETSKY<sup>1</sup>, and WOLFRAM HERGERT<sup>2</sup> — <sup>1</sup>Faculty of Physics, Moscow State University, 119899 Moscow, Russia — <sup>2</sup>Fachbereich Physik, Martin-Luther-Universität, D06099 Halle, Germany

During the last decade many experimental and theoretical studies have been performed on Co/Cu heterostructures which are of great interest for spintronic applications. While the formation of thin Co films during thermal deposition on Cu(100) and Cu(111) has been investigated and understood at the atomic scale [1,2], our knowledge about growth process of Co on Cu(110) is still missing.

Here, performing atomic-scale simulations we study the growth of Co on Cu(110) in the early stages of heteroepitaxy. The energetics of various diffusion processes relevant for this system is investigated by means of molecular dynamics simulations and density functional theory. We show that the interface intermixing occurs at room temperature [3]. Our results reveal that embedded Co atoms serve as nucleation centers for substituted Cu atoms. Surface diffusion of expelled Cu adatoms rules an elongated along the [1-10] direction shape of nanoislands consisting mainly of Cu atoms [3].

- [1] F. Nouvertne et al., Phys. Rev. B 60, 14382 (1999).  
 [2] N.N. Negulyaev et al., Phys. Rev. B 77, 125437 (2008).  
 [3] O.V. Stepanyuk et al., Phys. Rev. B 78, 113406 (2008).

O 42.80 Wed 17:45 P2

**Preparation and electrical characterization of BaO, SrO and Ba<sub>0.7</sub>Sr<sub>0.3</sub>O thin films on Si(001)** — ●DIRK MÜLLER-SAJAK<sup>1</sup>, ALEXANDR COSCEEV<sup>2</sup>, HERBERT PFNÜR<sup>1</sup>, and KARL R. HOFMANN<sup>2</sup> — <sup>1</sup>Leibniz-Universität Hannover, Inst. f. Festkörperphysik — <sup>2</sup>Leibniz-Universität Hannover, Bauelemente der Mikro- und Nanoelektronik

In context with the search for alternative gate oxides in CMOS technology, we have grown high-k BaO, SrO and Ba<sub>0.7</sub>Sr<sub>0.3</sub>O films of thickness between 5 and 20 nm on clean Si(001) using molecular beam epitaxy of pure metals in ambient oxygen pressure. Especially the BaSr mixture oxide is of high interest, because it grows epitaxially and crystalline on Si(001).

Using Si(001) samples with thick SiO<sub>2</sub> films in combination with lithography, windows of clean Si(001) have been fabricated. Our thin films were only generated on these small squares using a tungsten mask. After preparation, the oxides were capped with 350nm Au and electrically characterized ex-situ.

From capacity-voltage (CV) measurements dielectric constants near the values for volume material were obtained. Furthermore we found very low hysteresis (<5mV) and flatband voltages close to that of the work function difference between Si and Au (+0.65eV). Due to the stoichiometry of these films and well defined interfaces, low leakage current densities (<10<sup>-5</sup>A/cm<sup>2</sup>) have been found by current-voltage (IV) measurements. The density of residual defect states at the interface have been derived from CV measurements and will be discussed.

O 42.81 Wed 17:45 P2

**Nucleation of Cu on Cu(001) by pulsed laser deposition** — ●ANDREAS DOBLER and THOMAS FAUSTER — Lehrstuhl für Festkörperphysik, Universität Erlangen-Nürnberg, Staudtstr. 7, 91058 Erlangen

For submonolayer homoepitaxial growth, nucleation theory allows to extract the critical island size by scaling island densities with the deposition rate. Pulsed laser deposition provides instantaneous deposition rates up to 10<sup>4</sup> ML/s and particle energies up to hundreds of eV.

We measured island densities after pulsed laser deposition of Cu on Cu(001) at 300 K. For best focus conditions ( $I \approx 10$  J/cm<sup>2</sup>), we varied the average deposition rate  $F$  from 10<sup>-5</sup> to 10<sup>-2</sup> ML/s at 1 Hz repetition rate. The saturation island density scales as  $n_x \propto F^p$  with an exponent near the value for thermal deposition of  $p = 0.4$ . However, the experimental island density is two orders of magnitude lower than expected by considering the instantaneous flux. This result is in good agreement with a theoretical study of nucleation for pulsed fluxes considering dimer mobility [1].

- [1] N. Combe and P. Jensen, Phys. Rev. B 57 (1998) 15553

O 42.82 Wed 17:45 P2

**Adsorption Geometry and Molecular Orbital Structure of Fluorinated Cobalt Phthalocyanine (F16CoPc) Layers on HOPG Substrate.** — ●MAHMOUD ABDEL-HAFIEZ<sup>1</sup>, MARIUS TOADER<sup>1</sup>, THIRUVANCHERIL G.GOPAKUMAR<sup>2</sup>, AFSHIN ABBASI<sup>1</sup>, and MICHAEL HIETSCHOLD<sup>1</sup> — <sup>1</sup>Solid Surfaces Analysis Group and Theo-

retical Physics Group, Institute of Physics, Chemnitz University of Technology, D-09107,-Chemnitz, Germany — <sup>2</sup>Christian-Albrechts-Universität zu Kiel, Institute of Experimental and Applied Physics, D-24118 Kiel, Germany

The adsorption geometry and electronic structure of isolated fluorinated Cobalt Phthalocyanine (F16CoPc) molecules adsorbed on the basal plane of HOPG (highly oriented pyrolytic graphite) substrate was studied. Monolayers were prepared using organic molecular beam epitaxy (OMBE) under UHV conditions at room temperature and investigated at 40 K using an Omicron VT-STM. At a thickness of around one monolayer, F16CoPc forms perfect quadratic phase superstructures on HOPG films. Adsorption geometry of molecules within the adlayer shows the influence of fluorine atoms on the packing. Single molecule calculations are employed to understand the type of interactions between F16CoPc and the substrate, as well as the effects of fluorine atoms on the geometric configurations of the adsorbed F16CoPc molecules.

O 42.83 Wed 17:45 P2

**Structure and energetics of bimetallic surface confined alloys** — ●ANDREAS BERGBREITER<sup>1</sup>, RALF T. RÖTTER<sup>1</sup>, ALBERT K. ENGSTFELD<sup>1</sup>, HARRY E. HOSTER<sup>1</sup>, AXEL GROSS<sup>2</sup>, and R. JÜRGEN BEHM<sup>1</sup> — <sup>1</sup>Institute of Surface Chemistry and Catalysis, Ulm University, D-89069 Ulm — <sup>2</sup>Institute for Theoretical Chemistry, Ulm University, D-89069 Ulm

The atomic distribution in a number of A<sub>x</sub>B<sub>1-x</sub>/B type surface alloys was determined by STM imaging with chemical contrast and statistically evaluated. Whereas in the systems Au<sub>x</sub>Pt<sub>1-x</sub>/Pt(111), Ag<sub>x</sub>Pt<sub>1-x</sub>/Pt(111), and Pd<sub>x</sub>Ru<sub>1-x</sub>/Ru(0001) we find preferences for larger homoatomic aggregates, the atom distribution in Pt<sub>x</sub>Ru<sub>1-x</sub>/Ru(0001) and Ag<sub>x</sub>Pd<sub>1-x</sub>/Pd(111) is very close to a random one [1]. In Ag<sub>x</sub>Pd<sub>1-x</sub>/Pd(111), our data show a small tendency towards clustering for  $x_{Ag} < 0.5$ , whereas at  $x_{Ag} > 0.5$  this is reversed to a slight preference for heteroatomic neighborhoods. Based on these experimental results, we have derived effective cluster interaction energies for all surface alloys [2]. These allow us to calculate phase diagrams for the surface alloys that we compare to predictions from theoretical work and to the behaviour of the corresponding bulk systems. We also discuss in how far the different atom distributions affect chemical and catalytic properties of the surface alloys.

- [1] H.E. Hoster et al., Phys.Chem.Chem.Phys 10 (2008) 3812.  
 [2] A. Bergbreiter et al., Phys.Chem.Chem.Phys 9 (2007) 5127.

O 42.84 Wed 17:45 P2

**Heterogeneously Catalysed Process for HCl Oxidation over Stabilised RuO<sub>2</sub>(110)** — ●STEFAN ZWEIDINGER<sup>1</sup>, JAN PHILIPP HOFMANN<sup>1</sup>, MARCUS KNAPP<sup>1</sup>, DANIELA CRIHAN<sup>1</sup>, ARI PAAVO SEITSONEN<sup>2</sup>, KEES-JAN WESTSTRATE<sup>3</sup>, EDWIN LUNDGREN<sup>3</sup>, JESPER ANDERSEN<sup>3</sup>, MICHAEL SCHMID<sup>4</sup>, PETER VARGA<sup>4</sup>, and HERBERT OVER<sup>1</sup> — <sup>1</sup>Physikalisch-Chemisches Institut, Justus-Liebig Universität Gießen, Heinrich-Buff-Ring 58, D-35392 Gießen — <sup>2</sup>IMPMC, CNRS & Université Pierre et Marie Curie, 4 place Jussieu, case 115, F-75252 Paris — <sup>3</sup>Dept. of Synchrotron Radiation Research, Lund University, Sölvegatan 14, S-22362 Lund — <sup>4</sup>Institut für Allgemeine Physik, TU Wien, Wiedner Hauptstraße 8-10, A-1040 Wien

High-resolution core-level shift spectroscopy and temperature-programmed reaction experiments together with density functional theory calculations reveal that the oxidation of HCl with oxygen producing Cl<sub>2</sub> and water proceeds on the chlorine-stabilised RuO<sub>2</sub> (110) surface via a one-dimensional Langmuir-Hinshelwood mechanism [1]. The recombination of two adjacent chlorine atoms on the catalyst's surface constitutes the rate-determining step in this novel Deacon-like process. The stability of RuO<sub>2</sub>(110) is related to the selective replacement of bridging O atoms at the catalyst surface by chlorine atoms [2], as evidenced by high-resolution core-level shift spectroscopy, scanning tunnelling microscopy and density functional theory simulations.

- [1] Crihan, D. et al.; Angew. Chemie Int. Ed. 2008, 47, 2131-2134.  
 [2] Zweidinger, S. et al.; J. Phys. Chem. C 2008, 112, 9966-9969.

O 42.85 Wed 17:45 P2

**Nanoporous Gold: XPS and In-situ XPS Investigation** — ●KARIFALA DUMBUYA<sup>1</sup>, ARNE WITTSTOCK<sup>2,3</sup>, VOLKMAR ZIELASEK<sup>2</sup>, JÜRGEN BIENER<sup>3</sup>, ALEX HAMZA<sup>3</sup>, MARCUS BÄUMER<sup>2</sup>, MICHAEL GOTTFRIED<sup>1</sup>, and HANS-PETER STEINRÜCK<sup>1</sup> — <sup>1</sup>Universität Erlangen-Nürnberg, Lehrstuhl für Physikalische Chemie II, Egerlandstr. 3, 91058 Erlangen, Germany — <sup>2</sup>Institute for Applied and Physical

Chemistry, University of Bremen, Leobener Strasse NW2, 28359 Bremen, Germany — <sup>3</sup>Nanoscale Synthesis and Characterization Laboratory, Lawrence Livermore National Laboratory, P.O. Box 808, Livermore, California 94550, United States of America

Recent reports [1] have revealed that monolithic nanoporous gold (npAu) exhibits remarkably high catalytic activity for CO oxidation. This observation is surprising because the traditional catalyst is of the oxide-supported type. The specific particle-support interactions, which apparently play important roles in the standard Au catalyst, are absent for the nanoporous Au. If this is the case, then why does it display such high activity? The answer is most likely related to traces of residual Ag in the npAu. To highlight the role played by each metal in the catalytic process, we have investigated npAu with respect to changes in the chemical and electronic states of both metals with and without CO and O<sub>2</sub> using in-situ XPS (1 mbar) and XPS, respectively. Our results confirm previous XPS results in that segregation of Ag occurs in the surface region. HP-XPS data suggests that this residual Ag plays a significant role in activating molecular oxygen. [1] V. Zielasek et al., *Angew. Chem. Int. Ed.* 2006, 45, 8241-8244.

O 42.86 Wed 17:45 P2

**Nanoporous Gold: XPS and In-situ XPS Investigation** — ●KARIFALA DUMBUYA<sup>1</sup>, ARNE WITTSTOCK<sup>2,3</sup>, VOLKMAR ZIELASEK<sup>2</sup>, JÜRGEN BIENER<sup>3</sup>, ALEX HAMZA<sup>3</sup>, MARCUS BÄUMER<sup>2</sup>, MICHAEL GOTTFRIED<sup>1</sup>, and HANS-PETER STEINRÜCK<sup>1</sup> — <sup>1</sup>Universität Erlangen-Nürnberg, Lehrstuhl für Physikalische Chemie II, Egerlandstr. 3, 91058 Erlangen, Germany — <sup>2</sup>Institute for Applied and Physical Chemistry, University of Bremen, Leobener Strasse NW2, 28359 Bremen, Germany — <sup>3</sup>Nanoscale Synthesis and Characterization Laboratory, Lawrence Livermore National Laboratory, P.O. Box 808, Livermore, California 94550, United States of America

Recent reports [1] have revealed that monolithic nanoporous gold (npAu) exhibits remarkably high catalytic activity for CO oxidation. This observation is surprising because the traditional catalyst is of the oxide-supported type. The specific particle-support interactions, which have been shown to play important roles in the standard Au catalyst, are absent for the nanoporous Au. This being the case, then why does it display such high activity? The answer is most likely related to traces of residual Ag in the npAu. To highlight the role played by each metal in the catalytic process, we have investigated npAu with respect to changes in the chemical and electronic states of both metals with and without CO and O<sub>2</sub> using in-situ XPS (1 mbar) and XPS, respectively. Our results confirm previous XPS results in that segregation of Ag occurs in the surface region. HP-XPS data suggests that this residual Ag plays a significant role in activating molecular oxygen. [1] V. Zielasek et al., *Angew. Chem. Int. Ed.* 2006, 45, 8241-8244.

O 42.87 Wed 17:45 P2

**Nanostructuring of Cu Planar Surfaces With Pt For The Investigation of Hydrogen Related Reactions** — ●ODYSSEAS PASCHOS<sup>1</sup>, HOLGER WOLFSCHMIDT<sup>1</sup>, RAINER BUSSAR<sup>1,2</sup>, and ULRICH STIMMING<sup>1,2</sup> — <sup>1</sup>Department of Physics E19, Technische Universität München, James-Frank-Str. 1, 85748, Garching, Germany — <sup>2</sup>Bavarian Center for Applied Energy Research (ZAE Bayern), Walther-Meißner Str. 6, 85748, Garching, Germany

Recent advances in electrochemistry show that nanostructuring surfaces with metallic catalysts can enhance their electrocatalytic activity. This is advantageous for various applications such as fuel cells and electrolyzers, since it can improve their performance with simultaneous decrease in the amount of precious metal catalysts that is used. Previous work on Pd decorated Au(111) surfaces showed that by decreasing the Pd amount on Au(111), an increase of the activity for hydrogen evolution reaction (HER) occurred for very small coverages. A similar trend was observed for the case of Pt nanostructured Au(111) surfaces. However more research needs to be done in order to obtain a better understanding of this effect. The choice of the substrate material is an important factor for the design of the catalyst structure. In this work we will present results on hydrogen related reactions for Pt nanostructured Cu surfaces. Pt deposited on Cu results in a compressed lattice of Pt and hence the electrochemical behavior of the catalyst system is altered compared to bulk Pt and Pt deposited on Au(111). The results will be compared to the Pt/Au(111) system and hence useful conclusions can be drawn for the choice of substrate material.

O 42.88 Wed 17:45 P2

**Vibrational Spectroscopy of Adsorbates on Roughened Cu(1 1 1)** — ●OLAF SKIBBE, DIANA VOGEL, and ANNEMARIE PUCCI —

Kirchhoff-Institut für Physik, Universität Heidelberg, Im Neuenheimer Feld 227, 69120 Heidelberg

Rough surfaces are known to provide properties different from those found on low-index pristine single crystal surfaces. These defect determined properties are often responsible for the chemical activity of the surface in heterogeneous catalysis. In this work we present vibrational spectra taken with high-resolution electron energy loss spectroscopy (HREELS) of different adsorbates (e.g. CO, C<sub>2</sub>H<sub>4</sub>) on roughened Cu(111). The roughening was performed by evaporating small amounts of copper on the cooled Cu(111) surface. In addition, we performed measurements of the work function change by using the highly monochromated electron beam of the HREELS in the retarding potential method. The structure of the  $I(U)$  curve can be assigned to different morphologies of the substrate.

O 42.89 Wed 17:45 P2

**Pressure gap in electrochemically induced oxygen spillover at Pt/YSZ electrodes** — ●ARAFAT TOGHAN, LIZ RÖSKEN, and RONALD IMBIHL — Institut für Physikalische Chemie und Elektrochemie, Leibniz-Universität Hannover, Callinstr.3-3a, D-30167 Hannover, Germany

Upon application of a pumping voltage to Pt electrodes on the oxygen-ion conducting solid electrolyte YSZ (yttria-stabilized zirconia) we observe the spillover of discharged oxygen atom onto the Pt surface. The spillover which represents the basis of the electrochemical promotion of heterogeneously catalyzed reactions has been investigated in the past at low pressure, at  $p < 10^{-4}$  mbar. We extend here these studies up to 1 mbar using in situ XPS at BESSY. We use (111) oriented YSZ single crystals, oriented Pt (111) electrodes were prepared by sputtering of Pt target on the surface of a single crystal YSZ (111) using magnetron sputtering technique in inert argon atmosphere at room temperature. The electrodes were characterized by scanning electron microscope(SEM) and by photoelectron emission microscopy(PEEM).

O 42.90 Wed 17:45 P2

**Study of atomic adsorption on graphite monolayer by computer simulation** — ●VITALIY GORBENKO — Classical Private University, Zaporozh'ye, Ukraine

Understanding of chemical interaction of various atoms with graphite and carbon-based structures is both scientifically and technologically important [1]. The calculations by semiempirical (PM3,PM6), ab-initio (Hartree-Fock) and density functional theory (DFT) methods have been used for study of main properties of the interaction and changes in electronic density of nanographite layers. The MOPAC2007 and GAMESS program packages have been used.

In graphite layers every carbon atom is bounded with three other carbon atoms via sp<sup>2</sup> hybridization. Breaking the pi-bonds and producing additional sigma-bond is the main mechanism of chemisorption of atoms on graphite monolayers. The three typical adsorption sites have been found. Namely, first is single carbon atom, next is bridge between nearest carbon atoms and last is center of hexagonal carbon cell. Cluster geometry, total energy, atom bonds orders, value of the electron density, atom orbital populations and molecular localized orbitals were obtained. The obtained results of calculations will be detailed and discussed.

[1] J.C. Meyer, A. K. Geim, M. I. Katsnelson, K. S. Novoselov, T. J. Booth, S. Roth, *Nature Lett.* 2007; 446:60.

O 42.91 Wed 17:45 P2

**Reaction of Methanol on functionalized Ruthenium** — ●PAWEL GAZDZICKI and PETER JAKOB — Fachbereich Physik, Philipps-Universität Marburg, D-35032 Marburg, Germany

Infrared Absorption Spectroscopy and Temperature-Programmed Desorption were used to study the adsorption and reaction of methanol on various functionalized Ru(0001) surfaces. The used substrates were the clean Ru(0001) surface, Ru(0001) precovered with 0.5 and 1 ML D, Ru(0001)-(2 × 2)-O, Ru(0001)-(2 × 1)-O and a pseudomorphic Cu monolayer on the Ru(0001) surface.

From the vibrational modes of the isotopes CH<sub>3</sub>OH and CH<sub>3</sub>OD clear evidence for intact adsorption at  $T = 80$  K has been found for all investigated substrates. This finding contradicts previous studies which suggested an OH (OD) bond scission upon adsorption of methanol on Ru(0001) and Ru(0001)-(2 × 2)-O, even at low temperatures, as well as recombinative desorption at elevated  $T$ .

The thermal evolution varies considerably for the individual surfaces with the prominent methoxy (CH<sub>3</sub>O) species being produced on clean

Ru(0001) and Cu/Ru(0001) only. On the oxygen (pre)covered surfaces methanol predominantly desorbs without reaction; a small fraction decomposes directly to form CO and H without forming any detectable intermediates. Finally, 1 ML D/Ru(0001) largely passivates the surface and methanol adsorption is fully reversible.

O 42.92 Wed 17:45 P2

**Chemical trends in the metal-substrate interaction for adsorbed Pt atoms** — ●CHONG GAO and AXEL GRÖSS — Institut für Theoretische Chemie, Universität Ulm, \*D-89069 Ulm, Germany

Catalysts typically consist of small metal particles deposited on an oxide substrate. In this context, the so-called strong metal support interaction (SMSI) has been discussed intensively [1] which significantly influences the catalytic properties of group VIII metals. Using density functional theory, we have performed a systematic study of chemical trends in the metal-support interaction. As a first step, we considered a single Pt atom adsorbed on TiO<sub>2</sub>, Si and Au substrates, thus making also contact to systems that are of interest in electrocatalysis. As a probe of the chemical reactivity, we determined the electronic structure of the adsorbed Pt atoms and evaluated CO adsorption energies on these metal-support systems. The results are compared to recent results of the local reactivity of surface alloy systems [1,2].

[1] S. Sakong, C. Mosch, and A. Groß, *Phys. Chem. Chem. Phys.* **9**, 2216 (2007).

[2] Y. Gohda and A. Gross *Surf. Sci.* **601**, 3702 (2007).

O 42.93 Wed 17:45 P2

**Pushing and Pulling a Sn Ion through an Adsorbed Phthalocyanine Molecule** — ●YONGFENG WANG<sup>1</sup>, JÖRG KRÖGER<sup>1</sup>, RICHARD BERNDT<sup>1</sup>, and WERNER A. HOFER<sup>2</sup> — <sup>1</sup>Institut für Experimentelle und Angewandte Physik, Christian-Albrechts-Universität zu Kiel, D-24098 Kiel, Germany — <sup>2</sup>Surface Science Research Center, University of Liverpool, Liverpool L69 3BX, United Kingdom

Molecule-based functional devices on surfaces may take advantage of bistable molecular switches. The conformational dynamics and efficiency of switches are radically different on surfaces compared to liquid phase. We present a design of molecular layers, which enables bistable switching on a surface, and, for the first time, demonstrate control of a single switch in a dense and ordered array at the spatial limit. Up and down motion of a central Sn ion through the frame of a phthalocyanine molecule is achieved via resonant electron or hole injection into molecular orbitals.

O 42.94 Wed 17:45 P2

**Micrometer-scale parallel studies on microstructured model catalysts** — ●MATTHIAS ROOS, STEFAN KIELBASSA, MENHILD EYRICH, JOACHIM BANSMANN, and R. JÜRGEN BEHM — Institute of Surface Chemistry and Catalysis, Ulm University, D-89069 Ulm

To study mesoscopic effects in catalytic reactions, a spatially resolving scanning mass spectrometer was developed, which allows to quantitatively determine reaction rates above model catalysts. Using microstructured model systems with catalytically active fields separated by inert areas, transport effects will be evaluated from the variation in local reaction rates with size and separation of the active fields [1,2]. Experimental data on microstructured Pt films on SiO<sub>2</sub> are presented, and compared with results of simulations. Moreover, first measurements on Au/TiO<sub>2</sub> model catalyst are shown.

[1] M. Roos et al., *Rev. Sci. Instrum.* **78** (2007) 084104

[2] S. Kielbassa et al., *Langmuir* **20** (2004) 6644

O 42.95 Wed 17:45 P2

**DFT Studies of TiO<sub>2</sub> (110) and Cu Surfaces** — ●PIOTR KOWALSKI<sup>1</sup>, BERND MEYER<sup>2</sup>, and DOMINIK MARX<sup>1</sup> — <sup>1</sup>Lehrstuhl für Theoretische Chemie, Ruhr-Universität Bochum, D-44780 Bochum — <sup>2</sup>Interdisziplinäres Zentrum für Molekulare Materialien und Computer-Chemie-Centrum, Department Chemie und Pharmazie, Friedrich-Alexander-Universität Erlangen-Nürnberg

Using DFT-based ab-initio calculations in combination with a thermodynamic formalism we investigate the properties of TiO<sub>2</sub> (110) and Cu surfaces. We have calculated the relative stability of various structural models of the nonpolar, mixed-terminated TiO<sub>2</sub> (110) surface in contact with a surrounding gas phase at finite temperature and pressure. Adsorption and desorption of H, H<sub>2</sub>O, CO, simple alcohols as well as the formation of O vacancies were considered. Assuming thermodynamic equilibrium between the surface and an oxygen, hydrogen and water containing atmosphere, we constructed a phase diagram of the

lowest free energy surface structures. Cu surfaces are interesting from technological point of view as methanol, a key material for the synthesis of organic materials, is made catalytically from gas containing CO, CO<sub>2</sub> and H<sub>2</sub> in presence of a Cu/ZnO/Al<sub>2</sub>O<sub>3</sub> catalyst. It is believed that the morphological changes of the Cu particles on the ZnO support due to a strong metal-support interaction (wetting/dewetting) is the source of higher catalytic activity. We use DFT-based ab-initio calculations to identify the reactive sites on the Cu particles. In particular we investigate the adsorption of hydrogen and dissociated formic acid on clean as well as defective (steps/terraces) Cu surfaces.

O 42.96 Wed 17:45 P2

**The interaction of HCOOH with oxygen-terminated ZnO(000-1)** — ●HENGSHAN QIU, YUEMIN WANG, and CHRISTOF WÖLL — Physical Chemistry I, Ruhr-University Bochum, 44780 Bochum, Germany

Zinc oxide is one of the most important metal oxides due to its electrical, optical and catalytic properties as well as potential applications [1]. The clean, adsorbate-free polar O-terminated ZnO(000-1) surface is electrostatically unstable due to uncompensated surface charges and adopts a (1x3) structure with an abundance of oxygen vacancies [1]. It has been proposed that these vacancy sites exhibit high catalytic activity toward methanol synthesis and formate species could be one of the important intermediates in this process. In this work, the interaction of HCOOH with O-ZnO(000-1) has been studied by high resolution electron energy loss spectroscopy (HREELS) and thermal desorption spectroscopy (TDS). Exposing ZnO(000-1) surface to HCOOH at 100 K leads to the formation of physisorbed multilayers, chemisorbed monolayer and bidentate formate species. The latter can only be formed at oxygen vacancies through a dissociative adsorption of HCOOH with the ionized H diffusing into the bulk. Heating the sample to higher temperatures induces a thermally activated conversion from the bidentate to a monodentate formate species. At 550 K further decomposition occurs releasing CO, CO<sub>2</sub> and H<sub>2</sub>. In addition, an adsorbate-induced Zn desorption was also observed along with the formate dissociation. [1] Ch. Wöll, *Prog. Surf. Sci.* **82** (2007) 55.

O 42.97 Wed 17:45 P2

**In-situ investigations of adsorbed benzene on silver modified Pt(322) surfaces** — ●SANDRA KÜNZEL<sup>1</sup>, MATTHIAS SCHÖPPKE<sup>1</sup>, REGINE STREBER<sup>2</sup>, MICHAEL PETER ANDREAS LORENZ<sup>2</sup>, HANS-PETER STEINRÜCK<sup>2</sup>, and REINHARD DENECKE<sup>1</sup> — <sup>1</sup>Wilhelm-Ostwald-Institut für Physikalische und Theoretische Chemie, Universität Leipzig, Linnestraße 2, 04103 Leipzig — <sup>2</sup>Lehrstuhl für Physikalische Chemie II, Universität Erlangen-Nürnberg, Egerlandstraße 3, 91058 Erlangen

In a previous study the site-specific adsorption of benzene on Ni(111) has been investigated by in-situ x-ray photoelectron spectroscopy (XPS) [1]. In an attempt to study lateral confinement on the adsorption properties of larger molecules, we applied such detailed analysis of C 1s core levels (excited by synchrotron radiation at BESSY II) to benzene adsorption on stepped Pt(322). The effective terrace width was modified from five atomic rows to zero by different amounts of Ag (from 0.2 to 1 ML) deposited at 300 K, which form monatomic rows along the step edges [2]. Adsorption of benzene on clean Pt(322) at 190 to 300 K yields only a single C 1s peak with no indication of specific step related adsorption. Increasing amounts of Ag result in a monotonous decrease of benzene adsorption at 300 K (no adsorption on Ag). Since complete site blocking was already observed for Ag coverages exceeding 0.6 ML (i.e. three monolayers), a horizontal adsorption geometry and, thus, a minimum free Pt area required can be proposed.

This work was supported by BMBF (05 ES3XBA/5).

[1] C. Papp et al., *Phys. Rev. B* **73** (2006) 235426.

[2] P. Gambardella et al., *Phys. Rev. B* **61** (2000) 2254.

O 42.98 Wed 17:45 P2

**Pulsed laser modification of the steel-polymer interface** — ●CHRISTIAN HOLZHEU, MATTHIAS LASKE, and OTHMAR MARTI — University of Ulm, Institute of Experimental Physics

Laser treatment of stainless steel and the resulting material changes are studied. The irradiation of steel surfaces with short laser pulses improves the adhesion of polymers and especially of fluorinated polymers. Several experiments helped to elucidate the main parameters responsible for polymer adhesion. A setup for laser conditioning under well defined atmospheres was developed. Chemical changes and changes in surface topography caused by laser treatment are analyzed and compared with relevant adhesion data. Measuring the reflectance

by the surface allowed to get a relative measure of chemical changes at the surface of the material. For quantitative material characterization GDOES (Glow Discharge Optical Emission Spectroscopy) is used. The durability of the steel before and after laser treatment is evaluated in long time tests applying mechanical pulses.

O 42.99 Wed 17:45 P2

**excited states of the chromophores within many-body perturbation theory** — ●YUCHEN MA and MICHAEL ROHLFING — Fachbereich Physik, Universität Osnabrück, Germany

Although the chromophores of photoactive yellow proteins and rhodopsin proteins have been the subject of numerous spectroscopic investigations because of their unique biochemistry and photophysical properties, the position in energy of their excited states are still not well-defined in theory. We use the *ab-initio* many-body perturbation theory (GW approximation and Bethe-Salpeter equation) to study the excited states of these chromophores, which taking into account electronic exchange, correlation, and electron-hole interaction effects.

Calculations show that the resonant-antiresonant coupling beyond the commonly employed Tamm-Dancoff approximation is needed for an accurate description of the lowest  $\pi \rightarrow \pi^*$  excitations, which affects the excitation energy by up to 0.4 eV. The huge exchange interaction between the electron and hole leads to the unnegligible coupling between the resonant transition and the antiresonant counterpart. The lowest  $n \rightarrow \pi^*$  excitation for the chromophores of photoactive yellow proteins is composed from free electron-hole transitions with very different quasiparticle transition energies. An accurate description of the lowest  $n \rightarrow \pi^*$  excitation requires inclusion of the dynamics effect in the electron-hole screening, which affects the excitation energy by up to 0.3 eV.

O 42.100 Wed 17:45 P2

**Perturbative approach for electronic excitations in adsorption on metal surfaces** — ●PETER KRATZER and MATTHIAS TIMMER — Fachbereich Physik - Theoretische Physik and Centre for Nanointegration (CeNIDE), Universität Duisburg-Essen, Lotharstr. 1, 47048 Duisburg, Germany

When molecules or atoms adsorb on a metal surface electronic excitations will appear. We have developed and implemented a new method, which is able to calculate the spectra of these excitations. Here, we present the method, which is based on first-order time-dependent perturbation theory, and ground-state density-functional theory (DFT) calculations. It is simple enough to be applied to a wide class of adsorbates and surfaces, while at the same time allowing us to extract system-specific information. We show results for the adsorption of atomic hydrogen isotopes on-top the Al(111) surface. The experimentally observed isotope effect can be explained. At the same time, the method avoids many of the problems of earlier approaches.

It can be implemented with reasonable effort within existing DFT codes, as a post-processing tool [1].

[1] <http://arXiv.org/abs/0810.5248>

O 42.101 Wed 17:45 P2

**Quasiparticle band-structures and lifetimes in noble metals using GW approximation** — ●ZHIJUN YI<sup>1</sup>, YUCHEN MA<sup>1</sup>, MICHAEL ROHLFING<sup>1</sup>, VIATCHESLAV SILKIN<sup>2</sup>, and EVGENI CHULKOV<sup>2</sup> — <sup>1</sup>Universität Osnabrück, Osnabrück, Germany — <sup>2</sup>Donostia International Physics Centre, San Sebastian, Spain

We present the calculations of quasiparticle bandstructures and lifetimes for noble metals Cu and Ag within the GW approximation. For Cu, Both the calculated positions of the *d* bands and the width of the *d* bands is within 0.1 eV compared to the experimental results. For Ag, partial core correction should be included in the pseudopotential to get reliable positions of the *d* bands. The calculated lifetime agree with the experiment in the energy region away from the Fermi level, but deviates from the experimental results near the Fermi level where short range interactions which GW approach fails to describe play an important role. For a better description of the lifetime near the Fermi level, higher terms beyond the GW approximation in the many body perturbation theory need to be considered.

O 42.102 Wed 17:45 P2

**Structural Dependence of Optical Properties of Tellurium** — ●STEPHAN BLANKENBURG<sup>1,2</sup>, WOJCIECH WELNIC<sup>1</sup>, and LUCIA REINING<sup>1</sup> — <sup>1</sup>Laboratoire des Solides Irradiés, École Polytechnique, Paris, France — <sup>2</sup>Theoretische Physik, Universität Paderborn, Paderborn, Germany

The further miniaturization of electronic and optoelectronic devices needs the understanding of fundamental material properties to open up new avenues for the nano-fabrication process. Essential steps for understanding the basic mechanisms are the experimental and theoretical study of well-defined model systems [1,2]. In this context, tellurium with its several chemical and physical properties is one of the elemental materials of interest. Due to the discrepancies between the theoretical and experimental determined optical parameters in the literature of Te [3,4], we used time-dependent density-functional theory to reveal the origin of this effect. The puzzling interplay between structural parameters and optical properties as well as the transition to one-dimensional Te nanowires are analyzed in detail.

[1] W. Welnic, et. al., Nature Materials 5, 56 (2006).

[2] W. Welnic, S. Botti, L. Reining, M. Wuttig, PRL 98, 236403 (2007).

[3] S. Tsuchihashi, et. al., Phys. Rev. 3, 177 (1969).

[4] P. Ghosh, M. Upadhyay, U. V. Waghmare, PRB 75, 245437 (2007).

O 42.103 Wed 17:45 P2

**Solving the Bethe-Salpeter equation for Wannier-Mott like excitons in InN, ZnO, and MgO.** — ●FRANK FUCHS, CLAUDIA RÖDL, ANDRÉ SCHLEIFE, JÜRGEN FURTHMÜLLER, and FRIEDHELM BECHSTEDT — Institut für Festkörpertheorie und -optik, Friedrich-Schiller-Universität Jena, Max-Wien-Platz 1, 07743 Jena, Germany

The accurate calculation and parameter-free prediction of optical spectra including excitonic effects is highly desirable for both fundamental and applied research. Excitonic effects can be treated in the framework of many-body perturbation theory and the Bethe-Salpeter equation (BSE), by solving an eigenvalue problem for the electron-hole Hamiltonian  $\hat{H}$ .

In this study we investigate the formation of Wannier-Mott like excitonic states below the optical absorption edge for InN, ZnO, and MgO. Using a recently developed numerically efficient method [1] it is possible to obtain converged results for the binding energies of the first shells of Wannier-Mott excitons.

The results are critically compared to the predictions based on the Wannier-Mott two-band model and available experimental data. In comparison to the latter the computed binding energies, if converged, appear to be significantly overestimated. We discuss this with respect to a deficiency in the underlying approximation of a static screening and investigate the possibility to go beyond.

[1] F. Fuchs, C. Rödl, A. Schleife, and F. Bechstedt Phys. Rev. B 78, 085103 (2008)

O 42.104 Wed 17:45 P2

**2nd-order Møller-Plesset perturbation theory applied to extended systems** — ●ANDREAS GRÜNEIS, MARTIJN MARSMAN, and GEORG KRESSE — Faculty of Physics, University Vienna, and Center for Computational Materials Science, Sensengasse 8/12, A-1090, Vienna, Austria

The use of wave function based methods, such as Møller-Plesset perturbation theory, to add electronic correlation to the Hartree-Fock (HF) approximation is common practice in the computational quantum chemistry of molecular systems. Due to the computational cost involved, however, these methods have hardly been applied to extended systems.

Recently, we have implemented 2nd-order Møller-Plesset (MP2) perturbation theory within the framework of the full-potential Projector-Augmented-Wave (PAW) method, using periodic boundary conditions and a plane wave basis set.

The present implementation allows for the calculation of total energies as well as quasiparticle energies. In order to determine the accuracy of this method we calculated lattice constants, bulk moduli, band gaps, and atomization energies of several semiconducting and insulating systems, including hexagonal Ice. Compared to HF, HF+MP2 yields an improved description of the aforementioned structural properties.

Regarding band gaps, HF+MP2 band gaps present an improvement over the corresponding HF results. Nevertheless, the underestimated static dielectric screening properties of the employed HF wave functions are reflected in underestimated band gaps.

O 42.105 Wed 17:45 P2

**Optical Spectra and Band Structure of Anatase and Rutile TiO<sub>2</sub>** — ●ANDREAS GREULING<sup>1</sup>, PATRICK RINKE<sup>2</sup>, and MICHAEL ROHLFING<sup>1</sup> — <sup>1</sup>Universität Osnabrück, Barbarastr.7,D-49069,Osnabrück — <sup>2</sup>University of California, Santa Barbara

TiO<sub>2</sub> is a semiconductor which is used in many applications (e.g. in biotechnology, cosmetic industry, paint industry, in catalysis or photocatalysis). Therefore, the (optical) properties of TiO<sub>2</sub> are of great interest. As these are still not fully understood in theory we address its excited electronic states and optical spectra with ab initio methods beyond DFT.

We present results of first principles calculations for anatase and rutile TiO<sub>2</sub>. Starting from the electronic ground state, which is calculated within DFT(LDA), we describe the single particle excitations with an GWA approach. We use Gaussian basis-sets because this results in reasonable computational cost. Then we calculate the electron-hole interaction and solve the Bethe-Salpeter Equation (BSE) in order to obtain coupled electron-hole excitations. Based on the resulting data we evaluate the optical spectra and compare them with experimental data.

O 42.106 Wed 17:45 P2

**IRRAS studies on a new emitter material for OLEDs** — ●TOBIAS GLASER<sup>1</sup>, MARTIN BINDER<sup>1</sup>, ANNEMARIE PUCCI<sup>1</sup>, CHRISTIAN LENNARTZ<sup>2</sup>, and CHRISTIAN SCHILDKNECHT<sup>2</sup> — <sup>1</sup>Kirchhoff-Institut für Physik, Universität Heidelberg — <sup>2</sup>BASF SE, 67056 Ludwigshafen

A new emitter material for organic light emitting devices (OLEDs) called CN-PMBIC is investigated by infrared (IR) spectroscopy. Experiments were performed under UHV conditions with a commercial FT IR spectrometer flanged to the chamber. Thin films of the organic material were deposited by vapor sublimation on different substrates. Especially infrared reflection absorption spectroscopy (IRRAS) is a well-suited method to investigate the growth of the organic films. Furthermore, the influence of Ca on CN-PMBIC was studied at room temperature and at 100 K. Ca plays an important role as cathode material in OLED fabrication. The evaporation of Ca onto a film of CN-PMBIC gives rise to new IR features that strongly depend on the sequence in which the various materials are deposited and on the sample temperature. The new features are supposed to be related to dynamic charge transfer effects.

O 42.107 Wed 17:45 P2

**Design of composite materials via textured polymer brushes** — ●MANUELA PLUNTKE<sup>1</sup>, SABINE LETSCHE<sup>2</sup>, DIRK VOLKMER<sup>2</sup>, and OTHMAR MARTI<sup>1</sup> — <sup>1</sup>Institute of Experimental Physics, Ulm University, Albert-Einstein-Allee 11, 89069 Ulm — <sup>2</sup>Institute of Inorganic Chemistry II, Ulm University, Albert-Einstein-Allee 11, 89069 Ulm

Acidic matrix macromolecules are involved in the production of biomaterials such as bone and nacre. Therefore polyelectrolyte brushes exposing a multitude of acidic groups are attractive tools to control the growth of biogenic minerals.

To obtain crystalline thin mineral films we deposit inorganic material in a lithographically structured organic matrix of polymer brushes grown by surface-initiated atom-transfer radical polymerisation. The initial metastable amorphous thin film is converted into a polycrystalline phase by thermal treatment.

To find optimal conditions for the specific deposition of different minerals we varied the matrix properties by altering the functional groups of the brushes and the experimental parameters.

Our current studies focus on the analysis of the brush swelling behaviour in the mineralization media by AFM as well as on the mechanical properties of the materials.

After all our investigations contribute to the understanding of the interactions between the inorganic minerals and the organic matrix molecules and offer attractive perspectives for potential applications like optical information processing and regenerative medicine.

O 42.108 Wed 17:45 P2

**Experimentelle Untersuchungen der Adsorption und des Kristallwachstums von Komponenten epikutikularer Wachse** — ●ALEXANDER HOMMES<sup>1,2</sup>, WILHELM BARTHLOTT<sup>3</sup> und KLAUS WANDEL<sup>2</sup> — <sup>1</sup>FGAN, Wachtberg, Germany. — <sup>2</sup>Institut für Theoretische und Physikalische Chemie, Surfaces and Interfaces, University of Bonn, Germany. — <sup>3</sup>Nees-Institut für Biodiversität der Pflanzen, University of Bonn, Germany.

Im Rahmen dieser Arbeit wurde das konzentrationsabhängige Phasenverhalten von adsorbiertem Octacosan-1-ol und Octacosan-1-ol Derivaten an der fest/flüssig und fest/gas Grenzfläche eines artifiziellen Substrats mittels AFM/STM/REM untersucht. Octacosan-1-ol ist Hauptbestandteil der epikutikularen Wachse auf Weizenblättern, und bildet somit die äußerste Barriere zur Umwelt und bestimmt die Hydrophobizität der Blattoberfläche. Die Nukleations- und Wachstumsbedingun-

gen auf der nativen Oberfläche führen zur Ausbildung von kristallinen "Platelets", die aufgrund einer komplexen mikro- und nanoskopische Architektur einen Superhydrophoben Effekt auslösen. Um diesen Effekt grundlegend zu verstehen und in einem technischen Prozeß nutzbar zu machen, muß ein Verständnis zum Wachstum von organischen Kristallen auf Oberflächen entwickelt werden. Hierzu werden verschiedene, in epikutikularen Wachsen enthaltene Moleküle auf artifiziellen Oberflächen adsorbiert und das Kristallwachstum beobachtet. Die erhaltenen Erkenntnisse sind nach dem "bottom up Prinzip", von der Einzelmoleküluntersuchung über Nukleation, Aggregatbildung bis hin zum makroskopischen Kristallwachstum gegliedert.

O 42.109 Wed 17:45 P2

**On the fate of hydrogen by formation of thiol-based self-assembled monolayers: A critical in situ photoelectron spectroscopy result** — ●LAXMAN KANKATE, ANDREY TURCHANIN, and ARMIN GÖLZHÄUSER — Fakultät für Physik, Universität Bielefeld, 33615 Bielefeld

Self-assembled monolayers (SAMs) of thiols on gold are vastly utilized for the functionalization of surfaces and interfaces in interdisciplinary research for many years. However, a seminal question on the fate of the hydrogen of the S-H groups upon SAM formation has not been answered unambiguously<sup>1</sup>. It is generally believed that the S-H bond scission takes place and the released hydrogen either sticks to the surface or desorbs in the molecular form. Some studies, however, suggest that the S-H bond scission does not occur at all. Here, we present the experimental results which clearly show that the atomic hydrogen forms upon thiol SAM formation and interacts with the monolayer terminus. Vapour phase deposition was utilized to grow 4'-nitro-1,1'-biphenyl-4-thiol, 4-nitrophenylthiol and bis-(4,4'-nitrobiphenyl)-disulphide SAMs on Au surfaces. Using in situ x-ray photoelectron spectroscopy (XPS) we found that the terminal nitro group of the thiol SAMs are partially reduced upon the self-assembly into the amino group. On the contrary, the disulphide SAMs form without any reduction.

[1] J.C. Love, L.A. Estroff, J.K. Kriebel, R.G. Nuzzo, G.M. Whitesides, Chem. Rev. 105 (2005) 1103

O 42.110 Wed 17:45 P2

**Study of azobenzene-containing self-assembled monolayers with surface plasmon resonance spectroscopy** — ●OLENA FILINOVA, ULRICH JUNG und OLAF MAGNUSSEN — Institut für Experimentelle und Angewandte Physik, Leibnizstraße 19, 24098 Kiel

Azobenzene-containing molecules can be switched between the trans and cis isomers by UV and visible light. Adsorbate layers of such molecular switches on surfaces are of great interest for the formation of functional nanosystems. Using surface plasmon resonance spectroscopy we have studied the kinetics of the photoisomerization processes for self-assembled monolayers containing azobenzene bound by thiol- and triazatriangulenium groups to Au surface. Using an Hg-lamp with bandpass filter the trans-cis photoswitching was monitored as a function of wavelength and radiation power. These measurements allowed to optimize the conditions for photoswitching and to determine the time constants for the first order kinetics of this processes, which allowed to estimate quantum yields of the photoisomerization reactions in the range 10<sup>-5</sup> to 10<sup>-3</sup>.

O 42.111 Wed 17:45 P2

**Reactive Sites for the Deposition of Calcium on Semiconducting Polymers** — ●FABIAN BEBENSEE<sup>1</sup>, JACK HESS BARICUATRO<sup>2</sup>, JUNFA ZHU<sup>3</sup>, JAMES SHARP<sup>2</sup>, WANDA LEW<sup>2</sup>, HANS-PETER STEINRÜCK<sup>1</sup>, J. MICHAEL GOTTFRIED<sup>1</sup>, and CHARLES T. CAMPBELL<sup>2</sup> — <sup>1</sup>Lehrstuhl für Physikalische Chemie II, Universität Erlangen-Nürnberg, Egerlandstraße 3, D-91058 Erlangen, Germany — <sup>2</sup>Department of Chemistry, University of Washington, Seattle, WA 98195, USA — <sup>3</sup>National Synchrotron Radiation Laboratory, University of Science and Technology of China, Hefei, Anhui 230029, China

Systems composed of semiconducting polymers and low work function metals - used as the cathode - are of great interest in the field of organic electronics, e.g., organic solar cells and organic light emitting diodes. The key parameter in the performance of such devices is the interface between the active polymer and the electrode. We investigated the deposition of calcium on several semiconducting polymers, including CN-MEH-PPV and P3HT, using a set of complementary experimental techniques (ISS, HR-XPS, adsorption microcalorimetry). The focus of this study is on the different adsorption or reaction sites for Ca on the polymer surface and the energetics of the interface formation. The considerable differences in the behavior of the polymers are linked to the

presence of different heteroatoms. Support by the DAAD, the NSF, and the Excellence Cluster "Engineering of Advanced Materials" at the University of Erlangen-Nürnberg is gratefully acknowledged.

O 42.112 Wed 17:45 P2

**High energy photoelectron spectroscopy of HBC-C14** — ●VAJIHEH ALIJANI<sup>1</sup>, S. SHAHABEDIN NAGHAVI<sup>1</sup>, ANDREI GLOSKOVSKI<sup>1</sup>, GERHARD H. FECHER<sup>1</sup>, CLAUDIA FELSER<sup>1</sup>, KATERINA MEDYANYK<sup>2</sup>, and GERD SCHÖNHENSE<sup>2</sup> — <sup>1</sup>Institute of Inorganic and Analytical Chemistry, Johannes Gutenberg - University, 55099 Mainz — <sup>2</sup>Institute of Physics, Johannes Gutenberg - University, 55099 Mainz

A charge transfer (CT) complex is defined as an electron donor /— electron acceptor complex, characterized by electronic transitions to an excited state. In this excited state, there is a partial transfer of a charge from the donor to the acceptor. CT complexes are good candidates as photovoltaic cells, transistors and superconductors. Thin films of HBC-C14 were prepared on Si/SiO<sub>x</sub> substrate by spin coating and characterised by profilometry and atomic force microscopy. The films were investigated by X-Ray photoelectron spectroscopy with laboratory XPS source and synchrotron excitation. The excitation energy was varied in the range from 1.4 keV to 8 keV. We show that high energy photoelectron spectroscopy at intermediate energies is better suited than at very high energies for studies of organic thin films. The reason is the enhanced contribution of the Si/SiO<sub>x</sub> substrate to the photoemission signal at higher photon energies. This is caused by very large inelastic electron mean free path that becomes comparable with the film thickness of few tens of nm at high kinetic energies of photoelectrons.

Funded by DFG through Transregio SFB TRR 49 (Project B8).

O 42.113 Wed 17:45 P2

**Valence band spectroscopy on plasma treated wood surfaces** — ●LOTHAR KLARHÖFER<sup>1</sup>, EVGENIJ PACHOMOW<sup>1</sup>, SEBASTIAN MATHES<sup>1</sup>, WOLFGANG MAUS-FRIEDRICH<sup>1</sup>, and WOLFGANG VIÖL<sup>2</sup> — <sup>1</sup>Institut für Physik und Physikalische Technologien, Leibnizstraße 4, D-38678 Clausthal-Zellerfeld, Germany — <sup>2</sup>HAWK FH Hildesheim/Holzwinden/Göttingen, Fakultät Naturwissenschaften und Technik, Von-Ossietzky-Straße 99, 37085 Göttingen

Wood has been plasma treated using a dielectric barrier discharge at atmospheric pressure in ambient air, in order to improve the wettability of the surface. Chemical changes due to plasma treatment were studied by several surface sensitive techniques like XPS, UPS and MIES.

The functional groups of cellulose were identified in the valence band by fingerprints from glucose and cellobiose. The fingerprints for lignin were obtained by coniferyl alcohol, cinnamyl alcohol, phenol and benzene.

The plasma treatment in ambient air has different effects to the surface of cellulose and lignin respectively. An oxygen containing plasma reduces the cellulose surface, causes the loss of hydroxyl groups and the formation of C=O double bonds.

The lignin surface oxidizes in an oxygen containing plasma which leads to the removal of the hydrophobic phenyl groups, which react preferred with the plasma species. The destruction of the phenyl groups and therefore the molecule backbone causes the removal of the lignin from the surface, leaving a polar and rich on oxygen surface with goof wetting behaviour.

O 42.114 Wed 17:45 P2

**A study of the Cobalt Phthalocyanine-Ag-Si(111) interface** — ●FEI SONG<sup>1,2</sup>, JUSTIN WELLS<sup>1,3</sup>, ZHESHEN LI<sup>1</sup>, KARSTEN HANDRUP<sup>1</sup>, SHINING BAO<sup>2</sup>, KARINA SCHULTE<sup>4</sup>, LOUISE MAYOR<sup>4</sup>, EDWARD PERKINS<sup>4</sup>, JANINE SWARBRICK<sup>4</sup>, LAUGE GAMMELGAARD<sup>5</sup>, MARJA AHOLA-TUOMI<sup>6</sup>, and PHILIP HOFMANN<sup>1</sup> — <sup>1</sup>University Aarhus, DK — <sup>2</sup>Zhejiang University, Hangzhou, CN — <sup>3</sup>Norwegian University of Science and Technology, Trondheim, N — <sup>4</sup>University of Nottingham, UK — <sup>5</sup>CARPES A/S, Kgs. Lyngby, DK — <sup>6</sup>University of Turku, FI

We describe the electronic and structural properties of the interface between Cobalt phthalocyanine(CoPc) molecules and a Si(111) surface, which is passivated by a monolayer of silver. Different photoemission-based techniques such as valence band UPS, XPS and NEXAFS are used, and the system is also investigated using nano-scale four point probes. Valence band UPS indicates a stronger bonding for the first monolayer of molecules than for subsequent monolayers. This is accompanied by a structural change from flat-lying to standing. For thicker layers, we infer the charge transfer and band alignment. Finally, the thickness-dependent surface conductance is related to these

observations.

O 42.115 Wed 17:45 P2

**Infrared and Raman spectroscopy of ultrathin organic films in a liquid cell** — ●NADJA BECKER<sup>1</sup>, DENNIS AULICH<sup>1</sup>, NORBERT ESSER<sup>1</sup>, JÖRG RAPPICH<sup>2</sup>, and KARSTEN HINRICH<sup>1</sup> — <sup>1</sup>ISAS - Institute for Analytical Sciences, Department Berlin, Albert-Einstein-Str. 9, 12489 Berlin, Germany — <sup>2</sup>Helmholtz Zentrum Berlin für Materialien und Energie GmbH, Abt. SE1, Kekuléstr. 5, 12489 Berlin, Germany

Thickness and structure of organic films is investigated by non-destructive, optical in-situ-methods. Besides molecular identification, Raman spectroscopy and infrared ellipsometry are shown to reveal complementary vibrational informations of thin films. The same in-situ cell [1] was used for characterisation of protein adsorption and the study of polymer films in contact with aqueous solutions.

Reference: [1] Y. Mikhaylova, L. Ionov, J. Rappich, M. Gensch, N. Esser, S. Minko, K.-J. Eichhorn, M. Stamm, K. Hinrichs, Anal. Chem. 79, 7676 (2007)

O 42.116 Wed 17:45 P2

**Nano-Mechanical Detection of (Bio-)Molecular Recognition** — ●K. GRUBER<sup>1</sup>, C. ROHR<sup>1</sup>, J. KOESER<sup>2</sup>, U. HUBLER<sup>2</sup>, T. SOBEV<sup>3</sup>, F. C. SIMMEL<sup>3</sup>, and B. A. HERMANN<sup>1</sup> — <sup>1</sup>Dept. of Physics / CeNS, LMU Munich and WMI, 85748 Garching, Germany — <sup>2</sup>Concentris GmbH, 4012 Basel, Switzerland — <sup>3</sup>Dept. of Physics, TU Munich, 85748 Garching, Germany

Based on the development of the atomic force microscope, the cantilever array technique monitors physical, chemical and biochemical processes taking place on the surface of wafer-thin and extremely sensitive silicon springs. These reactions can be measured directly without fluorescent or radioactive labels, and can be followed in real-time allowing analysis of reaction dynamics and determination of e.g. kinetic constants. The goal is to understand the chemical transduction process of a (bio-)molecular key-lock-recognition in a deflection signal by performing well defined experiments.

The hybridization signals of two 70% to 80% homologous single-stranded DNA sequences could be clearly distinguished. Each half of one cantilever array was functionalized with one of the two DNA strands. Hence, only those cantilever that bear the exact complementary to a matching single strand, offered in the sample solution, show deflection. The experiment could be successfully reproduced for several independently functionalized cantilever arrays. As one possible application, we demonstrated that a thrombin catching DNA-aptamer[1] could be successfully bound onto a cantilever surface.

[1] F. C. Simmel et al., Angew. Chem. Int. Ed. 2004 43, 3549 (2004)

O 42.117 Wed 17:45 P2

**Influence of supporting substrate on the shape of deposited size-selected nanoparticles** — ●CHRISTIAN KLEINHANS, WOLFGANG ROSELLEN, FURKAN BULUT, KERSTIN GEBHARDT, and MATHIAS GETZLAFF — Institute of Applied Physics, University Düsseldorf

The structure of supported clusters, significantly affecting their electronic and magnetic properties, is of large interest in today's physics, especially from a technological point of view for future applications. With a continuously working, UHV-compatible arc cluster ion source (ACIS), Fe-, Co- and FeCo-alloy-clusters have been produced and subsequently mass filtered using an electrostatic quadrupole-deflector-unit. The sizes range from 5 to 15nm. The deposition of these preformed free clusters onto a ferromagnetic Ni-thin-film prepared on a W(110)-substrate was performed under soft-landing conditions. For comparison, the clusters were additionally deposited on the bare W(110) surface. Due to the different surface energies, changes in the shape of the clusters are to be expected. The determination of size and shape of the nanoparticles was carried out by means of STM and TEM. We will also discuss the temperature dependence concerning the different nanoparticle-substrate systems.

O 42.118 Wed 17:45 P2

**Crystal structure of iron oxide nano particles synthesized form ferritin** — ●MICHAEL KRISPIN, ALADIN ULLRICH, and SIEGFRIED HORN — Lehrstuhl für Experimentalphysik II, Universität Augsburg, D-86135 Augsburg

We have investigated the local crystal structure of nanosized iron oxides by extended x-ray absorption fine structure (EXAFS). Iron oxide

nanoparticles of different diameters were produced by thermal treatment of horse spleen ferritin molecules and remineralized apo-ferritin molecules, respectively. The size was determined by atomic force microscopy (AFM) as well as transmission electron microscopy (TEM). The structure of these particles was compared to various iron oxide and ferrihydrite references. The Fourier transformed (FT) EXAFS spectra of the iron oxide nanoparticles differ significantly from  $\alpha$ -Fe<sub>2</sub>O<sub>3</sub> and  $\gamma$ -Fe<sub>2</sub>O<sub>3</sub> reference spectra and change systematically as a function of particle diameter, signalling a corresponding evolution of the structure. A possible explanation could be the occurrence of a mixture of  $\alpha$ -Fe<sub>2</sub>O<sub>3</sub> and  $\gamma$ -Fe<sub>2</sub>O<sub>3</sub> phases in a core-shell model, i.e. the particle consists of a  $\alpha$ -Fe<sub>2</sub>O<sub>3</sub> core and  $\gamma$ -Fe<sub>2</sub>O<sub>3</sub> like shell. A decrease of core to shell ratio with decreasing particle size may then explain the changes in the measured FT-EXAFS. Indeed, EXAFS oscillations of samples can be fitted by a linear combination of the EXAFS oscillations of the measured  $\alpha$ -Fe<sub>2</sub>O<sub>3</sub> and  $\gamma$ -Fe<sub>2</sub>O<sub>3</sub> reference powders. This picture is supported by the fact, that x-ray diffraction (XRD) measurements on annealed native ferritin show that the  $\alpha$  and  $\gamma$  phases coexist.

O 42.119 Wed 17:45 P2

**Electronic properties of size selected Ag clusters on C<sub>60</sub> and HOPG surfaces** — ●BEN WORTMANN<sup>1</sup>, STEFANIE DUFFE<sup>1</sup>, LUKAS PATRYARCHA<sup>1</sup>, BERND VON ISSENDORFF<sup>2</sup>, and HEINZ HÖVEL<sup>1</sup> — <sup>1</sup>Technische Universität Dortmund, Experimentelle Physik I, 44221 Dortmund, Germany — <sup>2</sup>Universität Freiburg, Fakultät für Physik, Hermann-Herder Straße 3, 79104 Freiburg, Germany

We deposited mass selected Ag clusters, which are expected to form geometrically magic icosahedra, on 1.5 ML C<sub>60</sub>/HOPG at low temperatures. On 1 and 2 ML C<sub>60</sub> we observed very narrow cluster height distributions for Ag<sub>309±3</sub> and Ag<sub>923±9</sub>. The clusters on 1 and 2 ML C<sub>60</sub> kept their original height for more than 12 hours at room temperature [1, 2]. To get information on the electronic structure of the clusters, scanning tunnelling spectroscopy measurements were performed at 5 K for Ag<sub>309±3</sub> and Ag<sub>923±9</sub>/C<sub>60</sub>/HOPG. We observed spectra with identical features for individual clusters with the same selected size. Additionally we investigated the electronic properties of size selected clusters with ultraviolet photoemission spectroscopy (UPS). Using C<sub>60</sub> as buffer layer for the cluster deposition, the dominant UPS signal of C<sub>60</sub> masks the signal of the clusters. For this reason the Ag clusters were deposited and investigated on bare HOPG at 100 K. The low temperature decreases the mobility of the clusters on HOPG and reduces coalescence. One aim of these studies is the comparison to UPS spectra of size selected clusters in free beam [3].

[1] S. Duffe et al., EPJD **45**, 3 (2007) [2] S. Duffe et al., submitted for publication [3] O. Kostko et al., PRL **98**, 043401 (2007)

O 42.120 Wed 17:45 P2

**Growth of magnetic clusters on a moiré pattern of graphene on Ru(0001)** — ●SIMON ALTENBURG, MARTIN ZIEGLER, JÖRG KRÖGER, and RICHARD BERNDT — Christian-Albrechts-Universität zu Kiel, D-24098 Kiel, Germany

Large areas of highly ordered single layer graphene were grown on a Ru(0001) surface by controlled segregation of Carbon from the bulk. The resulting moiré superstructure was atomically resolved by scanning tunnelling microscopy. We find that the moiré pattern acts as a template for the growth of Co clusters: Depositing Co onto the graphene layer gives rise to Co islands whose lateral dimensions are determined by the moiré pattern. The dependence of the Co island dimensions on deposition temperature and coverage was investigated. Funding by the Deutsche Forschungsgemeinschaft through SFB 668 is acknowledged.

O 42.121 Wed 17:45 P2

**Growth and Characterization of Pt Nanoparticles on CeO<sub>2</sub>(111) Films on Cu(111) by STM** — ●THORSTEN STAUDT<sup>1</sup>, YAROSLAVA LYKHACH<sup>1</sup>, LUTZ HAMMER<sup>2</sup>, M. ALEXANDER SCHNEIDER<sup>2</sup>, and JÖRG LIBUDA<sup>1</sup> — <sup>1</sup>Lehrstuhl für Physikalische Chemie II, Friedrich-Alexander-Universität Erlangen-Nürnberg — <sup>2</sup>Lehrstuhl für Festkörperphysik, Friedrich-Alexander-Universität Erlangen-Nürnberg

Precious metal nanoparticles supported on ceria films are widely used in many important applications, including three-way automotive catalysts and the catalytic oxidation of hydrocarbons. The use of ceria is motivated by its unique ability to store and release oxygen, while it is well known that metal particles supported on oxides can exhibit different chemical reactivity depending upon their size and structure.

Here we present a scanning tunnelling microscopy study on the growth of Pt nanoparticles on CeO<sub>2</sub>(111) films. These films are grown

by physical vapour deposition (PVD) of cerium on a Cu(111) substrate in O<sub>2</sub> at 520 K. The recipe has been adopted from the one suggested by Matolin and coworkers [1] and modified by the use of a higher oxidation temperature to form atomically flat terraces. LEED measurements reveal a well-ordered film with a (1.5x1.5) superstructure in orientation to the underlying substrate. A Volmer-Weber growth mode of ceria is identified by STM measurements. In a next step we investigate the nucleation behaviour and growth of Pt nanoparticles, prepared by PVD. Finally, the thermal stability of these particles is studied and it is found that they are transformed into flat islands upon annealing. [1] V. Matolin et al., Thin Solid Films **516** (2008) 6120-6124

O 42.122 Wed 17:45 P2

**Towards an understanding of the vibrational spectrum of the neutral Au<sub>7</sub> cluster** — ●LUIS MANCERA and DAVID M. BENOIT — Nachwuchsgruppe Theorie - SFB 569, University of Ulm, Albert-Einstein-Allee 11, D-89081 Ulm, Germany

Most experimental vibrational studies on neutral gold nanoclusters have focused on charged particles. For neutral clusters, such studies have been limited in the past to Au<sub>2</sub> and Au<sub>3</sub>. Only very recently, vibrational spectra of a few small neutral gold clusters in gas-phase have been reported, using far-infrared multiple-photon dissociation (FIR-MPD) spectroscopy [1]. Among them, Au<sub>7</sub> receives a particular attention since it is in a size regime in which anions and cations are known to adopt planar structures. In this contribution, we address the prediction of the vibrational spectrum of the Au<sub>7</sub> cluster from first principles. Since discrepancies between experimental and theoretical spectra are often attributed to anharmonic effects, we also investigate the vibrational spectrum of this cluster, using the vibrational self-consistent field method (VSCF), which includes anharmonic coupling between vibrational modes. Besides anharmonicity, we discuss other issues affecting the prediction of the spectrum, such as polymorphism and the theoretical description of the underlying potential energy surface.

[1] P. Gruene, D. M. Rayner, B. Redlich, A. F. G. van der Meer, J. T. Lyon, G. Meijer, and A. Fielicke, Science **321**, 674 (2008)

O 42.123 Wed 17:45 P2

**HICS – Highly charged ion collisions with surfaces** — ●CHRISTIAN HAAKE, THORSTEN PETERS, JOHANNES HOPSTER, ANDREAS WUCHER, and MARIKA SCHLEBERGER — Universität Duisburg-Essen, Fachbereich Physik, 47057 Duisburg, Germany

A new ion beam installation with the name HICS (highly charged ions collisions with surfaces) has been constructed to investigate the mechanisms of energy dissipation in a substrate after the impact of highly charged ions. The set-up offers high charge states (up to Ar<sup>16+</sup> or Xe<sup>44+</sup>) and adjustable kinetic energies which can be less than 100 eV/q. These low energies are achieved by a deceleration system which uses a device we call an ion escalator. An evaporation chamber for sample preparation is mounted and a load lock system offers *in situ* transport to other vacuum systems. To analyse the irradiation effects a time-of-flight system for secondary and neutral mass spectrometry (SIMS/SNMS) is installed. Inner Electronic excitations can be detected with metal-insulator-metal junctions. These detectors offer the possibility to study excitations below the work function which limits the external emission of electrons. First data measured with Ag-AlO<sub>x</sub>-Al detectors will be presented.

O 42.124 Wed 17:45 P2

**Photochromic silver nanoparticles fabricated by nanosphere lithography** — ●MELANIE MEIXNER, ALEXANDER SPRAFKE, FLORIAN HALLERMANN, MAXIMILIAN REISMANN, MATTHIAS WUTTIG, and GERO VON PLESSEN — Institute of Physics (IA), RWTH Aachen University, 52056 Aachen, Germany

Photochromic materials change their color under irradiation with light. In previous work [1], we have studied the photochromic transformation of silver nanoparticles embedded in transition-metal oxides prepared by dc-sputter deposition, such as TiO<sub>x</sub>, ZrO<sub>x</sub> and HfO<sub>x</sub>. The silver nanoparticles are highly inhomogeneous in shape, size and spatial distribution. The photochromic effect is based on spectral hole burning in the inhomogeneously broadened particle-plasmon band. This hole burning is probably caused by photoemission of electrons from the resonantly excited particles.

In the present work, we show that TiO<sub>x</sub>-embedded silver nanoparticles with improved photochromic properties can be fabricated through a combination of electron-beam evaporation and nanosphere lithography. Nanosphere lithography is a method to produce hexagonal arranged and equally shaped particles [2]. The good reproducibility of

this approach allows us to analyze the photochromic transformation in a more quantitative way than was possible with samples prepared by sputter deposition.

[1] C. Dahmen et al., Appl. Phys. Lett. 88 ,011923 (2006)

[2] J. C. Hulthen et al., J Vac Sci Technol A 13 pp. 1553-1558 (1995)

O 42.125 Wed 17:45 P2

**Exposure of Single-Molecule-Magnets Mn<sub>6</sub>Cr and Mn<sub>7</sub> to Soft X-Rays** — FABIAN MERSCHJOHANN<sup>1</sup>, ●ANDREAS HELMSTEDT<sup>1</sup>, AARON GRYZIA<sup>1</sup>, ANDREAS WINTER<sup>1</sup>, SEBASTIAN STEPPELER<sup>1</sup>, NORBERT MÜLLER<sup>1</sup>, ARMIN BRECHLING<sup>1</sup>, MARC D. SACHER<sup>1</sup>, ULRICH HEINZMANN<sup>1</sup>, CARL-GEORG FREIHERR V. RICHTHOFEN<sup>2</sup>, THORSTEN GLASER<sup>2</sup>, SÖNKE VOSS<sup>3</sup>, MIKHAIL FONIN<sup>3</sup>, and ULRICH RÜDIGER<sup>3</sup> — <sup>1</sup>Fak. f. Physik, Uni Bielefeld — <sup>2</sup>Fak. f. Chemie, Uni Bielefeld — <sup>3</sup>Fak. f. Physik, Uni Konstanz

Mn<sub>6</sub>Cr and Mn<sub>7</sub> are two representatives of the new 7-core Single-Molecule-Magnets (SMM) with a large spin moment. Adsorbed on surfaces their electronic configuration may change depending on the substrate material. Possible modifications of the electronic configuration can be studied element-specificly by X-ray absorption spectroscopy and by measuring the spin-polarization of photoelectrons ejected by circularly polarized synchrotron radiation. Drawback of the above mentioned methods is the bad stability of the SMM during X-ray exposure. The SMM degrade due to photoreduction with increasing time of exposure. The trivalent metallic components (here Mn and Cr) become divalent ones. This degradation process was observed by using very

small photon fluxes at Maxlab III. Within about one hour of X-Ray exposure the degradation saturates. The rate of degradation depends on the substrate material as well as on the SMM-concentration on the substrate. Beneath these results we will present first spin-resolved photo-emission measurements of SMM-crystals.

O 42.126 Wed 17:45 P2

**Investigation of hot electrons below the surface** — ●JOHANNES HOPSTER<sup>1</sup>, THORSTEN PETERS<sup>1</sup>, CHRISTIAN HAAKE<sup>1</sup>, DETLEF DIESING<sup>2</sup>, ANDREAS WUCHER<sup>1</sup>, and MARIKA SCHLEBERGER<sup>1</sup> — <sup>1</sup>Fachbereich Physik, Universität Duisburg-Essen, Lotharstrasse 1, 47057 Duisburg, Germany — <sup>2</sup>Physikalische Chemie, Universität Duisburg-Essen, 45117 Essen, Germany

In many physical processes energetic (hot) charge carriers play a significant role. Hot electrons may be produced in different ways, e.g. by energetic ions, laser beams or directly by a monoenergetic electron beam. Our aim is to investigate the spatial and temporal development of the electron energy distribution below the surface. To detect the hot charge carriers thin film metal insulator metal junctions (MIMs) are used. The measured yield of electron transmission through the insulator barrier depends on the initial excitation energy, the top electrode thickness, the material of the top electrode and the barrier height. By applying a bias voltage between the two metal electrodes energy dispersive measurements are possible. Corresponding data that has been obtained on various MIMs will be presented.

## O 43: Invited Talk (Jürg Osterwalder)

Time: Thursday 9:30–10:15

Location: HSZ 02

### Invited Talk

O 43.1 Thu 9:30 HSZ 02

**Measuring spin polarization vectors with ARPES** — ●JÜRGEN OSTERWALDER<sup>1</sup>, HUGO DIL<sup>1,2</sup>, FABIAN MEIER<sup>1,2</sup>, JORGE LOBO-CHECA<sup>3</sup>, LUC PATTHEY<sup>2</sup>, and VLADIMIR N. PETROV<sup>4</sup> — <sup>1</sup>Physik-Institut, Universität Zürich, CH-8057 Zürich — <sup>2</sup>Swiss Light Source, Paul Scherrer Institut, CH-5232 Villigen — <sup>3</sup>Department Physik, Universität Basel, CH-4056 Basel — <sup>4</sup>St. Petersburg Technical University, 195251 St. Petersburg, Russia

Combining an angle-resolved photoelectron spectrometer equipped with a three-dimensional spin polarimeter [1] and a new two-step fitting routine [2] we can measure absolute spin polarization vectors for individual bands intersected in a particular set of ARPES data. This procedure is crucial when analyzing strongly overlapping peaks or weak

signals sitting on a large unpolarized background, especially in the presence of non-collinear spins. It is robust against strong intensity variations due to matrix element effects because it references the spin polarization contribution of each band to the measured peak intensity. The method is applied to two-dimensional systems where spin-orbit effects lead to spin splittings and complex momentum-dependent spin structures. Presented case studies include surface alloys of Bi and Pb on Ag(111) that show a giant Rashba effect, as well as ultrathin Pb layers on Si(111), where by introducing the electron spin as an additional tag Rashba splittings of the order of 15 meV could be measured. We find in all cases that the states are 100% spin polarized. [1] M. Hoesch et al., J. Electron Spectrosc. Relat. Phenom. 124, 263 (2002). [2] F. Meier et al., Phys. Rev. B 77, 165431 (2008).

## O 44: Metal substrates: Adsorption of organic / bio molecules VI

Time: Thursday 10:30–13:00

Location: SCH A118

O 44.1 Thu 10:30 SCH A118

**Self-Assembly Induced Chirality in CoTPP on Cu(110)** — ●ABEL ROBIN, PHILIP DONOVAN, RASMITA RAVAL, MATTHEW STEPHEN DYER, and MATS PERSSON — University of Liverpool, Liverpool, U.K.

We describe the adsorption of Co(II) tetraphenylporphyrin (CoTPP) on Cu(110) using a combination of STM and periodic DFT. Porphyrins' electronic, magnetic and catalytic properties make them an attractive target for introducing organised functionality at surfaces.

We show that CoTPP forms highly ordered 2D arrays on Cu(110). Importantly, the self-assembled structures exhibit chirality on both organisational and molecular levels, creating equal and opposite mirror domains. The expression of chirality in adsorbed porphyrin systems has only been observed rarely. Here we delineate important factors driving chiral expression in a per se non-chiral system.

DFT shows a strong energetic preference for molecules adsorbing in bridge sites, accompanied by a significant charge exchange between the macrocycle and the substrate. Optimised intermolecular and molecule-substrate interactions rotate and tilt the phenyls, endowing the porphyrins with a propeller-like, thus chiral, conformation. These propeller-like molecules assemble along two non-symmetry directions, leading to large chiral domains mirrored across the main copper axes.

For the predominant structure we distinguish two sets of diametrically opposite phenyls possessing distinct interactions with the sub-

strate. Because of this anisotropy, assembly along one chiral direction is less flexible than along the other. Our DFT calculated images correspond well with the STM images for this structure.

O 44.2 Thu 10:45 SCH A118

**SPA-LEED study on metal-free phthalocyanine sub-monolayers on Ag(111)** — ●PATRICK BAYERSDORFER<sup>1</sup>, INGO KRÖGER<sup>1</sup>, FRIEDRICH REINERT<sup>1,2</sup>, and CHRISTIAN KUMPF<sup>1,3</sup> — <sup>1</sup>Universität Würzburg, Experimentelle Physik II, D-97074 Würzburg — <sup>2</sup>FZ Karlsruhe, Gemeinschaftslabor für Nanoanalytik, D-76021 Karlsruhe — <sup>3</sup>FZ Jülich GmbH, IBN-3, D-52425 Jülich

The geometrical alignment of organic molecules in the first adlayer on a surface strongly influences interface properties like surface dipoles or charge transfer, but it also plays an important role for the growth of further molecular layers. Phthalocyanines (Pcs) deposited on a silver surface play a prominent role in this context since they exhibit an unusual adsorption behaviour. We use high-resolution low energy electron diffraction (SPA-LEED) in order to investigate geometrical aspects of metal-free Pc (H<sub>2</sub>Pc) sub-monolayers on Ag(111). At room temperature (RT) and up to a coverage of 0.75 ML no long range ordered structures occur. The molecules arrange themselves randomly on the surface and maximize the distance to their neighbours. Between 0.75 ML and 0.91 ML a commensurate superstructure is formed

followed by a series of continuously changing point-on-line structures above 0.91 ML. The latter superstructures were already observed for metal Pcs in our group (CuPc, SnPc, TiOPc, see contributions of I. Kröger, M. Häming and M. Kochler). They proof the existence of a dominant intermolecular repulsion between the molecules on Ag(111). However, in contrast to the metal Pcs, H2Pc exhibits a commensurate structure also at RT which indicates a reduced intermolecular repulsion.

O 44.3 Thu 11:00 SCH A118

**Determining the diffusion coefficients of large organic molecules on a metal surface from tunneling current fluctuations** — ●JULIAN IKONOMOV, CHRISTOPH H. SCHMITZ, and MORITZ SOKOLOWSKI — Institut für Physikalische und Theoretische Chemie, Universität Bonn, Wegelerstr. 12, 53115 Bonn, Deutschland

The diffusion of organic molecules on surfaces has so far been mostly investigated by molecule tracking using the video STM technique [1]. This method requires small molecule coverages and small diffusion coefficients. Here we present a new technique suitable for higher temperatures and arbitrarily coverages based on the temporal increase in the tunneling current that occurs when a molecule diffuses under the STM tip. For our measurements, we have chosen the model system perylene-3,4,9,10-tetracarboxylic acid dianhydride (PTCDA) on Ag(100). The PTCDA molecules form highly ordered two-dimensional islands surrounded by gas-like phase [2]. In order to determine the diffusion coefficients, we used a continuum model to describe the diffusion of the molecules under the tip. Due to the finite size of the molecule it is even possible to obtain the spatial anisotropy of the diffusion coefficient. From the density of the peaks in the current-time spectra, one may in addition quantitatively estimate the tip-molecule interaction and the mean local coverage.

Funded by the DFG through SFB 624.

[1] M. Schunack et al., *Phys. Rev. Lett.*, **88** (2002) 156102.

[2] J. Ikonov et al., *Surf. Sci.*, **602** (2008) 2061.

O 44.4 Thu 11:15 SCH A118

**Nature of Free-Electron-Like States in PTCDA molecules Adsorbed on an Ag(111) Surface** — ●MATS PERSSON and MATTHEW DYER — Surface Science Research Centre, University of Liverpool, L69 3BX Liverpool, UK

Advances in molecular assembly experiments on metal surfaces and potential applications arising from them call for a better understanding of the electronic structure at the interface of metals and organic systems. There is a high interest in delocalized electronic states, because of their potential use in molecular and opto-electronics applications. Recently, unoccupied, free-electron-like states arising in mono layers of 3,4,9,10-perylene-tetracarboxylic acid dianhydride (PTCDA) molecules adsorbed on an Ag(111) surface at energies close to the Fermi energy have been observed by scanning tunneling and photoemission spectroscopies [1,2]. So as to reveal the nature of these delocalized states we have carried out a density functional study of the electronic structure and local density of states of these systems. We show that the observed free-electron state originates from a Shockley surface state (SS) at the zone centre of the bare surface. The SS is shifted up by the interaction with the organic overlayer. [1] R. Temirov *et al.*, *Nature* **444**, 350 (2006). [2] C. H. Schwalb *et al.*, *Phys. Rev. Lett.* **101**, 146801 (2008).

O 44.5 Thu 11:30 SCH A118

**PTCDA chemisorbed on Ag(110): Dispersion interactions and charge equilibration** — ●REINHARD SCHOLZ<sup>1</sup> and AFSHIN ABBASI<sup>2</sup> — <sup>1</sup>Walter Schottky Institut, TU München, Germany — <sup>2</sup>Institut für Physik, TU Chemnitz, Germany

The chemisorption of PTCDA on Ag(110) is analysed with 2<sup>nd</sup> order Møller-Plesset perturbation theory (MP2), accounting therefore for the main part of the dispersion interactions at an *ab initio* level. Irrespective of the size of the rigid silver cluster used as a substrate model, the optimized geometry consists of a nearly flat perylene core, surrounded by carboxylic oxygens closer to the substrate, but with anhydride atoms at a larger height. The charge equilibration between adsorbate and substrate involves charge injection from the oxygen atoms into the substrate, and back transfer of two electrons into the former LUMO of the free molecule. Surprisingly, the resulting negative charge of the adsorbate has a very small contribution in the core region where the main part of the LUMO is localized, but instead accumulates on the end groups. It can be shown in detail that a rehybridization of molecular  $\sigma$  and  $\pi$  states results in a decoupling of several  $\pi$  states

on the oxygen atoms from the aromatic core, as opposed to the free molecule, where the  $\pi$  states delocalize over the entire molecule. These decoupled  $\pi$  states on the end groups are forming the binding Ag-O orbitals injecting electronic charge from the molecule into the substrate. Compared to the dominating mechanisms discussed above, the hybridization between orbitals in the core region and the underlying substrate plays only a minor role for the charge balance.

O 44.6 Thu 11:45 SCH A118

**Interface states investigated by PES, IPES and 2PPE: the example of PTCDA/Ag** — ●ACHIM SCHÖLL<sup>1</sup>, STEFAN KRAUSE<sup>1</sup>, SÖNKE SACHS<sup>1</sup>, JOHANNES ZIROFF<sup>1</sup>, CHRISTIAN SCHWALB<sup>2</sup>, MANUEL MARKS<sup>2</sup>, ULRICH HÖFER<sup>2</sup>, EBERHARD UMBACH<sup>3</sup>, and FRIEDRICH REINERT<sup>1</sup> — <sup>1</sup>Uni Würzburg, Experimentelle Physik II, D-97074 Würzburg — <sup>2</sup>Philipps-Uni Marburg, Physik und Materialwissenschaften, D-35032 Marburg — <sup>3</sup>FZ Karlsruhe, D-76021 Karlsruhe

We have studied the occupied and unoccupied states at the PTCDA/Ag interface, enabling us to draw a comprehensive picture of the interfacial electronic structure [1]. The strong, unambiguously covalent, interaction leads to hybrid orbitals (interface states), involving at least LUMO, HOMO, and HOMO-1, and Ag 5s- and 4d-states. The LUMO is pulled below  $E_F$  resulting in a new occupied state. High-resolution photoemission (PES) data reveal that on Ag(111) this state is partially filled leading to a "metallic" phase. Inverse PES (IPES) and two-photon photoemission (2PPE) reveal a new unoccupied state 0.6 eV above  $E_F$ , which disperses with an effective mass of 0.39  $m_e$  at the  $\Gamma$ -point. The short lifetime (54 fs) indicates a large penetration into the metal. This state is interpreted as predominantly due to an adsorption induced upshift of the Ag(111) Shockley state[2].

These interface states are expected to have notable influence on the charge carrier injection properties at an interface, particularly if their wave function penetrates the metal as well as the molecular layer.

[1] Y. Zou et al., *Surf. Science*, 2006. 600(6)1240.

[2] C.H. Schwalb et al., *Phys. Rev. Lett.*, 2008. 101(14).

O 44.7 Thu 12:00 SCH A118

**PTCDA induced faceting of a vicinal Ag(111) surface: an in-situ LEEM study** — ●THOMAS SCHMIDT<sup>1</sup>, FLORIAN POLLINGER<sup>2</sup>, HELDER MARCHETTO<sup>1</sup>, STEFAN SCHMITT<sup>2</sup>, FLORIAN C. MAIER<sup>2</sup>, ALESSANDRO SALA<sup>1</sup>, FRIEDRICH T. REINERT<sup>2</sup>, EBERHARD UMBACH<sup>2,3</sup>, and HAJO FREUND<sup>1</sup> — <sup>1</sup>Fritz-Haber-Institut, Abt. CP, 14195 Berlin — <sup>2</sup>Universität Würzburg, EP II, 97074 Würzburg — <sup>3</sup>Forschungszentrum Karlsruhe, 76021 Karlsruhe

Adsorption of organic molecules on vicinal metal surfaces is known to promote faceting and self-organized ordering on mesoscopic scales[1]. In the temperature range between 400 K and 620 K the adsorption of PTCDA on a Ag(10 8 7) surface has been studied in-situ and in real-time by LEEM (low energy electron microscopy) and LEED, using the SMART microscope[2]. The deposition of one organic layer leads to grating-like structures. The direct observation reveals a two-step process: first, facets with an angle of ca. 25° inclination are formed with (111) orientated areas in between, whereas only the facets are covered by PTCDA. In a second step the bare (111) areas are covered by PTCDA, forming a complete monolayer. The temperature dependence of the structure sizes and the influence of inhomogeneity in the initial substrate step density are discussed.

[1] S. Schmitt, Dissertation Würzburg, 2007.

[2] R. Fink et al. *J. Electr. Spectrosc. Rel. Phen.* **84** (1997) 231-250.

O 44.8 Thu 12:15 SCH A118

**Current-induced switching of PTCDA on Ag(111)** — ●OLGA NEUCHEVA, CHRISTIAN WEISS, RUSLAN TEMIROV, and FRANK STEFAN TAUTZ — Institut für Bio- und Nanosysteme (IBN-3) and JARA-Fundamental of Future Information Technology, Forschungszentrum Jülich, 52425 Jülich, Germany

A low temperature scanning tunneling microscope (LT-STM) has been used to investigate electron transport through a single PTCDA molecule on Ag(111). Under certain conditions, one of the carboxylic oxygen atoms of the PTCDA molecule establishes a chemical bond with the STM tip, forming a covalently bound single molecular junction [1]. In this contribution, we investigate the process of contact formation as a function of parameters such as distance, bias voltage and electrical current through the molecular junction. In a narrow distance and voltage interval, bistable switching of the oxygen atom between a high- and low-conductance state is observed. The implications of this observation are discussed. [1] Temirov R., Lassise A., Anders F.B., et al., *Nanotechnology* **19** (2008) 065401

O 44.9 Thu 12:30 SCH A118

**Influence of dispersion interactions on the adsorption geometry of NTCDA on a (110)-oriented silver substrate** — ●AFSHIN ABBASI<sup>1</sup>, MICHAEL SCHREIBER<sup>1</sup>, and REINHARD SCHOLZ<sup>2</sup> — <sup>1</sup>Institut für Physik, Technische Universität Chemnitz, D-09107 Chemnitz, Germany — <sup>2</sup>Walter Schottky Institut, Technische Universität München, Am Coulombwall 3, D-85748 Garching, Germany

We investigate the adsorption of NTCDA on Ag(110) with second-order Møller-Plesset perturbation theory (MP2) and density functional theory (DFT), using rigid metal clusters of different size as a model for the substrate. In each method, the adsorption geometry depends only weakly on the size of the metal cluster, but both microscopic approaches differ significantly: MP2 gives a nearly flat adsorbate, whereas the lack of dispersion interaction in DFT results in a strongly bended geometry, placing the aromatic core at a much larger distance from the topmost substrate layer with respect to the oxygen groups. Irrespective of the microscopic approach, the carboxylic oxygens interact more strongly with the substrate than the anhydride oxygens, placing them about 0.2 Å closer to the topmost silver layer. On the largest substrate cluster containing 34 silver atoms in three consecutive crystal planes, MP2 places the carbon atoms at an average height of 2.57 Å above the topmost silver layer, about 0.3 Å closer than in the strongly bended geometry obtained with DFT. From these findings, we conclude that the chemisorption geometry of NTCDA on Ag(110) cannot be quantified without the dispersion interactions included at the MP2 level.

O 44.10 Thu 12:45 SCH A118

**"Soft" metallic contact to isolated C<sub>60</sub> molecules** — ●HENDRIK GLOWATZKI<sup>1</sup>, BENJAMIN BRÖKER<sup>1</sup>, RALF-PETER BLUM<sup>1</sup>, OLIVER T. HOFMANN<sup>2</sup>, ANTJE VOLMER<sup>3</sup>, RALPH RIEGER<sup>4</sup>, KLAUS MÜLLEN<sup>4</sup>, EGERT ZOJER<sup>2</sup>, JÜRGEN P. RABE<sup>1</sup>, and NORBERT KOCH<sup>1</sup> — <sup>1</sup>Humboldt-Universität zu Berlin, Institut für Physik, Berlin, Germany — <sup>2</sup>Technische Universität Graz, Institut für Festkörperphysik, Graz, Austria — <sup>3</sup>BESSY, Berlin, Germany — <sup>4</sup>MPI for Polymer Research, Mainz, Germany

We investigated the electronic as well as the structural properties of Hexaazatriphenylene-hexanitrile (HATCN) and C<sub>60</sub> on Ag(111) by using ultraviolet photoelectron spectroscopy (UPS) and scanning tunneling microscopy (STM) accordingly. HATCN was used as buffer layer to decouple the test-molecule C<sub>60</sub> from the metal substrate. Photoemission revealed metallic behavior of HATCN on Ag(111) which calculations confirmed to be due to partial filling the LUMO of chemisorbed HATCN. From STM a regular honeycomb-structure was found. Using C<sub>60</sub> as test-molecule on top of this layer the holes within the honeycombs were acting as adsorption centers leading to laterally spacing between C<sub>60</sub> molecules as observed by STM. At the same time UPS revealed virtually bulk like electronic properties of C<sub>60</sub> on metallic HATCN/Ag(111) which is in strong contrast to the bare C<sub>60</sub>-Ag(111) interface being significantly altered by charge transfer. This opens up new possibilities in probing the undisturbed properties of individual molecules on metal substrates. This work is financially supported by European Community project "IControl" (EC-STREP-033197).

## O 45: Heterogeneous catalysis

Time: Thursday 10:30–13:00

Location: SCH A215

O 45.1 Thu 10:30 SCH A215

**Interaction of CO<sub>2</sub> and CH<sub>4</sub> with MgO/CeO<sub>2</sub>/Cu(111) and Pt/CeO<sub>2</sub>/Cu(111) model catalyst surfaces** — ●YAROSLAVA LYKHACH, THORSTEN STAUDT, MICHAEL P. A. LORENZ, REGINE STREBER, ANDREAS BAYER, HANS-PETER STEINRÜCK, and JÖRG LIBUDA — Lehrstuhl für Physikalische Chemie II, Friedrich-Alexander-Universität Erlangen-Nürnberg, Egerlandstraße 3, D-91058 Erlangen

We have studied the interaction of CO<sub>2</sub> and CH<sub>4</sub> with CeO<sub>2</sub> based model catalyst. Toward this aim, we employ epitaxially grown CeO<sub>2</sub> films on Cu(111) as well-ordered model supports [1]. Morphology and growth of the deposited films were characterized by means of STM and LEED. The CeO<sub>2</sub>/Cu(111) substrates were modified by deposition of MgO or Pt. The reaction behaviour of CO<sub>2</sub> on MgO/CeO<sub>2</sub>/Cu(111) was investigated by XPS. The interaction of CH<sub>4</sub> was studied on CeO<sub>2</sub>/Cu(111) and Pt/CeO<sub>2</sub>/Cu(111) in supersonic beam assisted experiments. Different carbonaceous species formed on the surfaces were monitored by XPS as a function of exposure, sample temperature and MgO or Pt particle sizes. Upon stepwise annealing removal of carbon is observed. While the Pt particles are recovered, significant reduction of CeO<sub>2</sub> substrate is observed at temperatures significantly lower than for clean Pt/CeO<sub>2</sub>/Cu(111). This indicates active participation of CeO<sub>2</sub> in removal of carbonaceous species via reverse-spillover of oxygen from the CeO<sub>2</sub> support to Pt.

[1] V. Matolin et al., Thin Solid Films 516 (2008) 6120-6124.

O 45.2 Thu 10:45 SCH A215

**Studies on the substrate mediated vibrational excitation of CO/Si(100) by means of SFG spectroscopy** — XU HAN, KRISTIAN LASS, ●THORSTEN BALGAR, and ECKART HASSELBRINK — Universität Duisburg-Essen, Fachbereich Chemie, 45117 Essen, Germany

Vibrational excitations of adsorbates play an important role in chemical reaction dynamics. In the past decade CO on solid surfaces was chosen as adequate model system for studying vibrational relaxation dynamics [1 - 3]. Our work is focused on the energy dissipation of vibrationally excited CO adsorbed on a silicon surface by means of IR/Vis sum frequency generation (SFG) spectroscopy [4, 5]. Here we present studies on substrate mediated excitation of vibrational modes of CO on Si(100) induced by UV radiation. We suppose the observation of highly excited internal stretch vibrations of CO caused by hot electrons generated within the silicon substrate.

[1] A. Tadjeddine, A. Le Rille, O. Pluchery, F. Vidal, W.Q. Zheng, A. Peremans, Phys. Status Solidi A 175 (1999) 89 [2] H. Ueba, Prog. Surf. Sci. 55 (1997) 115 [3] M. Buck, M. Himmelhaus, J. Vac. Sci.

Technol. A 19 (2001) 2717 [4] K. Lass, X. Han, E. Hasselbrink, J. Chem. Phys. 123 (2005) 051102 [5] K. Lass, X. Han, E. Hasselbrink, Surf. Sci. 600 (2006) 4275

O 45.3 Thu 11:00 SCH A215

**From electrons to reactive flow: Coupling first-principles kinetic Monte Carlo with continuum level simulations** — ●SEBASTIAN MATERA and KARSTEN REUTER — Fritz-Haber-Institut der Max-Planck-Gesellschaft, Faradayweg 4-6, D-14195 Berlin

First-principles kinetic Monte Carlo (kMC) simulations have evolved into an important tool in the modeling of heterogeneous catalytic processes. The success of the approach relies on the accurate treatment of two central aspects for the reactive surface chemistry: A first-principles description of the involved elementary processes and an evaluation of their statistical interplay that fully accounts for the correlations, fluctuations and spatial distributions of the chemicals at the catalyst surface. Particularly for technologically more relevant environments, i.e. ambient pressures and elevated temperatures with concomitant higher product formation rates, a third aspect in form of the heat and mass flow in the system becomes increasingly important. We investigate these effects by coupling first-principles kMC simulations self-consistently with continuum level simulations for the gas and solid phase transport, considering a stagnation point flow geometry as a model for recent *in situ* measurements over single-crystal model catalysts. Applying our method to the CO oxidation over RuO<sub>2</sub>(110) [1], we demonstrate how the build-up of temperature and pressure gradients over the active surface influence the observed catalytic activity and surface composition.

[1] K. Reuter and M. Scheffler, Phys. Rev. B **73**, 045433 (2006).

O 45.4 Thu 11:15 SCH A215

**XPS, TDS and STM Characterization of Carbonate Species and O-α on Ag(111)** — ●R. REICHEL, S. BÖCKLEIN, S. GÜNTHER, and J. WINTTERLIN — Ludwig-Maximilians-Universität, 81377 München, Germany

The interaction between Ag surfaces and oxygen is extremely complex and characterized by several different oxygen species. For this reason there is no general agreement about the role of these species in the Ag-catalyzed ethylene epoxidation. Carbonate is one of the species, and it is formed on silver at high pressures. Another one is atomic oxygen on reconstructed Ag surfaces, such as the (4×4)O reconstruction on Ag(111). An important role in recent reaction models is played by the so called O-α, O atoms on the non-reconstructed Ag surface.

Using XPS, TDS and STM we have investigated carbonate and other oxygen species on Ag(111). The species obtained sensitively depend on the preparation conditions, especially on very low impurities of CO<sub>x</sub>. Instead of the formation of O-α by exposure of Ag(111) to oxygen at room temperature we could identify three different species. Besides the (4×4)O we observed carbonate and CO<sub>2,ad</sub>. Those two can be distinguished in TDS and can be discriminated from the postulated O-α by XPS. Carbonate could be decomposed by heating to 475 K forming the (4×4)O. Thus it shows the behaviour of O-α described in literature, and the O-α species may have to be reinterpreted. CO<sub>2,ad</sub> however may be mistaken for carbonate. In STM we followed the decomposition of (4×4)O-patches under exposure of CO<sub>2</sub>, and CO<sub>2,ad</sub> is formed instead of carbonate.

O 45.5 Thu 11:30 SCH A215

**Morphology of alloy catalysts in an oxidizing environment: Structure-sensitivity of ethylene epoxidation over Ag-Cu particles** — ●SIMONE PICCINI<sup>1</sup>, CATHERINE STAMFFL<sup>1</sup>, and MATTHIAS SCHEFFLER<sup>2</sup> — <sup>1</sup>University of Sydney, Sydney, Australia — <sup>2</sup>Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, Germany

Ag-Cu alloys have been proposed as catalysts for ethylene epoxidation due to their superior selectivity compared to pure silver, the predominant catalyst for this reaction [1]. By means of density-functional theory and atomistic thermodynamics, we study the surface structure and morphology of Ag-Cu particles in thermodynamic equilibrium with an oxygen atmosphere. Contrary to the common assumption of the formation of a 2D surface alloy, we find that at temperatures and pressures of interest for practical applications the particles can display a variety of structures, including thin Cu-surface-oxides in coexistence with clean Ag. At variance with pure Ag in UHV, we find that under reactive conditions the (111) facet is not dominant. We identify different reaction pathways that will compete and/or synergetically interplay in the catalysis. In general, the reaction mechanism is structure-dependent and often the reaction does not proceed through the formation of stable intermediates, in contrast to clean Ag and the 2D alloy. Analyzing the competing reactions, we discuss how the addition of Cu improves the selectivity and stress the overall importance of accounting for the effect of ambient conditions.

[1] S. Linic et al. *J. Catal.* 224, 148 (2004)

O 45.6 Thu 11:45 SCH A215

**Carbon in palladium catalysts** — ●NICOLA SERIANI, FLORIAN MITTENDORFER, and GEORG KRESSE — University of Vienna, Austria

A carbon-rich film at the surface of a palladium catalyst is thought to be responsible for the high selectivity observed in partial hydrogenation reactions [1]. The exact nature of this phase is still unclear. We have employed density functional theory as implemented in VASP to investigate the Pd-C configuration space and the thermodynamic stability of possible phases. Bulk carbides, intercalated graphite, diamond-like phases and dissolved carbon have been considered. The calculated core level shifts and formation energies exclude the formation of a bulk carbide, as suggested in Ref. [1]. A more complex picture involving graphite and dissolved carbon arises from our calculations. The results shed light on the complex Pd-C interactions important for partial hydrogenation catalysis.

[1] D. Teschner et al., *Science* 320, 86 (2008).

O 45.7 Thu 12:00 SCH A215

**Bifunctional Nanostructured Model Catalysts: Metal/Oxide Interaction Controls Initial NO<sub>x</sub> Storage Mechanism** — ●THORSTEN STAUDT<sup>1</sup>, AINE DESIKUSUMASTUTI<sup>1</sup>, ZHIHUI QIN<sup>2</sup>, MARKUS HAPPEL<sup>1</sup>, YAROSLAVA LYKHACH<sup>1</sup>, MATHIAS LAURIN<sup>1</sup>, FRIEDEMANN ROHR<sup>3</sup>, SHAMIL SHAIKHUTDINOV<sup>2</sup>, and JÖRG LIBUDA<sup>1</sup> — <sup>1</sup>Lehrstuhl für Physikalische Chemie II, Friedrich-Alexander-Universität Erlangen-Nürnberg — <sup>2</sup>Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin — <sup>3</sup>Umicore AG & Co. KG, Hanau

In order to get detailed insights into the underlying mechanism and microkinetics, we investigated the initial NO<sub>x</sub> uptake on a model nitrogen storage and reduction (NSR) catalyst. This model system is prepared under UHV conditions by co-deposition of noble metal particles (Pd) and Ba-containing oxide particles, representing the storage compound, onto an ordered alumina film on a NiAl(110) substrate.

Using a combination of vibrational spectroscopy (IRAS), molecular-beam methods (MB) and scanning tunnelling microscopy (STM), we were able to show that the reaction mechanism is critically controlled by the metal-oxide interaction between the active noble metal particles and the NO<sub>x</sub> storage compound [1][2]. We suggest that a reverse

spillover of activated oxygen species from the NO<sub>x</sub> storage compound to the noble metal is facilitated by the strong interaction between both components. A partial oxidation of the metal particles and a simultaneous stabilization of surface nitrite intermediates are a consequence of this process. [1] A. Desikusumastuti et al., *ChemPhysChem* 9 (2008), 2191-2197 [2] A. Desikusumastuti et al., *Surf. Sci. Lett.* in press

O 45.8 Thu 12:15 SCH A215

**Infrared spectroscopic studies of syngas adsorption on ZnO nanoparticles** — ●HESHMAT NOEI<sup>1</sup>, HENGSHAN QIU<sup>2</sup>, YUEMIN WANG<sup>1,2</sup>, CHRISTOF WÖLL<sup>2</sup>, and MARTIN MUHLER<sup>1</sup> — <sup>1</sup>Industrial Chemistry, Ruhr-University Bochum, 44780 Bochum, Germany — <sup>2</sup>Physical Chemistry I, Ruhr-University Bochum, 44780 Bochum, Germany

Zinc oxide is an important material with a wide range of applications in catalysis. Presently, the most prominent application of ZnO is industrial methanol synthesis from syngas (CO<sub>2</sub>/CO/H<sub>2</sub>) over Cu/ZnO catalysts. The study of syngas adsorption on ZnO surfaces is of fundamental importance in understanding the microscopic processes occurring in methanol synthesis. In this work, the interaction of CO and CO<sub>2</sub> with ZnO nanoparticles has been studied by ultra-high vacuum Fourier-transform infrared spectroscopy (UHV-FTIRS) together with diffuse reflectance IR spectroscopy (DRIFTS). Based on the corresponding HREELS data obtained from single-crystal surfaces, the IR results on ZnO powder samples can be understood on the atomic level. Exposing ZnO to CO<sub>2</sub> leads to the formation of a number of carbonate species on different facets. For CO adsorption on clean ZnO powder one dominant band is observed at 2189 cm<sup>-1</sup> and assigned to CO bound to Zn sites on ZnO(10-10). Furthermore, the FTIRS data demonstrated that the binding energy of CO is dramatically increased when ZnO is pre-modified by CO<sub>2</sub>. This unexpected effect results from the formation of tridentate carbonate species on the nonpolar (10-10) surfaces, which increase the Lewis acidity of neighboring Zn<sup>2+</sup> cations.

O 45.9 Thu 12:30 SCH A215

**Reactivity of Hydrogen Related Reactions of Platinum Nanoparticles on Graphite** — ●TINE BRÜLLE<sup>1</sup>, HOLGER WOLFSCHMIDT<sup>1</sup>, and ULRICH STIMMING<sup>1,2</sup> — <sup>1</sup>Department of Physics E19, Technische Universität München, James-Franck-Straße 1, D-85748 Garching, Germany — <sup>2</sup>Bavarian Center for Applied Energy Research (ZAE Bayern) Division 1, Walter-Meißner-Straße 6, D-85748 Garching, Germany

A present challenge in electrocatalysis is to identify novel, highly active catalysts. Former experimental investigations of the systems Pd/Au(111) [1,2] and Pt/Au(111) [3,4] show that with decreasing amount of the catalyst material the specific catalytic activity increases considerably with respect to hydrogen oxidation reaction (HOR) and hydrogen evolution reaction (HER). In order to improve the understanding of such an enhanced catalytic activity, hydrogen based reactions were investigated for platinum supported on HOPG (highly oriented pyrolytic graphite). For that purpose, the HOPG surface was structured with nanoparticles of platinum using electrochemical pulse techniques. First results on the catalytic activity of Pt/HOPG regarding HOR and HER are presented and compared to the results of the bimetallic systems Pd/Au(111) and Pt/Au(111).

[1] Kibler, L. A. *ChemPhysChem* 7 (2006) 985 [2] Pandelov, S.; Stimming, U. *Electrochimica Acta* 2007, 52, 5548 [3] Wolfschmidt, H.; Buřar, R.; Stimming, U. *J. Phys. Condens. Matter*, 2008, 20/37, 374127 [4] Wolfschmidt, H.; Buřar, R.; Stimming, U. submitted for publication

O 45.10 Thu 12:45 SCH A215

**Similarities and Differences of the Reactivity of Pt/Au(111) and Pd/Au(111) towards HER, HOR, ORR and MOR** — ●HOLGER WOLFSCHMIDT<sup>1</sup>, RAINER BUSSAR<sup>1,2</sup>, and ULRICH STIMMING<sup>1,2</sup> — <sup>1</sup>TU München, Garching, Deutschland — <sup>2</sup>ZAE Bayern, Garching, Deutschland

Nanoparticles and nanostructures often show a different behavior compared to the bulk material. Especially in the field of catalysis high reactivity and low amounts of catalyst are required. Thereby, well known noble metal catalysts such as Pt and Pd were electrochemically deposited onto inert Au(111) supports. These nanostructured model surfaces allow investigating the effects of particle dispersion, particle size and the influence of the substrate material. The following reactions were investigated: I.) hydrogen evolution reaction (HER), II.) hydrogen oxidation reaction (HOR), III.) oxygen reduction reaction (ORR) and IV.) methanol oxidation reaction (MOR). Electrochemical

methods such as pulse techniques and cyclic voltammetry were used to determine the electrocatalytic properties. The morphology of the model electrodes and the amount of noble metal was obtained with EC-STM. It was found that with decreasing amount of Pd and Pt deposited onto Au(111) the specific activity towards hydrogen related

reactions increases by up to three orders of magnitude. In contrast to the strong enhancement for the hydrogen reactions the ORR shows an increasing electrocatalytic activity with increasing amount of noble metal as one would expect. The specific reactivity of Pt on Au(111) for the MOR seems to behave also in an expected way.

## O 46: Time-resolved spectroscopies I

Time: Thursday 10:30–13:00

Location: SCH A315

O 46.1 Thu 10:30 SCH A315

**Heat transport beyond thermodynamic equilibrium** — ●MARTIN KAMMLER, ANJA HANISCH-BLICHARSKI, BORIS KRENZER, SIMONE MÖLLENBECK, PAUL SCHNEIDER, and MICHAEL HORN-VON HOEGEN — Department of Physics, Universität Duisburg-Essen, 47048 Duisburg, Germany

The heat transport of a thermal excited film into the substrate is determined by the thermal boundary resistance at the interface and well described by the Acoustic Mismatch Model (AMM) and Diffuse Mismatch Model (DMM), both well-accepted bulk models. For ultra thin films we observe a deviation for the AMM model.

After excitation of an ultra thin epitaxial Bi(111) film with fs-laser pulses the heat transport into the silicon substrate is determined by studying the cooling process with ultrafast time resolved electron diffraction in RHEED geometry using the Debye Waller effect. For Bi on Si(111) the observed exponential temperature decay time is well described by the AMM and DMM up to only 2.5 nm thin films but not for Bi/Si(001). Here, we observe a slight saturation of the cooling process with a decay constant  $\tau = 500$  ps on films thinner than 6 nm; the heat is trapped!

O 46.2 Thu 10:45 SCH A315

**Freezing Hot Electrons in Crystalline NH<sub>3</sub> and D<sub>2</sub>O on Metal Surfaces** — ●JULIA STÄHLER<sup>1,2</sup>, MICHAEL MEYER<sup>1</sup>, UWE BOVENSIEPEN<sup>1</sup>, CORNELIUS GAHL<sup>3</sup>, and MARTIN WOLF<sup>1,4</sup> — <sup>1</sup>Freie Universität Berlin, Fachbereich Physik, Arnimallee 14, 14195 Berlin — <sup>2</sup>University of Oxford, Department of Physics, Clarendon Laboratory, Parks Road, Oxford OX1 3PU, United Kingdom — <sup>3</sup>Max-Born-Institut für Nichtlineare Optik und Kurzzeitspektroskopie, Max-Born-Str. 2A, 12489 Berlin — <sup>4</sup>Fritz-Haber-Institut der MPG, Abteilung Physikalische Chemie, Faradayweg 4-6, 14195 Berlin

Electron transfer across molecule-metal interfaces is crucial in technologically highly relevant fields as, for instance, the design of nanoscale electronic devices and solar cells. Knowledge of the impact of the molecular structure and morphology on the interfacial electron dynamics is hereby essential for the development of efficient and reliable appliances. We use time-resolved two-photon photoelectron (2PPE) spectroscopy to study the electron transfer and solvation dynamics at the NH<sub>3</sub>/Cu(111) and the D<sub>2</sub>O/Ru(001) interface. We show that (i) the electron dynamics are significantly influenced by crystallization of the adlayer, (ii) the structural reorganization results in electron lifetimes on the order of minutes, and (iii) the microscopic and structural properties of the solvent determine the energetic relaxation even on macroscopic timescales. In addition, we present the first direct observation of electron trapping in pre-existing traps and demonstrate that the remarkably long lifetimes cannot be attributed to a purely morphological transition.

O 46.3 Thu 11:00 SCH A315

**Vibrational response of D<sub>2</sub>O molecules on Ru(001) upon electron injection observed with time-resolved sum-frequency generation** — ●CHRISTIAN FRISCHKORN, JURAJ BDZOCH, JAN ZACHARIAS, and MARTIN WOLF — Fachbereich Physik, Freie Universität Berlin, Arnimallee 14, 14195 Berlin

Electrons as excess charges in polar solvents result in molecular motion within the solvent to stabilize the new charge distribution known as electron solvation. We employ time-resolved broadband-IR-VIS SFG (sum frequency generation) spectroscopy as a powerful technique to study the changes in the vibrational spectra of the D<sub>2</sub>O water layers upon electron injection from a Ru(001) surface. Unlike in time-resolved photoemission experiments where the electron binding energy is traced and the solvent response is inferred subsequently, SFG vibrational spectroscopy *directly* monitors the molecular reorientation induced by the excess charge. If the Ru surface is excited with 266-nm (4.65 eV)

photons, excess electrons injected into the adsorbate layer induce – dependent on layer morphology and layer thickness– drastic changes in the vibrational spectra of the OD stretch vibration. While in amorphous ice layers only weak changes are observed, a SFG signal increase by several orders of magnitude (enhancement factor  $\sim 10^3 - 10^4$ ) is found in crystalline D<sub>2</sub>O layers. The physical and chemical processes involved will be discussed.

O 46.4 Thu 11:15 SCH A315

**Lifetime reduction of surface states caused by impurity scattering** — ●SWANTJE HEERS, PHIVOS MAVROPOULOS, SAMIR LOUNIS, and STEFAN BLÜGEL — Institut für Festkörperforschung and Institute for Advanced Simulation, Forschungszentrum Jülich, 52425 Jülich, Germany

In order to describe the dynamics of charge transport, localization and quantum information on metal surfaces it is of crucial importance to understand the temporal evolution of quasiparticles (electrons and holes) in surface states, characterized by a lifetime  $\tau$ . This lifetime is strongly reduced by scattering at impurities, vacancies and adatoms. Using the Korringa-Kohn-Rostoker Green function method [1], the elastic scattering rate  $1/\tau$  can be calculated for adatoms as well as impurities and vacancies in and below the surface. We have performed calculations for the Cu(111) surface of finite-thickness slabs, investigating the lifetime of the Cu(111) surface state for the whole series of 3d transition metals as impurities. The thickness of the slab is varied, ranging from six to forty atomic layers. Our formalism allows us to separate the lifetime reduction induced by scattering to bulk states from scattering to surface states. We show that trends through the 3d series are qualitatively different for adatoms, compared to impurities in the surface. This work was supported by the ESF EUROCORES Programme SONS under contract N. ERAS-CT-2003-980409 and the Priority Programme SPP1153 of the DFG grant Bl 444/8-1.

[1] N. Papanikolaou, R. Zeller, P. H. Dederichs *J. Phys.: Condens. Matter* **14**, 2799 (2002).

O 46.5 Thu 11:30 SCH A315

**Mechanical Oscillations of Nanostructures** — ●RICHARD TAUBERT<sup>1</sup>, FLORIAN HUDERT<sup>2</sup>, ALBRECHT BARTELS<sup>2,3</sup>, and THOMAS DEKORSY<sup>2</sup> — <sup>1</sup>Universität Stuttgart — <sup>2</sup>Universität Konstanz — <sup>3</sup>Gigaoptics GmbH, Konstanz, Deutschland

Understanding the mechanical properties of nanostructures has been a field of large interest during the last years. We present a method to investigate the phonon dynamics in nanostructures by time-resolved optical measurements. A new technique, Asynchronous Optical Sampling (ASOPS) is used to carry out pump-probe spectroscopy. Instead of using one laser and a mechanical delay line to generate pump- and probe-beams, two separated lasers, whose repetition rates are slightly detuned by several kHz are used. This allows the measurement of mechanical oscillations with GHz line width and a signal-to-noise ratio of  $10^7$  within 100 seconds of measurement time.

Time-resolved measurements on metallic and semiconductor superlattices as well as metallic nano-triangles and nano-tetrahedrons are presented. The measurements on the superlattices clearly resolve the first-order back-folded longitudinal acoustic phonons at the zone center. Furthermore, it is possible to do precise layer thickness and superlattice-period measurements. The mechanical oscillations of metallic triangles and pyramids with different edge lengths are observed and the influence of geometry, size and substrate are investigated.

O 46.6 Thu 11:45 SCH A315

**Fano line profiles in two-photon photoemission of image-potential states on Si(100)** — ●CHRISTIAN EICKHOFF<sup>1,2</sup>, JENS KOPPRASCH<sup>1,2</sup>, CORNELIUS GAHL<sup>1</sup>, and MARTIN WEINELT<sup>1,2</sup> — <sup>1</sup>Max-

Born-Institut, Max-Born-Straße 2a, 12489 Berlin, Germany — <sup>2</sup>Freie Universität Berlin, Fachbereich Physik, Arnimallee 14, 14195 Berlin, Germany

We have studied the surface states on Si(100) by time-, energy- and angle-resolved two-photon photoemission spectroscopy. Tuning the photon energy of the pump pulse between 4.5 and 5.4 eV allows us to populate unoccupied states up to the Si(100) vacuum level. Besides the occupied dangling-bond state  $D_{up}$ , we have identified the Rydberg-like series of image-potential states. Lifetimes and binding-energies of  $n=1, 2$  and  $3$  will be presented. Significant variation of both the 2PPE peak positions and intensities were found when tuning the photon energy across the  $D_{up}$  to  $n = 1$  and  $D_{up}$  to  $n = 2$  transitions. Below resonance we observe the  $D_{up}$  initial state with the kinetic energy following the pump pulse photon energy. Above resonance the  $D_{up}$  intensity is significantly reduced and the peak position reflects the respective image-potential-state resonances. Around the resonance the lowering in energy of the expected peak position and the intensity variations can be explained by a Fano-like resonance, caused by interference between transitions from  $D_{up}$  to the discrete image-potential-state resonances and the bulk continuum in combination with the finite bandwidth of the laser pulses.

O 46.7 Thu 12:00 SCH A315

**Two-photon photoemission spectroscopy of image potential states on Ag(001): Momentum-dependent lifetimes and quantum beats** — ●MARIO KIEL, KLAUS DUNCKER, and WOLF WID-DRA — Martin-Luther Universität Halle-Wittenberg, Halle, Germany

Using a novel all-fiber based oscillator/amplifier system operating at a repetition rate of 1.5 MHz which pumps two noncollinear optical parametric amplifiers with tunable pulses ( $<30$  fs) in the range of 500-950 nm, the  $n=1, 2$  and  $3$  image potential states on Ag(001) have been investigated by time and momentum-resolved two-color two-photon photoemission spectroscopy (2PPE). Lifetimes of 55, 165 and 380 fs at  $k_{||}=0$  have been determined for these states, respectively, similar to previous work [1]. The lifetime of the  $n=1$  state reveals a quadratic momentum-dependence of the decay rate. This leads to a shortening to 26 fs at  $k_{||}=0.4 \text{ \AA}^{-1}$  which can be described by a linear 34 meV/eV decay rate increase with excess kinetic energy which is comparable to results on Cu(001) [2]. It clarifies the controversy regarding the existence of additional decay channels on Ag(001) vs. Cu(001) derived from intrinsic linewidth measurements [3].

Quantum beat spectroscopy is used to determine the energy difference between the  $n=3$  and  $4$  states to 35 meV based on the 2PPE signal oscillation with a periodicity of 118 fs.

[1] I. L. Shumay, *et al.*; PRB **58** (1998), 13974

[2] W. Berthold, *et al.*; PRL **88** (2002), 056805

[3] G. Ferrini, *et al.*; PRB **67** (2003), 235407

O 46.8 Thu 12:15 SCH A315

**Chirped-pulse two-photon photoemission from Cu(111): experiment and theory** — ●ALEXANDER FISCHER<sup>2</sup>, FELIX STEEB<sup>2</sup>, STEFAN MATHIAS<sup>2</sup>, MARTIN WIESENMEYER<sup>1</sup>, MARTIN AESCHLIMANN<sup>2</sup>, and MICHAEL BAUER<sup>1</sup> — <sup>1</sup>IEAP, Sektion Physik, Christian-Albrechts-Universität zu Kiel, 24908 Kiel — <sup>2</sup>Department of Physics and Research Center OPTIMAS, University of Kaiserslautern, 67663

In the study of ultrafast processes at surfaces using femtosecond light sources the effect of the spectral phase of the excitation pulse has been considered only in a few publications, yet [1,2]. For instance, Petek *et al.* investigated the spectral changes in the 2PPE signal from the Cu(111) Shockley surface state as induced by a controlled variation of the spectral phase of the excitation light. In this case the findings

were attributed to the specific ultrafast dynamics of the involved intermediate state and not to the chirp of the laser pulse. Here we report on an extension of these earlier studies, which considers next to the peak position further spectral signatures such as the peak FWHM and asymmetry. Additionally we develop a theoretical model, which enable us to reproduce and interpret our observations in a quantitatively very satisfactory manner. It reproduces almost perfectly the experimental observed changes in the surface state 2PPE signal for a non resonant excitation scheme under consideration of the complete spectral phase of the laser pulse, especially the interaction of GVD and TOD[3].

[1] H. Petek, *et al.*, Phys. Rev. Lett. **79** 4649 (1997) [2] M. Merschdorf, *et al.*, Phys. Rev. B **70**, 1934401 (2004) [3] M. Bauer, *et al.*, The nature of a nonlinear excitation..., New J. of Phys., in print

O 46.9 Thu 12:30 SCH A315

**Observation of Surface Plasmon Propagation with Attosecond Accuracy** — ●NIEMMA MOHAMADIE BUCKANIE<sup>1</sup>, NICOLAI RASS<sup>1</sup>, and FRANK-JOACHIM MEYER ZU HERINGDORF<sup>1,2</sup> — <sup>1</sup>Universität Duisburg-Essen, Institut für Experimentelle Physik, Lotharstraße 1, 47057 Duisburg — <sup>2</sup>Center for Nano Integration Duisburg-Essen (CeNIDE), 47057 Duisburg

Surface Plasmon Polaritons (SPP) are collective oscillations of the electron gas in metallic systems that propagate along nano-particle surfaces. SPPs can be imaged by Photoemission Electron Microscopy (PEEM), using ultra short femtosecond laser pulses [1]. For the observation of the SPP wave propagation, time resolved techniques, i.e., pump-probe techniques must be applied, where delay times of attosecond accuracy between the pump and the probe pulse are required. The necessary interferometer to generate the time delay must then be stable in the attosecond time regime for the duration of the experiments, i.e., over several hours. To achieve these requirements, we designed and built an actively stabilized Mach-Zehnder-Interferometer (MZI) that has the ability to control time delays between the pump and the probe pulse in the attosecond time regime and that has a long-time stability of 15 as. With this MZI the SPP propagation in Ag islands on Si(111) is directly observed.

[1] L.I. Chelaru and F.-J. Meyer zu Heringdorf, *Surf. Sci.* **601** (2007) 4541–4545

O 46.10 Thu 12:45 SCH A315

**Correlated positron-electron emission from surfaces** — ●FRANK O. SCHUMANN, GRANT VAN RIESSEN, MICHAEL BIRKE, CARSTEN WINKLER, and JÜRGEN KIRSCHNER — Max-Planck Institut für Mikrostrukturphysik, Weinberg 2, 06120 Halle

Electrons in a solid do not move independent from each other. The Pauli principle demands that two electrons with parallel spins can not be at the same location. The Coulomb interaction makes it energetically unfavorable for electrons to be close to each other. This constitutes the concept of the exchange-correlation (xc) hole. Our electron pair emission studies demonstrate that this concept is an experimental reality. In these experiments a primary electron or photon hits a surface and emits an electron pair. In order to disentangle the different contributions to the xc-hole, one should use as primary particle a positron and study the positron-electron pair emission. In this case one does not need to consider the Pauli principle. Because of this motivation we performed the first experiment, which demonstrates that the impact of a positron causes indeed the emission of a positron-electron pair. We used the NEPOMUC facility together with a pair of hemispherical analyzers operated with a coincidence circuit. As target we selected a LiF(100) surface, which was hit with 85 eV primary positrons. We find that the emission of positron-electron pairs is time correlated.

## O 47: Methods: Scanning probe techniques II

Time: Thursday 10:30–12:30

Location: SCH A316

O 47.1 Thu 10:30 SCH A316

**Investigation of Locally Stored Charges in Silica by Kelvin Probe Force Microscopy** — ●CARSTEN MAEDLER, HARALD GRAAF, and CHRISTIAN VON BORCZYKOWSKI — Center of Nanostructured Materials and Analytics, Chemnitz University of Technology, D-09107 Chemnitz, Germany

The storage and dissipation of positive and negative charges in thin

silicon oxide films were studied in a local manner using Kelvin Probe Force Microscopy. The charges were injected into the oxide by applying a voltage between an electric conductive tip and the silicon beneath the oxide while the tip was in close proximity to the silicon oxide surface. The method used for investigation of the charges, Kelvin Probe Force Microscopy allows the simultaneous imaging of the electrical and topographical properties of a surface. Various patterns were created, where

the smallest achieved structures were about 100 nm wide. Because silanol groups are supposed to be the main trapping site for charges we studied the charging properties of silica with various pre-treatment and thus different amounts of silanol groups. A different approach is to passivate the surface with hydrophobic monolayers. We achieved a considerable decrease in charge spreading by the attachment of a layer of Octadecyltrichlorosilane forming a hydrophobic monolayer on the silica surface.

O 47.2 Thu 10:45 SCH A316

**Towards a quantitative tunneling spectroscopy: Using differential barrier heights for a deconvolution of the tip and sample density of states** — ●HOLGER PFEIFER, BERNDT KOSLOWSKI, ANNA TSCHETSCHETKIN, and PAUL ZIEMANN — Institut für Festkörperphysik, Universität Ulm, D-89069 Ulm, Germany

Based on the recently developed method for recovering the electronic density of states (DOS) from scanning tunneling spectroscopy (STS) data [1], we analytically calculate the differential barrier ( $\partial_z \partial_V I$ ) for an energy-dependent DOS of either the sample or the tip. It turns out that (i) considering a peaked DOS the sign of the peak reveals whether this peak belongs to the sample or the tip, and (ii) the formula for the differential barrier can be rewritten to form an additional Volterra integral equation of the second kind for both the DOS of sample and tip, respectively. Additionally to the equations obtained earlier from the differential conductivity ( $\partial_V I$ ), these equations can be exploited by using the Neumann approximation to optimize iteratively the recovered DOS' being then self-consistent with the WKB approximation and measured data ( $I$ ,  $\partial_V I$ , and  $\partial_z \partial_V I$ ). By comparing these results with experimental data obtained on Nb(110) we analyze how far the proposed scheme enables deconvolution of the DOS' of sample and tip.

[1] B. Koslowski, Ch. Dietrich, A. Tschetschetkin, P. Ziemann, Phys. Rev B 75, 035421 (2007)

O 47.3 Thu 11:00 SCH A316

**Dynamic Force Microscopy with Small Amplitudes at Ambient Conditions** — ●ELISABETH KÖSTNER and FRANZ J. GIESSIBL — Institut für Experimentelle und Angewandte Physik, Universität Regensburg, 93040 Regensburg

Yamada et al. [1] have shown that it is possible to obtain atomic resolution on cleaved mica in water with frequency-modulation force microscopy. These impressive results have been acquired with a very sophisticated setup. This setup enabled them to get a very low deflection noise density, which is decisive for atomic resolution in their measurement scheme.

In our case we tried to image surfaces at ambient conditions with quartz tuning fork based cantilevers. We tried to simplify our setup by using stiff cantilevers (spring constant of some thousand N/m) with small amplitudes (some nanometers) and—most importantly—a higher Q factor. Some first results made in amplitude-modulation force microscopy mode with this setup are presented showing atomic resolution on graphite in air.

[1] T. Fukuma, K. Kobayashi, K. Matsushige, and H. Yamada, Appl. Phys. Lett. 87, 034101 (2005)

O 47.4 Thu 11:15 SCH A316

**Structural investigations of membrane electrode assemblies (MEA) in fuel cells via environmental scanning electron microscopy (ESEM)** — ●SUSANNE ZILS<sup>1</sup>, NATHALIE BENKER<sup>2</sup>, and CHRISTINA ROTH<sup>1</sup> — <sup>1</sup>Institute for Materials Science, TU Darmstadt, Petersenstr. 23, 64287 Darmstadt, Germany — <sup>2</sup>Institute of Applied Geosciences, TU Darmstadt, Schnittspahnstraße 9, 64287 Darmstadt, Germany

Detailed studies to investigate the contact between the ion- and electron-conducting parts of a MEA of a polymer electrolyte membrane fuel cell (PEMFC) have only been performed by SEM and TEM up to now. These methods exclude the investigation of MEAs under realistic conditions. To obtain significant information of the structure under quasi in-situ conditions ESEM is used in this work. This technique allows for studying the MEAs under different temperatures as well as under different relative humidities.

The ESEM measurements were carried out with a Quanta 200F (FEI company, Netherlands) equipped with a field emission gun and an energy dispersive X-ray detector for elemental analysis.

During the experiments, relative humidities between 5% and 100% at defined temperatures have been adjusted. Images and movies have been recorded to investigate structural changes in the electrodes as well as on the interface between the polymer electrolyte membrane and the

electrodes. Further experiments shall allow us to investigate the influence of ice formation on the electrode structure and the membrane electrode interface.

O 47.5 Thu 11:30 SCH A316

**Distance and material dependence of the near-field thermal heat transfer** — ●ROBERT BERGANSKI, ACHIM KITTEL, and ULI F. WISCHNATH — Energy and Semiconductor Research Laboratory - University of Oldenburg

The heat transfer between the probe and the sample is measured by means of a Near-field Scanning Thermal Microscope (NSThM) which is based on a commercial scanning tunneling microscope. In our setup the standard STM-Probe is replaced by a miniaturized coaxial thermocouple, which records the change in the temperature at the tip. Thus the heat transfer can be measured while the distance between the probe and the sample surface will be varied by a few tens nanometers. The investigated heat transfer relies on evanescent modes of the thermal transfer between the tip at room temperature and the sample at about 110K. All other interfering distant dependent heat transfer mechanisms are excluded by using ultra high vacuum conditions. In the present contribution the focus lies on the material dependence of these evanescent modes which are reaching a few nanometers into the vacuum. The influence of the dielectric properties of the sample material on the heat transfer is studied by varying the material of the sample surface.

O 47.6 Thu 11:45 SCH A316

**Transport of product gases in a scanning mass spectrometer setup** — ●MATTHIAS ROOS<sup>1</sup>, DAN ZHANG<sup>2</sup>, JOACHIM BANSMANN<sup>1</sup>, OLAF DEUTSCHMANN<sup>2</sup>, and R. JÜRGEN BEHM<sup>1</sup> — <sup>1</sup>Institute of Surface Chemistry and Catalysis, Ulm University, D-89069 Ulm — <sup>2</sup>Institute for Chemical Technology and Polymer Chemistry, University of Karlsruhe, D-76131 Karlsruhe

The transport and distribution of reaction products above microstructured catalytically active samples was studied by spatially resolved scanning mass spectrometry and by combined Monte Carlo simulations and Fluid Dynamics calculations. For CO oxidation on planar Pt microstructures, the spatial distribution of CO<sub>2</sub> product gas was probed via a thin quartz capillary, which leads the gases to a quadrupole mass spectrometer. To obtain reasonable lateral resolution, the capillary orifice was located a few micrometers above the sample surface during measurement. In this geometry, shadowing by the capillary results in a local reduction of the reactant partial pressures underneath the capillary. To quantitatively analyse the reaction rates, the three-dimensional distribution of CO<sub>2</sub> product gas was modeled, considering the flow of educt gases, and their local variation of the pressure and the gas temperature.

O 47.7 Thu 12:00 SCH A316

**HarmoniX microscopy: A new scanning probe microscopy technique for high resolution mapping of material properties** — ●UDO VOLZ — Veeco Instruments GmbH Dynamostraße 19 D-68165 Mannheim

HarmoniX microscopy is a brand new mode of Scanning Probe Microscopy which provides fast and high resolution nanoscale mapping of material properties such as elasticity, adhesion, and dissipation. HarmoniX imaging utilizes special Tapping Mode probes that are designed for high bandwidth measurements of the forces acting on the probe tip. The variation in tip-sample forces during one period of the tapping oscillation is reconstructed by analyzing the full spectrum of motion of the probe. From the measured force-distance curves the material properties of the sample are then determined independently for each pixel of the image. HarmoniX microscopy is working at typical Tapping Mode imaging speeds and is thus hundreds of times faster than other quantitative material mapping techniques such as force volume imaging, but it retains the high resolution, non-destructive qualities of Tapping Mode Imaging.

O 47.8 Thu 12:15 SCH A316

**Nanometer Resolution of Materials Properties with Scanning Microwave Microscopy** — ●MATTHIAS FENNER, WENHAI HAN, and HASSAN TANBAKUCHI — Agilent Technologies, 61476 Kronberg, Germany

Advances in scanning probe microscopy have led to the introduction of new tools for local characterization of surfaces and materials at the nanoscale, beyond basic topography and structure. We are proposing a

new technique that was realized by combining Agilent's core competencies in the interdisciplinary fields of electronic test and measurement, nanotechnology, and life sciences. This new scanning microwave microscopy (SMM) platform enables the simultaneous measurements of AFM data and traditional microwave network analysis. SMM measures the electrical properties of a material (i.e. dielectric properties,

capacitance, and complex impedance), providing researchers in polymer science, semiconductors, and bioscience a new analytical tool for advancing research. This presentation will review our SMM implementation and an explanation of the technical challenges in developing this new technology. We will show the latest results followed by potential benefits this new technology might bring other scientific disciplines.

## O 48: Focused Session: Spin-Orbit Interaction at Surfaces: From the Rashba Effect to Topological States of Matter I

Time: Thursday 10:30–13:00

Location: HSZ 02

**Topical Talk** O 48.1 Thu 10:30 HSZ 02  
**The Rashba and quantum size effects in ultrathin Bi films** — ●TORU HIRAHARA — Department of Physics, University of Tokyo, Japan

Semimetal bismuth (Bi) is one of the most extensively studied elements in solid state because of its extreme physical properties. For example, Bi has been employed to examine the quantum size effect (QSE) in thin films or nanowires due to its extraordinary large Fermi wavelength. An oscillation in the conductivity or the Hall coefficient with film thickness due to the QSE was predicted theoretically [1]. Furthermore since Bi is a very heavy element, spin-orbit coupling (SOC) effects play a dominant role in the electronic and transport properties, which can be found in the large atomic splitting (1.5 eV), or the anti-localization behavior in magnetotransport measurements [2].

When the system downsizes to the nanometer scale, it can be expected that the contributions from the surface states will make the system more intriguing. In this talk, I will present our recent results obtained for a well-defined ultrathin Bi film [3] utilizing the state-of-art spin- and angle- resolved photoemission spectroscopy, first-principles calculations, and surface-sensitive conductivity measurements. Particular focus will be given on the QSE and SOC effect at the surface (Rashba effect).

[1] V. B. Sandomirskii, Sov. Phys. JETP 25, 101(1967). [2] F. Komori et al., 52, 368(1983). [3] T. Nagao et al., Phys. Rev. Lett. 93, 105501 (2004).

**Topical Talk** O 48.2 Thu 11:00 HSZ 02  
**Giant Spin-Splitting on Metallic and Semiconducting Surfaces** — ●CHRISTIAN R. AST — Max-Planck-Institut für Festkörperforschung, Stuttgart, Germany

One of the goals in the emerging field of spintronics is to manipulate the electron spin without the use of magnetic fields. This can be achieved at surfaces and interfaces where the inversion symmetry is broken so that a strong spin-orbit interaction can lift the spin-degeneracy (Rashba-Bychkov Model). Such a spin-splitting can further be enhanced by additional contributions from an in-plane inversion asymmetry as has been found for the Bi/Ag(111) surface alloy. The observed spin-splitting in this system is more than an order of magnitude stronger than in the Au(111) surface state. This introduces a new component in the mechanism of the Rashba-type spin-splitting. The strength of the splitting can be tuned by mixing different elements in the surface alloy. In particular, this concept can be transferred onto a semiconducting substrate in order to make it more interesting for the broad field of spintronics.

**Topical Talk** O 48.3 Thu 11:30 HSZ 02  
**Exploring the Rashba spin-orbit splitting by *ab initio* theory** — ●GUSTAV BIHLMAYER — Institut für Festkörperforschung & Institute for Advanced Simulation, Forschungszentrum Jülich, 52425 Jülich

Since the discovery of a Rashba-type spin-orbit splitting of the surface state of Au(111), many new manifestations of this effect have been discovered, e.g. on surfaces of magnetic or semimetallic elements, in surface alloys and even in quantum-well states of thin metallic films. These systems offer the possibility to study phenomena beyond the usual Rashba-type effect, leading to splittings that are no longer linear in the momentum and show complex spin-orientation patterns in surface states [1]. We also observe unconventional Fermi surface topologies [2], and will discuss new ways to tune the effect to meet specific requirements [3]. Employing first-principles calculations, the origin of these intriguing phenomena will be analyzed. In particular, I will focus on the appearance of a spin-splitting in thin Bi [4] and Pb films, which offers a view on the shape of the wavefunction of the surface-

and quantum-well states in these films.

[1] G. Bihlmayer, E. V. Chulkov, and S. Blügel, Phys. Rev. B **75**, 195414 (2007)

[2] O. Krupin, G. Bihlmayer, K. Starke, S. Gorovikov et al., Phys. Rev. B **71**, 201403 (R) (2005)

[3] Yu. M. Koroteev, G. Bihlmayer, E. V. Chulkov, and S. Blügel, Phys. Rev. B **77**, 045428 (2008)

[4] T. Hirahara, T. Nagao, I. Matsuda, G. Bihlmayer et al., Phys. Rev. Lett. **97**, 146803 (2006)

O 48.4 Thu 12:00 HSZ 02  
**Giant Rashba spin-orbit splitting in the unoccupied quantum-well band-structure of Bi/Cu(111)** — ●M. AESCHLIMANN<sup>1</sup>, S. MATHIAS<sup>1</sup>, A. RUFFING<sup>1</sup>, F. DEICKE<sup>1</sup>, M. WIENMAYER<sup>2</sup>, G. BIHLMAYER<sup>3</sup>, E.V. CHULKOV<sup>4,5</sup>, YU.M. KOROTEEV<sup>4,6</sup>, and M. BAUER<sup>2</sup> — <sup>1</sup>Department of Physics and Research Center OPTIMAS, University of Kaiserslautern, 67663 Kaiserslautern, Germany — <sup>2</sup>IEAP, Christian-Albrechts-Universität zu Kiel, 24908 Kiel, Germany — <sup>3</sup>FZ Jülich, 52425 Jülich, Germany — <sup>4</sup>DIPC, 20018 San Sebastián/Donostia, Spain — <sup>5</sup>Departamento de Física de Materiales, UPV/EHU, Apdo 1072, 20080 San Sebastián, Spain — <sup>6</sup>Institute of Strength Physics and Materials Science, RAS, 634021, Tomsk, Russia

The unoccupied electronic structure of the Bi surfactant layer (0.5 ML coverage) on Cu(111) is investigated by angle-resolved two-photon photoemission (AR-2PPE). An unoccupied quantum-well state is observed exhibiting a large spin-orbit splitted band with a Rashba energy of  $E_R \simeq 134$  meV and a wave number offset of  $k=0.09$  1/Å. This enhancement of the spin splitting is surprisingly high given the fact that the ultrathin Bi film on Cu(111) does not show surface alloying. We therefore carried out first principle calculations to unravel the origin of the large spin-splitting, potentially caused by corrugation or the influence of the interface potential onto the ultrathin Bi film, giving rise to a quantum-size induced giant spin-orbit splitting. Such a scenario would directly allow for another possibility to tailor spin-orbit splitting (next to surface alloying) by means of thin film nanofabrication.

O 48.5 Thu 12:15 HSZ 02  
**Electronic Structure of the Bi/Cu(111) surface alloy and its modification upon Na adsorption** — ●HENDRIK BENTMANN<sup>1</sup>, HOLGER SCHWAB<sup>1</sup>, FRANK FORSTER<sup>1</sup>, GUSTAV BIHLMAYER<sup>2</sup>, LUCA MORESCHINI<sup>3</sup>, MARCO GRIONI<sup>3</sup>, and FRIEDRICH REINERT<sup>1,4</sup> — <sup>1</sup>Universität Würzburg, Experimentelle Physik II, Am Hubland, D-97074 Würzburg, Germany — <sup>2</sup>Institut für Festkörperforschung, Forschungszentrum Jülich, D-52425 Jülich, Germany — <sup>3</sup>Ecole Polytechnique Fédérale de Lausanne (EPFL), Institut de Physique des Nanostructures, CH-1015 Lausanne, Switzerland — <sup>4</sup>Forschungszentrum Karlsruhe, Gemeinschaftslabor für Nanoanalytik, D-76021 Karlsruhe, Germany

Employing angle-resolved photoelectron spectroscopy (ARPES) we have investigated the electronic structure of the long-range ordered surface alloy Bi-Cu(111)( $\sqrt{3} \times \sqrt{3}$ )R30° and its modification after Na adsorption. On the clean alloy we observe a spin-split surface state band with an energy maximum approximately 230 meV above the Fermi level. By doping the surface alloy with Na we are able to tune the position of Fermi level relative to the surface state continuously. Our data provides direct information about electronic states above the Fermi level. This allows for an unambiguous deduction of the surface electronic structure and the Rashba parameters. The experimental findings are fully confirmed by first principles calculations.

O 48.6 Thu 12:30 HSZ 02

**Rashba effect in unoccupied states: Two-photon photoemission experiments and first-principles calculations for Bi/Cu(111)** — PING YU, CHENG-TIEN CHIANG, AIMO WINKELMANN, HOSSEIN MIRHOSSEINI, ARTHUR ERNST, SERGEY OSTANIN, •JÜRGEN HENK, and JÜRGEN KIRSCHNER — Max Planck Institute of Microstructure Physics, Halle, Germany

Surface alloys of Bi and noble metals on fcc(111) surfaces exhibit Rashba-split occupied  $sp_z$  surface states which have been thoroughly investigated by photoemission experiments and electronic-structure calculations. Their unmatched splitting is attributed to the interplay between an in-plane potential gradient and the conventional out-of-plane image-potential gradient. However, the splitting of a set of  $p_x p_y$  surface states remained unresolved so far because these unoccupied states cannot be accessed by conventional photoemission.

By angle-resolved two-photon photoemission experiments and first-principles calculations we study in detail the unoccupied  $p_x p_y$  states on  $\sqrt{3} \times \sqrt{3}R30^\circ$ -Bi/Cu(111). Their experimental dispersion in the relevant energy range, band maxima (at  $E_F + 1.4$  eV), and momentum offset ( $0.03 \text{ \AA}^{-1}$ ) agree with the theoretical predictions. Due to their symmetry, these states are expected to be particularly respon-

sive to an in-plane gradient. The abovementioned mechanism and its implications on dispersion and spin polarization are discussed.

O 48.7 Thu 12:45 HSZ 02

**Unconventional Fermi surface spin patterns in the (Bi/Pb/Sb)/Ag(111) surface alloy** — •FABIAN MEIER<sup>1,2</sup>, VLADIMIR PETROV<sup>3</sup>, LUC PATTHEY<sup>2</sup>, JÜRIG OSTERWALDER<sup>1</sup>, and HUGO DILL<sup>1,2</sup> — <sup>1</sup>Physik Institut Universität Zürich, CH — <sup>2</sup>Swiss Light Source PSI, CH — <sup>3</sup>Physics Institute St Petersburg, RU

By a controllable change in the stoichiometry of the long range ordered mixed surface alloy (Bi/Pb/Sb)/Ag(111) the Rashba and Fermi energy can be tuned over a wide range. We show by spin and angle-resolved photoemission spectroscopy that the spin structure of the individual surface state bands remain unaffected despite the random intermixing of the adatoms. We further report on the observation of unconventional Fermi surface spin textures. These spin textures are found when the Fermi energy lies between the crossing point and the apex of the Rashba type Kramer's pair. The results will be discussed in the context of spin transport.

## O 49: Ab-initio approaches to excitations in condensed matter II

Time: Thursday 10:30–13:30

Location: SCH 251

O 49.1 Thu 10:30 SCH 251

**Effects of electron-phonon interaction beyond mean-field approximation in the non-adiabatic dynamics of photo-excited short polyacetylene chains** — •LORENZO STELLA — London Centre for Nanotechnology, London, United Kingdom — University College London, London, United Kingdom

Conjugated polymers, of which polyacetylene is the simplest example, combine good mechanical and electronic properties that may be exploited in future technological applications. To this end, a proper description of photo-generation of charged and neutral excitations is crucial. In particular, if quantum vibrational modes (phonons) can be excited, the adiabatic approximation is no longer applicable and this will affect the transfer of energy from the electronic excitations. I show here that neglecting quantum fluctuations of atoms can lead to a qualitatively wrong account of the relaxation dynamics of photo-excited short polyacetylene chains. Indeed, even at zero temperature, quantum fluctuations of the molecular degrees of freedom can trigger the decay of an excited electronic state, through spontaneous emission of phonons: within a mean-field approach, such a process cannot be described at all. A proper study of this quantum phenomenon is given here by an improved version of Correlated Electron-Ion Dynamics (CEID) which includes quantum fluctuations of atoms about their mean-field trajectories in a converging perturbative way. This method is stable, efficient and provides a smooth evolution for both electronic and molecular degrees of freedom. Implications of the obtained results on the efficiency of conjugated polymer devices are also discussed.

O 49.2 Thu 10:45 SCH 251

**Fully relativistic one-step theory of photoemission: chemical disorder and correlation** — •JAN MINAR, JURGEN BRAUN, and HUBERT EBERT — Dep. Chemie und Biochemie, LMU München, Germany

We present a generalized version of the fully relativistic one-step model of photoemission, which takes into account chemical disorder and electronic correlation on an equal footing. The electronic structure input is calculated within the Coherent Potential Approximation (CPA) alloy theory. The spectroscopic analysis itself is based on the configurationally averaged photocurrent first proposed by [1]. Both, electronic structure and photoemission calculations have been performed by use of the upgraded version of the Munich SPR-KKR program package [2]. The formalism is applicable to arbitrary two-dimensional systems and photon energies ranging from the ultraviolet to the hard X-ray regime. Strong electronic correlations are treated by the LSDA-DMFT approach, selfconsistently implemented in the SPR-KKR program. Here, we discuss spectroscopic data from binary intermetallic  $\text{Ni}_x\text{Pd}_{1-x}$ ,  $\text{Ag}_x\text{Au}_{1-x}$  and ternary Heusler  $\text{Co}_2\text{Mn}_{1-x}\text{Fe}_x\text{Si}$  and  $\text{Co}_2\text{Cr}_{1-x}\text{Fe}_x\text{Al}$  alloys as function of the concentration  $x$ .

1. P. J. Durham, J. Phys. F: Met. Phys. **11** 2475 (1981).
2. H. Ebert et al., The munich SPR-KKR package, version 3.6,

<http://olymp.cup.uni-muenchen.de/ak/ebert/SPRKKR> (2008).

O 49.3 Thu 11:00 SCH 251

**Transforming Nonlocality into a Frequency Dependence: A Shortcut to Spectroscopy** — •MATTEO GATTI<sup>1,2,3</sup>, VALERIO OLEVANO<sup>1,4</sup>, ILYA TOKATLY<sup>1,3</sup>, and LUCIA REINING<sup>1,2</sup> — <sup>1</sup>European Theoretical Spectroscopy Facility (ETSF) — <sup>2</sup>LSI - Ecole Polytechnique, Palaiseau, France — <sup>3</sup>Universidad del País Vasco, San Sebastian, Spain — <sup>4</sup>Institut Néel, Grenoble, France

Measurable spectra are often derived from contractions of many-body Green's functions. In this way, one calculates hence more information than needed. Here we present and illustrate an in principle exact approach to construct effective potentials and kernels for the direct calculation of electronic spectra. In particular, a dynamical but local and real potential yields the spectral function needed to describe photoemission. We discuss for model solids the frequency dependence of this photoemission potential stemming from the nonlocality of the corresponding self-energy. We also show that our approach leads to a very short derivation of a kernel of time-dependent (current-)density functional theory that is known to well describe absorption and energy-loss spectra of a wide range of materials.

O 49.4 Thu 11:15 SCH 251

**Kohn-Sham scheme for frequency dependent linear response** — •RYAN REQUIST and OLEG PANKRATOV — Lehrstuhl für Theoretische Festkörperphysik, Universität Erlangen-Nürnberg

Due to the so-called causality paradox, the Kohn-Sham scheme in time dependent density functional theory cannot be derived from a stationary principle of the form  $\delta A/\delta n = 0$ , where  $A[n]$  is the density functional for the quantum mechanical action. As Vignale has recently shown [1], the density-functional formulation of the action principle contains boundary terms. Therefore, the exact exchange-correlation potential cannot be calculated from the functional derivative of a universal functional. However, we find that the second-order quasienergy,  $K_v^{(2)}$ , satisfies a stationary principle  $\delta K_v^{(2)}/\delta n_\omega^{(1)} = 0$ , where  $n_\omega^{(1)}$  is the linear response density induced by a harmonic perturbation with frequency  $\omega$ . This is not inconsistent with Vignale's result because boundary terms vanish in this case. The stationary principle can serve as a basis for the linear response Kohn-Sham scheme. The first-order exchange-correlation potential  $v_{xc}^{(1)}$  is the functional derivative of the exchange-correlation part of  $K_v^{(2)}$ . With the same approach, we also find a stationary principle and linear response Kohn-Sham scheme in the time dependent extension of reduced density matrix functional theory, in which the basic variable is the one-body reduced density matrix.

- [1] G. Vignale, Phys. Rev. A, **77**, 062511 (2008).

O 49.5 Thu 11:30 SCH 251

**Time-dependent density functional study of  $S_1 \leftarrow S_0$  tran-**

sition of 2,3-benzofluorene — ●DAVOUD POULADSASZ<sup>1</sup>, GAEL ROUILLE<sup>2</sup>, FRIEDRICH HUISKEN<sup>2</sup>, MICHAEL SCHREIBER<sup>1</sup>, and REINHARD SCHOLZ<sup>3</sup> — <sup>1</sup>Institut für Physik, Technische Universität Chemnitz — <sup>2</sup>Labor Astrophysik, Friedrich-Schiller-Universität Jena — <sup>3</sup>Walter Schottky Institut, Technische Universität München

We have recently studied the  $S_1(^1A')$  ←  $S_0(^1A')$  absorption spectrum of 2,3-benzofluorene (Bzf) [1]; the potential energy surfaces of the  $S_n = 0, 1, 2$  states of Bzf have been investigated with calculations based on the time-dependent density functional theory (TD-DFT). At the B3LYP/TZ level of theory, TD-DFT does not deliver a realistic difference between the excited  $S_1$  and  $S_2$  potential energy surfaces, a problem which can be avoided by introducing a reference geometry where this difference coincides with the observation. In this geometry, an expression for the Herzberg-Teller corrected intensities of the vibronic bands is proposed, allowing a straightforward assignment of the observed  $a'$  modes below 900  $\text{cm}^{-1}$ , including realistic calculated intensities. For vibronic bands at higher energies, the agreement between calculated and observed modes is deteriorated by substantial Dushinsky rotations and nonparabolicities of the potential energy surface  $S_1$ . We consider our calculations to be the best approach to an ab initio study realized for Bzf until now since only parametrized force fields had been used before.

[1] A. Staicu, G. Rouillé, Th. Henning, F. Huisken, D. Pouladsasz, and R. Scholz, J. Chem. Phys. **129**, 074302 (2008)

O 49.6 Thu 11:45 SCH 251

**Ab-initio Study of the Electronic and Optical Properties of MnO, FeO, CoO, and NiO** — ●CLAUDIA RÖDL, FRANK FUCHS, JÜRGEN FURTHMÜLLER, and FRIEDHELM BECHSTEDT — Institut für Festkörpertheorie und -optik, Friedrich-Schiller-Universität Jena, Max-Wien-Platz 1, 07743 Jena, Germany

Although the electronic properties of MnO, FeO, CoO, and NiO have been studied for decades, the description of the one-particle excitation spectrum of these materials remains a challenge. Quasiparticle calculations using a perturbative treatment of Hedin's *GW* approximation based on (semi)local approaches to exchange and correlation in the subjacent density-functional calculation fail to reproduce the experimental photoemission spectra.

For this reason, we use the non-local HSE03 exchange-correlation functional to obtain a reasonable starting point for a quasiparticle calculation within first-order perturbation theory and compare to results obtained within the computationally less expensive *GGA+U* scheme. The respective value for the on-site interaction  $U$  is determined by a fit to the more sophisticated HSE03+ $G_0W_0$  band structure.

Furthermore, we examine the optical properties of these materials. Accounting for their antiferromagnetic ordering, we solve the spin-polarized Bethe-Salpeter equation (BSE) and calculate optical absorption spectra including excitonic and local-field effects.

O 49.7 Thu 12:00 SCH 251

**Influence of free carrier absorption on the optical spectrum of ZnO** — ●ANDRÉ SCHLEIFE<sup>1,2</sup>, EMMANOUIL KIOUPAKIS<sup>2</sup>, PATRICK RINKE<sup>2</sup>, CLAUDIA RÖDL<sup>1</sup>, FRANK FUCHS<sup>1</sup>, CHRIS G. VAN DE WALLE<sup>2</sup>, and FRIEDHELM BECHSTEDT<sup>1</sup> — <sup>1</sup>Institut für Festkörpertheorie und -optik, Jena, Germany — <sup>2</sup>Materials Department, University of California, Santa Barbara, USA

For optoelectronic devices such as light emitting or laser diodes as well as solar cells an important aspect is the availability and controllability of transparent conducting materials. Zinc oxide as a transparent conducting oxide is strongly in the focus of scientific interest.

In this ab-initio study we investigate the impact of electrons in conduction bands on the optical properties. By employing density functional theory within a generalized-gradient approximation and making use of the projector-augmented wave method, we compute all-electron wave functions. They allow the calculation of optical transition matrix elements. We explicitly elucidate the Burstein-Moss shift due to the occupancy of conduction bands as well as the absorption caused by conduction-conduction band transitions on the level of the random-phase approximation within the independent quasiparticle approximation. Both effects are analyzed regarding their dependence on the free carrier concentration.

Consequences for the transparency of zinc oxide will be discussed including the dependence on the free carrier concentration.

O 49.8 Thu 12:15 SCH 251

**Tailoring High-Order Harmonics: A Computational Approach Based on Time-Dependent Density-Functional The-**

**ory** — ●ALBERTO CASTRO<sup>1</sup>, ALI AKBARI<sup>2</sup>, ANGEL RUBIO<sup>2</sup>, and EBERHARD GROSS<sup>1</sup> — <sup>1</sup>Freie Universität Berlin, Berlin, Germany — <sup>2</sup>University of the Basque Country, San Sebastián, España

Atoms and molecules react in complex manners when they are irradiated with high-intensity electromagnetic pulses: multi-photon, tunnelling and over-the-barrier ionisation, laser driven photo-induced isomerisations or fragmentations, and high harmonic generation are some of the non-linear effects that are observed. The so-called pulse shaping techniques can be used to design pulses that produce a desired effect. A technologically appealing possibility is to tailor the harmonic emission spectrum: enhancement of some given orders, suppressions of others, etc. We have undertaken the task of exploring this possibility from a theoretical point of view, by making use of time-dependent density-functional theory to describe the electrons, a real-space numerical representation, and various optimization techniques.

O 49.9 Thu 12:30 SCH 251

**Optical properties of molecular crystals: Periodicity meets molecular deformation patterns** — ●REINHARD SCHOLZ and LINUS GISSLEN — Walter Schottky Institut, Technische Universität München, Am Coulombwall 3, 85748 Garching, Germany

In the calculation of the dielectric properties of molecular pigments, one has to reconcile the deformation of an excited molecule with the periodicity of the crystal. For a set of six perylene-based chromophores, we demonstrate that the excited geometry can be obtained most reliably when applying DFT to a modified occupation of the frontier orbitals, whereas the deformations obtained in TD-DFT remain systematically too small. In the crystalline state, electron and hole transfer mix neutral molecular excitations with charge transfer (CT) states, and as the largest transfer parameters occur along the stacking direction, they can easily be determined by *ab initio* calculations of a stacked dimer. The transition dipoles of molecular excitations and CT states can be derived from TD-DFT applied to a stacked dimer. These DFT-based calculations leave two essential parameters of the system undetermined: The transfer of a neutral excitation to its neighbours, and the energetic difference between neutral excitations and CT states. Albeit estimates for these quantities can be obtained from *ab initio* schemes, they are most precisely obtained from an exciton model accounting for the mixing of neutral molecular excitations and CT states, together with the deformation patterns of excited and charged molecular states. From the calculated lineshapes, one can derive quite precise energies of the CT states, a key parameter for device applications.

O 49.10 Thu 12:45 SCH 251

**The multiconfigurational time-dependent Hartree-Fock method for excited states: Theory and application to conjugated polymers** — ●RAFAEL P. MIRANDA<sup>1</sup>, ANDREW P. HORSFIELD<sup>2</sup>, and ANDREW J. FISHER<sup>1</sup> — <sup>1</sup>Department of Physics and Astronomy, University College London, London, United Kingdom — <sup>2</sup>Department of Materials, Imperial College London, London, United Kingdom

The solution of the time-dependent Schrödinger equation for systems of interacting electrons is generally a prohibitive task, for which approximate methods are highly desirable. One of the simplest schemes, known as the time-dependent Hartree-Fock (TDHF) approximation, consists in restricting the electronic wavefunction to a single Slater determinant. However, several physical processes of interest involve excited states which can not be properly described by a single determinant. For instance, in a photoexcitation process, absorption of a photon creates an open-shell singlet state, and thus devising a scheme which retains the proper spin symmetry requires two Slater determinants. In this work, we extend the TDHF method to such multiconfigurational states. Based on a time-dependent variational principle, we derive the optimal equations of motion for the single-particle molecular orbitals. This method, together with a classical description of the ionic degrees of freedom (mean-field approximation), is then applied to study the dynamics of photoexcitations in conjugated polymers. We show the relaxation of electron-hole pairs to form excitons and charged polarons, and discuss the modifications to the relaxation process predicted by the inclusion of the Coulomb interaction between the carriers.

O 49.11 Thu 13:00 SCH 251

**Reduction of the number of orbital products and computation of molecular spectra from the Gross-Petersilka-Grabo equation** — ●DIETRICH FOERSTER and PETER KOVAL — CPMOH, Université de Bordeaux 1, 351 cours de la Libération, 33405 Talence, France

Electronic excitations in molecular systems live in a space of orbital products the dimension of which is too large for effective computation.

To circumvent this well known difficulty, we identify a smaller subspace of linearly independent "dominant directions" that span the original space of products with exponential accuracy.

As a first application, we compute molecular spectra by solving, in this subspace of reduced dimensions, the Gross-Petersilka-Grabo equations rather than the equations of Casida.

Possible applications of our method include the study of excitons in molecular systems.

Reference: D. Foerster, "Elimination, in electronic structure calculations, of redundant orbital products", J. Chem. Phys. **128** (2008) 43108.

O 49.12 Thu 13:15 SCH 251

**Product basis set in TDDFT: molecular absorption spectra**

**within linear response.** — ●PETER KOVAL and DIETRICH FOERSTER — CPMOH, Universite de Bordeaux 1, 351 Cours de la Liberation, 33405, Talence, France

We propose a new basis set [1] and corresponding method [2] to calculate of the Kohn-Sham density response function  $\chi_0(\omega, \mathbf{r}, \mathbf{r}')$ . Computational cost of our method scales comparatively cheaply with the number of atoms  $N$ .

Here we discuss the application of our technique to the computation of molecular absorption spectra. Spectra are calculated directly in  $O(N^2)$  operations from the Gross-Petersilka-Grabo equations [3].

References:

[1] Foerster D, J. Chem. Phys. **128** 034108 (2008)

[2] Foerster D, Phys. Rev. B **72** 073106 (2005)

[3] Petersilka M, Gossmann U J and Gross E K U, Phys. Rev. Lett. **76** 1212 (1996)

## O 50: Invited Talk (Mahbube Hortamani)

Time: Thursday 14:00–14:45

Location: HSZ 02

**Invited Talk**

O 50.1 Thu 14:00 HSZ 02

**Si-based spintronics from first principles** — ●MAHBUBE HORTAMANI — Max Planck Institute of Microstructure Physics — Fritz-Haber-Institut der Max-Planck-Gesellschaft

An important step is implementation of spin-based electronic functionality in Silicon devices. Remarkable progress made during the last two years [1] gives confidence that this is within reach, although significant challenges still remain. For example Si-based magnetic materials with a transition temperature higher than room temperature do not exist yet.

Here we discuss the specific aspects associated with ferromagnetic MnSi films on the Si substrate and determine how the electronic struc-

ture and the magnetic properties of these films and Silicon conspire to render a magnetic Si-based heterojunction.

Atomic-level insight is a necessary prerequisite to understand the mechanisms of basic physical processes such as surface diffusion and epitaxial growth. These processes are probed within the framework of density functional theory. Magnetic interactions of MnSi films at finite temperature are studied by means of a Heisenberg model. We predict the formation of a thin ferromagnetic film of MnSi in B2 (cesium chloride) crystal structure on the Si(001) surface with a Curie temperature around room temperature .

[1] Ian Appelbaum, B.Q. Huang, and D.J. Monsma, Nature 447, 295 (2007)

## O 51: Surface chemical reactions I

Time: Thursday 16:15–19:15

Location: SCH A01

O 51.1 Thu 16:15 SCH A01

**Ab initio molecular dynamics simulation of electronic energy dissipation: A comparison of H/Si(001), H/Al(111), and HCl/Al(111)** — GEORG KRUGEL, MICHAEL GROTEMEYER, JAN VAN HEYS, MICHAEL LINDENBLATT, and ●ECKHARD PEHLKE — Institut für Theoretische Physik und Astrophysik, Universität Kiel, Germany

The energy transfer to solid surfaces during chemisorption and surface scattering is of considerable relevance. Energy dissipation via electron-hole pair excitation has attracted much recent interest, see e.g. [1]. To identify the electronic dissipation mechanisms, we carry through ab initio molecular dynamics simulations. The time-dependent Kohn-Sham equations of the electrons are integrated numerically, while the positions of the ions follow from Ehrenfest dynamics. The time-dependent electronic state of the system is compared to the electronic ground state at the respective frozen-in ionic positions. This yields detailed information on the electronic excitations along the trajectory. This method has been applied to chemisorption of H-atoms on Al(111), with results consistent with the time-dependent Newns-Anderson model by Mizielinski and Bird [2]. In case of H/Si(001) we find an energy transfer into electron-hole pairs after one round-trip of the atom in front of the surface comparable to H/Al(111). We explain this unexpected result on the basis of the electronic structure. In case of HCl/Al(111) we find a significant coupling of the HCl molecular vibration to electron-hole pair excitations in the Al-substrate.

[1] A.M. Wodtke *et al.*, Prog. Surf. Sci. **83**, 167 (2008).

[2] D.M. Bird *et al.*, Surf. Sci. **602**, 1212 (2008).

O 51.2 Thu 16:30 SCH A01

**Real-space investigation of high-barrier diffusion of hydrogen on Si(001)** — ●M. DÜRR<sup>1,2</sup>, C. H. SCHWALB<sup>1</sup>, and U. HÖFER<sup>1</sup> — <sup>1</sup>Fachbereich Physik und Zentrum für Materialwissenschaften, Philipps-Universität Marburg, D-35032 Marburg — <sup>2</sup>Fakultät Angewandte Naturwissenschaften, Hochschule Esslingen, D-73728 Esslingen

Due to the strong corrugation of Si(001) with its dimer row reconstruc-

tion, various diffusion channels exist already on the flat, clean surface. Among the possible processes, diffusion between two dimer rows is associated with the highest diffusion barrier; as a consequence, it has not been observed by means of standard STM experiments up to now.

To probe this high-barrier pathway in real space, we used a combination of STM and nanosecond laser heating [1,2]. STM images taken after different numbers of heating pulses represent snapshots of the surface configurations frozen at various stages of the diffusion process. In this way hydrogen diffusion associated with rates as high as  $10^8 \text{ s}^{-1}$  could be monitored with atomic resolution at 1400 K. We observe that diffusion across the dimer rows is almost as effective as diffusion along the dimer rows. The experiment thus demonstrates the importance of this high-barrier process at elevated temperatures. Considering the large Si-Si distance between the dimer rows, the observed diffusion rate is surprisingly high. It is interpreted in terms of a strong concerted movement of hydrogen and the Si lattice.

[1] M. Dürr *et al.*, Science **296**, 1838 (2002).

[2] C. H. Schwalb *et al.*, Phys. Rev. B **75**, 085439 (2007).

O 51.3 Thu 16:45 SCH A01

**STM investigations of an electron induced switching process in azobenzene-based structures** — ●JÖRG HENZL and KARINA MORGENSTERN — Universität Hannover, Institut für Festkörperphysik, Abt. Oberflächen, Appelstr. 2, 30167 Hannover

The cis- trans isomerization of azobenzene molecules in gas phase and in solution is a well studied phenomenon. But only in the recent years first studies of azobenzene molecules adsorbed on single crystal surfaces have been emerged. This system is of particular interest not only from a fundamental point of view but also because of its possible applications in nanotechnology as a molecular switch.

Here we present low temperature scanning tunnelling microscopy measurements of 4-anilino-4'-nitroazobenzene on the Au(111)-surface. Upon adsorption at 250 K the molecules form both meandering lines of single molecules which are guided by the Au(111)-herringbone re-

construction, and a chiral star-shaped structures consisting of six molecules each.

A switching process within a single molecule inside the star-shaped structures is induced by placing the tip of the scanning tunnelling microscope above one molecule and applying a bias voltage of 2.5 V. The other molecules of the star-shaped structure remain unaffected during this manipulation. This reversible and bistable switching process will be discussed in greater detail in this talk.

O 51.4 Thu 17:00 SCH A01

**Theoretical cluster studies on the catalytic sulfidation of MoO<sub>3</sub>** — ●XUERONG SHI<sup>1,2</sup>, JIANGUO WANG<sup>2</sup>, and KLAUS HERMANN<sup>1</sup> — <sup>1</sup>Theory Department, Fritz-Haber-Institut der MPG, Faradayweg 4-6, D-14195 Berlin and Sfb 546 "Transition Metal Oxide Aggregates", Berlin (Germany). — <sup>2</sup>State Key Laboratory of Coal Conversion, Institute of Coal Chemistry, Chinese Academy of Sciences, Taiyuan, Shanxi 030001, P. R. China

Sulfidation of molybdenum trioxide, MoO<sub>3</sub>, yielding local surface regions of molybdenum disulfide, MoS<sub>2</sub>, is an essential step to improve the hydrotreating activity of Mo catalysts. Therefore, theoretical studies of sulfided MoO<sub>3</sub> surfaces can contribute to an understanding of detailed reaction mechanisms at corresponding catalyst surfaces. We apply density functional theory together with large cluster models to obtain information about the behavior of oxygen and sulfur adsorbates at local sections of the MoO<sub>3</sub>(010) surface with and without oxygen vacancies. In all cases, adsorbed oxygen is found to bind more strongly with the substrate than sulfur with binding distances that are shorter than those for the sulfur adsorbate. S/O exchange reactions at the substrate surface are always energetically preferred over sulfur adsorption. In addition, the first and second sulfur substitution takes place preferentially at the singly coordinated oxygen site O(1). Finally, the calculations show that pre-adsorbed hydrogen can facilitate the sulfidation process at the MoO<sub>3</sub>(010) surface.

O 51.5 Thu 17:15 SCH A01

**Theoretical investigations on the electrochemical hydrogen evolution on Pt-hydride surfaces** — ●FEDOR STRIGUNOV, JOHN KEITH, and TIMO JACOB — Institut für Elektrochemie, Universität Ulm, 89081 Ulm

Noble metals are a common component of electrodes that drive electrochemical reactions. Despite their nobility, electrode surfaces may take on many different structures or morphologies under electrochemical environments. Using periodic density functional theory, we calculated the surface free energies for several different surfaces of a variety of bulk Pt-hydride morphologies. In combination with the extended ab initio thermodynamics approach [1,2] we present a first phase diagram showing under which experimental temperature, activity, and electrode potential conditions hydrogen is present on the surface and which Pt-hydride surface orientation and structure is stabilized. On the basis of the most relevant Pt-hydride surfaces we then evaluated the adsorption of atomic hydrogen as well as the barriers for hydrogen evolution. This data will be used as the grounds for further understanding reactions on electrochemical electrodes.

[1] M. Scheffler, J. Dabrowski, *Phil. Mag.*, **A 58**, 107 (1988). [2] T. Jacob, *J. Electroanal. Chem.*, **607**, 158, (2007).

O 51.6 Thu 17:30 SCH A01

**CO oxidation on planar Au/TiO<sub>2</sub> model catalysts: activation energy and influence of reaction atmosphere** — ●MENHILD EYRICH, STEFAN KIELBASSA, JOACHIM BANSMANN, and R. JÜRGEN BEHM — Institute of Surface Chemistry and Catalysis, Ulm University, D-89069 Ulm

The high interest in oxide supported Au catalysts and in particular in the low-temperature CO oxidation reaction on these catalysts, in combination with the still unknown reaction mechanism, has stimulated model studies on planar model catalysts. Analogously to the respective powder catalysts, also the activity of the planar model catalysts strongly depends on the catalyst preparation. Here we report results of reaction measurements on differently reduced Au/TiO<sub>2</sub>(110) model catalysts. The activation energy for CO oxidation on these model systems was determined, and the influence of the reactant gas composition (CO/O<sub>2</sub> ratio) on the catalytic activity was evaluated. The results will be compared to the findings for other Au/TiO<sub>2</sub> (model) catalysts, and possible reasons for the significant reactivity enhancement for reduced model catalysts will be discussed.

O 51.7 Thu 17:45 SCH A01

**Interaction of Thin Nickel Oxide Layers with Carbon Oxides**

— ●MICHAEL PETER ANDREAS LORENZ<sup>1</sup>, REGINE STREBER<sup>1</sup>, CHRISTIAN PAPP<sup>1</sup>, MARIE-MADELEINE WALZ<sup>1</sup>, ANDREAS BAYER<sup>1</sup>, SANDRA KÜNZEL<sup>2</sup>, REINHARD DENECKE<sup>2</sup>, and HANS-PETER STEINRÜCK<sup>1</sup> — <sup>1</sup>Lehrstuhl für Physikalische Chemie II, Universität Erlangen-Nürnberg, Egerlandstr. 3, 91058 Erlangen — <sup>2</sup>Wilhelm-Ostwald-Institut für Physikalische und Theoretische Chemie, Universität Leipzig, Linnéstr. 2, 04103 Leipzig

NiO is an important material in heterogeneous catalysis. Under ambient conditions, reaction with CO<sub>2</sub> can easily lead to the formation of carbonates, which could block active sites and thereby influence the catalytic reactivity. Behm and Brundle [1] reported carbonate formation on Ni(100) by simultaneously dosing molecular oxygen and CO<sub>2</sub>. We have now studied the interaction of CO<sub>2</sub> and also CO on an oxidised Ni(111) surface in great detail by in situ XPS applying synchrotron radiation at BESSY II. For both, characteristic peaks develop in the O 1s and C 1s spectra, albeit with different intensities, indicating the formation of carbonate layers. Similar results are obtained for thick oxidised Ni layers (~2 ML) grown on Cu(111). In contrast, thin oxidised Ni layers (~0.5 ML) on Cu(111) exhibit a significantly reduced reactivity towards carbonate formation. The decomposition of the carbonate species was determined in situ by XPS during heating. This work was supported by BMBF (05 ES3XBA/5) and the DFG through the Cluster of Excellence "Engineering of Advanced Materials".

[1] R. J. Behm, C. R. Brundle, *Surf. Sci.* 255 (1991) 327

O 51.8 Thu 18:00 SCH A01

**The Surface Selective Chlorination of RuO<sub>2</sub>(110)** — ●JAN PHILIPP HOFMANN<sup>1</sup>, STEFAN ZWEIDINGER<sup>1</sup>, MARCUS KNAPP<sup>1</sup>, ARI PAAVO SEITSONEN<sup>2</sup>, KARINA SCHULTE<sup>3</sup>, EDVIN LUNDGREN<sup>3</sup>, JESPER ANDERSEN<sup>3</sup> and HERBERT OVER<sup>1</sup> — <sup>1</sup>Physikalisch-Chemisches Institut, Justus-Liebig Universität Gießen, Heinrich-Buff-Ring 58, D-35392 Gießen — <sup>2</sup>IMPMC, CNRS & Université Pierre et Marie Curie, 4 place Jussieu, case 115, F-75252 Paris — <sup>3</sup>Dept. of Synchrotron Radiation Research, Lund University, Sölvegatan 14, S-22362 Lund

Chlorinated ruthenium dioxide plays an important role in the heterogeneously catalysed oxidation of hydrogen chloride to chlorine (Deacon process)[1]. High resolution core level shift spectroscopy (HRCLS) and temperature programmed reaction (TPR) experiments together with density functional theory (DFT) calculations were used to elucidate the chlorination mechanism of ruthenium dioxide RuO<sub>2</sub>(110) by hydrogen chloride exposure on the atomic scale. The surface selective chlorination proceeds via the diffusion of chlorine atoms in surface vacancies, which are formed by the desorption of water. H<sub>2</sub>O is produced either by the dissociative adsorption of HCl adjacent to a surface hydroxyl group or by the chlorine assisted recombination of two neighbouring surface hydroxyl groups [2].

[1] Crihan, D. et al.; *Angew. Chemie Int. Ed.* 2008, 47, 2131-2134.

[2] Hofmann, J. P.; Zweidinger, S.; Knapp, M.; Seitsonen, A. P.; Schulte, K.; Andersen, J. N.; Lundgren, E.; Over, H.; *J. Phys. Chem. C*, submitted.

O 51.9 Thu 18:15 SCH A01

**HREELS study of Cu clusters deposited on the O-terminated ZnO(000-1) surface** — ●HENGSHAN QIU, YUEMIN WANG, and CHRISTOF WÖLL — Physical Chemistry I, Ruhr-University Bochum, 44780 Bochum, Germany

The interaction of metal clusters and films with oxide substrates plays a key role as regards the microscopic mechanisms of many processes in heterogeneous catalysis. In this work, the interaction of Cu clusters with the O-terminated ZnO(000-1) surface was studied by high-resolution energy loss spectroscopy (HREELS), together with thermal desorption spectroscopy (TDS) and low-energy electron diffraction (LEED). It was found that Cu deposition on O-ZnO leads to the formation of well-defined islands with the Cu(111) facets. For the small clusters the partial oxidation of Cu<sup>0</sup> into Cu<sup>+</sup> was clearly identified by the characteristic changes in the C-O stretch frequencies of CO molecules adsorbed on the Cu atoms. Upon heating the Cu atoms undergo, instead of desorption, diffusion into the O-ZnO bulk. The doping of ZnO by Cu leads to the formation of shallow donor states, in which the electrons can be thermally excited into the conduction band and, as a result, give rise to the plasmon-induced broadening of the quasielastic peak in HREELS [1]. From the observed temperature dependence, the donor level ionization energy was determined. This unexpected doping effect of ZnO by Cu has important consequences for its chemical activity, as confirmed by detailed studies on CO<sub>2</sub> adsorption. [1] H. Qiu, B. Meyer, Y. Wang, Ch. Wöll, *Phys. Rev. Lett.*

in press (2008).

O 51.10 Thu 18:30 SCH A01

**Adsorption and diffusion of H and NH<sub>x</sub> as key steps of the NH<sub>x</sub> dehydrogenation reaction at the V<sub>2</sub>O<sub>5</sub> (010) surface** — ●MATHIS GRUBER and KLAUS HERMANN — Fritz-Haber-Institut der MPG, Faradayweg 4-6, D-14195 Berlin and Sfb 546, Berlin (Germany)

Various selective oxidation reactions as the Selective Catalytic Reduction (SCR) of NO<sub>x</sub> or the ammoxidation of propane/propene to acrylonitrile are processed on vanadium based metal-oxide catalysts in the presence of ammonia. In the reactions the intermediates NH<sub>2</sub>, NH<sub>3</sub>, and NH<sub>4</sub> are involved indicating that the adsorption and dehydrogenation of NH<sub>x</sub>,  $x < 4$ , are important steps. We have performed theoretical studies of corresponding reaction steps where the catalyst is simulated by a finite section of the V<sub>2</sub>O<sub>5</sub> (010) surface. The calculations apply density-functional theory combined with clusters modeling the adsorbate system. The substrate lowers corresponding dehydrogenation energies considerably compared with values for the gas phase reaction. However, the lowering is too small to make dehydrogenation of NH<sub>3</sub> likely to happen. Our results on the role of oxygen vacancies for the dehydrogenation indicate that such surface defects become important for the reaction. Besides the energetics also the diffusion at the surface influences the reaction. A Nudged Elastic Band (NEB) routine has been implemented to evaluate diffusion paths and barriers. Hydrogen diffusion on the surface will be discussed and additional examples for NH<sub>x</sub> diffusion will be shown. Based on these results possible reaction scenarios for the dehydrogenation reaction will be presented.

O 51.11 Thu 18:45 SCH A01

**PrO<sub>2-x</sub>/Si(111) – A model system for praseodymium oxide based catalysts** — ●ANDREAS SCHAEFER<sup>1</sup>, SEBASTIAN LAMBERTI<sup>1</sup>, VOLKMAR ZIELASEK<sup>1</sup>, JENS FALTA<sup>2</sup>, THOMAS SCHRÖDER<sup>3</sup>, and MARCUS BÄUMER<sup>1</sup> — <sup>1</sup>Institut für Angewandte und Physikalische Chemie, D-28359 Universität Bremen — <sup>2</sup>Institut für Festkörperphysik, D-28334 Universität Bremen — <sup>3</sup>IHP microelectronics, D-15236 Frankfurt (Oder), Germany

Praseodymium (Pr) oxides are promising candidates for applications in catalysis and microelectronics due to their variable valency along with a high oxygen mobility. Thin films of the oxide prepared on a Si(111) surface in an UHV environment provide a simplified two-

dimensional model system of the oxide catalyst. Such a model system allows insight into the atomic details of oxygen transport and transfer when exposed to adsorbed molecules. Additionally, details on the defect structure of such oxide films can be obtained, which is a crucial point for applications in microelectronics. The films were prepared by molecular beam epitaxy of hex-Pr<sub>2</sub>O<sub>3</sub> and subsequent *ex-situ* annealing in oxygen atmosphere to obtain cubic PrO<sub>2</sub>. Here we report on a study on cleaning, reduction and reoxidation of a PrO<sub>2-x</sub> ( $x = 0-0.5$ ) starting film to obtain a surface with defined oxidation state and stoichiometry. Annealing experiments with and without gas dosage during heating will be compared as well as H<sub>2</sub> and O<sub>2</sub> plasma treatment. The surfaces have been studied using x-ray photoelectron spectroscopy and low-energy electron diffraction. First thermal desorption spectra of CO adsorbed on the differently prepared surfaces are presented.

O 51.12 Thu 19:00 SCH A01

**Ferrocene Affinity Label for the Electrochemical Detection of Enzymes down to a Single Molecule Level** — ●CLAUDIA BAIER, ALICE SCHLICHTIGER, JÖRG EPPINGER, and ULRICH STIMMING — TU München, Garching, Deutschland

The research field of biosensors and bioelectronics offers a large potential for the development of functional devices. In this presentation, we show that we are able to electrochemically detect enzymes which are originally not redox-active such as papain and trypsin by using ferrocene affinity labels. These ferrocene-based affinity labels are ideally suited since they combine the electrochemically active ferrocene moiety which is stable under physiological conditions with the selectivity and activity sensing properties of the affinity label concept. The redox-labeled enzymes are immobilized on highly oriented pyrolytic graphite (HOPG) and are electrochemically investigated using cyclic voltammetry and impedance measurements. Furthermore, we established a nano-scale readout i.e. the detection of direct electron transfer processes on a single molecule level by in-situ SPM visualization. Therefore, potential dependent in-situ electrochemical scanning tunneling microscopy (EC-STM) studies and first results of scanning electrochemical potential microscopy (SECPM) will be presented. SECPM, which is the latest invention of the electrochemical SPM techniques, uses the electrochemical potential at the solid/liquid interface as feedback signal by measuring the potential difference between a potentiometric tip and the potential controlled working electrode.

## O 52: Metal substrates: Adsorption of organic / bio molecules VII

Time: Thursday 15:00–19:15

Location: SCH A118

O 52.1 Thu 15:00 SCH A118

**Understanding the electronic transport across single phthalocyanine molecules** — ●ANNIKA BORK<sup>1</sup>, ALBERT F. TAKÁCS<sup>1,2</sup>, FLORIAN WITT<sup>1</sup>, STEFAN SCHMAUS<sup>1,2</sup>, TIMOFEY BALASHOV<sup>1</sup>, MARTIN BOWEN<sup>3</sup>, ERIC BEAUREPAIRE<sup>3</sup>, and WULF WULFHEKEL<sup>1,2</sup> — <sup>1</sup>Physikalisches Institut, Universität Karlsruhe (TH) — <sup>2</sup>CFN-DFG Centrum für Funktionelle Nanostrukturen — <sup>3</sup>Institut de Physique et Chimie des Matériaux de Strasbourg

Regarding the increasing miniaturization of electronic devices, molecular electronics is a field of growing interest. Here, we present STM and STS results on hydrogen (H<sub>2</sub>Pc), cobalt (CoPc) and manganese (MnPc) phthalocyanines deposited on a clean Cu(111) surface as well as on bilayer cobalt islands on Cu(111). By laterally positioning the STM tip over a single molecule and approaching the tip towards the surface we were able to investigate the conductance of the molecules. Our results show that the molecules tend to lift from the surface and jump into contact with the STM tip. On Cu(111) we found that the conductance through H<sub>2</sub>Pc, CoPc and MnPc is about 0.1 G<sub>0</sub> whereas the conductance of H<sub>2</sub>Pc and CoPc on the cobalt islands is about 3 times higher. By performing STS measurements the orbitals of the H<sub>2</sub>Pc and CoPc can be obtained. In both cases we can observe a shift of the HOMO to the Fermi edge, which explains the increased conductance on the cobalt islands. Further, inelastic STS revealed a soft phonon excitation located on the sidegroups, that is the underlying mechanism of the jump into contact.

O 52.2 Thu 15:15 SCH A118

**Systematic study of phthalocyanine (sub-)monolayer phases by high-resolution PES and NEXAFS** — ●M.

HÄMING<sup>1</sup>, C. SCHEUERMANN<sup>1</sup>, E. UMBACH<sup>1,2</sup>, A. SCHÖLL<sup>1</sup>, and F. REINERT<sup>1,2</sup> — <sup>1</sup>Universität Würzburg, Experimentelle Physik II — <sup>2</sup>Forschungszentrum Karlsruhe, 76021 Karlsruhe

The interaction at metal-organic interfaces is crucial for electronic devices, since it influences the morphology and the electronic structure at the interface, and consequently the charge transport through metal-organic contacts. Therefore we investigate the interaction and interplay between the geometric and electronic structure at a metal-organic model interface. We study systematically various (sub-)monolayers phases of flat lying phthalocyanine on the Ag(111) surface by high-resolution photoemission spectroscopy (PES) and near edge x-ray absorption fine structure spectroscopy (NEXAFS). We observe evidence for chemisorption of the molecules in all spectra (valence band, NEXAFS and core levels). Moreover, already small differences in the adsorption geometry between the different phases change the respective spectra and the work function significantly. For example, an increase in coverage leads to a weaker interface bond. Consistent changes in the valence band and NEXAFS spectra indicate that consequently the occupation of the former molecular LUMO level, which is partly occupied due to the chemisorption, is altered. Our investigation demonstrates that the electronic structure at interfaces is very sensitive to relatively small changes in the interaction, and that high-resolution PES and NEXAFS are powerful techniques to study these correlations.

O 52.3 Thu 15:30 SCH A118

**Temperature and thickness dependent adsorption studies of azobenzene molecules on Cu(100)** — ●ALEX KRÜGER, MARTEN PIANTEK, CRISTINA NAVIO, JORGE MIGUEL, MATTHIAS BERNIEN, and WOLFGANG KUCH — Institut für Experimentalphysik, Freie Univer-

sität Berlin

Here we present a study of the influence of temperature and coverage on the ordering of dimetacyano-azobenzene (DMC) ultrathin layers adsorbed on Cu(001). Near-edge X-ray absorption fine structure (NEXAFS) and X-ray photoelectron spectroscopy (XPS) provided information on the molecular geometry relative to the substrate and on the nature of molecule adsorption to the surface, respectively. From XPS data we determine that DMC molecules evaporated onto Cu(001) at room temperature are chemisorbed, but a dramatic change in the angle-dependent C- and N-K edge NEXAFS between 0.5 and 1 ML (monolayer) indicates that strong intermolecular interactions provoke a conformational change. On a second step, we studied the temperature dependence of 1 ML DMC on Cu(001). At 150 K, about half of the molecules are physisorbed in a planar conformation parallel to the surface. As the temperature increases, the NEXAFS data shows a strong change in the molecular conformation at 230 K, concurrent with the formation of a bond between one of the azo nitrogen atoms to the surface, as seen by XPS. These results are supported by density functional theory calculations. We conclude that both intermolecular and molecule-substrate interactions can give rise to the observed conformational change.

O 52.4 Thu 15:45 SCH A118

**Adsorption energy and geometry of adsorbed organic molecules on Au(111) probed by surface-state photoemission** — ●JOHANNES ZIROFF<sup>1</sup>, FRANK FORSTER<sup>1</sup>, and FRIEDRICH REINERT<sup>1,2</sup> — <sup>1</sup>Universität Würzburg, Experimentelle Physik II, D-97074 Würzburg, Germany — <sup>2</sup>Forschungszentrum Karlsruhe, Gemeinschaftslabor für Nanoanalytik, D-76021 Karlsruhe, Germany

The modification of the Au(111) surface states by an adsorbed monolayer of large  $\pi$ -conjugated molecules (PTCDA, NTCDA, CuPc) was investigated by high-resolution angle-resolved photoelectron spectroscopy. We determined binding energy, band mass, and Rashba-splitting and discuss the results in the context of rare-gas adsorption on noble metals. This comparison allows the determination of the bonding strength of the adsorbates, found to be physisorptive with derived binding energies per molecule of 2.0 eV for PTCDA and 1.5 eV for NTCDA. We will also present a superstructure model for the NTCDA/Au(111) system, deduced from low energy electron diffraction images in combination with band-backfolding of the Tamm and Shockley states. The coverage dependent evolution of the surface states was also investigated for the three molecules, giving evidence for a dilute-phase growth of the CuPc molecule on the Au(111) surface.

O 52.5 Thu 16:00 SCH A118

**Investigation of meso-Tetraphenylporphyrin Molecules using Scanning Tunneling Microscopy** — ●VINÍCIUS CLAUDIO ZOLDAN<sup>1,2</sup>, KHALIL ZAKERI<sup>1</sup>, CHUNLEI GAO<sup>1</sup>, ANDRÉ AVELINO PASA<sup>2</sup>, and JÜRGEN KIRSCHNER<sup>1</sup> — <sup>1</sup>Max Planck Institute of Microstructure Physics, Halle, Germany — <sup>2</sup>Laboratório de Filmes Finos e Superfícies, Universidade Federal de Santa Catarina, Brazil

Due to their distinct physicochemical properties and potential for molecular architecture, porphyrins represent a group of molecules which has attracted a great technological and fundamental interest. The meso-Tetraphenylporphyrin (H<sub>2</sub>-TPP) and meso-Tetraphenylporphyrin-Cobalt II (Co-TPP) molecules were grown on Ag(111) and Cu<sub>3</sub>Au(100) substrates. In the case of Ag(111), self-organized monolayer was observed, as has been reported [1]. The growth of single molecules were achieved on Cu<sub>3</sub>Au(100) at room temperature. The chemical sensitivity through bias-dependent imaging of both molecules has been measured using low temperature Scanning Tunneling Microscopy/Spectroscopy (STM/STS). The STS results show one characteristic peak near 0.6 eV for H<sub>2</sub>-TPP molecules, whereas for the Co-TPP molecules two peaks were observed at energies of -0.5 and -1.1 eV. Moreover, the dehydrogenation of the individual H<sub>2</sub>-TPP and Co-TPP molecules was realized with a local ramp-voltage from the STM tip. The energy needed for the dehydrogenation is found to be 2.0 and 3.5 eV for H<sub>2</sub>-TPP and Co-TPP, respectively.

Comanici et al. *Langmuir*. **24**, 1897 (2008)

O 52.6 Thu 16:15 SCH A118

**Interaction between coordinated metal ions and a metal substrate: Differently substituted cobalt porphyrins on Ag(111)** — ●YUN BAI, FLORIAN BUCHNER, MARTIN SCHMID, INA KELLNER, FLORIAN VOLLNHALS, HUBERTUS MARBACH, HANS-PETER STEINRÜCK, and J. MICHAEL GOTTFRIED — Universität Erlangen-Nürnberg, Lehrstuhl für Physikalische Chemie II, Egerlandstr. 3,

91058 Erlangen, Germany

Adsorbed metalloporphyrins are of increasing interest due to their potential applications in heterogeneous catalysis and in sensor systems. Previous studies from our group have suggested the existence of an electronic interaction between the metal centers of the adsorbed porphyrin complexes of iron and cobalt and the underlying substrate surface, which plays an important role in modifying the electronic structure and, thereby, the reactivity of these metal centers.[1,2] However, with the previously used tetraphenylporphyrin (TPP) ligands, the adsorbed complexes undergo saddle-shape distortion, which could also influence the electronic structure. To separate the effects of distortion on the one hand and the coupling to the substrate on the other, we have studied cobalt octaethylporphyrin, which adsorbs in a flat, undistorted conformation on Ag(111). Comparison of our XPS, UPS, and STM results with previous CoTPP data [1,2] confirms that indeed the metal center plays an essential role in the electronic interaction between the porphyrin complexes and the substrate. Supported by the DFG through SFB 583.

1. T. Lukaszczuk et al., *J. Phys. Chem. C* **111** (2007) 3090.

2. K. Flechtner et al., *J. Am. Chem. Soc.* **129** (2007) 12110.

O 52.7 Thu 16:30 SCH A118

**Electronic and magnetic coupling of iron and copper phthalocyanine to ferromagnetic Co(100) surfaces** — ●FELIX SCHMIDT<sup>1</sup>, JENS SAUTHER<sup>1</sup>, EHESAN ALI<sup>2</sup>, STEFAN LACH<sup>1</sup>, PETER OPPENEER<sup>2</sup>, and CHRISTIANE ZIEGLER<sup>1</sup> — <sup>1</sup>Department of Physics, University of Kaiserslautern, Erwin Schrödinger Str. 56, D-67663 Kaiserslautern, Germany — <sup>2</sup>Department of Physics and Materials Science, Box 530, Uppsala University, S-75121 Uppsala, Sweden

Metallo-phthalocyanines are organic semiconductors which show in certain cases promising magnetic properties, advertising them for use in organic spintronics. Here, copper (CuPc) and iron phthalocyanine (FePc) were grown on ultra thin layers of Co(100) substrates with well known highly spin-polarized electron injection capability. Photoelectron spectroscopy (XPS) reveals different interactions between the pyrrolic nitrogen atoms and the cobalt surface for the two phthalocyanines. The analysis of the different multiplet structures appearing for the nitrogen core levels in the submonolayer regime and UPS investigations of the valence band electronic structure of the Co dominated region near the Fermi level indicates a particularly electronic coupling and a rehybridisation of the molecular orbitals with the cobalt orbitals. In order to clarify the influence of the two different central atoms on the electronic- and subsequently the magnetic coupling to the Co substrate, theoretical calculations using the GGA and GGA+U methodologies on a structure of Fe/Cu-phthalocyanine adsorbed on a 3-layered cobalt surface were performed indicating a ferromagnetic coupling between FePc and Co.

O 52.8 Thu 16:45 SCH A118

**Investigation of the electronic structure of CuPc on Cu(100) interfaces using ARUPS with polarized light** — ●MICHAEL WIESSNER<sup>1</sup>, MARC HAEMING<sup>1</sup>, FRANK FORSTER<sup>1</sup>, ACHIM SCHÖLL<sup>1</sup>, and FRIEDRICH REINERT<sup>1,2</sup> — <sup>1</sup>Universität Würzburg, Experimentelle Physik II, D-97074 Würzburg — <sup>2</sup>Forschungszentrum Karlsruhe, Gemeinschaftslabor für Nanoanalytik, D-76021 Karlsruhe

The understanding of the electronic structure at metal-organic interfaces is crucial for electronic devices since it determines the charge transport through metal-organic contacts. Particularly if chemical interaction occurs, as it is the case between most aromatic organic molecules and metals, the hybridization of molecule and metal wave functions effects both the energy position and the symmetry of the involved orbitals. Consequently, the dipole matrix element, i.e. the intensity of a photoemission signal, will be influenced. This phenomenon can thus be utilized as a sensitive probe for the interfacial interaction and the character of the involved molecular and metal states.

We report on an investigation of the adsorption of ultra-thin Cu-phthalocyanine films on Cu(100) surfaces by means of angular resolved photoemission spectroscopy (ARPES) with polarized light. By using a monochromatized *HeI $\alpha$*  source with a high degree of polarization and with variable polarization direction we observe polarization-dependent intensities for signals from the substrate, from the adsorbate molecules, and from interface states which are generated due to the chemisorption. The evaluation of these variations in intensity shows that the applied method is a useful tool for understanding the interaction mechanisms.

O 52.9 Thu 17:00 SCH A118

**Fingerprints of large organic molecules: on the interior**

**of tetraphenyl-porphyrins in scanning tunneling microscopy** — FLORIAN BUCHNER<sup>1,3</sup>, KARL-GEORG WARNICK<sup>2,3</sup>, THORSTEN WÖLFLE<sup>2,3</sup>, WOLFGANG HIERINGER<sup>2,3</sup>, ANDREAS GÖRLING<sup>2,3</sup>, HANS-PETER STEINRÜCK<sup>1,3</sup>, and •HUBERTUS MARBACH<sup>1,3</sup> — <sup>1</sup>Lehrstuhl für Physikalische Chemie II — <sup>2</sup>Lehrstuhl für Theoretische Chemie — <sup>3</sup>Interdisciplinary Center of Molecular Materials (ICMM), Universität Erlangen-Nürnberg, Egerlandstr. 3, D-91056 Erlangen

The appearance of a constant current scanning tunneling microscopy (STM) image is determined by both the topography and the electronic structure of the investigated object. The discrimination of these effects and the understanding of the bias dependent appearance of different adsorbed species represents a major challenge. We investigate an intermixed tetraphenylporphyrin (TPP) layer consisting of 2HTPP, CoTPP and FeTPP molecules on Ag(111), to allow for a direct in situ comparison. By a combined experimental and theoretical analysis, we find that at lower bias voltages the appearance of CoTPP in the STM image is dominated by electronic effects, while at high bias a combination of both electronic and topographic effects is observed. For 2HTPP and FeTPP the images are dominated by topographic effects. The detailed interpretation of the bias dependence is performed by means of high quality density-functional calculations, which allow to reproduce the experimentally observed STM images with very high accuracy and to trace back the observed features to individual molecular orbitals. Supported by the DFG through SFB 583.

O 52.10 Thu 17:15 SCH A118

**Portrait of a potential barrier: electron tunneling at metal-organic interfaces** — •LUCIA VITALI<sup>1</sup>, GIACOMO LEVITA<sup>2</sup>, ROBIN OHMANN<sup>1</sup>, ALESSIO COMISSO<sup>3</sup>, ALESSANDRO DE VITA<sup>3</sup>, and KLAUS KERN<sup>1</sup> — <sup>1</sup>Max-Planck Institute for Solid State Research, Stuttgart, Germany — <sup>2</sup>INFN Democritos, University of Trieste, Italy — <sup>3</sup>Physics Department, King's College, London

Organic semiconductors constitute the basis of a fast developing microelectronics and are successfully making the first steps towards high performance nanoscale devices. Further improvements and the design of new molecular-based electronic circuits require a better understanding of the charge transport and injection mechanisms. At present, one of the major constraints is given by the electron potential barrier forming at the molecule-metal interface. Here, by means of a low temperature scanning tunneling microscope (STM), we visualize this metal-molecule interface on a local scale. We found that the molecular interaction with the substrate leads to the formation of a potential barrier which is non-uniform across the molecule. This reflects the relation between the chemical composition and the interaction with the metal surface.

O 52.11 Thu 17:30 SCH A118

**Adsorption of metal-phthalocyanines on the Ag(111) surface** — •INGO KRÖGER<sup>1</sup>, CHRISTOPH STADLER<sup>1</sup>, PATRICK BAYERSDORFER<sup>1</sup>, FLORIAN POLLINGER<sup>1</sup>, ANDREAS STAHL<sup>1</sup>, FELIX ERFURTH<sup>1</sup>, BENJAMIN STADTMÜLLER<sup>1</sup>, CHRISTIAN KUMPF<sup>1,2</sup>, and FRIEDRICH REINERT<sup>1,3</sup> — <sup>1</sup>Universität Würzburg, Experimentelle Physik II, 97074 Würzburg — <sup>2</sup>Forschungszentrum Jülich GmbH, IBN-3, D-52425 Jülich — <sup>3</sup>Forschungszentrum Karlsruhe GmbH, Gemeinschaftslabor für Nanoanalytik, D-76021 Karlsruhe

The sub-monolayer growth of metal-phthalocyanines (MePc) on the Ag(111) surface exhibits a rich phase diagram consisting of 2D gas-like phases, commensurate phases and - most interestingly - continuous series of phases with point-on-line coincidence with the substrate. The latter are caused by a repulsive molecule-molecule interaction which can be tuned (and even suppressed) by changing coverage and/or temperature. Therefore these adsorbate systems represent model systems for investigating the interplay of molecule-molecule and molecule-substrate interaction as well as geometric and electronic structure. In this talk we present an overview of the phase diagrams for CuPc, SnPc, TiOPc and H2Pc. The data was obtained using spot profile analysis low energy electron diffraction (SPA-LEED) and X-ray standing waves (XSW). Comparing these systems gives insight in the molecular adsorption geometry as well as the influence of the central metal atom on the molecule-substrate and the molecule-molecule interactions.

O 52.12 Thu 17:45 SCH A118

**STM and STS study of F<sub>16</sub>CoPc adsorbed onto Ag(110) surface** — •MARIUS TOADER<sup>1</sup>, THIRUVANCHERIL G. GOPAKUMAR<sup>2</sup>, MAHMOUD ABDEL-HAFIEZ<sup>1</sup>, and MICHAEL HIETSCHOLD<sup>1</sup> — <sup>1</sup>Chemnitz University of Technology, Solid Surfaces Analysis Group, D-09107 Chemnitz, Germany — <sup>2</sup>Christian-Albrechts-Universität zu Kiel, Institute

of Experimental and Applied Physics, D-24118 Kiel, Germany

In this work the adsorption of cobalt(II) hexadecafluorophthalocyanine (F<sub>16</sub>CoPc), one of the few organic n-type semiconductors, onto silver (110) surface prepared by OMBD is investigated using UHV VT-STM from Omicron operating at 40 K. The asymmetry of the metal substrate is found to act as a template for the organic adlayer which grows preferentially along the [1-10] crystallographic axis leading to a commensurate structure with well defined pinning centers. The proposed structural model is strongly sustained by the molecular self assembly at the defects proximity and especially at the domain boundaries where a mirror structure is induced. The perturbed electronic properties like HOMO-LUMO gap, induced new states close to the Fermi level are illustrated using STS. Single molecule DFT calculations are implemented to understand the mechanism responsible for the organic-metal interface formation from STS.

O 52.13 Thu 18:00 SCH A118

**Dimerization Boosts One-Dimensional Mobility of Conformationally Adapted Porphyrins on a Hexagonal Surface Atomic Lattice** — •MAXIMILIAN EICHBERGER<sup>1</sup>, MATTHIAS MARSCHALL<sup>2</sup>, JOACHIM REICHERT<sup>2</sup>, ALEXANDER WEBER-BARGIONI<sup>1</sup>, WILLI AUWÄRTER<sup>2</sup>, RICHARD L. C. WANG<sup>3</sup>, HANS J. KREUZER<sup>3</sup>, YAN PENNEC<sup>1</sup>, AGUSTIN SCHIFFRIM<sup>1,2</sup>, and JOHANNES V. BARTH<sup>2</sup> — <sup>1</sup>Department of Physics & Astronomy, University of British Columbia, Vancouver, Canada — <sup>2</sup>Physik Department, TU München, Germany — <sup>3</sup>Department of Physics and Atmospheric Science, Dalhousie University, Halifax, Canada

We employed temperature-controlled fast-scanning tunneling microscopy to monitor the diffusion of tetrapyrrolylporphyrin molecules on the Cu(111) surface. The data reveal unidirectional thermal migration of conformationally adapted monomers in the 300-360 K temperature range. Surprisingly equally oriented molecules spontaneously form dimers that feature a drastically increased one-dimensional diffusivity. The analysis of the bonding and mobility characteristics indicates that this boost is driven by a collective transport mechanism of a metallosupramolecular complex.

O 52.14 Thu 18:15 SCH A118

**The Adsorption of Porphine on Copper (110)** — •MATTHEW STEPHEN DYER, ABEL ROBIN, SAM HAQ, RASMITA RAVAL, and MATS PERSSON — University of Liverpool, Liverpool, U. K.

Porphyrin molecules and related phthalocyanines have come under a lot of interest in recent years as potential components for molecular-scale devices with various applications. By studying the simplest porphyrin, porphine (H<sub>2</sub>-P), and its interaction with a clean copper surface we obtain physical insight relevant for larger, more complicated systems.

We present the results of scanning tunnelling microscopy (STM) and reflection absorption infrared spectroscopy (RAIRS) experiments, along with density functional theory (DFT) calculations, which show that H<sub>2</sub>-P is chemisorbed on Cu(110) with the centre above the short-bridge site. Considerable charge transfer occurs upon adsorption from the metal into the unoccupied orbitals of the molecule.

An unexpected and very interesting result is that copper adatoms are observed to reside in the vicinity of H<sub>2</sub>-P molecules in STM images. DFT calculations show that there is an energetic preference of about 25 meV for copper adatoms to reside in certain sites on the surface close to H<sub>2</sub>-P molecules. There is no chemical bond formed between the molecule and the adatom, rather the attraction is probably due to a substrate-mediated interaction.

O 52.15 Thu 18:30 SCH A118

**Adsorption Geometry of Non-Planar Phthalocyanines on Cu(111): Orientation of the Electric Dipole Moment** — •A. GERLACH<sup>1</sup>, S. DUHM<sup>2</sup>, T. HOSOKAI<sup>1</sup>, F. SCHREIBER<sup>1</sup>, N. KOCH<sup>2</sup>, O. HOFMANN<sup>3</sup>, E. ZOJER<sup>3</sup>, T.-L. LEE<sup>4</sup>, and J. ZEGENHAGEN<sup>4</sup> — <sup>1</sup>Institut für Angewandte Physik, Universität Tübingen, Germany — <sup>2</sup>Institut für Physik, Humboldt-Universität zu Berlin, Germany — <sup>3</sup>Institut für Festkörperphysik, Technische Universität Graz, Austria — <sup>4</sup>European Synchrotron Radiation Facility, Grenoble, France

The orientation of polar organic molecules on metal surfaces has important implications for the electronic properties of the first molecular layer. We have studied the orientational ordering of chlorogallium phthalocyanines (GaClPc) on Cu(111) using the X-ray standing wave technique, photoelectron spectroscopy and DFT calculations.

The XSW data indicate that for low coverages the majority of

GaClPc molecules adsorb in a 'Cl-down' configuration with a chlorine bonding distance of 1.88 Å. Since the gallium atoms are located at 4.21 Å, we find a Ga-Cl bond length close to the gas phase value. For higher coverages the XSW data indicate a co-existence of the 'Cl-down' and 'Cl-up' configuration on Cu(111).

Due to the alignment of the GaClPc molecules in the sub-monolayer regime their dipole moments are expected to contribute to the decrease of the work function. The non-monotonic change of the work function with increasing GaClPc coverage observed in UPS measurements can be traced back to the different adsorption geometries of GaClPc. The analysis is further supported by quantum chemical calculations.

O 52.16 Thu 18:45 SCH A118

**High-resolution ARUPS study of thin CuPc films on noble metal (111) surfaces** — ●MARIO KOCHLER<sup>1</sup>, JOHANNES ZIROFF<sup>1</sup>, FRANK FORSTER<sup>1</sup>, HATICE KARACUBAN<sup>2</sup>, and FRIEDRICH REINERT<sup>1,3</sup> — <sup>1</sup>Universität Würzburg, Experimentelle Physik II, Am Hubland, D-97074 Würzburg, Germany — <sup>2</sup>Universität Duisburg Essen, Fachbereich Physik, D-47057 Duisburg, Germany — <sup>3</sup>Forschungszentrum Karlsruhe, Gemeinschaftslabor für Nanoanalytik, D-76021 Karlsruhe, Germany

The large  $\pi$ -conjugated organic molecule copper phthalocyanine (CuPc) is widely applied in the promising field of organic electronics, for instance as donor material in solar cells. For these applications the electronic structure of the organo-metallic interface is of particular interest. We present high-resolution ARUPS data of epitaxial CuPc films on Au, Ag and Cu (111). The valence band features, i.e. the highest occupied molecular orbital (HOMO), the former lowest unoccupied molecular orbital (F-LUMO) and a sharp resonance right at

the Fermi level, are specific for each substrate. The differences in the electronic structure are a result of the increasing interaction strength between the molecules and the substrate, ranging from physisorption on Au to strong chemisorption on Cu. We correlate the coverage dependent change of the HOMO binding energy to the individual adsorption strength. The intermediate bonding strength on Ag (111) causes a partially filled F-LUMO that gives rise to the sharp resonance at the Fermi level. We will discuss these features on the background of the different growth modes of CuPc on noble metal surfaces.

O 52.17 Thu 19:00 SCH A118

**STM observations of the interaction of NO and CO with adsorbed metalloporphyrin molecules** — ●KNUD SEUFERT, WILLI AUWÄRTER, JOACHIM REICHERT, and JOHANNES V. BARTH — Physik Department, TU München, Germany

The reactivity of metalloporphyrins towards small gas molecules is of fundamental interest as it plays for example a key role in the transport of respiratory gases in biological systems. Here we present a comparative low temperature STM and STS study of the interaction of CO and NO with Cobalt-tetraphenylporphyrins (CoTPP) anchored on a Ag(111) surface. The response of CoTPP to the exposure of CO and NO is clearly different: In the CO case, the CoTPP can be dressed by one or two CO ligands, the geometric and electronic structure of CoTPP is mostly preserved. The attachment of NO to CoTPP drastically modifies the topographic appearance of CoTPP. The two-fold symmetry of CoTPP resulting from an adsorption-induced distortion is lost upon NO coordination. These experiments were systematically extended to further metalloporphyrins and a Cu(111) surface, to get more information on the underlying bond characteristics.

## O 53: Nanostructures at surfaces: Dots, particles, clusters III

Time: Thursday 15:00–18:30

Location: SCH A215

O 53.1 Thu 15:00 SCH A215

**One-Dimensionally Ordered Metal Cluster Arrays on Carburized W(110)** — ●MAGDALENA BACHMANN, MARTIN GABL, NORBERT MEMMEL, and ERMINALD BERTEL — Institute of Physical Chemistry, University of Innsbruck, A-6020 Innsbruck, Austria

The growth of noble (Ag, Au) and transition metal (Co) nanodots on the carburized tungsten (15x12)C/W(110) surface is studied by scanning tunneling microscopy (STM). At elevated temperatures for all metals small clusters are observed which are arranged with the periodicity defined by the template structure (1.4 x 3.1 nm<sup>2</sup>). The same adsorption sites are occupied by transition and noble metal clusters. Apart from these similarities also marked differences exist, in particular at higher coverages, when more material is deposited than can be adsorbed on the favorable cluster adsorption sites in each unit cell. Close to room temperature excess cobalt atoms nucleate as "interstitial" Co clusters, whereas Ag forms double-layer islands overgrowing the nanodots. At elevated temperatures in case of Co monolayer-high islands are observed, filling the free space between the clusters, whereas in case of Ag a transport of excess Ag atoms to clean tungsten terraces takes place, resulting in regular cluster growth on carbon-covered patches. Obviously, for Co the difference in adsorption strength between the more and the less favourable sites within each unit cell is less pronounced. The present results for Au contradict to some extent a recent STM study by Varykhalov et al. [Phys. Rev. B 77, 035412 (2008)]. Reasons for these discrepancies will be discussed.

O 53.2 Thu 15:15 SCH A215

**Ag island and cluster growth and thermal stability on C<sub>60</sub> films** — ●LUKAS PATRYARCHA<sup>1</sup>, STEFANIE DUFFE<sup>1</sup>, MICHAEL MOSELER<sup>2,3,4</sup>, and HEINZ HÖVEL<sup>1</sup> — <sup>1</sup>Technische Universität Dortmund, Experimentelle Physik I — <sup>2</sup>Universität Freiburg, Fakultät für Physik — <sup>3</sup>Fraunhofer-Institut für Werkstoffmechanik, Freiburg — <sup>4</sup>Freiburger Materialforschungszentrum

In former experiments for Ag<sub>309</sub>/C<sub>60</sub>/HOPG and Ag<sub>309</sub>/C<sub>60</sub>/Au(111) a substrate dependent cluster stability was observed [1]. In order to compare with these data, here at T<50 K Ag atoms with an effective coverage of 0.5 monolayers (ML) were evaporated on Au(111) functionalized with 1.5 ML C<sub>60</sub> and imaged with STM at 77 K. Cluster growth on 1 and 2 ML C<sub>60</sub> was observed directly after evaporation with STM at 77 K. After 45 min at 215 K most of the clusters grown

on 1 ML decayed. The atomistic calculations for Ag<sub>309</sub>/C<sub>60</sub>/Au(111) [1] suggest that Ag atoms moved through 1 ML C<sub>60</sub> to the Au(111) surface and formed Ag monolayer islands below the C<sub>60</sub> film. Primary clusters with a height of about 1,3 nm and 1,7 nm were formed on 2 ML C<sub>60</sub> and stayed stable for 14 days at room temperature. In an additional experiment 4 ML Ag were evaporated. Also in this case no long-time stable clusters at T>265 K on 1 ML C<sub>60</sub> were observed while clusters on 2 ML grew. By approximating the cluster shape with an ellipsoid a width-height-factor was calculated, so cluster growth effects and the change of the effective cluster coverage remaining on the surface after each annealing step could be identified.

[1] S. Duffe et al., submitted for publication

O 53.3 Thu 15:30 SCH A215

**X-ray evidence for mesoscopic relaxations in Cobalt nanoislands on Cu(001)** — OLEG MIRONETS<sup>1</sup>, ●HOLGER L. MEYERHEIM<sup>1</sup>, CHRISTIAN TUSCHE<sup>1</sup>, VALERY S. STEPANYUK<sup>1</sup>, ELEENA SOYKA<sup>1</sup>, PAUL ZSCHACK<sup>2</sup>, HAWOONG HONG<sup>2</sup>, NICOLE JEUTTER<sup>3</sup>, ROBERTO FELICI<sup>3</sup>, and JÜRGEN KIRSCHNER<sup>1</sup> — <sup>1</sup>MPI f. Mikrostrukturphysik, D-06120 Halle (Germany) — <sup>2</sup>APS, Argonne National Laboratory, Argonne, IL 60439 (USA) — <sup>3</sup>ESRF, F-38043 Grenoble (France)

Surface x-ray diffraction (SXRD) combined with scanning tunneling microscopy (STM) and molecular dynamics (MD) calculations provides evidence that monolayer thick Co nanoislands on Cu(001) experience large relaxations called mesoscopic misfit (MM). In small Co islands consisting of several tens of atoms only, the average bond length is reduced to 2.40-2.45 Å (bulk: 2.51 Å). The SXRD analysis is based on the determination of the Co-adlayer position on Cu(001) by probing the intensity distribution along the crystal truncation rods [1]. In contrast to the case of large islands (>>100 atoms), where Co-atoms reside in hollow sites separated by 2.56 Å, Co-atoms in mesoscopic misfitted islands also occupy positions off the hollow sites. The MM is identified by giant static disorder of the Co-atoms representing the distribution of adsorption sites around the hollow site position. MD calculations are in excellent agreement with the SXRD derived results.

[1] O. Mironets, H. L. Meyerheim, C. Tusche, V.S. Stepanyuk, E. Soyka, P. Zschack, H. Hong, N. Jeutter, R. Felici, and J. Kirschner, Phys. Rev. Lett. 100, 096103 (2008)

O 53.4 Thu 15:45 SCH A215

**Effect of confined surface electrons on atomic motion on nanoislands** — ●LARISSA NIEBERGALL<sup>1</sup>, ALEXEY S. SMIRNOV<sup>2,3</sup>, NIKOLAY N. NEGULYAEV<sup>2</sup>, WOLFRAM HERGERT<sup>2</sup>, ALEXANDER M. SALETSKY<sup>3</sup>, and VALERI S. STEPANYUK<sup>1</sup> — <sup>1</sup>Max Planck Institute of Microstructure Physics, 06120 Halle, Germany — <sup>2</sup>Physics Department, Martin-Luther-University, 06099 Halle, Germany — <sup>3</sup>Faculty of Physics, Moscow State University, 119899 Moscow, Russia

Several fascinating phenomena occur if surface electrons are confined to closed nanostructures [1-3]. The first experimental investigation of the quantum confinement of surface electrons on nanoscale islands on (111) noble metal surfaces by means of STM has been performed by Li et al. [3]. These studies revealed the validity of the confinement picture down to the smallest of island sizes. Here, the quantum confinement of surface electrons on top of nanoscale islands and around them is studied by means of the first-principles Korringa-Kohn-Rostocker Greens function method [4]. Our kinetic Monte Carlo simulations reveal that confinement-induced electronic states around and on top of nanoislands significantly affect atomic diffusion [4]. Formation of empty zones and orbits of adatom motion is shown. We demonstrate that the quantum confinement dramatically influences the growth process of nanoislands at low temperatures [4].

1. N. N. Negulyaev et al., Phys. Rev. Lett. 101, 226601 (2008)
2. V. S. Stepanyuk et al., New J. Phys. 9, 388 (2007)
3. J. Li et al., Phys. Rev. Lett. 80, 3332 (1998)
4. A. S. Smirnov et al., Phys. Rev. B 78 041505R (2008)

O 53.5 Thu 16:00 SCH A215

**Reduction of the critical temperature in ultrathin superconducting lead nanocrystals** — CHRISTOPHE BRUN<sup>1</sup>, I-PO HONG<sup>1</sup>, FRANÇOIS PATTHEY<sup>1</sup>, I.YU. SKLYADNEVA<sup>2,3</sup>, R. HEID<sup>4</sup>, P. M. ECHENIQUE<sup>2,5</sup>, K. P. BOHNEN<sup>4</sup>, E. V. CHULKOV<sup>2,5</sup>, and ●WOLFDIETER SCHNEIDER<sup>1</sup> — <sup>1</sup>Ecole Federale de Lausanne (EPFL), CH-1015 Lausanne, Switzerland — <sup>2</sup>Donostia International Physics Center (DIPC), 2018 San Sebastian/Donostia, Basque Country, Spain — <sup>3</sup>Inst. Strength Physics and Mat. Sci., 634021, Tomsk, Russia — <sup>4</sup>Forschungszentrum Karlsruhe, Inst. f. Festkörperphysik, D-76021 Karlsruhe, Germany — <sup>5</sup>Departamento de Física de Materiales and Centro Mixto CSIC-UPV/EHU, Facultad de Ciencias Químicas, 20080 San Sebastian/Donostia Basque Country, Spain

The energy gap of superconducting Pb nanocrystals grown on a Si(111) substrate was probed *in situ* layer-by-layer between 5 to 60 monolayers by low-temperature scanning tunneling spectroscopy. The critical temperature  $T_c$  was found to decrease from its bulk value as a function of inverse island thickness, in quantitative agreement with *ex situ* magnetic susceptibility measurements, however, in stark contrast to previous scanning probe results. *Ab initio* density functional calculations of the electron-phonon coupling constant support the experimental findings and show that the decrease of  $T_c$  mainly originates from a concomitant decrease of the electronic density of states at the Fermi level.

O 53.6 Thu 16:15 SCH A215

**Gas Sensitivity in Nanoporous Crystalline Metal Oxides: Dependence on Coordination Number** — ●JULIA DRAEGER<sup>1</sup>, MARKUS ULRICH<sup>1</sup>, CLAUS-DIETER KOHL<sup>2</sup>, STEFANIE RUSS<sup>3</sup>, and ARMIN BUNDE<sup>1</sup> — <sup>1</sup>Institut für Theoretische Physik III, Justus-Liebig-Universität, Heinrich-Buff-Ring 16, 35392 Giessen — <sup>2</sup>Institut für Angewandte Physik, Justus-Liebig-Universität, Heinrich-Buff-Ring 16, 35392 Giessen — <sup>3</sup>Institut für Theoretische Physik, Freie Universität Berlin, Arnimallee 14, 14195 Berlin

We use a percolation model to study numerically and analytically the influence of gas adsorption on the conductance of thin films of nanoporous crystalline metal oxides. We model the layers by a network of intergranular contacts with conductances that depend on the amount of adsorbed gas molecules. For a given layer thickness, average grain size and coordination number we estimate the critical gas concentration  $N_c$  below which the nanoporous structure is insulating due to the absence of a percolating cluster of conducting grains. Above  $N_c$ , which decreases strongly with the coordination number, the conductance increases rapidly. In order to obtain a low threshold  $N_c$ , it is advantageous to consider films consisting of several monolayers with low coordination number.

O 53.7 Thu 16:30 SCH A215

**Metal-organic networks as templates for Fe and Co nanostructures** — ●UTA SCHLICKUM<sup>1</sup>, REGIS DECKER<sup>1</sup>, FLORIAN KLAPPENBERGER<sup>2</sup>, GIORGIO ZOPPELLARO<sup>3</sup>, SVETLANA KLYATSKAYA<sup>3</sup>,

MARIO RUBEN<sup>3</sup>, JOHANNES BARTH<sup>2</sup>, and HARALD BRUNE<sup>1</sup> — <sup>1</sup>Institut de Physique des Nanostructures, EPF-Lausanne, Switzerland — <sup>2</sup>Physik Department E20, Technische Universität München, Germany — <sup>3</sup>Institut für Nanotechnologie, Forschungszentrum Karlsruhe, Germany

Recently we demonstrated the capability to form extremely regular metal-organic honeycomb nanomeshes using linear dicyanitrile molecules in combination with Co atoms on Ag(111). The size of the network unit cell can be adjusted by the length of the employed linear molecular bricks [1]. In this contribution we present a new approach to steer the growth of metal-nanostructures using these metal-organic networks as templates. When depositing Fe or Co atoms onto the template, the metal atoms adsorb exclusively on top of the metal-organic network avoiding the open hexagonal cavities. In addition, the nucleation sites for Fe clusters can be shifted from the organic ligands towards the metal coordination nodes by changing the deposition temperature. Therefore, by tuning the honeycomb mesh size and the deposition temperature we can control the adsorption sites, the shape and the spacing of the small metal-clusters.

- [1] U. Schlickum et al., Nano Lett. 3813 (2007)

O 53.8 Thu 16:45 SCH A215

**Silver cluster growth on highly oriented molecular films** — ●GÜNTHER WEIDLINGER<sup>1</sup>, LIDONG SUN<sup>1</sup>, MICHAEL HOHAGE<sup>1</sup>, SINA GUSENLEITNER<sup>2</sup>, STEPHEN BERKEBILE<sup>2</sup>, MICHAEL RAMSEY<sup>2</sup>, and PETER ZEPPENFELD<sup>1</sup> — <sup>1</sup>Institut für Experimentalphysik, Johannes Kepler Universität Linz, Altenberger Straße 69, A-4040 Linz — <sup>2</sup>Institut für Physik, Fachbereich Experimentalphysik, Karl-Franzens-Universität Graz, Universitätsplatz 5, A-8010 Graz

Para-sexiphenyl (p-6P) was deposited on the Cu(110)-(2x1)O surface at room temperature under UHV conditions. The structure of the (2x1)-reconstructed substrate served as a template for the growth of a highly ordered molecular film. The sequential deposition of p-6P films was monitored by means of Reflectance Difference Spectroscopy (RDS) showing a high optical anisotropy at the HOMO-LUMO transition energy, which is characteristic for the growth of a well-oriented molecular layer. Following the growth of this molecular layer, Ag clusters were prepared on the p-6P film by means of physical vapor deposition. The cluster growth can be monitored by the RD signal related to the particle plasmon resonance of the Ag clusters. Ex-situ AFM studies of these samples reveal that the Ag clusters are distributed homogeneously on the p-6P layer. Furthermore, photoelectron emission spectroscopy measurements show that the p-6P features are absent in the corresponding spectra, indicating that the Ag clusters are on top of the p-6P layer.

O 53.9 Thu 17:00 SCH A215

**Modification of SrTiO<sub>3</sub> single-crystalline surface after plasma flow treatment** — ●ALEXANDR A. LEVIN<sup>1</sup>, NIKOLAY A. KULAGIN<sup>2</sup>, TORSTEN WEISSBACH<sup>1</sup>, TILMANN LEISEGANG<sup>1</sup>, ENRICO LANGER<sup>3</sup>, and DIRK C. MEYER<sup>1</sup> — <sup>1</sup>Institut für Strukturphysik, Technische Universität Dresden, 01062 Dresden, Germany — <sup>2</sup>Kharkiv National University for Radioelectronics, av. Shakespeare 6-48, 61045 Kharkiv, Ukraine — <sup>3</sup>Institut für Festkörperphysik, Technische Universität Dresden, 01062 Dresden, Germany

Surface of pure and transition metal-doped SrTiO<sub>3</sub>(STO) single crystals before and after hydrogen plasma-flow treatment (energy of 5...20 J/cm<sup>2</sup>) is investigated by wide-angle X-ray diffraction (WAXRD), fluorescence X-ray Absorption Near Edge Structure (XANES) and scanning electron microscopy (SEM) techniques. Plasma treatment results in the formation of a textured polycrystalline layer at the surface of the single-crystalline samples with different orientation. The formation of the quasi-ordered structures consisting of nanoscale-sized pyramids is observed by SEM. XANES evidences the change of the valency of the part of Ti<sup>4+</sup> to Ti<sup>3+</sup> due to the plasma treatment. The data obtained together with results of X-ray spectroscopy measurements [1] gives evidences of the change of stoichiometry of the STO samples resulting in a change of their physical properties after plasma treatment [2].

- [1] N.A. Kulagin, A.A. Levin, E. Langer, D.C. Meyer, I. Doichinovich, Ya. Purich. Crystallography Reports 53 (N6) (2008) 1061-1067 [2] J.-C. Krupa, N.A. Kulagin. Physics of Laser Crystals. Kluwer Academic Publisher. Brussels, 2003

O 53.10 Thu 17:15 SCH A215

**Generation of phononic temperature waves during short pulse laser nanostructuring experiments on metals** — ●DMITRY IVANOV and BAERBEL RETHFELD — Technical University of Kaiser-

slautern, Physics Department, Erwin Schroedinger Str. 46, 67663 Germany

In this work we demonstrate the generation of phononic temperature waves in short pulse (pico- and femto-seconds) laser nanostructuring experiments on a metal surface. The existence of such waves was predicted based on numerical calculations with the atomistic-continuum model. This model describes the kinetics of transient nonequilibrium laser-induced processes at the atomic level and fast electron heat conduction in continuum. The analysis of obtained numerical data allowed to deduce the macroscopic parameters of observed thermal waves. The description of wave-like behavior within the frames of the diffusion equation is considered and the comparative analyzes between the continuum and the atomistic-continuum calculations is presented. The characteristic time of thermal wave relaxation was found to be on the level of 50 ns.

O 53.11 Thu 17:30 SCH A215

**Thermodynamics and sintering kinetics of Pt-Rh nanoalloys from lattice Monte Carlo simulations** — ●JOHAN POHL, MATHIAS NALEPA, and KARSTEN ALBE — Institut f. Materialwissenschaft, TU Darmstadt, Petersenstr. 23, 64287 Darmstadt, Germany

Pt-Rh nanoparticles play an important role as catalytically active material in many devices, but an in depth understanding of the thermodynamics and kinetics of this nanoalloy is, however, still lacking.

We have therefore studied the thermodynamics and kinetics of Pt-Rh nanoparticles in the framework of a bond-order simulation mixing model. First, the bulk phase-diagram is calculated that includes ordered low-temperature phases as predicted from first-principles calculations. Next, the role of finite-size effects for the phase stability in nanoparticles is investigated by semi-grand canonical Monte-Carlo simulations and thermodynamic integration, while order parameters of the finite and bulk phases are discussed. Finally, the model is extended to account for the kinetics of vacancy and surface diffusion.

Simulations of the sintering process of free particles of different sizes as well as sintering on a substrate with varying metal-substrate interaction are presented and compared with results from sintering theory.

O 53.12 Thu 17:45 SCH A215

**Surface enhanced Raman scattering of polymer molecules** — MANUEL GONÇALVES and ●OTHMAR MARTI — Universität Ulm - Inst. für Experimentelle Physik, Albert-Einstein-Allee 11, 89069 Ulm, Deutschland

Localized surface plasmons may enhanced the near-fields several orders of magnitude. The near-field enhancement depends strongly on shape and material of the metallic nanostructure. These enhancements permit to obtain Raman spectra of few of single molecules. However, spectral fluctuations and blinking were observed for single molecules adsorbed on metallic nanoparticles.

Surface enhanced Raman scattering (SERS) has been observed on polymer films, cast on silver nanostructures. Polymers as polybutadiene (PB), polybutadiene-block-polyisoprene (PB-b-PIP), poly(methyl methacrylate) (PMMA), and the elastomer polydimethylsiloxane (PDMS) were investigated. These materials present low fluorescence when illuminated with laser light of wavelength  $\lambda = 532$  nm, comparing to dye-molecules as Rhodamine 6G, usually used in SERS measurements. On the other hand, polymer molecules have long chains and may have many orientations close to rough metal surface. Therefore, averaged SERS spectra are expected for films. Nevertheless,

SERS spectra with spectral fluctuations and blinking were observed.

The highest Raman enhancements occur at the edges and corners of the metallic particles. The near-field enhancements obtained from FEM based calculations confirm the experimental observations.

O 53.13 Thu 18:00 SCH A215

**Energy dissipation during hyperthermal deposition of non-IPR fullerenes on HOPG** — STEFAN-SVEN JESTER, DANIEL LÖFFLER, PATRICK WEIS, ●ARTUR BÖTTCHER, and MANFRED KAPPE — Institut für Physikalische Chemie, Universität Karlsruhe, 76131 Karlsruhe, Germany

Low energy cluster beam deposition, LECBD, has been used to generate thin films comprising monodisperse non-IPR fullerenes,  $C_n$ ,  $50 < n < 60$ , on HOPG. The topography of the resulting  $C_n$  films has subsequently been studied by AFM. Deposition experiments were carried out at hyperthermal incident kinetic energies,  $E_0$  (1-40 eV) and elevated surface temperatures  $T_s$  (300-700 K). Initial sticking of  $C_n$  cages is governed by the lateral density of step edges, which act as pinning and nucleation centers for migrating cages. Thus, in the early deposition stages, the surface exhibits large areas of empty terraces, while the step edges themselves are well-decorated. The terraces in turn become decorated by dendritic  $C_n$  islands in later deposition stages. Both, the mean size of these 2D islands and the mean distance between nearest islands,  $\delta$ , scale with the size of the terraces. When increasing the primary kinetic energy, the fractal-like islands become smaller and less dendritic in shape. The mean initial sticking coefficient decays exponentially with increasing  $E_0$ . Instead of the dendritic islands generated at room temperature, densely packed islands terminated by smooth rims are observed at elevated temperatures. The findings are rationalized by a model which describes the friction-conditioned energy losses in the sliding movement of the cages on terraces.

O 53.14 Thu 18:15 SCH A215

**Pt dimers landing on Cu(001): an *ab initio* approach** — ●GEORGE PAL, GEORG LEFKIDIS, and WOLFGANG HÜBNER — Fachbereich Physik, Technische Universität Kaiserslautern, P.O.Box 3049, 67653 Kaiserslautern, Germany

We present real-space first-principles calculations for the adsorption of not only one but also two Pt clusters on a non-magnetic Cu(001) substrate. Considering that the interaction of adsorbates on surfaces is a local phenomenon, a representation of the substrate by a large cluster of 74 Cu atoms allows one to treat the electronic structures of both systems, i.e., the adsorbate and the surface, on equal footing. Using highly correlated quantum chemistry, we investigate different scenarios of soft-landing of Pt dimers on the substrate, for which we also optimize the Pt-Pt distance, and we compute the electronic excited states, which yields the optical absorption spectrum, on top of the electronic configuration at equilibrium geometry.

By analyzing the absorption spectra and the electronic densities of states we are able not only to characterize the interactions between the adsorbates and the substrate, but also to identify the surface-mediated interactions among the dimers. The latter is very important for technological applications since in experimental setups metallic substrates can alter the properties of the adsorbates, thus leading to new physics.

[1] Y. Pavlyukh, J. Berakdar and W. Hübner, Phys. Rev. Lett. **100**, 116103 (2008)

[2] G. Pal, G. Lefkidis and W. Hübner, submitted to J. Phys. Chem.

## O 54: Nano-optics of metallic and semiconducting nanostructures (experiments II)

Time: Thursday 15:00–18:30

Location: SCH A216

O 54.1 Thu 15:00 SCH A216

**Negative-index bi-anisotropic photonic metamaterial by direct laser writing and silver shadow evaporation** — ●MICHAEL S. RILL<sup>1</sup>, CHRISTINE E. KRIEGLER<sup>1</sup>, MICHAEL THIEL<sup>1</sup>, GEORG VON FREYMAN<sup>1,2</sup>, STEFAN LINDEN<sup>1,2</sup>, and MARTIN WEGENER<sup>1,2</sup> — <sup>1</sup>Institut für Angewandte Physik and DFG-Center for Functional Nanostructures (CFN), Universität Karlsruhe (TH), Wolfgang-Gaede-Str. 1, 76131 Karlsruhe — <sup>2</sup>Institut für Nanotechnologie, Forschungszentrum Karlsruhe in der Helmholtz-Gemeinschaft, 76021 Karlsruhe, Germany

Metamaterials are artificially fabricated structures composed of sub-

wavelength metallic building blocks (“photonic atoms”) that show – unlike natural substances – magnetism at optical frequencies [1].

Here, we present a novel blueprint of a negative-index metamaterial [2]. Our structure is realized using 3D direct laser writing, SiO<sub>2</sub> atomic layer deposition and silver shadow evaporation. The comparison of measured linear optical spectra with theory shows good agreement and reveals a negative real part of the refractive index  $n$  at around 3.85  $\mu\text{m}$  wavelength – despite the fact that the metamaterial structure is bi-anisotropic [3,4] due to the lack of inversion symmetry along its surface normal.

[1] V.M. Shalaev, Nature Photon. **1**, 41 (2007).

- [2] M.S. Rill *et al.*, Opt. Lett., accepted.  
 [3] M.S. Rill *et al.*, Nature Mater. **7**, 543 (2008).  
 [4] R. Marques *et al.*, Phys. Rev. B **65**, 144440 (2002).

O 54.2 Thu 15:15 SCH A216

**Surface enhanced infrared spectroscopy using interacting gold nanowires** — ●FRANK NEUBRECH<sup>1</sup>, DANIEL WEBER<sup>1</sup>, HONG SHEN<sup>2</sup>, MARC LAMY DE LA CHAPELLE<sup>3</sup>, and ANNEMARIE PUCCI<sup>1</sup> — <sup>1</sup>Kirchhoff-Institut für Physik, Heidelberg, Deutschland — <sup>2</sup>Universite Troyes, Troyes, France — <sup>3</sup>Universite Paris 13, Bobigny, France

We performed surface enhanced infrared spectroscopy (SEIRS) of molecules adsorbed on gold nanowires using synchrotron light of the ANKA IR-beamline at the Forschungszentrum Karlsruhe (Germany). Arrays of gold nanowires with interparticle spacings down to 30nm were prepared by electron beam lithography. The interparticle distance was reduced further by wet-chemically increasing the size of the gold nanowires. The growth of the wires was proofed using IR spectroscopy as well as scanning electron microscopy.

After this preparation step, appropriate arrays of nanowires with an interparticle distance down to a few nanometers were selected to demonstrate the surface enhanced infrared spectroscopy of one monolayer octadecanethiol (ODT). As know from SEIRS studies using single gold nanowires, the spectral position of the antenna-like resonance in relation to the absorption bands of ODT (2850cm<sup>-1</sup> and 2919cm<sup>-1</sup>) is crucial for both, the lineshape of the molecular vibration and the signal enhancement. In contrast to single nanowires studies, a further increase of the enhanced signals is expected due to the interaction of the electromagnetic fields of the close-by nanowires.

O 54.3 Thu 15:30 SCH A216

**Bimetallic core-shell nanoparticles: In-situ controlled manipulation of plasmonic properties and material composition** — ●THOMAS HÄRTLING<sup>1</sup>, NADJA C. BIGALL<sup>2</sup>, ALEXANDER EYCHMÜLLER<sup>2</sup>, and LUKAS M. ENG<sup>1</sup> — <sup>1</sup>Institut für Angewandte Photophysik, TU Dresden, 01062 Dresden — <sup>2</sup>Physikalische Chemie und Elektrochemie, TU Dresden, 01062 Dresden, Germany

Due to their distinct physical and chemical properties, metal nanoparticles are crucial components of various nanotechnological applications. For most of them, the particle material composition is a key parameter defining the optical, magnetic, and catalytic particle properties. Here we report on the in-situ controlled manipulation of this material composition at the surface of single bimetallic core-shell nanoparticles by optically induced metal deposition. Two strategies are followed to illustrate the capabilities of this photochemical approach. On the one hand, single core particles without a localized surface plasmon (LSP) resonance in the VIS are decorated with a plasmonically active shell, which renders the particles visible in the optical microscope. Vice versa, the light scattered from a LSP resonant particle is used to monitor the photochemical deposition of a nonresonant metal shell. These two approaches are demonstrated by the fabrication of Au@Pt and Cu@Au particles, respectively, leading to different, in-situ controlled optical and chemical particle properties. The presented method is applicable to an extremely wide range of material combinations and thus paves the way for the optically in-situ controlled fabrication and manipulation of multi-composite nanostructures.

O 54.4 Thu 15:45 SCH A216

**Wave-Particle Duality of Single Surface Plasmon Polaritons** — ●BERNHARD GROTZ<sup>1</sup>, ROMAN KOLESOV<sup>1</sup>, GOPALAKRISHNAN BALASUBRAMANIAN<sup>1</sup>, RAINER STÖHR<sup>1</sup>, AURÉLIEN NICOLET<sup>1</sup>, PHILIP HEMMER<sup>2</sup>, FEDOR JELEZKO<sup>1</sup>, and JÖRG WRACHTRUP<sup>1</sup> — <sup>1</sup>Physikalisches Institut, Universität Stuttgart, Germany — <sup>2</sup>Department of Electrical and Computer Engineering, Texas A&M University, College Station, USA

When light interacts with metal surfaces it excites electrons which can form propagating excitation waves called surface plasmon polaritons (SPP). These collective electronic excitations have many applications due to their ability to produce strong electric fields, localized to sub-wavelength distance scales. However many potential applications, in particular those related to quantum networks, require a deep understanding of fundamental quantum properties of SPPs. Remarkably these collective electron states preserve many key quantum mechanical properties of the original photons used to excite them, like entanglement and sub-poissonian statistics. Here we experimentally show that single surface plasmon polaritons also exhibit wave and particle properties similar to those of single photons. Furthermore, we demonstrate that a detailed analysis of spectral interference pattern provides

a new method to characterize dimensions of metallic waveguides with nanometer accuracy.

O 54.5 Thu 16:00 SCH A216

**Optical characterisation of ripple formation through oblique incidence ion sputtering of Ag(001)** — ●FRANK EVERTS, HERBERT WORMEESTER, and BENE POELSEMA — Solid State Physics, MESA+ Institute for Nanotechnology, University of Twente, Enschede, The Netherlands

Oblique incidence ion sputtering leads to the formation of ripple patterns on the surface of many materials. The temporal evolution of these ripple patterns can be measured in-situ with Reflection Anisotropy Spectroscopy (RAS). The periodicity of the ripple pattern supports the excitation of surface plasmons on a Ag(001) surface. This enables a rather straightforward interpretation of the measured optical spectrum. Ion sputtering at a polar angle of incidence with the normal of 70 deg. and beyond, provides a RAS spectrum that is characterized by a single peak, related to the periodicity between the ripples. Sputtering at a polar angle of incidence with the normal of 61 deg. also leads to an additional feature in the RAS spectrum that is attributed to an average periodicity of the ripple length, next to the peak that is related to the periodicity perpendicular to the ripples. The analysis of the optical spectra will be discussed in relation to the results of Low Energy Electron Diffraction (LEED) images obtained after sputtering.

O 54.6 Thu 16:15 SCH A216

**Photoluminescence enhancement of Sm<sup>3+</sup> ions in the vicinity of noble-metal nanoparticles** — ●FLORIAN HALLERMANN, ANDREAS SCHMITZ, and GERO VON PLESSEN — Institute of Physics (IA), RWTH Aachen University, 52056 Aachen, Germany

The photoluminescence intensity of an optical emitter changes when placed in close proximity to a noble-metal nanoparticle, due to two contributions. First, the optical near-field of the nanoparticle leads to a change in excitation rate of the emitter. Secondly, the emission efficiency is changed due to an optical energy transfer from the emitter to the metal nanoparticle, which provides additional radiative and non-radiative decay channels. In this work we investigate the photoluminescence of Sm<sup>3+</sup> ions, which are embedded in SiO<sub>2</sub>. The photoluminescence spectrum of ions in proximity to single silver and gold nanoparticles is measured. The influence of the spectral position of the nanoparticle plasmon peak on the photoluminescence yield will be discussed and compared with model calculations.

O 54.7 Thu 16:30 SCH A216

**Optical characterization of metal-dielectric-metal resonant systems** — ANDREAS ENGLISCH, ●STEFAN GRIESING, and UWE HARTMANN — Experimental Physics, Saarland University, P.O. Box 15 11 50, D-66041 Saarbrücken, Germany.

Reflectivity and Raman measurements were carried out on the sandwich systems consisting of substrate-metal mirror-dielectric 1/4 resonator-metallic thin film, introduced in [1]. The thickness of the metallic cover layer has been varied from 1nm to 40nm. Its morphology was investigated by SEM and AFM. Measurements showed that the reflectivity of the system can be dramatically reduced for a certain spectral region. For a given thickness of the dielectric layer, the system exhibits a close-to-zero reflectivity for a cover layer being just at the percolation threshold, corresponding to a mass thickness of about 3nm. By varying the thickness of the cover layer, the width and position of the spectral regime of decreased reflectivity can be tuned. In contrast, by varying the thickness of the dielectric layer at a given thickness of the cover layer, the spectral position of the reflectivity minimum can be shifted due to the 1/4 condition. Raman measurements carried out on optical systems with percolating metallic cover layer revealed an intensity enhancement of up to four orders of magnitude. This result is compared with a model based on the effective refractive indices of the individual layers and local field enhancements of the metallic nanoparticles.

[1] J. Sukmanowski et al., J. Appl. Phys. 97, 104332 (2005).

O 54.8 Thu 16:45 SCH A216

**Raman scattering from single gold nanostars** — ●CALIN HRELESCU, TAPAN K. SAU, ANDREY ROGACH, FRANK JÄCKEL, and JOCHEN FELDMANN — Photonics and Optoelectronics Group, Physics Department und CeNS, Ludwig-Maximilians-Universität München, Amalienstraße 54, 80799 München, Germany

We report on surface-enhanced Raman scattering (SERS) from single

star-shaped gold nanoparticles coated with self-assembled monolayers of 4-mercaptobenzoic acid. SERS is observed without the formation of gold nanoparticle aggregates or resonant excitation of the analyte. Total Raman scattering enhancement factors for single nanostars are comparable to those of nanoparticle assemblies exhibiting coupled plasmon resonances. This renders gold nanostars promising for Raman imaging applications in complex environments such as cells or membranes.

O 54.9 Thu 17:00 SCH A216

**Enhanced LED emission by metal nanoparticles** — ●TINO GÖHLER<sup>1</sup>, ANDREAS HILLE<sup>1</sup>, STEFAN GRAFSTRÖM<sup>1</sup>, LUKAS M. ENG<sup>1</sup>, and REINER WINDISCH<sup>2</sup> — <sup>1</sup>Technische Universität Dresden, 01069 Dresden, Germany — <sup>2</sup>OSRAM Opto Semiconductors GmbH, 93055 Regensburg, Germany

The external quantum efficiency of light emitting-diodes (LEDs) based on AlGaAs is limited by internal total reflection because of the of high refractive index ( $n=3.6$ ). Metal nanoparticles (MNPs) can be used as dipole scatterers in order to enhance the emission of LEDs.

We investigate the enhancement produced by single gold MNPs onto red LEDs ( $\lambda_{\text{emission}} = 645 \text{ nm}$  FWHM=20 nm) by using a confocal imaging set-up. The enhancement depends strongly on the particle size and on the surrounding medium (air  $n=1.0$ , immersion oil  $n=1.5$ ). While in air particles of all sizes investigated (80-150 nm) enhance the LED emission, we observed a strong size dependence when embedding the particle in immersion oil. Here, the surrounding medium shifts the plasmon resonance of the particles such that it overlays the LED emission spectrum for larger particles. Then absorption leads to suppression rather than enhancement of the emission.

O 54.10 Thu 17:15 SCH A216

**Phase contrast imaging in near-field superlensing** — ●THOMAS TAUBNER<sup>1,2</sup>, JON SCHULLER<sup>2</sup>, MARK BRONGERSMA<sup>2</sup>, CHRIS FIETZ<sup>3</sup>, GENNADY SHVETS<sup>3</sup>, and RAINER HILLENBRAND<sup>4</sup> — <sup>1</sup>I. Physikalisches Institut, RWTH Aachen, Germany — <sup>2</sup>Department of Material Science, Stanford University, USA — <sup>3</sup>Department of Physics, UT Austin, USA — <sup>4</sup>Max-Planck-Institut für Biochemie, Martinsried, Germany

Here we study the optical imaging properties of novel near-field imaging device called a SiC superlens. A superlens is a planar device that allows for subwavelength imaging by employing coupled surface waves on a thin slab of a negative-permittivity material. As opposed to previous intensity-only measurements, we now perform amplitude and phase-measurements of the near-fields in the image plane of a superlens by mapping the field distribution with a scattering-type near-field optical microscope (s-SNOM). When investigating the spectral properties of the SiO<sub>2</sub>/SiC/SiO<sub>2</sub> superlens, we observe a sign change in the phase of the transmitted near-fields when tuning the illumination wavelength over the superlenses resonance condition.

This change will be explained by the dispersion relation of the superlens, in combination with a fundamental interference effect. When operating a superlens off-resonance, the interference of evanescent fields causes the intensity contrast to decrease. This can be compensated for with phase-sensitive imaging to practically maintain the spectral range of high-resolution operation. Our results are important for future spectroscopic applications of superlenses and other devices such as hyperlenses or 2D plasmon lenses.

O 54.11 Thu 17:30 SCH A216

**Spectroscopy of Individual “Artificial Atoms”** — ●MARTIN HUSNIK<sup>1</sup>, NILS FETH<sup>1,2</sup>, MATTHIAS WOLFRAM KLEIN<sup>1</sup>, MICHAEL KÖNIG<sup>3</sup>, JENS NIEGEMANN<sup>3</sup>, KURT BUSCH<sup>2,3</sup>, STEFAN LINDEN<sup>1,2</sup>, and MARTIN WEGENER<sup>1,2</sup> — <sup>1</sup>Institut für Angewandte Physik, Universität Karlsruhe (TH), 76131 Karlsruhe, Germany — <sup>2</sup>Institut für Nanotechnologie, Forschungszentrum Karlsruhe in der Helmholtz-Gemeinschaft, 76021 Karlsruhe, Germany — <sup>3</sup>Institut für Theoretische Festkörperphysik, Universität Karlsruhe (TH), 76131 Karlsruhe, Germany

Metamaterials exhibiting a magnetic response at optical wavelengths have recently attracted much attention [1]. The magnetic response depends on both the design of the individual building blocks (“artificial atoms”) and on electromagnetic coupling effects between the “artificial atoms”. Thus for future developments, investigation of the individual “artificial atoms” is crucial.

Here, we present absolute extinction cross-section spectra of individual split-ring resonators (SRR) measured by means of a modulation

technique [2,3]. The extinction cross-section at the fundamental magnetic resonance is found to be eight times the geometrical area covered by the SRR. The experimental results are in excellent agreement with microscopic calculations and can be understood by a simple electric-circuit model.

- [1] V. M. Shalaev et al., Nature Photon. **1**, 41 (2007).
- [2] A. Arbouet et al., Phys. Rev. Lett. **93**, 127401 (2004).
- [3] M. Husnik et al., Nature Photon. **2**, 614 (2008).

O 54.12 Thu 17:45 SCH A216

**Transform limited focusing of few cycle optical pulses using all-reflective optics** — ●DIYAR SADIQ, BJOERN PIGLOSIEWICZ, MANFRED MASCHKE, WJATSCHESLAW SCHMIDT, ROBERT POMRAENKE, PARINDA VASA, and CHRISTOPH LIENAU — Institut für Physik, Carl von Ossietzky Universität, 26129 Oldenburg, Germany

The availability of high-intensity few-cycle optical pulses from turn-key laser oscillators is important for various applications in the emerging field of extreme nonlinear optics. This requires focussing few-cycle pulses down to - or even beyond - the diffraction limit. Using conventional microscope objectives this is highly challenging due to their complex spatio-temporal dispersion properties. All-reflective objectives, minimizing chromatic dispersion, are expected to have much more favorable focussing characteristics. So far, however, little is known about the spatio-temporal distribution of electromagnetic fields of few-cycle pulses in the focus of such an all-reflective-objective. Here, we demonstrate focussing 6-fs, 2.25-cycle optical pulses from an 80-MHz repetition rate Ti-sapphire oscillator down to a diffraction-limited spot size of less than  $1 \mu\text{m}$  while maintaining the pulse duration. Three-dimensional mapping of the spatial intensity profile near the focus is performed using a scanning near-field optical microscope. The time profile of the focussed pulse is characterized by interferometric autocorrelation measurements using second harmonic generation or - with sub-100-nm spatial resolution - using electron generation at sharp metallic tips. Progress towards direct space- and time-resolved electric field measurements will be reported.

O 54.13 Thu 18:00 SCH A216

**Near-field radiative heat transfer between a spheroid and a surface** — ●OLIVER HUTH, FELIX RÜTING, and SVEND-AGE BIEHS — Institut für Physik, Carl von Ossietzky Universität Oldenburg

A near-field scanning thermal microscope has been developed at Oldenburg University. This instrument measures the heat transfer between the tip of a sensor and the surface of a sample with a different temperature at nanometer distances. Our objective is to describe this near-field heat transfer theoretically, and to compare the theory to the measured data. To this end, the foremost part of the sensor can be modelled as a small sphere. Then the heat transfer between the sphere and the sample is calculated within the framework of Rytov's fluctuational electrodynamics. Actually, however, the shape of the sensor's tip deviates from a sphere, which requires more refined strategies for modelling the tip. An analytically tractable generalisation of the sphere model is obtained by considering general spheroids, which allows one to assess the influence of the tip's shape on the magnitude of the heat transfer. In this talk we present first results of such calculations, together with comparisons to results given by the sphere model.

O 54.14 Thu 18:15 SCH A216

**Near-field radiative heat transfer between a sphere and a nano-structured surface** — ●FELIX RÜTING, OLIVER HUTH, and SVEND-AGE BIEHS — Institut für Physik Carl von Ossietzky Universität Oldenburg

We study the near-field radiative heat transfer between a probe and a structured sample at nanometer distances. The probe is modeled as a nanosphere by means of a dipole model, while the surface of the sample is treated by a perturbative ansatz based on the Rayleigh hypothesis and the Ewald-Oseen theorem. We obtain characteristic signatures of the heat transfer between a sphere and a simple model geometry, computed numerically up to the second order in the profile. The validity of the approximations employed is ascertained. Furthermore, we show that signals measured with a near-field scanning thermal microscope (NSThM) operated in constant-distance mode are in good qualitative agreement with the theoretical results already to the first order in the surface profile, even though the theoretical model is subject to restrictions which are not obeyed in the experiment.

## O 55: Time-resolved spectroscopies II

Time: Thursday 15:00–16:15

Location: SCH A315

O 55.1 Thu 15:00 SCH A315

**Quantum-beat spectroscopy of image-potential resonances** — ●MANUEL MARKS, CHRISTIAN SCHWALB, KAI SCHUBERT, and ULRICH HÖFER — Fachbereich Physik und Zentrum für Materialwissenschaften, Philipps-Universität Marburg, D-35032 Marburg

Previous 2PPE studies of image-potential states on metal surfaces have largely concentrated on states that are located in a gap of the projected bulk band. In these cases, the states decay by inelastic electron-hole-pair excitation. In many situations of more practical interest, however, the resonant charge transfer at metal interfaces is more important. In this contribution we report the first results of a systematic 2PPE investigation of the image-potential states of Ag(111) where the states ( $n \geq 2$ ) are degenerate with the upper  $sp$ -band of the metal. Although one might expect a rapid delocalization of electrons excited to these image-potential resonances, a whole series could be observed by coherent excitation of resonances up to quantum number  $n = 7$ , just like in the well-studied case of the gap states of Cu(100). The binding energies  $E_n$  deduced from quantum-beat spectroscopy fit well to a Rydberg series with a quantum defect  $a = 0.062$ . The inelastic lifetimes of the resonances show good agreement with the  $n^3$ -scaling law. Surprisingly, the absolute values of the experimental lifetimes are longer than expected theoretically. A major difference between the Cu(100) image-potential states and the Ag(111) image-potential resonances is a considerably shorter dephasing time of the latter.

O 55.2 Thu 15:15 SCH A315

**Decoupling of image-potential states by Ne adlayers** — ●NICO ARMBRUST<sup>1</sup>, JENS GÜDDE<sup>1</sup>, ULRICH HÖFER<sup>1</sup>, and PETER FEULNER<sup>2</sup> — <sup>1</sup>Fachbereich Physik und Zentrum für Materialwissenschaften, Philipps-Universität Marburg, D-35032 Marburg — <sup>2</sup>Physik-Department E20, TU München, D-85748 Garching, Germany

The influence of neon adlayers on the image-potential states of Cu(100) has been investigated by time-resolved two-photon photoemission (2PPE). Ne represents a particularly interesting case for studies of the decoupling of image-potential states because its large negative electron affinity of -1.3 eV is expected to result in a large tunnelling barrier even for very thin Ne adlayers. We find that the adsorption of one monolayer of Ne reduces the binding energies of the first two image-potential states by about 30% to  $E_1 = 438$  meV and  $E_2 = 139$  meV and that the inelastic lifetime of the  $n = 1$  state increases from 40 fs to 300 fs. We compare these results with model calculations using a one-dimensional potential that has been developed for adlayers of the heavier rare-gases [1]. We further report on the observation of laser-induced desorption of the Ne films which is surprisingly efficient not only for the UV pump pulses ( $\hbar\omega_{UV} = 4.66$  eV), but also for the near-infrared probe pulses ( $\hbar\omega_{IR} = 1.53$  eV).

[1] W. Berthold *et al.*, Appl. Phys. A **78**, 131 (2004)

O 55.3 Thu 15:30 SCH A315

**The role of exchange scattering in the spin-dependent lifetime of hot electrons** — ●ANDREAS GORIS<sup>1,2</sup>, ILJA PANZER<sup>1,2</sup>, KRISTIAN DÖBRICH<sup>1</sup>, MARTIN PICKEL<sup>1</sup>, ANKE B. SCHMIDT<sup>3</sup>, MARKUS DONATH<sup>3</sup>, and MARTIN WEINELT<sup>1,2</sup> — <sup>1</sup>Max-Born-Institut, 12489 Berlin — <sup>2</sup>Freie Universität Berlin, 14195 Berlin — <sup>3</sup>Physikalisches Institut, Universität Münster, 48149 Münster

We have identified a  $\Delta_1$  surface resonance of minority character on cobalt thin films on Cu(001) at 0.45 eV below the Fermi level in spin-resolved photoemission and two-photon photoemission (2PPE) [1]. With a laser pulse ( $h\nu = 1.5$  eV) we excite electrons above the Fermi level and create photoholes in the surface resonance. A second UV laser pulse is used to probe lifetimes and spin-polarization of the excited electrons. While the hot electron lifetime shows only weak spin

dependence ( $\tau_{\uparrow} = 30$  fs;  $\tau_{\downarrow} = 22$  fs at  $E - E_F = 0.25$  eV), we find a long-living tail with predominantly majority character for energies up to 0.45 eV above  $E_F$ . By quenching the minority surface resonance with oxygen adsorption, the long-living tail of majority electrons vanishes. This strongly suggests that exchange scattering dominates hot electron decay and leads to the discrepancy between measured and calculated hot electron lifetimes [2,3]: the minority photohole is filled by a minority electron and in exchange a majority electron is excited above  $E_F$ , thereby adapting  $\tau_{\uparrow}$  and  $\tau_{\downarrow}$ .

[1] A. B. Schmidt *et al.*, J. Phys. D **41** No 16, 164003 (2008)[2] Aeschlimann *et al.*, Phys. Rev. Lett. **79**, 5158 (1997)[3] Zhukov *et al.*, Phys. Rev. Lett. **93**, 096401 (2004)

O 55.4 Thu 15:45 SCH A315

**Ultrafast dynamics of occupied quantum well states in Pb/Si(111)** — ●LAURENZ RETTIG, PATRICK S. KIRCHMANN, MARTIN WOLF, and UWE BOVENSIEPEN — Freie Universität Berlin, Fachbereich Physik, Arnimallee 14, 14195 Berlin

We investigated the ultrafast response of occupied quantum well states (QWS) in the two-dimensional model system Pb/Si(111) to an intense optical excitation using time-resolved photoemission spectroscopy (tr-PES). Employing pump photon energies of 1.5 eV and absorbed fluences up to  $200 \mu\text{J}/\text{cm}^2$  a significant part of the valence electrons can be excited. The effect on the QWS is probed with 6.0 eV photon energy. We find a pronounced shift of up to 40 meV of the binding energy of the highest occupied QWS to higher binding energies, i.e. an energetic stabilization. A detailed analysis reveals that this shift is established within the laser pulse duration of  $\sim 80$  fs where most of the excess energy resides in the electronic system. Therefore, this gain in binding energy can be attributed to an electronic effect. The shift can be explained by a transient reduction of the electronic screening of the ion core potentials due to the excitation of electrons into unoccupied parts of the discrete QWS band structure. This can lead to a spatial redistribution of the electron density within the metal film, hence reducing the electron density at the core sites. Furthermore, a careful analysis of the transient binding energy reveals a small (2 meV) periodic modulation of the binding energy at a frequency of 2.18(5) THz which we attribute to a coherent longitudinal high energy phonon excitation within the lead film.

O 55.5 Thu 16:00 SCH A315

**Unoccupied band-structure and hot electron lifetimes in Pb quantum-wells** — ●ANDREAS RUFFING<sup>1</sup>, STEFAN MATHIAS<sup>1</sup>, FREDERIK DEICKE<sup>1</sup>, MARTIN WIESENMEYER<sup>2</sup>, MICHAEL BAUER<sup>2</sup>, and MARTIN AESCHLIMANN<sup>1</sup> — <sup>1</sup>Department of Physics and Research Center OPTIMAS, University of Kaiserslautern, 67633 Kaiserslautern — <sup>2</sup>Institut für Experimentelle und Angewandte Physik, Christian-Albrechts-Universität zu Kiel, D-24908 Kiel, Germany

Metallic quantum wells (QW) have been studied extensively in the recent past motivated by their potential to tune condensed matter properties via control of the quantum mechanical boundary conditions in these low-dimensional systems. Additional to the tuneability, these systems show interesting features in the electronic structure, such as avoided crossings, band gaps or modifications due to interaction with the substrate. All these features dominantly influence the decay dynamics of excited carriers. Our goal is to gain further knowledge in femtosecond hot electron dynamics by investigating these electronic features with time-resolved two-photon photoemission (2PPE) and a two-dimensional analyzer for parallel energy ( $E$ ) and momentum ( $k_{\parallel}$ ) detection. A prominent example of these systems are thin Pb films, which we investigated on a Cu(111) substrate. We will show the unoccupied band structure and discuss the according electron dynamics by means of angular resolved hot electron lifetime maps  $\tau(E, k_{\parallel})$ .

## O 56: Metal substrates: Epitaxy, growth and adsorbates

Time: Thursday 15:00–19:15

Location: SCH A316

O 56.1 Thu 15:00 SCH A316

**The Cu(110) surface state anisotropy as a probe for the initial stages of homoepitaxial growth** — ●MICHAEL HOHAGE, LIDONG SUN, ALEXANDER DORNINGER, and PETER ZEPPENFELD — Institut für Experimentalphysik, Johannes Kepler Universität Linz, A-4040 Linz, Austria

Reflectance Difference Spectroscopy (RDS) revealed that the Cu(110) surface state anisotropy is an extremely sensitive probe to study adsorption and growth. The high sensitivity originates from the quenching of surface state contribution to the optical anisotropy at 2.1 eV, due to surface state scattering at adsorbates or point defects. Here, we apply this phenomenon to the investigation of the homoepitaxial growth of Cu on Cu(110). The transition from a step-flow growth at high temperatures to a 3D-island growth and finally to a re-entrant layer-by-layer growth at low temperatures can be easily observed. In addition, we were able to study the morphological changes occurring upon annealing after depositing 0.04 ML Cu at 10 K, by monitoring the partial recovery of the surface state anisotropy. The recovery proceeds mainly in two steps: (i) the onset of the adatom diffusion and nucleation of tiny clusters (90 K to 120 K) and (ii) the onset of adatom detachment and ripening of the clusters (> 190 K). Detailed analysis of the data with the help of a kinetic-Monte-Carlo code allows simulating the experimental results quantitatively and permits to quantify the effective cross-section of small ad-clusters for depolarization of the surface state.

O 56.2 Thu 15:15 SCH A316

**Evidence for Cu dimer mobility on Cu(001)** — ●ANJA MICHL, ANDREAS DOBLER, and THOMAS FAUSTER — Lehrstuhl für Festkörperphysik, Universität Erlangen-Nürnberg, Staudtstr. 7, 91058 Erlangen  
We investigated the homoepitaxial submonolayer growth of Cu on Cu(001) at 300 K. The density of stable Cu islands  $n_x$  was measured by scanning tunneling microscopy after thermal deposition at pressures below  $5 \times 10^{-11}$  mbar.

Variation of coverage  $\theta$  and particle flux  $F$  lead to a characteristic behavior of  $n_x \propto \theta^{0.20 \pm 0.05}$  for  $\theta \leq 0.11$  ML and  $n_x \propto F^{0.40 \pm 0.02}$  at saturation for  $F = 10^{-5}$  to  $10^{-2}$  ML/s. This result is not compatible with standard models of nucleation which predict an exponent  $i/(i+2)$  for the flux dependence with the atom number  $i$  of the largest unstable islands.

A recent theoretical study [1] concludes that dimer mobility is dominant at 300 K in the experimentally available range of flux. The predicted behavior  $n_x \propto \theta^{1/5}$  and  $n_x \propto F^{2/5}$  is in excellent agreement with our experimental results.

[1] P. A. Mulheran and M. Basham, Phys. Rev. B **77** (2008) 075427

O 56.3 Thu 15:30 SCH A316

**Non adiabatic processes during homoepitaxy of silver and gold films** — ●DOMOCOS KOVACS<sup>1</sup>, ECKART HASSELBRINK<sup>2</sup>, and DETLEF DIESING<sup>2</sup> — <sup>1</sup>Institut für Experimentalphysik, Universität Duisburg Essen — <sup>2</sup>Institut für Physikalische Chemie, Universität Duisburg Essen

Thin film metal-insulator-metal (MIM) tunnel junctions have been employed in the last years in the investigation of electronic excitations induced by particles at metal surfaces. Such type of junctions act simultaneously as target and detector: While the electronic excitation is produced by the irradiation of the top metal layer, the excited charge carriers (electrons and holes) are detected in the bottom metal layer as an internal emission current. A major advantage offered by the present method in comparison with the methods measuring the external emission is the possibility of detecting excited charge carriers of very low energy (< 5 eV). We show that a MIM junction is suitable for the investigation of the electronic effects accompanying the adsorption of metal atoms from the gas phase onto the surface of a metal film consisting of the same atomic species. Thus, we show that the adsorption of Au(Ag) Atoms at the surface of the top Au(Ag) film of a Au(Ag)-TaO<sub>x</sub>-Ta tunnel junction generates hot charge carriers which are finally detected in the bottom Ta film. The relatively large emission yield, of the order of  $10^{-4}$  electrons per incident atom, measured for 15-20 nm Au(Ag) films, indicates that the binding energy of 3-4 eV/atom, released during adsorption, is primarily transferred into the electronic system.

O 56.4 Thu 15:45 SCH A316

**The temperature dependence of film stress in epitaxial Co monolayers on Pt(111)** — ●SAFIA OUAZI<sup>1,2</sup>, ZHEN TIAN<sup>2</sup>, ANITA DHAKA<sup>2</sup>, DIRK SANDER<sup>2</sup>, HARALD BRUNE<sup>1</sup>, and JÜRGEN KIRSCHNER<sup>2</sup> — <sup>1</sup>Institut de Physique des Nanostructures, EPFL, Station 3, CH-1015 Lausanne, Switzerland — <sup>2</sup>Max-Planck-Institut für Mikrostrukturphysik, Weinberg 2, D-06120 Halle, Germany

We perform combined stress and low energy electron diffraction (LEED) studies to investigate the correlation between film strain and stress during the deposition of several monolayer thin Co films on Pt(111) in the temperature range 250 to 400 K. The quantitative analysis of our cantilever stress measurements indicates a tensile stress of +4.3 GPa in the thickness range between 3 to 7 ML for the investigated growth temperature range. LEED indicates a Moiré-like diffraction pattern, where our quantitative analysis of the in-plane lattice spacing gives a film strain of +1.2% from 1 to 7 ML. We apply continuum elasticity and calculate +5 GPa for the strain-induced film stress, in close agreement with the experimental value. In thinner films, the measured film stress is found to depend sensitively on the growth temperature. We ascribe this strong temperature dependence of the initial stress to the thermally activated Co incorporation into Pt, which relieves surface stress. We discuss our results in view of STM [1], LEED [2], and SXRD[3] studies, and indicate the implication of Pt-Co intermixing for the magnetic anisotropy of this system.

[1] Varga et al., phys. Stat. sol. 187 (2001) 97 [2] Tsay et al., Surf. Sci. 96 (1998) 313 [3] Ferrer et al., Phys. Rev. B 56 (1997) 9848

O 56.5 Thu 16:00 SCH A316

**Growth of ultra-thin Ag films on Ni(111)** — ●AXEL MEYER<sup>1</sup>, JAN INGO FLEGE<sup>1</sup>, SANJAYA SENANAYAKE<sup>2</sup>, FAISAL ALAMGIR<sup>3</sup>, and JENS FALTA<sup>1</sup> — <sup>1</sup>Institute of Solid State Physics, University of Bremen, 28359 Bremen, Germany — <sup>2</sup>Chemistry Department, Brookhaven National Laboratory, Upton, NY 11973-5000, USA — <sup>3</sup>Georgia Institute of Technology, Atlanta, GA 30332-0245, USA

The physical and chemical properties of ultra-thin metal films on metallic substrates strongly depend on their morphology and the structure of the buried interface. Hence, detailed knowledge of the growth mechanisms is essential for the creation of new functional materials with novel characteristics. In this contribution, we present a comprehensive structural study of the growth and properties of epitaxial Ag films on Ni(111) by in-situ low energy electron microscopy (LEEM).

For lower temperatures, the growth of the Ag film proceeds in a Stranski-Krastanov mode after completion of the wetting layer, while for higher temperatures layer-by-layer growth is observed. Quantitative information about the film structure were obtained by analyzing the intensity-voltage (I-V) dependence of the local electron reflectivity (IV-LEEM). The corresponding I(V) spectra showed intensity oscillations depending on local thickness of the Ag film due to the quantum size effect (QSE). Modeling of the I(V) spectra was performed both within the framework of a one-dimensional Kronig-Penney model and multiple scattering IV-LEED calculations. The results of both approaches concerning the variation of the layer spacings and interface characteristics for different temperatures and film thicknesses will be discussed.

O 56.6 Thu 16:15 SCH A316

**Floating of PtRu and PdRu surface alloys on Ru(0001) studied by STM and AES** — ●ANDREAS BERGBREITER, HARRY E. HOSTER, and R. JÜRGEN BEHM — Institute of Surface Chemistry and Catalysis, Ulm University, D-89069 Ulm

According to previous studies by scanning tunnelling microscopy (STM) with chemical contrast and Auger electron spectroscopy (AES), deposition of submonolayer Pt (Pd) on Ru(0001) and subsequent annealing to  $T = 1300$  K (1150 K) results in atomically smooth and laterally equilibrated PtRu (PdRu) surface alloys on Ru(0001) confined to the outermost layer [1]. To verify whether or not these surface alloys reflect local equilibrium, the prepared alloys were deliberately buried by > 1 ML of vapor deposited Ru. After surface analysis by STM and AES, these samples were again annealed to the respective surface alloy formation temperature. Both STM and AES confirm that the initially formed surface alloy is recovered by this final annealing step, i.e., both types of surface alloys exhibit a surfactant-like floating

behavior. We discuss, in how far this behaviour depends on the transport mechanism involved in the surface alloy formation process, and for which types of surface alloys a similar inherent stability is to be expected.

[1] H.E. Hoster et al., Phys.Chem.Chem.Phys. 10 (2008) 3812.

O 56.7 Thu 16:30 SCH A316

**Atom distribution and interactions in  $\text{Ag}_x\text{Pt}_{1-x}$  and  $\text{Au}_x\text{Pt}_{1-x}$  surface alloys on Pt(111)** — ●RALF T. RÖTTER, ANDREAS BERGBREITER, HARRY E. HOSTER, and R. JÜRGEN BEHM — Institute of Surface Chemistry and Catalysis, Ulm University, D-89069 Ulm

The atom distributions in  $\text{Ag}_x\text{Pt}_{1-x}/\text{Pt}(111)$  and  $\text{Au}_x\text{Pt}_{1-x}/\text{Pt}(111)$  surface alloys were studied by high resolution UHV-STM. These surfaces were prepared by submonolayer Ag (Au) metal deposition on Pt(111), followed by annealing at 900 K or 1000 K, respectively, which in both cases results in surface confined 2D alloys, with equilibrated distribution of the components. Both systems show a tendency towards two-dimensional clustering, which fits well to their known bulk immiscibility. Effective cluster interactions (ECIs) will be derived by a quantitative evaluation of the 2D atom distributions in the surface alloys [1]. By comparing the ECIs for PtAg and PtAu on Pt(111), and considering that Ag and Au have almost similar lattice constants, the results allow conclusion on the physical origin of the tendency for clustering.

[1] A. Bergbreiter et al., Phys.Chem.Chem.Phys. 9 (2007) 5127.

O 56.8 Thu 16:45 SCH A316

**Growth on nanopatterned gold surfaces** — ●YASMINE NAHAS<sup>1,2</sup>, VINCENT REPAIN<sup>1</sup>, and SYLVIE ROUSSET<sup>1</sup> — <sup>1</sup>Laboratory Material and Quantum Phenomena, University Paris 7, UMR 7162, 10 rue Alice Domon et Léonie Duquet, 75205 Paris, France — <sup>2</sup>Physikalisches Institut, Universität Karlsruhe (TH), Wolfgang-Gaede-Str., D-76131, Karlsruhe, Germany

The magnetic properties of nanometer size objects cause a large interest in technological applications as well as in the fundamental point of view. Ordered growth allows to obtain controlled size and density structures, as shown by the Co/Au(788) system and others [1]. Although basic mechanisms for this ordered growth have been found out, the complexity of atomistic processes on surfaces (and especially on nanopatterned ones) makes the behaviour of such system generally very surprising. I will show variable temperature experiments of the growth of various elements (Fe, Pt, Co, Au) on different naturally patterned surfaces (Au(111) and Au(788)). I will extract some common features to these systems but I will also explain how the thermodynamic properties of each element (crystallographic phase, lattice parameter, binary phase diagram ...) have a strong influence on some characteristics of the nucleation and growth process. Finally, results on the ordered growth of codeposited iron and platinum atoms will be shown. Different experiments varying the relative concentration of iron and the substrate temperature will be discussed in the framework of the nucleation and growth kinetic theory.

[1] V. Repain et al., J. Phys.: Condens. Matter. 18 (2006) S17-S28

O 56.9 Thu 17:00 SCH A316

**Novel mechanism of growth of atomic wires on (110) surfaces driven by intermixing** — OLEG V. STEPANYUK<sup>1</sup>, ●NIKOLAY N. NEGULYAEV<sup>2</sup>, PAVEL A. IGNATIEV<sup>3</sup>, MAREK PRZYBYLSKI<sup>3</sup>, WOLFRAM HERGERT<sup>2</sup>, ALEXANDER M. SALETSKY<sup>1</sup>, and JÜRGEN KIRSCHNER<sup>3</sup> — <sup>1</sup>Faculty of Physics, Moscow State University, 119899 Moscow, Russia — <sup>2</sup>Fachbereich Physik, Martin-Luther-Universität, D06099 Halle, Germany — <sup>3</sup>Max-Planck-Institut für Mikrostrukturphysik, D06120 Halle, Germany

We reveal a novel mechanism of nanowire growth on fcc (110) metal surfaces, which is promoted by interface intermixing of deposited and substrate atoms. We present a theoretical investigation of the self-assembly of 1D nanostructures during room temperature thermal deposition of Fe and Co atoms on Pd(110) in the sub-monolayer regime. Calculations performed by means of density functional theory demonstrate that incorporation of the deposited Fe (Co) atoms into the top-most substrate layer is energetically and kinetically feasible at room temperature. Kinetic Monte Carlo simulations based on ab initio calculated diffusion barriers of relevant atomic processes indicate that the surface diffusion of expelled substrate atoms is responsible for the growth of atomic wires consisting mainly of Pd atoms. We suggest that

scanning tunneling spectroscopy could allow to distinguish between Fe (Co) and Pd atomic chains on Pd(110) to confirm our predictions.

O 56.10 Thu 17:15 SCH A316

**Kinetic Monte Carlo Simulations of Temperature Programmed Desorption** — ●THOMAS FRANZ — Faculty of Physics, University of Vienna

We present a simulation of Temperature Programmed Desorption (TPD) experiments using single- and multi-site models on the basis of Density Functional Theory (DFT) calculations. The system under consideration was O/Rh(111), for which adsorption in both fcc and hcp hollow sites was taken into account. The lateral interactions of the adsorbed oxygen atoms were determined by fitting to a set of DFT energies. The calculations of these energies were performed using the Vienna ab-initio simulation package (VASP). Applying Cross Validation, we maximized the predictive power of our parametrization. The calculated desorption spectra were compared with experimental data. We found that for the investigated system the application of a multi-site model is necessary to obtain good agreement with experiment.

O 56.11 Thu 17:30 SCH A316

**First-principles initial sticking coefficient for  $\text{O}_2$  at Pd(100)** — ●JÖRG MEYER and KARSTEN REUTER — Fritz-Haber-Institut, Faradayweg 4-6, D-14195 Berlin (Germany)

Although the first steps in the oxidation of metal surfaces are of fundamental importance e.g. in heterogeneous catalysis, first-principles investigations of the sticking behavior of oxygen molecules are still scarce and center on simple metals like Al(111) [1]. To address catalytically much more interesting transition metals, we apply a divide and conquer approach [2] to study sticking of oxygen on Pd(100): First, an analytical six dimensional potential energy surface (PES) is generated using a neural network to interpolate between several thousand energy data points obtained from density-functional theory in the generalized gradient approximation. After that, the initial sticking  $S_0$  as a function of initial kinetic energy  $E_0$  of the impinging oxygen molecules is calculated by evaluating a sufficiently large number of classical molecular dynamics trajectories on the previously constructed PES. We detail on technical aspects of the employed interpolation strategy, focussing on how symmetry of the (100) surface is exploited to reduce the necessary amount of input data and optimize the interpolation quality. In light of the good agreement of the obtained sticking curve  $S_0(E_0)$  with the sparse experimental data, we critically discuss the employed frozen-surface approximation and the importance of electronically non-adiabatic effects for this system.

[1] J. Behler et al., Phys. Rev. Lett. **94** (2005) 036104.

[2] A. Gross, Surf. Sci. Rep. **32** (1998) 291.

O 56.12 Thu 17:45 SCH A316

**Adsorption induced surface stress change of O and H on Pt(111)** — ●ZHEN TIAN, DIRK SANDER, and JÜRGEN KIRSCHNER — Max-Planck Institute of Microstructure Physics, 06120, Halle, Germany

Surface stress changes induced by adsorption of oxygen and hydrogen on clean Pt(111) surface are measured in a UHV system with an optical beam bending method. Combined low energy electron diffraction (LEED) and stress measurements identify a compressive surface stress change of  $-2.2$  N/m upon formation of a p(2×2)-O structure for an exposure of 120 L oxygen at  $5 \times 10^{-7}$  mbar at room temperature. The exposure of clean Pt(111) to  $\text{H}_2$  at  $P_{\text{H}_2} = 5 \times 10^{-7}$  mbar leads to a compressive surface stress change of  $-0.5$  N/m, which saturates after 5 L. We found that the magnitude of the H-induced surface stress change depends on the  $\text{H}_2$  partial pressure. Exposure at higher partial pressure induces larger compressive stress change, e.g. partial pressure of  $P_{\text{H}_2} = 5 \times 10^{-6}$  mbar induces a compressive stress change of  $-0.73$  N/m. These results are discussed in view of other experimental studies on surface stress[1] and calculations[2] on adsorbate-induced surface stress of Pt(111).

[1] A. Grossmann, W. Erley, and H. Ibach, Surf. Rev. Lett. **2** (1995) 543. [2] P. J. Feibelman, Phys. Rev. B, **56** (1997) 2175.

O 56.13 Thu 18:00 SCH A316

**Influence of C-adsorption on the segregation profile of  $\text{Pt}_{25}\text{Rh}_{75}(100)$**

— ●WOLFGANG LANDGRAF, TOBIAS KERSCHER, and STEFAN MÜLLER — Universität Erlangen-Nürnberg, Lehrstuhl für Theoretische Physik 2, Staudtstr. 7, D-91058 Erlangen

As found earlier by experiment [1] and theory [2], the (100) and (111) surfaces of the alloy system  $\text{Pt}_{25}\text{Rh}_{75}$  show a strong Pt enrichment in the top atomic layer and a Pt depletion in the layer underneath. However, from experiment [1], it appears that for the (100) orientation even a small amount of carbon impurity leads to a considerable decrease in the Pt top layer concentration. We applied density functional theory to analyze quantitatively the influence of C-adsorption on the segregation profile of  $\text{Pt}_{25}\text{Rh}_{75}(100)$ . Indeed, we find that the segregation profile tremendously change as function of the C-coverage: Already at  $\Theta = 0.5$  the configuration being lowest in energy consists of carbon atoms in hollow sites and pure Rh-layers in the near surface regime. The correlations between structural and energetic properties will be discussed. The corresponding energetics can be used for the construction of a cluster expansion Hamiltonian in order to predict the alloy's most stable segregation profile for arbitrary carbon coverage. Supported by Deutsche Forschungs-Gemeinschaft

[1] E. Platzgummer et al., Surf. Sci. **419**, 236 (1999).

[2] S. Müller, M. Stöhr, O. Wieckhorst, Appl. Phys. A. **82**, 415 (2006).

O 56.14 Thu 18:15 SCH A316

**CuO: template and/or surfactant** — ●THORSTEN WAGNER, THOMAS BRANDSTETTER, MARTIN OEHZELT, and PETER ZEPPEFELD — Johannes Kepler Universität Linz, Altenberger Str. 69, A-4040 Linz, Österreich

The Cu(110) surface can be structured readily by adsorbing oxygen: If the coverage of oxygen is less than  $\theta = 0.5$ , the  $(2 \times 1)$  reconstructed areas form stripes which are separated by unreconstructed copper areas. These stripes are uniformly distributed and parallel to the  $[001]$ -direction. To extend this one-dimensional template to a two-dimensional array we studied the adsorption of oxygen on a vicinal Cu(19191) surface by means of STM. The steps of this surface are perpendicular to the oxygen stripes. However, the formation of the oxygen reconstruction leads to step bunching and individual terraces are significantly broadened. Therefore the periodicity of the copper template is reduced.[1,2]

On the vicinal and the low index copper surface which were pre-structured by the CuO stripe phase silver was adsorbed at 660K. Although more than a monolayer of silver was added, the total area covered by the CuO phase was preserved. By means of STM, PEEM, and AES we have determined that the step bunches (forming (111) facets on the vicinal surface) are covered by silver. The experimental results suggest that CuO is acting as a surfactant.

[1] T. Brandstetter *et al.*, Phys. Rev. B **78** (2008) 075402

[2] T. Brandstetter *et al.*, Phys. Rev. B **76** (2007) 245420

O 56.15 Thu 18:30 SCH A316

**In-situ X-ray Study of the Oxidation of vicinal NiAl(671)** — ●CLAUS ELLINGER, VEDRAN VONK, NAVID KHORSHIDI, ANDREAS STIERLE, and HELMUT DOSCH — Max-Planck-Institut für Metallforschung, Heisenbergstr. 3, D-70569 Stuttgart

Vicinal surfaces with a regular stepped pattern are used to tailor the growth of oxide films or other epitaxial grown materials. In order to study the role of surface steps and kinks on the oxidation behaviour we investigated a vicinal NiAl(6,7,1) surface consisting of (110) terraces. It was chosen as the flat, oxidized NiAl(110) serves as important template for model catalysts and a tailoring of the ultra-thin alumina film

would open new ways for the growth of nano particles or nanowires. In the presented surface x-ray diffraction study we show that the regular stepped surface is preserved during the initial exposure of  $10^{-6}$  mbar of oxygen at 540 K while the formation of large (110) facets is observed during the annealing process. Thereby the faceting is induced by the ordering of the alumina. In addition, the preferential oxide growth of one out of two possible twin domains is found, probably caused by stress relief at the step edges of the vicinal surface.

O 56.16 Thu 18:45 SCH A316

**Dissociative adsorption of methane on surface oxide structures of PdPt alloys** — ●AREZOO DIANAT<sup>1</sup>, NICOLA SERIANI<sup>2</sup>, MANFRED BOBETH<sup>1</sup>, WOLFGANG POMPE<sup>1</sup>, and LUCIO COLOMBI CIACCHI<sup>3</sup> — <sup>1</sup>Institute for Materials Science, Dresden University of Technology, Germany — <sup>2</sup>Fakultät für Physik, Universität Wien, Austria — <sup>3</sup>Faculty of Production Engineering, University of Bremen, Germany

Oxides of Pd and Pt are known for their high activity in the catalytic combustion of methane. It was reported that bimetallic Pd-Pt oxide systems exhibit higher activity for  $\text{CH}_4$  combustion than PdO. To get some insight into the catalytic activity of PdPt we have studied the dissociative adsorption of  $\text{CH}_4$  on oxidised PdPt surfaces using DFT. First, the stability of various surface oxides was investigated, including oxygen adsorbed on the surface, subsurface oxygen, and thin oxide films. As base structures for the thin oxide films we have chosen PdO(101)/Pd(100),  $\alpha$ -PtO<sub>2</sub>/Pt(111) and Pt<sub>3</sub>O<sub>4</sub>/Pt(100), which show small lattice misfit between film and substrate. Adsorption energies for oxygen on the PdPt surface and in subsurface positions are higher than on the monometals. For thin oxide films, doping of Pd or Pt results in lower mean oxygen binding energies compared to pure Pd and Pt oxide films. The decomposition of  $\text{CH}_4$  to  $\text{CH}_3$  and H has been found to be endothermic on metal surfaces, but it becomes exothermic on oxidised surfaces. Among the considered monometallic oxide structures, Pt<sub>3</sub>O<sub>4</sub>/Pt(100) shows the highest  $\text{CH}_4$  adsorption energy. For some of the bimetallic oxide configurations considered, the  $\text{CH}_4$  adsorption energy was found to be higher than on the monometallic oxides.

O 56.17 Thu 19:00 SCH A316

**The Interaction of Hydrogen with the Cobalt(0001) Surface** — ZITA HÜSGES and ●KLAUS CHRISTMANN — Institut für Chemie und Biochemie der FU Berlin, 14195 Berlin

We report latest data on the interaction of hydrogen with the hexagonal Co(0001) surface in the temperature range between 90 K and 600 K as obtained by means of LEED, thermal desorption spectroscopy (TDS) and work function change measurements. Expectedly, hydrogen adsorbs spontaneously and dissociatively with an initial sticking probability around 0,1. The H atoms form two binding states having desorption energies between 80 and 100 kJ/mole. Interestingly, H adsorption causes only a slight decrease of the work function between 10 and 17 meV near saturation ( $\sim 0.7$  ML). Most notably, a H-induced  $c(2 \times 2)$  LEED phase forms around half a monolayer coverage, similar to the H/Ni(111) system. T and coverage dependent LEED intensity measurements suggest a critical temperature of the ordered H phase of about 240 K and a strongly asymmetric phase diagram that points to a H honeycomb structure. Our data will be discussed and compared with previous work on Co(0001)/H and on Ni(111)/H.

## O 57: Focused Session: Spin-Orbit Interaction at Surfaces: From the Rashba Effect to Topological States of Matter II

Time: Thursday 15:00–19:00

Location: HSZ 02

### Topical Talk

O 57.1 Thu 15:00 HSZ 02

**Rashba-type spin-orbit effects by spin-resolved photoemission** — ●OLIVER RADER — Helmholtz-Zentrum Berlin

In order to create spin currents in a solid, the Rashba effect can be instrumental. It requires neither a ferromagnetic material nor external magnetic fields. In this talk, we show that a quantum cavity for spin can be constructed from metals. Spin- and angle-resolved photoemission is used to study the dependence of the spin-orbit splitting of quantum-well states on parameters such as momentum and atomic number. In this context, we will also discuss the perspectives of graphene for spintronics.

### Topical Talk

O 57.2 Thu 15:30 HSZ 02

**Quantum spin Hall phases and topological surface states** — ●SHUICHI MURAKAMI — Department of Physics, Tokyo Institute of Technology, Tokyo, Japan — PRESTO, JST

Triggered by the research of the spin Hall effect [1], quantum spin Hall (QSH) effect [2,3] is studied intensively in recent years. The QSH system is an insulator in the bulk, while the boundary (i.e. edge in 2D and surface in 3D) supports gapless states carrying spin currents due to spin-orbit coupling. These edge or surface states remain gapless, and are robust against nonmagnetic impurities and surface roughness.

This robustness stems from bulk topological order characterized by the  $Z_2$  topological number. Namely, the bulk topological properties become manifest as an existence of the gapless boundary states.

The QSH effect occurs under a zero magnetic field unlike the quantum Hall effect. In some materials this effect occurs in nature without applying fields, as demonstrated theoretically and experimentally. In my talk I explain our theoretical proposal that the (111)1-bilayer bismuth ultrathin film shows the QSH effect [4]. I also discuss strategies to search for candidate materials showing the QSH effect.

[1] S. Murakami, N. Nagaosa, and S.-C. Zhang, *Science* 301, 1348 (2003). [2] C. L. Kane and E. J. Mele, *Phys. Rev. Lett.* 95, 146802; *ibid.* 95, 226801 (2005). [3] B. A. Bernevig and S.-C. Zhang, *Phys. Rev. Lett.* 96.106802 (2006). [4] S. Murakami, *Phys. Rev. Lett.* 97, 236805 (2006).

### Topical Talk

O 57.3 Thu 16:00 HSZ 02

**Observation of a new topological phase of quantum matter : Quantum Hall-like effect without magnetic field.** — ●ZAHID HASAN — Princeton University, Princeton, New Jersey, USA

Most quantum states of condensed-matter are categorized by the spontaneously broken symmetries. The remarkable discovery of charge quantum Hall effects (1980s) revealed that there exists an organizational principle of matter based not on the spontaneously broken symmetry but only on the topological distinctions in the presence of time-reversal symmetry breaking. In the past few years, theoretical developments suggest that new classes of topological states of matter might exist that are purely topological in nature in the sense that they do not break time-reversal symmetry hence can be realized without any applied magnetic field : "Quantum Hall-like effects without magnetic field". In this presentation, I report a series of experimental results documenting and demonstrating the existence of such a topologically ordered time-reversal-invariant state of matter and discuss the exotic electromagnetic and spin properties this novel phase of quantum matter might exhibit and outline their potential use.

O 57.4 Thu 16:30 HSZ 02

**Rashba type spin-orbit splitting of quantum well states in ultrathin Pb films** — ●HUGO DIL<sup>1,2</sup>, FABIAN MEIER<sup>1,2</sup>, JORGE LOBO-CHECA<sup>3</sup>, LUC PATTHEY<sup>2</sup>, GUSTAV BIHLMAYER<sup>4</sup>, and JÜRIG OSTERWALDER<sup>1</sup> — <sup>1</sup>Universität Zürich, CH — <sup>2</sup>Swiss Light Source, CH — <sup>3</sup>Universität Basel, CH — <sup>4</sup>Forschungszentrum Jülich, D

When the thickness of a metal layer approaches the electron coherence length, quantum well states (QWS) may form in the layer. It has been shown previously that QWS may show a spin splitting due to hybridization with interface[1] or surface states[2], which either decays with layer thickness or is sensitive to contamination. Here we will report the first observation of an intrinsic Rashba type spin-orbit splitting in metallic QWS by spin and angle-resolved photoemission[3]. The resulting band splitting is too small to be detected by spin integrated ARPES and highlights the possibilities of state-of-the-art spin resolved ARPES. It will be shown that the spin-orbit interaction takes place throughout the whole layer, but that the necessary asymmetry is induced by the two interfaces of the film. This opens up the possibility to manipulate the effect by interface engineering.

[1] C. Koitzsch et al. *PRL* 95, 126401 (2005)  
 [2] K. He et al. *PRL* 101, 107604 (2008); E. Frantzeskakis et al. *PRL* 101, 196805 (2008)  
 [3] H. Dil et al. *PRL* in press

O 57.5 Thu 16:45 HSZ 02

**Relativistic effects in the surface emission of layered intermetallic systems** — ●JURGEN BRAUN, JAN MINAR, SVEN BORNEMANN und HUBERT EBERT — Dep. Chemie und Biochemie, LMU München, Germany

In the framework of the fully relativistic version of the one-step model, the photoemission intensities resulting from layered intermetallic thin films will be presented. The electronic structure as well as the photoemission calculations have been performed for true semi-infinite systems using the upgraded version of the Munich SPR-KKR program package [1]. To guarantee for a quantitative description of the surface-sensitive spectral distribution special attention is paid on the image-potential behavior of the surface barrier, which is included as an additional layer in the photoemission formalism [2]. Here, we show the intensity distributions that result by excitation with ultraviolet radiation from Ag/Au(111), Ag/Au(110) and Au/Ni(111) surfaces. We discuss the variation in binding energy and spin-orbit splitting of the corresponding surface states as a function of the overlayer thickness

and compare our results with available experimental data.

1. H. Ebert et al., The Munich SPR-KKR package, version 3.6, <http://olymp.cup.uni-muenchen.de/ak/eibert/SPRKKR> (2008).  
 2. A. B. Schmidt et al., *J. Phys. D: Appl. Phys.* 41 164003 (2008).

O 57.6 Thu 17:00 HSZ 02

**Ab initio  $g$ -tensor calculation for paramagnetic surface states** — ●MARTIN ROHRMÜLLER<sup>1</sup>, UWE GERSTMANN<sup>1,2</sup>, and WOLF GERO SCHMIDT<sup>1</sup> — <sup>1</sup>Theoretische Physik, Universität Paderborn, 33095 Paderborn, Germany — <sup>2</sup>Institut de Minéralogie et de Physique des Milieux Condensés, Université Pierre et Marie Curie, Campus Boucaut, 140 rue de Lourmel, 75015 Paris, France

The effects of spin-orbit interaction provide an interesting possibility to investigate the electronic and microscopic structure at surfaces. The spin-orbit coupling determines e.g. the elements of the electronic  $g$ -tensors which can be observed in electron paramagnetic resonance (EPR) measurements. Based on double-perturbation theory we are able to calculate the  $g$ -tensor from first principles, using a recently developed gauge-including projector augmented plane wave (GI-PAW) approach [1] in the framework of density functional theory.

The presented approach is able to distinguish between different surface states. In combination with the corresponding experimental EPR data an unambiguous identification of the microscopic structure of adsorbed species becomes possible. This is demonstrated here for surface defects at hydrogen-passivated Si(001) and Si(111) surfaces.

[1] Ch.J. Pickard and F. Mauri, *Phys. Rev. Lett.* 88, 086403 (2002).  
 [2] U. Gerstmann, A. P. Seitsonen and F. Mauri, *phys. stat. sol. (b)* 245, 924 (2008).

O 57.7 Thu 17:15 HSZ 02

**Bi(114): A quasi one-dimensional metal with strong spin-orbit splitting** — ●PHILIP HOFMANN<sup>1</sup>, JUSTIN WELLS<sup>1,2</sup>, HUGO DIL<sup>3,4</sup>, FABIAN MEIER<sup>3,4</sup>, JORGE LOBO-CHECA<sup>3,4</sup>, VLADIMIR PETROV<sup>5</sup>, JÜRIG OSTERWALDER<sup>3</sup>, MIGUEL MORENO UGEDA<sup>6</sup>, ISABEL FERNANDEZ-TORRENTE<sup>6</sup>, JOSE IGNACIO PASCUAL<sup>6</sup>, EMILE RIENKS<sup>1</sup>, and MARIA FUGLSANG JENSEN<sup>1</sup> — <sup>1</sup>University of Aarhus, DK — <sup>2</sup>University of Science and Technology, Trondheim, N — <sup>3</sup>Universität Zürich-Irchel, CH — <sup>4</sup>Paul Scherrer Institut, CH — <sup>5</sup>St. Petersburg Technical University, RU — <sup>6</sup>Freie Universität Berlin, D

The (114) vicinal surface of the semimetal Bi is found to support a quasi one-dimensional, metallic surface state. As required by symmetry, the state is degenerate along the  $\bar{\Gamma}-\bar{Y}$  line of the surface Brillouin zone with a highest binding energy of  $\approx 100$  meV. In the  $\bar{\Gamma}-\bar{X}$  direction the degeneracy is lifted by the strong spin-orbit interaction, as directly shown by spin-resolved photoemission. This results in a Fermi surface consisting of two closely separated, parallel lines of opposite spin direction. We discuss these findings in the light of the recently discovered topological stability of surface states on BiSb topological insulators.

### short intermittance

O 57.8 Thu 17:45 HSZ 02

**Spin restrictions in the electron interference process on Bi(110)** — ●ANNA STROZECKA<sup>1</sup>, ASIER EIGUREN<sup>2</sup>, and JOSE IGNACIO PASCUAL<sup>1</sup> — <sup>1</sup>Institut für Experimentalphysik, Freie Universität Berlin, Arnimallee 14, 14195 Berlin, Germany — <sup>2</sup>Donostia International Physics Center (DIPC), Paseo Manuel de Lardizabal 4, E-20018 Donostia/San Sebastian, Spain

The surfaces of bismuth can be viewed as a quasi-two-dimensional metal with unique spin properties [1]. The strong spin-orbit interaction and the lack of the symmetry on the surface results in the splitting of the surface state bands with respect to the spin direction. The lack of the spin degeneracy strongly affects the quasiparticle interference [2]. We have studied in detail the interference patterns on Bi(110) surface by means of scanning tunneling microscopy. The observed patterns do not reflect directly the shape of the Fermi contour, as it is usually found for metals, but result from the spin-conserving scattering process. The investigation of the energy dependence of the interference reveals that at the energies away from the Fermi level highly anisotropic patterns arise. The origin of these new scattering events can be established by analyzing the dispersion of the spin split bands. The interpretation of the data is supported by spin-resolved DFT simulations.

[1] Ph. Hofmann, *Prog. Surf. Sci.* 81, 191 (2006)  
 [2] J. I. Pascual et al., *Phys. Rev. Lett.* 93, 196802 (2004)

O 57.9 Thu 18:00 HSZ 02

**Spin-orbit coupling effect on surface state ripples** — ●SAMIR LOUNIS, ANDREAS BRINGER, and STEFAN BLÜGEL — Institut für Festkörperforschung and Institut für Advanced Simulation, Forschungszentrum Jülich, D-52425 Jülich, Germany

Surfaces are an inversion asymmetric environment. In combination with the spin-orbit interaction, surface electrons experience a Rashba effect, which leads to spin-split surface states. Having an adatom on such a surface, surface states scatter at it. Interferences are created from which, surprisingly, the fingerprints of spin-orbit coupling cannot be seen with a scanning tunneling microscope (STM) [3]. Instead of a single adatom, Walls and Heller [4] proposed to use a corral of atoms to create extra spin-orbit coupling related modulations in the charge density. Resting on multiple scattering theory, we propose a different suggestion to visualize such effects using STM considering either a single adatom or a corral of adatoms.

This work is supported by the ESF EUROCORES Programme SONS under contract N. ERAS-CT-2003-980409 and the DFG Priority Programme SPP1153.

[1] S. Lashell, B.A. McDougall, E. Jensen, Phys. Rev. Lett. **77**, 3419 (1996).

[2] Yu. M. Koroteev, G. Bihlmayer, J.E. Gayone, E.V. Chulkov, S. Blügel, P.M. Echenique, Ph. Hofmann, Phys. Rev. Lett. **93**, 046403 (2004).

[3] L. Petersen and P. Hedegård, Surf. Sci. **49**, 459 (2000).

[4] J.D. Walls and E.J. Heller, Nano Letters **7**, 3377 (2007).

O 57.10 Thu 18:15 HSZ 02

**An ab-initio description of the magnetic shape anisotropy** — ●SVEN BORNEMANN, JAN MINAR, JÜRGEN BRAUN, and HUBERT EBERT — Department Chemie und Biochemie, LMU München, Germany

For magnetic transition metal systems with reduced dimensionality and low symmetry the shape anisotropy becomes a significant contribution to the magnetic anisotropy. In fact, it can reach the same order of magnitude as the spin-orbit induced anisotropy. So far, the shape anisotropy has been always treated as a classical interaction between magnetic dipoles while the spin-orbit anisotropy has been determined by relativistic band structure calculations. It is uncertain, however, whether such an inconsistent treatment of the two anisotropy contributions is still valid for low dimensional nano structures such as magnetic thin films, wires or clusters where the magnetic easy axis can depend strongly on the interplay between these two contributions.

As an alternative to the classical approach an ab-initio description of the shape anisotropy has been developed. This is achieved by including the Breit interaction, being the natural cause of the shape anisotropy, in the Dirac-equation set up within the framework of spin density functional theory. We have implemented this approach using the fully relativistic KKR band structure scheme. We will present the details of our implementation and show first results for the shape anisotropy of thin Fe films on Au(001) in comparison with the classical

treatment.

O 57.11 Thu 18:30 HSZ 02

**Spin-orbit induced exchange interactions in magnetic surfaces described by first-order perturbation theory** — ●MARCUS HEIDE, GUSTAV BIHLMAYER, and STEFAN BLÜGEL — Institut für Festkörperforschung (IFF) and Institute of Advanced Simulation (IAS), Forschungszentrum Jülich, Germany

When applying the spin-orbit coupling operator  $H_{so}$  as a perturbation to a Schrödinger-type equation, the first-order term  $\sum_{\nu} \langle \psi_{\nu} | H_{so} | \psi_{\nu} \rangle$  vanishes for all collinear magnetic structures. Thus, the magnetocrystalline anisotropy is at least a second-order effect in the spin-orbit coupling and cannot be calculated from the expectation values of  $H_{so}$ . However, in systems with low magnetic and spatial symmetry these expectation values do not necessarily vanish: Non-collinear magnetic structures in surface geometries allow for magnetic interactions of Dzyaloshinskii-Moriya type, that are first order in  $H_{so}$ . These interactions can have a significant impact on the magnetic structure of low-dimensional magnets [M. Bode *et al.*, Nature **447**, 190 (2007)].

In this talk, we investigate the role of the spin-orbit coupling in ultrathin Fe and Mn films on transition metal surfaces in the framework of density functional theory. Employing the FLEUR code ([www.flapw.de](http://www.flapw.de)), we compare the expectation values of  $H_{so}$  with the higher-order corrections and show that first-order perturbation theory is capable of estimating the antisymmetric exchange interactions in these systems. This allows to use simple models to relate these interactions to the electronic structure. This work is supported by DFG (BI 823/1-1) and ESF EUROCORES Programme SONS (ERAS-CT-2003-980409).

O 57.12 Thu 18:45 HSZ 02

**Non-collinear magnetism in two-dimensional FePt systems** — ●SVITLANA POLESYA, SVEN BORNEMANN, SERGIY MANKOVSKY, JAN MINAR, and HUBERT EBERT — Ludwig-Maximilians-Universität München, Department Chemie und Biochemie/Physikalische Chemie, München, Deutschland

The temperature dependent magnetism of a FePt monolayer and of a FePt two-dimensional (2D) alloy cluster on a Pt(111) substrate were investigated by means of Monte Carlo simulations. The calculations were based on the extended Heisenberg model accounting for isotropic exchange as well as the anisotropic Dzyaloshinski-Moriya (DM) exchange interaction. The DM coupling was found to be responsible for a non-collinear spin configuration in both alloy systems at low temperature. The Fe-Pt exchange turned out to play an important role stabilising the ferromagnetic order and appreciably influencing the critical temperature. For this reason a corresponding term in the model Hamiltonian was included describing the induced Pt magnetic moment as a function of the average magnetic moments of the surrounding Fe atoms. The role of the magnetic anisotropy on magnetic order in the 2D alloy systems was also investigated in detail.

## O 58: SYAI: Ab-initio approaches to excitations in condensed matter

Time: Thursday 15:00–18:30

Location: SCH 251

See SYAI for details about the program

## O 59: General Meeting of the Surface Science Division

Time: Thursday 19:30–20:00

Location: HSZ 02

Report of the Chairman of the DPG Surface Science Division

## O 60: Post Deadline Session followed by Surface Science "get-together"

Time: Thursday 20:00–21:00

Location: HSZ 02

O 60.1 Thu 20:00 HSZ 02

**Can molecular orbitals be simply reconstructed from photoemission data?** — ●PETER PUSCHNIG<sup>1</sup>, CLAUDIA AMBROSCH-DRAXL<sup>1</sup>, THOMAS SEYLLER<sup>2</sup>, STEPHEN BERKEBILE<sup>3</sup>, GEORG KOLLER<sup>3</sup>, FALKO P. NETZER<sup>3</sup>, and MICHAEL G. RAMSEY<sup>3</sup> — <sup>1</sup>Chair for Atomistic Modelling and Design of Materials, University Leoben — <sup>2</sup>Institut für Tech-

nische Physik II, Universität Erlangen-Nürnberg — <sup>3</sup>Surface Science Group, Institute of Physics, University Graz

We present a new and simple approach with the aim to determine the shape of molecular orbitals by means of angle-resolved photoemission (PE) experiments. It applies to molecular films ranging from mono-

layers up to multilayers and leads to images of individual molecular states with a spatial resolution of about 1 Å, thereby competing with state-of-the-art scanning probe techniques. We demonstrate how the PE intensity recorded over a hemispherical region generates reciprocal space maps of the initial state. This data provides unambiguous fingerprints of individual molecular orbitals and is used to reconstruct real space images of the frontier molecular orbitals in good agreement with density functional (DFT) calculations. With k-space maps obtained using the toroidal analyser at BESSY II we demonstrate the viability of the proposed method even for the strongly bound monolayer of para-sexiphenyl adsorbed on Cu(110). Here the reconstructed HOMO and ex-LUMO orbital can both be clearly recognized and compare well to the DFT results. The generality of the approach is then illustrated with examples from molecular films ranging from the small rod-like pentacene to the plate-like tetraphenylporphyrin.

O 60.2 Thu 20:15 HSZ 02

**Localization of Electronic States within a Moiré Pattern** — ●THIRUVANCHERIL G. GOPAKUMAR, NICOLAS NÉEL, JÖRG KRÖGER, and RICHARD BERNDT — Christian-Albrechts-Universität zu Kiel, D-24098 Kiel, Germany

Moiré patterns have been observed for various heteroepitaxial layers. Little is known about the electronic structure on a nanometre scale of these regular superlattices. We use a cryogenic scanning tunnelling microscope to probe the electronic properties of a moiré pattern observed from Co islands on Ag(111). Spatially resolved spectroscopy reveals that the moiré pattern gives rise to a striking localization of Co *d*-states. We use these states as an electronic template to guide the arrangement of magnetic molecules.

O 60.3 Thu 20:30 HSZ 02

**Polar catastrophe and how thin LaAlO<sub>3</sub> films on SrTiO<sub>3</sub>(001) deal with it** — ●ROSSITZA PENTCHEVA<sup>1</sup> and WARREN E. PICKETT<sup>2</sup> — <sup>1</sup>Dept. of Earth and Environmental Sciences, University of Munich — <sup>2</sup>Dept. of Physics, University of California at Davis

Even at the interface of conventional band insulators polar discontinuities can drive novel electronic behaviour: An example is the two-dimensional electron gas [1] and thickness dependent switching from insulating to conducting behaviour [2] reported in thin LaAlO<sub>3</sub> films on a SrTiO<sub>3</sub>(001)-substrate.

Density functional theory calculations reveal that a strong polar dis-

ortion creates the necessary screening and enables several unit cells of LaAlO<sub>3</sub> to sustain their ionic charges and remain insulating. However, the band gap of the system, defined by O 2*p* states at the surface and Ti 3*d* states at the interface decreases with each added LaAlO<sub>3</sub>-layer, before an insulator-to-metal transition and a crossover to an electronic reconstruction (as observed previously at the isolated interface [3]) takes place at around 5 monolayers of LaAlO<sub>3</sub>. The implications of two different, spatially separated types of carriers - holes at the surface and electrons at the interface - will be discussed.

A BaCaTec grant and a computational grant at the Leibniz Rechenzentrum are gratefully acknowledged.

[1] A.Ohtomo and H.Y.Hwang, *Nature* **427**, 423 (2004)[2] S.Thiel *et al.*, *Science* **313**, 1942 (2006)[3] R. Pentcheva and W.E. Pickett, *Phys. Rev. B.* **74**, 035112 (2006); *ibid.* **78**, 205106 (2008).

O 60.4 Thu 20:45 HSZ 02

**Photo resist free patterning by local oxidation of Ag surfaces** — ●SEBASTIAN GÜNTHER<sup>1</sup>, ROBERT REICHELT<sup>1</sup>, JOOST WINTERLIN<sup>1</sup>, ANDREA LOCATELLI<sup>2</sup>, MIGUEL NIÑO<sup>2</sup>, TEFKVİK MENTEŞ<sup>2</sup>, and ALEXEI BARINOV<sup>2</sup> — <sup>1</sup>Department Chemie, Ludwig-Maximilians-Universität München, Butenandtstr. 11, 81377 München, Germany — <sup>2</sup>Sincrotrone Trieste S.C.p.A., Area Science Park, 34012 Basovizza-Trieste, Italy

Traditional surface patterning processes usually make use of photo resists and require several preparation steps such as resist irradiation and development, etch or deposition steps and eventually lift off processes. Here, we report on a potential single step structuring process which can be used to chemically pattern Ag surface by a local oxidation reaction. In particular, we present our recent findings that low energy electron irradiation of Ag(111) or polycrystalline Ag during NO<sub>2</sub> adsorption at 300 K induces the formation of Ag oxide. Using a spatially confined electron beam, small Ag<sub>2</sub>O spots could be grown with sharp, ~ 100 nm wide, boundaries to the non irradiated metallic surface. The structure may be written as well by photon instead of electron irradiation, which makes the use of masks possible. Since the structure size will mainly depend on the sharpness of the irradiation electron beam or of the applied masks, the observed process has the potential of a single step nanostructuring process. Temperature treatment offers an easy way to manipulate the boundary between oxide and metallic silver by steering chemical fronts.

## O 61: Invited Talk (Claudia Ambrosch-Draxl)

Time: Friday 10:15–11:00

Location: HSZ 02

### Invited Talk

O 61.1 Fri 10:15 HSZ 02

**First-principles approaches towards organic film growth** — ●CLAUDIA AMBROSCH-DRAXL, PETER PUSCHNIG, and DMITRII NABOK — Chair of Atomistic Modelling and Design of Materials, University of Leoben, Austria

The technological applicability of organic semiconductors in optoelectronic devices strongly depends on the morphology of the active organic layer as well as on the interface between the thin organic film and the metal electrode. The cohesive properties of the organic materials as well as their interfaces with metal surfaces are key quantities in this context. Regarding first-principles calculations, only recently it has become possible to properly treat van der Waals interactions which thereby play a dominant role. The excellent agreement with ex-

periment for the so obtained cohesive energies of the oligo-acenes and oligo-phenyles allows to predict also the surface energies for a variety of organic materials. Moreover, it is shown that also the interaction between the molecule and the metal substrate is predominantly van-der-Waals like. Our results enable us to assess semi-empirical approaches to be used for complex situations where an ab-initio treatment is out of reach. Applying an empirical force-field method, we tackle the topic of film growth. The latter also requires the determination of the relevant processes and the corresponding energy barriers. As a first example, we have investigated the energetics driving mound formation of sexiphenyl molecules on mica as revealed by atomic-force microscopy. It turns out that the complex nature of the organic building block requires models that go beyond those of inorganic film growth.

## O 62: Surface chemical reactions II

Time: Friday 11:15–13:00

Location: SCH A01

O 62.1 Fri 11:15 SCH A01

**In-situ investigation of sulfur oxidation on a stepped Pt surface** — ●REGINE STREBER<sup>1</sup>, CHRISTIAN PAPP<sup>1</sup>, MICHAEL PETER ANDREAS LORENZ<sup>1</sup>, ANDREAS BAYER<sup>1</sup>, REINHARD DENECKE<sup>2</sup>, and HANS-PETER STEINRÜCK<sup>1</sup> — <sup>1</sup>Lehrstuhl für Physikalische Chemie II, Universität Erlangen-Nürnberg, Egerlandstr. 3, 91058 Erlangen — <sup>2</sup>Willhelm-Ostwald-Institut für Physikalische und Theoretische Chemie, Universität Leipzig, Linnéstr. 2, 04103 Leipzig

We studied the reaction of oxygen with preadsorbed sulfur on the stepped Pt(355) surface by in-situ high-resolution XPS applying synchrotron radiation at BESSY II. The reactivity strongly depends on surface temperature. At 250 K, dosing of molecular oxygen on the partially sulfur precovered surface leads to the coadsorption of atomic S and O, but almost no reaction, as concluded from the S 2*p* spectra. Upon heating this mixed layer to elevated temperatures, the subsequent formation of two new species is observed, which are assigned to

SO<sub>2</sub> and SO<sub>4</sub>. At 300 K, dosing of oxygen results in the partial formation of SO<sub>2</sub>, while at 350 K a consecutive reaction to SO<sub>4</sub> occurs. To determine the kinetic parameters of these reactions, the oxidation has been studied at different temperatures. In addition, the influences of the initial sulfur precoverage and of the oxygen pressure have been investigated. This work was supported by BMBF (05 ES3XBA/5) and the DFG through the Cluster of Excellence "Engineering of Advanced Materials".

O 62.2 Fri 11:30 SCH A01

**Structure Formation in Ultrathin V-Oxide films on Rh(111) under different Reaction Conditions** — ●FLORIAN LOVIS, MARTIN HESSE, and RONALD IMBIHL — Institut für Physikalische Chemie und Elektrochemie, Leibniz-Universität Hannover, Callinstr.3-3a, D-30167 Hannover, Germany

As a model system for vanadium-oxide based catalysts we prepared ultrathin vanadium oxide films on a Rh(111) surface. At 400°C 0.1 and 0.25 ML of vanadium were evaporated in oxygen with  $p(\text{O}_2)=2 \times 10^{-7}$  mbar. After characterization with LEED and Auger electron spectroscopy the films were subjected to the O<sub>2</sub> + H<sub>2</sub> reaction using photoemission electron microscopy (PEEM). After evaporation a large variety of differently ordered Rh(111)/V/O phases were identified in LEED. The O<sub>2</sub> + H<sub>2</sub> reaction was studied in the 10<sup>-8</sup> to 10<sup>-5</sup> mbar range at temperatures between 400 and 500°C. With PEEM we observe that under reaction conditions the film is no longer homogeneous but reaction fronts and stationary Turing-like patterns develop. In the evaporated V-film we find partially ordered patterns consisting of large islands of about 0,05 mm diameter. These islands are very stable and change only very slowly after turning off the gases. Under different reaction conditions we find small islands of roughly 0,02 mm diameter which in contrast to the large islands are quite dynamic and vary in diameter depending on the reaction conditions. The patterns induced by the reaction are discussed in the context of the concept of reactive phase separation. It is suspected that the attraction between oxygen and vanadium is the driving force for the condensation process.

O 62.3 Fri 11:45 SCH A01

**Non-adiabatic energy dissipation in metal homoepitaxy** — ●ULRICH HAGEMANN, KORNELIA HUBA, DAVID KRIX, and HERMANN NIENHAUS — Experimental Physics, University of Duisburg-Essen, Germany

The growth of metal films releases energies of typically a few eV per metal atom. By now, the energy is believed to be dissipated adiabatically by direct excitation of phonons. We present data which give strong evidence for the creation of electron-hole pairs during Mg homoepitaxy, i.e., for a non-adiabatic dissipation channel. To detect the generated hot charge carriers, large-area ultrathin metal film Mg/p-Si(001) Schottky diodes were fabricated. The homogeneous Schottky barrier height was determined as 0.52 eV and the reverse current could be reduced to below 1 nA at low temperatures. During exposure of the diodes to a thermal Mg atom beam internal currents in the 100 pA range are observed. The currents can be attributed to two mechanisms: first the internal exoemission process (chemicurrent effect) due to non-adiabatic energy dissipation and second the photocurrent due to the infrared radiation of the evaporator. By varying the evaporator temperature and the Mg film thickness the two current contributions can be distinguished. The chemicurrent during Mg homoepitaxy depends exponentially on the evaporation temperature yielding the Mg evaporation enthalpy of 1.3 eV. The strong exponential attenuation of the chemicurrent with increasing Mg film thickness further supports the concept of generation of ballistic charge carriers by the metal formation process.

O 62.4 Fri 12:00 SCH A01

**State resolved measurements of photodesorbed NO from Ag(111) surface** — ●DANIEL MULUGETA<sup>1</sup>, KAZUO WATANABE<sup>1</sup>, DIETRICH MENZEL<sup>1,2</sup>, and HANS-JOACHIM FREUND<sup>1</sup> — <sup>1</sup>Fritz-Haber-Institute der Max-Planck-Gesellschaft, Faradayweg 4-6, 14195 Berlin — <sup>2</sup>Physik-Department E20, Technische Universität München, 85747 Garching

The distribution of energy over the various degrees of freedom of photodesorbed molecules contains important information about the dynamics of the desorption event. We have performed state resolved (translation, rotation, vibration) measurements of NO photodesorbed from (NO)<sub>2</sub> adsorbed on Ag(111) at 60 K by nanosecond laser pulses (2.3, 3.5 or 4.7 eV) by using (1+1) resonant multiphoton ionization (REMPI) via the  $A^2\Sigma \leftarrow X^2\Pi$  transition. Both thermal and non-

thermal components are observed in state selective time of flight measurements. Rotational and vibration temperatures of about 430 K and 710 K, respectively, were found for NO photodesorbed with a velocity of about 960 m/s, regardless of the photon energy used. The translational energy distributions did not show major change with vibrational excitations. By contrast, the translational temperature showed a systematic increase with increasing rotational excitation. The results are interpreted in terms of an excitation-deexcitation mechanism via transient negative ions.

O 62.5 Fri 12:15 SCH A01

**Direct photochemical formation of N<sub>2</sub> from NO dimers on cold Ag(111)** — ●KI HYUN KIM<sup>1</sup>, KAZUO WATANABE<sup>1</sup>, DIETRICH MENZEL<sup>1,2</sup>, and HANS-JOACHIM FREUND<sup>1</sup> — <sup>1</sup>Fritz-Haber-Institut der Max-Planck-Gesellschaft, Faradayweg 4-6, 14195 Berlin, Germany — <sup>2</sup>Technische Universität München, 85747 Garching, Germany

Direct photochemical formation of N<sub>2</sub> has been identified for the first time in photoreactions of (NO)<sub>2</sub> adsorbed on Ag(111) at ~ 30 K, induced by UV and visible light. Mass selected time-of-flight signals of N<sub>2</sub>, N<sub>2</sub>O, and NO formed from (NO)<sub>2</sub> on Ag(111) by irradiating with 2.3, 3.5 and 4.7 eV laser beams (Nd:YAG laser) were measured. The results show that the translational temperature of the N<sub>2</sub> formed from (NO)<sub>2</sub> on Ag(111) is ~ 5700 K, while those of photodesorbed N<sub>2</sub>O and NO are ~ 1200 and 770 K, respectively, independent of incident photon energy. On the other hand the translational temperature of N<sub>2</sub> formed from adsorbed N<sub>2</sub>O on Ag(111) is only ~ 1400 K, i.e. much lower than that of N<sub>2</sub> formed from (NO)<sub>2</sub>.

We propose that the formation of fast N<sub>2</sub> from (NO)<sub>2</sub> on Ag(111) occurs via simultaneous cleavage of the two N-O bonds followed by the formation of an N-N triple bond of N<sub>2</sub>, and can be regarded as mutual abstraction of the N atom from each nitrosyl in (NO)<sub>2</sub>. The Ag surface reduces the N-N bond length of (NO)<sub>2</sub> to enable the formation of N<sub>2</sub> as well as of N<sub>2</sub>O; furthermore, the equilibrium surface distance of (NO)<sub>2</sub> is considerably shorter than that of N<sub>2</sub> which leads to the latter's high kinetic energy.

O 62.6 Fri 12:30 SCH A01

**Adsorption of Methanol on Ru(0001)** — ●PAWEL GAZDZICKI and PETER JAKOB — Fachbereich Physik, Philipps-Universität Marburg, D-35032 Marburg, Germany

Infrared Absorption Spectroscopy was used to study the adsorption and reaction of methanol on Ru(0001). From the vibrational modes of the isotopes CH<sub>3</sub>OH and CH<sub>3</sub>OD clear evidence for intact adsorption at  $T = 80$  K has been found. This finding contradicts previous studies which suggested an OH (OD) bond scission upon adsorption of methanol even at low temperatures as well as recombinative desorption at elevated  $T$ . Our conclusion is based on isotopic shifts of vibrational modes associated with the OH (OD) group of adsorbed CH<sub>3</sub>OH and CH<sub>3</sub>OD, respectively. The findings are corroborated by TPD experiments of CH<sub>3</sub>OH with coadsorbed D on Ru(0001). While clearly showing desorption of CH<sub>3</sub>OH, no desorption of CH<sub>3</sub>OD caused by the recombination of dissociated CH<sub>3</sub>OH and D was observed. At low coverages (< 0.1 ML) we suggest the presence of isolated methanol molecules which begin to cluster with increasing density by building hydrogen bonds. This clustering was also observed after annealing a low coverage methanol layer up to 100-120 K. At temperatures  $T = 170$ -200 K CH<sub>3</sub>OH decomposes (O-H bond cleavage) to form an upright methoxy species (CH<sub>3</sub>O). The final reaction products are CO and H which are formed at  $T > 220$  K.

In comparison, CH<sub>3</sub>OH adsorbed on pseudomorphic Cu/Ru(0001) produces the same species as on Ru(0001). Yet, the temperature range of the methoxy species is significantly larger, i.e. 200-300 K.

O 62.7 Fri 12:45 SCH A01

**A new transferable method to calculate electronic excitations in adsorption on metal surfaces** — ●MATTHIAS TIMMER and PETER KRATZER — Fachbereich Physik - Theoretische Physik and Centre for Nanointegration (CeNIDE), Universität Duisburg-Essen, Lotharstr. 1, 47048 Duisburg, Germany

Non-adiabatic effects in adsorption on metal surfaces include the excitation of electrons and holes, which can be observed as chemicurrents. We present a new quantitative method on the basis of ground-state density-functional theory (DFT) to calculate these excitation probabilities. The method uses first-order time-dependent perturbation theory, which is implemented using the evaluation of matrix elements between Kohn-Sham states of the rate of change of the Kohn-Sham potential between subsequent static DFT calculations. We can access the exci-

tation spectra directly. The method is applied to adsorption of atomic hydrogen isotopes on-top the Al(111) surface. Results can explain the experimental data for noble metal surfaces; in particular the observed isotope effect in H versus D adsorption is described. Moreover, the results are in quantitative agreement with computationally expensive calculations of the full dynamics within time-dependent DFT, with the

notable exception of effects due to spin dynamics.

The method presented is simple enough to be applied to a wide class of adsorbates and surfaces, while at the same time allowing us to extract system-specific information. It can be implemented with reasonable effort within existing DFT codes [1].

[1] <http://arXiv.org/abs/0810.5248>

## O 63: Semiconductor substrates: Adsorption

Time: Friday 11:15–13:00

Location: SCH A118

O 63.1 Fri 11:15 SCH A118

**Magnetic Molecules on GaN Studied by Low Temperature STM** — ●KENDAL CLARK, DANDA ACHARYA, VIOLETA IANCU, ERDUNG LU, ARTHUR SMITH, and SAW-WAI HLA — Ohio University, Physics and Astronomy Department, Athens, Ohio 45701, USA.

Spin electron interactions involving magnetic molecules and semiconductor surfaces are of great interest for the development of molecular spintronic devices. Due to its wide range of applications, GaN (0001) surface has received a special attention for the development of novel electronic devices. Here, we studied electronic and structural properties of TBrPP-Co molecules deposited on a freshly grown nitrogen polar GaN (0001) surface using a scanning tunneling microscopy and spectroscopy at 4.6 K under an ultra-high-vacuum condition. The TBrPP-Co molecule has a spin-active cobalt atom caged at the center of porphyrin unit and four bromo-phenyl groups are attached to its four corners. On GaN(0001), the molecules bind the surface through the bromo-phenyl units and form a saddle conformation, in which the central part of the molecule is bent by lifting the two pyrrole units of the porphyrin macrocycle. The molecules self-assemble and formed ordered clusters on GaN(0001) surface. Within the self-assembled molecular clusters, the molecules are aligned either parallel or 90 degree rotated to each other. In the presentation, we will discuss the spin-electron coupling of this molecule-surface system. This work is supported by the Ohio University BNNT, National Science Foundation NSF-DMR 0304314, NSF-PIRE: OISE 0730257, NSF-EMT: CCF-0622158, and the United States Department of Energy, DE-FG02-02ER46012 grants.

O 63.2 Fri 11:30 SCH A118

**Self assembled organic monolayers on silicon carbide** — ●MARCO HOEB, IAN D. SHARP, CARLOS A. DIAZ ALVAREZ, SEBASTIAN SCHOELL, MARTIN STUTZMANN, and MARTIN S. BRANDT — Walter Schottky Institut, Technische Universität München, Am Coulombwall 3, 85748 Garching, Germany

Because of its remarkable properties such as its biocompatibility or the possibility of bandgap engineering using its different polytypes, silicon carbide (SiC) is a promising substrate material for applications in the field of biosensors. One requirement for stable biosensors based on organic-inorganic hybrids is a covalent attachment of functional organic layers to the semiconductor surface. Here, we demonstrate high quality monolayers of 1-octadecene ( $C_{18}H_{36}$ ) on both Si- and C-polar 6H-SiC surfaces. Organic monolayer self-assembly in the well-known case of silicon is typically achieved via hydrosilylation, a process where a hydrogen-terminated surface is required. The double-bonded carbon atom of the alkane directly attaches to the silicon surface and results in a Si-C bond. In contrast, SiC surfaces are OH-terminated following etching in hydrofluoric acid and are, therefore, in principle not appropriate for this reaction. Nevertheless, the hydroxylated surfaces form dense and chemically stable alkene layers on both crystal faces. We show by X-ray photoelectron spectroscopy (XPS) and Fourier transform infrared (FTIR) spectroscopy that the bridging between the organic molecule and SiC occurs via an oxygen atom that is not present in the case of hydrosilylated silicon. We discuss this reaction in the framework of Markownikow addition.

O 63.3 Fri 11:45 SCH A118

**Long-lived excitonic desorption of NO from  $C_{60}/Cu(111)$**  — TIM HOGER and ●HELMUT ZACHARIAS — Westfälische Wilhelms-Universität Münster

The desorption of NO molecules from a  $C_{60}/Cu(111)$  surface is initiated by a 7 ns UV laser pulse (355 nm). The NO molecules are rotational state selectively detected by a frequency-doubled dye-laser (226 nm) by (1+1) REMPI. In a TOF mass spectrometer the arrival

time spectrum shows two channels, one fast direct one and a slow one. This is confirmed by measuring directly the velocity distribution of the desorbing NO. The fast channel refers to a DIET process with a hot rotational distribution and a moderate vibrational excitation with a strong rotational-translational coupling. In the slow channel the velocity distribution does not depend on the particular detection time after initiating the desorption by the 355 nm pump pulse. The recorded velocities are further faster than expected from the detection time. It is thus concluded that the desorption occurs time-delayed with respect to the excitation. The lifetime of this excitation can be estimated to approximately 125  $\mu$ s, in good agreement with lifetimes of triplet excitons in  $C_{60}$ . Triplet excitonic states in  $C_{60}$  are possible energy reservoirs for this desorption.

O 63.4 Fri 12:00 SCH A118

**STM study of the adsorption of coronene on Si(111)-(7x7)** — ●JESUS MARTINEZ-BLANCO, MAX KLINGSPORN, and KARSTEN HORN — Fritz Haber Institut, Berlin, Germany

The adsorption of organic molecules on silicon surfaces is of interest in the control of their preparation and processing for applications in device fabrication. The (7x7) reconstructed silicon (111) surface presents a rich array of electronically inequivalent reaction sites, due to its unique electronic properties of reactive adatoms, rest atoms, and corner holes on the surface, which has been investigated with respect to molecular adsorption, and provides a rich playground. Here we report on the adsorption of coronene ( $C_{24}H_{12}$ ) on the Si(111)-(7x7) surface. Coronene is a polycyclic aromatic hydrocarbon (PAH) consisting of seven peri-fused benzene rings. We use Scanning Tunneling Microscopy (STM) to investigate the local long range structure. Upon room temperature adsorption, we find that the coronene molecules preferentially adsorb on the unfaulted half of the 7x7 unit cell. Molecules adsorbed on different sites can be induced to move to the preferential sites by the action of the tip in repeated image scans. Imaging of the molecules is strongly bias dependent, and also critically depends on the adsorption site. We discuss the structure of coronene on Si(111)-(7x7) on the basis of our data and in comparison with STM studies of coronene on the Si(001)-(2x1) surface where long range order is not observed.

O 63.5 Fri 12:15 SCH A118

**Site-selective reactivity of ethylene on hydrogen pre-covered Si(001)** — ●GERSON METTE<sup>1</sup>, MICHAEL DÜRR<sup>1,2</sup>, and ULRICH HÖFER<sup>1</sup> — <sup>1</sup>Fachbereich Physik und Zentrum für Materialwissenschaften, Philipps-Universität Marburg, D-35032 Marburg — <sup>2</sup>Fakultät Angewandte Naturwissenschaften, Hochschule Esslingen, D-73728 Esslingen

The reactivity of a semiconductor surface is expected to correlate not only with the concentration of dangling bonds but also with the local electronic properties of the dangling-bond states. For  $H_2$  dissociation on Si(001), a strongly activated process, site-selective reactivity at locally distorted configurations was demonstrated, e.g. by pre-adsorption of atomic hydrogen [1]. In this study, site-selective adsorption of ethylene on Si(001) has been investigated by means of STM. Two ethylene adsorption geometries were found on clean Si(001) with ethylene adsorbed on one and two dimers, respectively. Distortion of the electronic configuration by pre-adsorption of atomic hydrogen is found to increase the reactivity of the two-dimer adsorption site by a factor of 50. Thus, locally distorted dangling-bond configurations show site-selective reactivity also in the case of barrierless, non-dissociative adsorption of an organic molecule. The results are discussed with respect to a precursor mediated adsorption pathway and the control of the adsorption barrier between precursor and chemisorbed state.

[1] M. Dürr and U. Höfer, Surf. Sci. Rep. **61**, 465 (2006)

O 63.6 Fri 12:30 SCH A118

**XPD-Measurement of the Si/SiO<sub>2</sub>-interface on Si(110)** — ●TOBIAS LÜHR<sup>1,2</sup>, DANIEL WEIER<sup>1,2</sup>, FRANK SCHÖNBOHM<sup>1,2</sup>, SVEN DÖRING<sup>1,2</sup>, ULF BERGES<sup>1,2</sup>, and CARSTEN WESTPHAL<sup>1,2</sup> — <sup>1</sup>Fakultät Physik - Technische Universität Dortmund, Otto-Hahn-Str. 4, D 44221 Dortmund, Germany — <sup>2</sup>DELTA - Technische Universität Dortmund, Maria-Goeppert-Mayer-Str. 2, D 44227 Dortmund, Germany

In the past, the investigation of the silicon (100) surface was in the center of many research activities. However, the structure of the interface for the Si(110)-surface is still unknown. In order to determine the structure of the oxidized Si(110)-surface XPS and angle-scanned XPD experiments were conducted. The experiments were performed at the synchrotron storage ring DELTA (Dortmund). In order to investigate the interface structure, we recorded high resolution photoemission spectra of the Si 2p signal with a photon energy of  $h\nu = 180\text{eV}$ . The spectra contain seven components which correspond to photoemission from emitters located in the interface region and in the bulk. Polar angle depending intensity plots of the recorded signals reveal the relative positions of their respective emitters in the interface. The Si<sup>1+</sup> and Si<sup>2+</sup> components are located in the same layer close to the bulk. The Si<sup>4+</sup> atoms are part of the silicon oxide film at the surface. The diffraction patterns clearly indicate a crystalline interface structure below the amorphous SiO<sub>2</sub>-layer. In order to determine the structure it is necessary to compare the experimental diffraction patterns with simulated XPD-patterns for structure models. A genetic algorithm was developed for the structure model optimization.

O 63.7 Fri 12:45 SCH A118

**Interaction of as-grown InN(0001) surfaces with oxygen** — ●ANJA EISENHARDT, MARCEL HIMMERLICH, JUERGEN A. SCHAEFER, and STEFAN KRISCHOK — Institut für Physik and Institut für Mikro- und Nanotechnologien, TU Ilmenau, P.O. Box 100565, 98684 Ilmenau, Germany

The interaction of oxygen with clean (2x2) reconstructed InN(0001) surfaces is investigated by in-situ photoelectron spectroscopy (XPS, UPS). InN thin films were grown by plasma assisted molecular beam epitaxy. Directly following the growth an in-situ characterization of the pure InN samples as well as the investigation of the oxidation of the non-contaminated surfaces without any preparation was performed. Differences between the core levels as well as the valence band spectra of the clean in-situ grown and the oxygen treated InN samples will be presented. The comparison of the valence band structure shows the appearance of two electronic structures at 5.2 eV and 10.3 eV that can be assigned to oxygen adsorbates due to the impurity-free preconditions. Furthermore, the oxygen exposure leads to the disappearance of the InN(0001)-(2x2) surface reconstruction as well as the related surface state close to the Fermi level. This can be explained by the distortion of the (2x2) adatom reconstruction. In XPS two different states are observed in the O1s emission. Based on the detected chemical shifts, the chemical state of the adsorbed oxygen will be discussed. Furthermore, the oxidation has only minor influence on the position of the valence band maximum and the work function.

## O 64: Metal substrates: Adsorption of inorganic molecules

Time: Friday 11:15–12:45

Location: SCH A215

O 64.1 Fri 11:15 SCH A215

**Angle Resolved Photoelectron Distribution of the 1 $\pi$  Resonance of CO/Pt(111)** — ●THORBEN HAARLAMMERT<sup>1</sup>, SEBASTIAN WEGNER<sup>1</sup>, GRIGORIUS TSILIMIS<sup>1</sup>, HELMUT ZACHARIAS<sup>1</sup> und ALEXANDER GOLOVIN<sup>2</sup> — <sup>1</sup>Physikalisches Institut, Westfälische Wilhelms Universität, Münster — <sup>2</sup>Institute of Physics, St. Petersburg State University

The CO 1 $\pi$  level of a c(4x2)-2CO / Pt(111) reconstruction shows a significant resonance when varying the photon energy between  $h\nu=23\text{eV}$  and  $h\nu=48\text{eV}$ . This resonance has not been observed in gas phase measurements or on the Pt(110) surface. To investigate the photoelectron distribution of the 1 $\pi$  level High Harmonic Radiation has been used. By conversion in rare gases like Argon, Neon, or Helium photon energies of up to 100 eV have been generated at repetition rates of up to 10 kHz. The single Harmonics have been separated and focused by a toroidal grating and directed to the sample surface. A time-of-flight detector with multiple anodes registers the kinetic energies of the emitted photoelectrons and enables the simultaneous detection of multiple emission angles.

The angular distributions of photoelectrons emitted from the CO 1 $\pi$  level have been measured for a variety of initial photon energies. Further the angular distributions of the CO 1 $\pi$  level photoelectrons emitted from a CO-Pt<sub>7</sub> cluster have been calculated using the MSX $\alpha$ -Method which shows good agreement with the experimental data.

O 64.2 Fri 11:30 SCH A215

**Coadsorption of CO and hydrogen on PtRu/Ru(0001) surface alloys** — ●THOMAS DIEMANT<sup>1</sup>, JOACHIM BANSMANN<sup>1</sup>, HUBERT RAUSCHER<sup>1,2</sup>, and R. JUERGEN BEHM<sup>1</sup> — <sup>1</sup>Institute of Surface Chemistry and Catalysis, Ulm University, D-89069 Ulm, Germany — <sup>2</sup>Institute for Health and Consumer Protection, Joint Research Centre, European Commission, I-21020 Ispra (VA), Italy

Due to their superior CO tolerance, bimetallic platinum-ruthenium catalysts are one of the most promising materials for the anodic hydrogen oxidation reaction in low-temperature polymer electrolyte fuel cells in the presence of small CO amounts. Therefore, the study of the adsorption properties of PtRu systems is of high interest. We have investigated the coadsorption of CO and hydrogen on PtRu/Ru(0001) surface alloy model systems by TPD and IR spectroscopy under UHV conditions. While hydrogen adsorption on the bimetallic surface alloys is already weakened in the absence of CO compared to the case of unmodified Ru(0001) [1], the addition of CO to the surface leads to a further significant weakening of hydrogen adsorption, caused by

the repulsive interaction between the adsorbed species. Furthermore, post-adsorbed CO displaces hydrogen to energetically less favourable Pt-rich adsorption sites. The implications of our results for fuel cell applications will be discussed.

[1] T. Diemant et al., J. Phys. Chem. C 112 (2008) 8381.

O 64.3 Fri 11:45 SCH A215

**Interaction of CO with PdAg/Pd(111) surface alloys** — YUNSHENG MA, ●JOACHIM BANSMANN, THOMAS DIEMANT, ALBERT ENGSTFELD, HARRY HOSTER, and BEHM BEHM — Institute of Surface Chemistry and Catalysis, Ulm University, D-89069 Ulm

The surface composition, distribution of different Pd ensembles and adsorption properties of PdAg/Pd(111) surface alloys have been investigated by Scanning Tunneling Microscopy (STM), Temperature Programmed Desorption (TPD) and High Resolution Electron Energy Loss Spectroscopy (HREELS) using CO as a probe molecule. The statistical analysis of atomic resolution STM images with chemical contrast reveals a nearly random distribution of the surface atoms on PdAg/Pd(111) surface alloys. The presence of Ag on the surface first suppresses the adsorption of CO on the preferred Pd threefold-hollow sites. For these sites, the adsorption energy does not change for small Ag coverages, indicative for a geometric (ensemble) effect. With increasing Ag surface concentration, CO mostly adsorbs on bridge sites of Pd dimers and top sites of Pd monomers surrounded by Ag atoms. At higher CO coverage, a transition of CO adsorption from bridge to top sites occurs on Pd dimers to accommodate more CO molecules, similar to the case on PdAu/Pd(111) surface alloys [1].

[1] M. Ruff et al., ChemPhysChem 8 (2007) 2068.

O 64.4 Fri 12:00 SCH A215

**CO adsorption on bimetallic PtRu/Ru(0001) surfaces - the influence of surface structure** — ●HEINRICH HARTMANN, THOMAS DIEMANT, JOACHIM BANSMANN, and R. JUERGEN BEHM — Institute of Surface Chemistry and Catalysis, Ulm University, D-89069 Ulm, Germany

To study the influence of the surface structure on the adsorption properties of PtRu/Ru(0001) surfaces, two types of bimetallic model systems with significantly different surface structure were prepared and studied by a combination of TPD and IR spectroscopy using CO and deuterium as probe molecules. While the first type of surface, a submonolayer Pt film on Ru(0001), shows Pt islands on the Ru substrate, the second type is a PtRu surface alloy with an almost random distribution of the components in the surface layer. For both surface

types, a marked weakening of the adsorption strength of both CO and deuterium is evidenced by TPD experiments. While the CO TPD measurements show only minor differences for the two surface types, the surface structure has a clear influence on the D<sub>2</sub> TPD spectra, which is most pronounced for intermediate Pt concentrations. These results demonstrate the special importance of ensemble effects for deuterium adsorption, where mixed threefold adsorption ensembles are occupied, while such effects are absent for CO with exclusive adsorption in on-top sites. For CO, the influence of ligand and strain effects for the CO adsorption on the bimetallic surfaces will be discussed.

O 64.5 Fri 12:15 SCH A215

**Ordered Iodine Adsorption as Fingerprint of (111) Orientation of Pt Thin Films** — ●BJÖRN BRAUNSCHWEIG, ALEXEJ MITIN, and WINFRIED DAUM — Institut für Physik und Physikalische Technologien, TU Clausthal, Leibnizstrasse 4, D-38678 Clausthal-Zellerfeld

Well-ordered Pt films deposited on re-usable substrates find applications such as inexpensive replacements for bulk single crystals or ultrathin transparent electrodes for spectro-electrochemical applications. While morphological properties of such films - roughness, atomic steps and spatial extent of atomically flat terraces - are easily imaged with the STM, atomic resolution of the Pt surface is often not attainable under environmental conditions. We demonstrate that the atomic surface structure of (111)-oriented Pt thin films deposited on  $\alpha$ -Al<sub>2</sub>O<sub>3</sub>(0001) substrates is clearly revealed after adsorption of ordered iodine adlayers. In comparative STM studies with Pt thin films and with (111)-oriented bulk single crystals we observed the same coexisting ( $4 \times 3\sqrt{3}$ )

and ( $\sqrt{43} \times \sqrt{43}$ ) iodine superstructures which indicates that our Pt films are highly ordered and (111)-oriented.

O 64.6 Fri 12:30 SCH A215

**Monte-Carlo lattice gas simulation of adsorption and desorption at disordered surface alloys** — ●MARKUS MAUKSCH<sup>1</sup>, ANDREAS BERGBREITER<sup>1</sup>, HARRY E. HOSTER<sup>1</sup>, YOSHIHIRO GOHDA<sup>2</sup>, AXEL GROSS<sup>2</sup>, and R. JÜRGEN BEHM<sup>1</sup> — <sup>1</sup>Institute of Surface Chemistry and Catalysis, Ulm University, D-89069 Ulm — <sup>2</sup>Institute of Theoretical Chemistry, Ulm University, D-89069 Ulm

The atom distribution in disordered surface alloys like PtRu/Ru(0001) or PdAg/Pd(111) is known from STM imaging with chemical contrast. The interaction of model adsorbates like H<sub>ad</sub> or CO with many of these surfaces were probed by thermal desorption and infrared spectroscopy [1]. Based on experimentally determined atom distributions in the surface alloys, we will model the adsorption properties of selected systems by lattice gas Monte-Carlo simulations including (i) site-specific molecule-substrate, (ii) molecule-molecule interaction energies and (iii) site-specific vibrational entropy [2]. Where available, molecule-substrate interactions are derived from DFT results, in other cases they are fitted to experimental data. The molecule-molecule interactions and site specific entropies are assumed to be close to those for Pt(111) [2] and Ru(0001) [3].

[1] H. Rauscher et al., Surf.Sci. 601 (2007) 4608.

[2] J.-S. McEwen et al., Surf.Sci. 545 (2003) 47.

[3] J.-S. McEwen et al., J.Chem.Phys. 126 (2007) 094701.

## O 65: Time-resolved spectroscopies III

Time: Friday 11:15–13:00

Location: SCH A315

O 65.1 Fri 11:15 SCH A315

**Transient electronic structure and melting of a charge density wave in TbTe<sub>3</sub>** — F. SCHMITT<sup>1</sup>, P. S. KIRCHMANN<sup>2</sup>, ●U. BOVENSIEPEN<sup>2</sup>, R. G. MOORE<sup>1,3</sup>, L. RETTIG<sup>2</sup>, M. KRENZ<sup>2</sup>, J.-H. CHU<sup>1</sup>, N. RU<sup>1</sup>, L. PERFETTI<sup>2</sup>, D. H. LU<sup>3</sup>, M. WOLF<sup>2</sup>, and Z.-X. SHEN<sup>1,3</sup> — <sup>1</sup>Stanford University, Department of Applied Physics, USA — <sup>2</sup>Freie Universität Berlin, Fachbereich Physik, Germany — <sup>3</sup>Stanford Synchrotron Radiation Laboratory, USA

Obtaining insight into cooperative effects is fascinating because, through self-coordination and collectivity, they can lead to instabilities with macroscopic impacts like phase transitions. The responsible interactions are of particular interest to understand these phenomena. We used femtosecond time- and angle-resolved photoelectron spectroscopy to analyze the electronic structure of the quasi-1D charge density wave (CDW) material TbTe<sub>3</sub> which exhibits an energy gap at the Fermi surface along the nesting direction. A Te derived mode at 3.6 THz can be monitored by binding energy variations at all electron momenta, incident fluence  $F$ , and temperatures ( $T=100, 300\text{K}$ ). A second mode at 2.3 THz is found only at low  $T$  and  $F$ , and exclusively at the Fermi surface. For higher  $F=2 \text{ mJ/cm}^2$  we find after 100 fs a closing of the energy gap and a recurrence of quasi-free electron like dispersion crossing the Fermi surface. This indicates unambiguously an ultrafast melting of the CDW state and identifies the 2.3 THz mode as the CDW amplitude mode. We expect that the information which is accessible with trARPES will greatly enhance the understanding of materials exhibiting cooperative phenomena.

O 65.2 Fri 11:30 SCH A315

**Ultrafast dynamics in Silicon studied at FLASH** — ●MARTIN BEYE<sup>1</sup>, ALEXANDER FÖHLISCH<sup>1</sup>, FLORIAN SORGENFREI<sup>1</sup>, BILL SCHLOTTER<sup>1</sup>, TORBEN BEECK<sup>1</sup>, ANNETTE PIETZSCH<sup>2</sup>, FRANZ HENNIES<sup>2</sup>, and WILFRIED WURTH<sup>1</sup> — <sup>1</sup>Department Physik, Universität Hamburg, Deutschland — <sup>2</sup>MAX-lab, Lund, Sweden

Soft X-ray spectroscopies at new light sources like the free electron LASER at Hamburg (FLASH), which provide pulses of some tens of fs length with unrivaled brilliances, provide new tools for the element specific analysis of ultrafast processes resolving local and long range symmetries. We present measurements on crystalline Silicon unraveling timescales of electronic and nuclear processes after specific excitations.

We either use an optical pump laser or the XUV pulses from FLASH to excite phonons, valence or core electrons, respectively. Their tempo-

ral evolution is tracked via X-ray emission spectroscopy of Silicon induced by variably delayed FLASH pulses. This shows the dynamics of the electronic system, resolves temporal changes in the bandstructure, in the electron distribution and of the orbital and crystal momentum.

Using the optical laser as a probe instead, we are sensitive to changes in the electronic structure around the bandgap and the long range structure of the crystal itself. We track those changes after X-ray excitation and their decay via different cascading electronic and phononic processes by analyzing transient reflectivity changes.

We acknowledge financial support from the BMBF priority program FSP301: "FLASH" and the GrK 1355 "Physics with new coherent light sources"

O 65.3 Fri 11:45 SCH A315

**Femtosecond melting of orbital order in magnetite** — ●NIKO PONTIUS<sup>1</sup>, TORSTEN KACHEL<sup>1</sup>, HERMANN A. DÜRR<sup>1</sup>, CHRISTIAN SCHÜSSLER-LANGEHEINE<sup>2</sup>, BILL SCHLOTTER<sup>3</sup>, MARTIN BEYE<sup>3</sup>, ALEXANDER FÖHLISCH<sup>3</sup>, and WILFRIED WURTH<sup>3</sup> — <sup>1</sup>Helmholtz-Zentrum Berlin, BESSY II, Albert-Einstein-Str. 15, 12489 Berlin — <sup>2</sup>Physikalisches Institut, Universität zu Köln, Zùlpicher Straße 77, 50937 Köln — <sup>3</sup>Institut für Experimentalphysik, Universität Hamburg, Luruper Chaussee 149, 22761 Hamburg

The Verwey transition in magnetite ( $Fe_3O_4$ ), discovered by Verwey in 1939 [1], takes place at  $T_V \approx 120\text{K}$  and becomes manifest in a metal-to-insulator transition as well as a structural phase transition, leading to the appearance of superstructure x-ray diffraction peaks. Recent soft x-ray diffraction (RSXD) experiments confirm charge and orbital order in the low temperature phase [2]. However, the microscopic origin of the transition is still controversial.

By using time-resolved RSXD we investigate the "melting" of charge and orbital order to get a more detailed insight into the driving forces of the transition, in particular the interplay of structural and electronic degrees of freedom. The Verwey transition is induced from below  $T_V$  by absorbing an infrared fs-laser pulse. The subsequent temporal evolution of the orbital order is probed by RSXD using fs x-ray pulses the free electron laser FLASH in Hamburg.

[1] E.J.W. Verwey, Nature 144, 327-328 (1939)

[2] J. Schlappa et al., Phys. Rev. Lett. 100, 026406 (2008)

O 65.4 Fri 12:00 SCH A315

**Direct measurement of core-level relaxation dynamics on a surface-adsorbate system** — ●STEFAN MATHIAS<sup>1</sup>, LUIS MIAJA-AVILA<sup>2</sup>, GUIDO SAATHOFF<sup>3</sup>, JING YIN<sup>2</sup>, CHAN LA-O-VORAKIAT<sup>2</sup>,

MICHAEL BAUER<sup>4</sup>, MARTIN AESCHLIMANN<sup>1</sup>, MARGARET MURNANE<sup>2</sup>, and HENRY KAPTEYN<sup>2</sup> — <sup>1</sup>University of Kaiserslautern, 67663 Kaiserslautern, Germany — <sup>2</sup>JILA and University of Colorado, Boulder, Colorado, 80309, USA — <sup>3</sup>Max-Planck-Institute of Quantum Optics, 85748 Garching, Germany — <sup>4</sup>Universität Kiel, 24908 Kiel, Germany

Electronic coupling in surface/adsorbate systems, which occurs on ultrafast time scales in the low femto- to attosecond regime, is fundamental to the understanding of surface chemistry. However, the dynamics of highly-excited adsorbate states have only been studied indirectly to-date. In this work, we present the first direct time-resolved observation of the lifetime of a core-excited state of an atom adsorbed onto a surface using high-harmonic generation (HHG) EUV light pulses. By combining the laser-assisted photoelectric effect (LAPE) on surfaces [1,2] with laser-assisted Auger decay on an adsorbate/surface system, we directly measure the lifetime of the  $4d^{-1}$  core level of Xenon on Pt(111) to be  $7 \pm 1$  fs [3]. This result opens up time domain measurements of highly-excited state dynamics in materials systems where, because of complex interactions, energy-resolved measurements provide incomplete information.

[1] L. Miaja-Avila et al., Phys. Rev. Lett. 97, 113604 (2006)

[2] G. Saathoff et al., Phys. Rev. A 77, 022903 (2008)

[3] L. Miaja-Avila et al., Phys. Rev. Lett. 101, 046101 (2008)

O 65.5 Fri 12:15 SCH A315

**Ultrafast dynamics in the 1T-TiSe<sub>2</sub> transition-metal dichalcogenide in the vicinity of the CDW phase transition** — ●MARTIN WIESENMAYER<sup>1</sup>, STEPHAN HILGENFELDT<sup>1</sup>, STEFAN MATHIAS<sup>2</sup>, TIMM ROHWER<sup>1</sup>, and MICHAEL BAUER<sup>1</sup> — <sup>1</sup>Institut für Experimentelle und Angewandte Physik, Universität Kiel, 24098 Kiel, Germany — <sup>2</sup>Department of Physics, TU Kaiserslautern, 67663 Kaiserslautern, Germany

The layered transition metal dichalcogenides (TMDC) have attracted considerable attention in the past due to a wide range of phenomena associated with their reduced dimensionality, such as charge density wave (CDW) instabilities and enhanced correlation effects. In this paper we report on a two-photon photoemission study of the TMDC compound 1T-TiSe<sub>2</sub>. Static 2PPE measurements reveal a strong quenching of the signal of the occupied Se 4p bands as the incident laser intensity increases. We find that the characteristic timescales associated with this quenching lie in the femtosecond to picosecond range, indicating the involvement and relevance of electronic excitations. Furthermore, the experiments show clear differences in the quenching behavior between the normal and the CDW state of 1T-TiSe<sub>2</sub>. Our results will be discussed under consideration of the highly disputed mechanism for the CDW transition of this compound.

O 65.6 Fri 12:30 SCH A315

## O 66: Organic, polymeric, biomolecular films – also with absorbates II

Time: Friday 11:15–12:45

Location: SCH A316

O 66.1 Fri 11:15 SCH A316

**In-situ infrared spectroscopic ellipsometry of the solid-liquid interface of mixed polymer brushes** — ●DENNIS AULICH<sup>1</sup>, EVA BITTRICH<sup>2</sup>, PETRA UHLMANN<sup>2</sup>, IGOR LUZINOV<sup>3</sup>, OLHA HOY<sup>3</sup>, KLAUS-JOCHEN EICHHORN<sup>2</sup>, MANFRED STAMM<sup>2</sup>, NORBERT ESSER<sup>1</sup>, and KARSTEN HINRICHS<sup>1</sup> — <sup>1</sup>ISAS - Institute for Analytical Sciences, Albert-Einstein-Str. 9, 12489 Berlin — <sup>2</sup>Leibniz-Institut für Polymerforschung Dresden e.V., Hohe Str. 6, 01069 Dresden — <sup>3</sup>Clemson University, 29634-0971, USA

For the control of protein adsorption, wettability and adhesion, functional surfaces based on ultrathin organic films attract more and more interests. Very promising representatives of functional surfaces are mixed polymer brushes. These polymer layers offer the possibility to switch the surface properties e.g. from a protein-repelling to a protein-adsorbing behaviour as a response to external stimuli like solvents, pH or temperature. In order to understand the complex mechanisms of surface functionalization and modification, the single mechanisms like switching of polymer brushes and the adsorption of protein layers have to be well understood. In our recent work we studied the selected mechanisms in-situ with infrared spectroscopic ellipsometry (IRSE). The reversible pH dependent switching of mixed polymer brush systems and mono polymer brushes as well were investigated in-situ in

**Kinetic Approach for Laser-excited Solids** — ●BANAZ OMAR and BAERBEL RETHFELD — Technical University of Kaiserslautern, Department of Physics, Erwin Schroedinger Str. 46, D-67663 Kaiserslautern, Germany.

The microscopic dynamical processes for ultrashort laser-excited solids have been investigated theoretically. The transient non-equilibrium evolution of electron distribution function due to excitation and the subsequent thermalization of the free electrons, as well as the dynamics of phonons are studied in metals. The microscopic collision processes, such as inverse bremsstrahlung absorption, electron-electron collision and electron-phonon interaction are considered in the collision terms of Boltzmann equation [1]. We apply our kinetic approach to the case of gold by taking the total electron density of states into account. A free-electron like conduction band is considered in the d-band, which lies within the conduction band at about 2.5 eV below the Fermi surface. In the case of dielectrics, impact ionization and multi-photon ionization generate free electrons in the conduction band and holes in the valance band. Intense short laser-pulse change a cold solid to a hot dense plasma. With increasing free electron density a dynamical collision frequency is required for quasi-particle collisions.

[1] B. Rethfeld, A. Kaiser, M. Vicanek, and G. Simon, Phys. Rev. B 65, 214303 (2002)

O 65.7 Fri 12:45 SCH A315

**Spectroscopy and dynamics of a surface-switchable phthalocyanine** — ●NILS HEINEMANN, OLEKSIY ANDREYEV, TILL LEISSNER, TIMM ROHWER, and MICHAEL BAUER — Institut für Experimentelle und Angewandte Physik, Christian-Albrechts-Universität Kiel

Molecular switching is a highly topical research field driven for instance by potential applications in molecular electronics.

The non-planar (shuttlecock-shaped) tin-phthalocyanine (SnPc) can adsorb in two different orientations on a surface due to its geometry. Wang et al. have demonstrated, that it is possible to induce a switching between these geometries with the tip of a scanning tunnelling microscope [1].

We present a two photon photoemission (2PPE) study of SnPc on Ag(111) suggesting the possibility of light-induced switching. The electronic structure of the adsorbate has been investigated and laser-induced, intensity dependent changes in the characteristic 2PPE spectra have been observed. We interpret this observation as a transient modification of the adsorbed molecules. Time-resolved 2PPE measurements show, that the characteristic relaxation dynamics take place on a femto- to picosecond time scale.

[1] Y. Wang, J. Kröger, R. Berndt, W. Hofer, *Probing structural and electronic properties of ultrathin SnPc films on Ag(111) at the single molecule level*, Angewandte Chemie (2008) (accepted)

O 66.2 Fri 11:30 SCH A316

**Photothermal fabrication of nanopatterned thiol-based organic monolayers on gold substrates** — ●MAREIKE MATHIEU, ALICE HUI, ECKART HASSELBRINK, and NILS HARTMANN — Fachbereich Chemie, Universität Duisburg-Essen and Center for Nanointegration Duisburg-Essen (CeNIDE), Universitätsstr. 5, 45141 Essen, Germany

In recent years nonlinear laser processing has been demonstrated as a facile means for nanopatterning of silane-based organic monolayers down to the sub 100 nm range [1,2]. Here we report on photothermal patterning of thiol-based monolayers. Gold-coated silicon substrates are functionalized with hexadecanethiol. Irradiation with a focused beam of an argon ion laser operated at a wavelength of 514 nm allows to locally remove the monolayer. Subsequently, the patterns are transferred into the gold film via selective etching in a ferri/ferrocyanide solution. Despite an  $1/e^2$  spot diameter of about 2.5  $\mu\text{m}$ , structures with lateral dimensions well below 500 nm are fabricated. The underlying nonlinear dependence of the patterning process on the laser intensity is traced back to the interplay between the laser-induced tran-

sient local temperature rise and the thermally activated desorption of the thiol molecules. A simple thermokinetic analysis of the data allows to estimate effective kinetic parameters of the patterning process. Respective values are in good agreement with data in the literature.

1. D. Dahlhaus, S. Franzka, E. Hasselbrink, N. Hartmann, *Nano Lett.* 6 (2006) 2358.

2. N. Hartmann, S. Franzka, J. Koch, B. N. Chichkov, A. Ostendorf, *Appl. Phys. Lett.* 92 (2008) 223111.

O 66.3 Fri 11:45 SCH A316

**Laser-assisted chemical lithography via local photothermal functionalization of silane-based organic monolayers** — ●BENJAMIN KLINGEBIEL, ANJA SCHRÖTER, and NILS HARTMANN — Fachbereich Chemie, Universität Duisburg-Essen (UDE) and Center for Nanointegration Duisburg-Essen (CeNIDE), Universitätsstraße 5, 45117 Essen

Photochemical routines are widely recognized as a versatile means to fabricate multifunctional patterned organic monolayers with laterally alternating chemical terminations. The lateral resolution, in turn, usually is limited to the micrometer and submicrometer length scales. A simple routine for nanopatterning of organic monolayers down to 100 nm and below relies on photothermal processes [1, 2]. For this purpose a focused laser beam is used to locally heat the substrate and initiate thermal decomposition of the monolayer. Here we report on a simple photothermal procedure for direct functionalization of organic monolayers. Surface-oxidized silicon samples are coated with alkylsiloxane monolayers. Local irradiation with a focused beam of an argon ion laser at a wavelength of 514 nm in gaseous bromine allows for direct functionalization of the monolayer. Mechanistic aspects and prospects of photothermal routines in micro- and nanofabrication of multifunctional organic monolayers are discussed.

1. D. Dahlhaus, S. Franzka, E. Hasselbrink, N. Hartmann, *Nano Lett.* 6 (2006) 2358.

2. N. Hartmann, B. Klingebiel, T. Balgar, S. Franzka, E. Hasselbrink, *Appl. Phys. A* 94 (2009) 95.

O 66.4 Fri 12:00 SCH A316

**Infrared spectroscopic ellipsometry for characterization of functionalized thin films** — ●D.M. ROSU<sup>1</sup>, G. SUN<sup>1</sup>, X. ZHANG<sup>2</sup>, J. RAPPICH<sup>2</sup>, J. JONES<sup>3</sup>, J.W.P. HSU<sup>3</sup>, U. SCHADE<sup>4</sup>, N. ESSER<sup>1</sup>, and K. HINRICH<sup>1</sup> — <sup>1</sup>Institute for Analytical Sciences, Albert-Einstein-Str. 9, 12489 Berlin, Germany — <sup>2</sup>Helmholtz-Zentrum Berlin für Materialien und Energie GmbH, Kekuléstraße 5, 12489 Berlin, Germany — <sup>3</sup>Sandia National Laboratories, Albuquerque, New Mexico 87185-1120 — <sup>4</sup>Helmholtz-Zentrum Berlin für Materialien und Energie GmbH, Albert-Einstein-Str. 15, 12489 Berlin, Germany

Organic thin films present a high interest due to their potential use in a large variety of applications: biosensors, microelectronic and optical devices. In the current work Infrared Spectroscopic Ellipsometry was used for chemical and structural characterisation of bifunctional surfaces as well as for investigation of the lateral homogeneity of organic monolayers for GaAs hybrid diodes[1]. The samples were studied using a lab FTIR ellipsometer and the FTIR synchrotron mapping ellipsometer located at the IR beamline at BESSY II[2]. The mapping system enables investigation of heterogeneous samples with monolayer

sensitivity and a lateral resolution below 1 mm<sup>2</sup>. Besides the molecular identification, evaluation of the measured spectra with simulations using optical layer models gives informations about thickness, homogeneity and orientation of the molecules.

[1] D.M. Rosu, et al., *Langmuir*, in print [2] M. Gensch, et al., *Infrared Phys. and Techn.* 49 (1-2) (2006) 39-44

O 66.5 Fri 12:15 SCH A316

**Magnetron sputtered hydrogenated (a-C:H) and oxygen containing (a-C:O) amorphous carbon coatings: surface characteristics, wettability and cell absorption behaviour** — ●FRIEDERIKE DANNEIL — Forschungszentrum Karlsruhe, Institut für Materialforschung I, Hermann-von-Helmholtz-Platz 1, 76344 Eggenstein-Leopoldshafen, Germany

Hydrogenated amorphous carbon (a-C:H) coatings are considered good potential materials for biomedical applications. Hydrogen-free, oxygen containing amorphous carbon (a-C:O) coatings exhibit promising haemocompatible properties but have not yet been investigated very detailed. The objective of this work is the characterization of the surface characteristics, surface properties, wettability and haemocompatibility both of a-C:H and a-C:O coatings prepared by reactive d.c. magnetron sputtering.

The coatings were deposited on Si wafer substrates by sputtering a graphite target in a mixture of methane and argon (Ar+CH<sub>4</sub>) and a mixture of oxygen and argon (Ar+O<sub>2</sub>), respectively. The reactive gas fractions were systematically varied during the experiments. For the surface characterization atomic force microscopy (AFM), Raman spectroscopy and X-ray photoelectron spectroscopy (XPS) were applied. The surface free energy was determined by contact angle measurements. A platelet adhesion test showed favourable behaviour of the a-C:O coatings for blood-contacting applications.

O 66.6 Fri 12:30 SCH A316

**Microscopic and fluorescence spectroscopic studies of organic molecules in contact to surfaces** — ●HEINRICH SÜDMEYER<sup>1</sup>, FRANZ-JOSEF SCHMITT<sup>1</sup>, JOACHIM BÖRNER<sup>1</sup>, MAX SCHOENGEN<sup>1</sup>, HANS-JOACHIM CAPPUS<sup>2</sup>, and HANS JOACHIM EICHLER<sup>1</sup> — <sup>1</sup>Institut für Optik und Atomare Physik, Technische Universität Berlin, Strasse des 17. Juni 135, 10623 Berlin — <sup>2</sup>Laser- und Medizin-Technologie GmbH, Fabekstrasse 60 - 62, 14195 Berlin

Specific amino acids contained in proteins show autofluorescence if excited in UV. Therefore the use of fluorescence markers is not necessary for high resolved fluorescence microscopy. On the other hand it is often necessary to immobilize proteins. But the photophysical and biochemical properties of organic molecules change due to surface contact. To understand these properties the change of protein conformations due to the surface contact must be analyzed. Combined microscopic and time correlated single photon counting methods (TCSPC) are very promising because the fluorescence depends on the conformational structure of the proteins and allows to analyze different quenching mechanisms. With TCSPC energy transfer processes between neighbouring amino acids, neighbouring molecules and between molecules and the surface can be analyzed. Due to the fluorescence kinetics it is also possible to separate the fluorescence of spectrally similar fluorescence emitters.

## O 67: Ab-initio approaches to excitations in condensed matter III

Time: Friday 11:15–12:45

Location: SCH 251

O 67.1 Fri 11:15 SCH 251

**Tackling localized *d*-states: a systematic investigation by  $GW@LDA+U$**  — ●HONG JIANG<sup>1</sup>, RICARDO I. GOMEZ-ABAL<sup>1</sup>, PATRICK RINKE<sup>2,1</sup>, and MATTHIAS SCHEFFLER<sup>1,2</sup> — <sup>1</sup>Fritz-Haber-Institut der MPG, Berlin — <sup>2</sup>University of California at Santa Barbara, CA 93106

First-principles modeling of systems with localized *d*-states is currently a great challenge in condensed matter physics. Density-functional theory (DFT) in the standard local-density approximation (LDA) proves to be problematic. This can be partly overcome by including local Hubbard *U* corrections (LDA+*U*), but itinerant states are still treated on the LDA level. Many-body perturbation theory in the *GW* approach offers both a quasiparticle perspective (appropriate for itinerant states) and an exact treatment of exchange (appropriate for lo-

calized states), and is therefore promising for these systems. Here we present a systematic investigation of the  $G_0W_0$  method based on LDA+*U* ( $G_0W_0@LDA+U$ ) for a series of prototype systems: 1) ZnS with semicore *d*-states, 2) ScN and TiO<sub>2</sub> with empty *d*-states and 3) late transition metal oxides (MnO, FeO, CoO and NiO) with partially occupied *d*-states. We show that for ZnS, ScN and TiO<sub>2</sub>, the  $G_0W_0$  band gap only weakly depends on *U*, but for the other transition metal oxides the dependence on *U* is as strong as in LDA+*U*. These different trends can be understood in terms of changes in the hybridization and screening. Our work demonstrates that  $G_0W_0@LDA+U$  with “physical” values of *U* provides a balanced and accurate description of both localized and itinerant states.

O 67.2 Fri 11:30 SCH 251

**Spin-wave excitations in itinerant ferromagnets from**

**many-body perturbation theory** — ●ERSOY SASIOGLU<sup>1</sup>, ARNO SCHINDLMAYR<sup>2</sup>, CHRISTOPH FRIEDRICH<sup>1</sup>, and STEFAN BLÜGEL<sup>1</sup> — <sup>1</sup>Institut für Festkörperforschung and Institute for Advanced Simulation, Forschungszentrum Jülich, 52425 Jülich, Germany — <sup>2</sup>Department Physik, Universität Paderborn, 33095 Paderborn, Germany

To study excitation spectra of magnetic materials from first principles we have developed a computational scheme based on many-body perturbation theory. The main quantity of interest is the dynamical transverse spin susceptibility, from which magnetic excitations, including single-particle spin-flip Stoner excitations and collective spin-wave modes as well as their lifetimes, can be obtained. In order to describe spin waves we include appropriate vertex corrections in the form of a multiple-scattering T-matrix, which describes the coupling of electrons and holes with different spin. To reduce the numerical cost for the calculation of the four-point T-matrix we exploit a transformation to maximally localized Wannier functions that takes advantage of the short spatial range of electronic correlation in the partially filled *d* or *f* orbitals of magnetic materials. Our implementation is based on the full-potential linearized augmented plane-wave (FLAPW) method. As an illustration, we present spin-wave spectra and dispersions for the elementary ferromagnets Fe, Co and Ni calculated with our scheme. The results are in good agreement with available experimental data.

O 67.3 Fri 11:45 SCH 251

**All-electron GW calculations for SrTiO<sub>3</sub>, BaTiO<sub>3</sub> and PbTiO<sub>3</sub>** — CHRISTOPH FRIEDRICH<sup>1</sup>, ●ANDREAS GIERLICH<sup>1</sup>, ARNO SCHINDLMAYR<sup>2</sup>, and STEFAN BLÜGEL<sup>1</sup> — <sup>1</sup>Institut für Festkörperforschung and Institute for Advanced Simulation, Forschungszentrum Jülich, 52425 Jülich, Germany — <sup>2</sup>Department Physik, Universität Paderborn, 33095 Paderborn, Germany

The GW approximation for the electronic self-energy, which combines bare exchange with the dynamical screening of the many-electron system within the random-phase approximation, yields quasiparticle band structures in very good agreement with experiment. While most implementations today employ the pseudopotential approximation, our recently developed realization (<http://www.flapw.de/spex>) is based on the all-electron full-potential linearized augmented-plane-wave (FLAPW) method, where core and valence electrons are treated on the same footing. Within this method a large variety of materials can be treated, including *d*- and *f*-electron systems, oxides and magnetic systems. In this work we present results for the perovskite transition-metal oxides SrTiO<sub>3</sub>, BaTiO<sub>3</sub> and PbTiO<sub>3</sub>, which are widely used in technical applications. Their band gaps are difficult to measure experimentally and have been under debate for a long time. Most *ab initio* studies so far were based on density-functional theory and showed a strong underestimation of the band gap. Here we present all-electron GW calculations that overcome this problem and yield band gaps very close to the best experimental estimates.

O 67.4 Fri 12:00 SCH 251

**Efficient all-electron GW calculations of complex semiconductors** — ●CHRISTOPH FRIEDRICH<sup>1</sup>, ARNO SCHINDLMAYR<sup>2</sup>, and STEFAN BLÜGEL<sup>1</sup> — <sup>1</sup>Institut für Festkörperforschung and Institute for Advanced Simulation, Forschungszentrum Jülich, 52425 Jülich, Germany — <sup>2</sup>Department Physik, Universität Paderborn, 33095 Paderborn, Germany

The GW approximation for the electronic self-energy yields quasiparticle band structures in very good agreement with experiment, but almost all implementations so far are based on the pseudopotential

approach, which limits their range of applicability. We have developed an implementation (SPEX, <http://www.flapw.de/spex/>) within the full-potential linearized augmented-plane-wave (FLAPW) method, which treats core and valence electrons on an equal footing. Within this method a large variety of materials can be treated, including *d*- and *f*-electron systems, oxides and magnetic systems. Our implementation employs a mixed product basis for the representation of wave-function products in the interstitial and muffin-tin regions. A basis transformation to the eigenfunctions of the Coulomb potential allows a reduction of the basis-set size without compromising the accuracy, thus leading to a considerable speed-up in computation time. To demonstrate the efficiency of the implementation we present results for complex semiconductors. Financial support from the Deutsche Forschungsgemeinschaft through the Priority Programme 1145 is gratefully acknowledged.

O 67.5 Fri 12:15 SCH 251

**X-ray absorption spectra of ice and water: a first principles study with the GW method** — XIFAN WU<sup>1</sup>, WEI CHEN<sup>2</sup>, and ●ROBERTO CAR<sup>1,2</sup> — <sup>1</sup>Department of Chemistry, Princeton University, Princeton, USA — <sup>2</sup>Department of Physics, Princeton University, Princeton, USA

We calculated the X-ray absorption spectra of ice and liquid water by adopting an approach based on the GW method to describe the excited electron in presence of a frozen core hole. We used the static Coulomb-hole and screened exchange approximation for the self-energy and used Maximally Localized Wannier functions to make GW calculations feasible in the large supercell needed to model a disordered system like water. The calculated spectra considerably improve the agreement with experiment, compared with previous DFT calculations. In particular, the three main features observed in experiments are well reproduced in terms of position and intensity for both ice and water. We also find that the difference between the ice and water spectra can be understood in terms of the electronic structures of these systems, manifested by a distorted, tetrahedral hydrogen bond network in the liquid.

O 67.6 Fri 12:30 SCH 251

**Electron-phonon coupling in graphite within the GW-approximation** — ●LUDGER WIRTZ<sup>1</sup>, MICHELE LAZZERI<sup>2</sup>, CLAUDIO ATTACALITE<sup>3</sup>, and FRANCESCO MAURI<sup>2</sup> — <sup>1</sup>IEMN, Lille France — <sup>2</sup>IMPMC, University "Pierre et Marie Curie", Paris, France — <sup>3</sup>European Theoretical Spectroscopy Facility, University of the Basque Country, San Sebastian, Spain

A seemingly trivial thing such as the phonon dispersion of graphite continues to present surprises. For most materials (both metals and insulators), density-functional perturbation theory using LDA or GGA gives phonon dispersions in close agreement with experimental results. For graphene and graphite, however, there is a pronounced failure of LDA and GGA for the highest optical phonon branch (HOB) around the Kohn-anomaly at the high-symmetry point K. We evaluate the electron-phonon coupling (EPC) between the pi-bands and the HOB in the GW-approximation. Non-local exchange-correlation effects renormalize the square EPC by almost 80%. This almost doubles the slope of the HOB around K and explains recent experimental results on graphite-phonons using inelastic x-ray scattering and double-resonance Raman spectroscopy. The short-coming of LDA and GGA may be partially fixed by the use of hybrid-functionals such as B3LYP (which partially contains exact Hartree-Fock exchange). The use of pure Hartree-Fock, however, leads to an extremely strong EPC and consequently to an instability of graphene under distortion along the HOB phonon.

## O 68: Invited Talk (Klaus Heinz)

Time: Friday 13:30–14:15

Location: HSZ 02

### Invited Talk

O 68.1 Fri 13:30 HSZ 02

**Surface Structure Analysis – Present Status and Future** — ●KLAUS HEINZ — Lehrstuhl für Festkörperphysik, Universität Erlangen-Nürnberg, Staudtstr. 7, 91058 Erlangen

The knowledge of the crystallographic structure of a surface, that is the positions of atoms within a certain slab of a surface, is essential for the quantitative understanding of its physical properties. Hereby, the item "surface" stands for clean and adsorbate covered surfaces as well as interfaces, which all are crucial components of nanostructures.

The current status of surface crystallography is reviewed including the limitations involved. Emphasis is on quantitative low-energy diffraction (LEED) but the strength of other and competing methods as, e.g., photoelectron diffraction (PED) and surface x-ray diffraction (SXRD) is also illuminated. Today's state of the art techniques which use TensorLEED combined with structural search routines as well as recent progress made by so called holographic-type direct methods or the valuable use of Patterson-type maps will be described. It will also be shown that a single method may be unable to resolve the (full)

structure one even to get only an idea about the proper model. Instead, the application of several methods can be necessary. These include in particular scanning tunneling microscopy (STM) with its real-space information and first-principles methods as density func-

tional theory (DFT) which minimizes the system's energetics rather than an R-factor. It will also be discussed whether or not crystallographic precision in the picometer range – which we are used to achieve for simple structures – is necessary for complex structural phases.

## O 69: Invited Talk (Martin Wolf)

Time: Friday 14:15–15:00

Location: HSZ 02

### Invited Talk

O 69.1 Fri 14:15 HSZ 02

**Transient Electronic Structure and Insulator-to-Metal Transitions Probed by Time-resolved Photoemission Spectroscopy**  
— ●MARTIN WOLF — Freie Universität Berlin, Dept. of Physics, Arnimallee 14, 14195 Berlin, Germany — Fritz-Haber-Institut d. MPG, Faradayweg 4-6, 14195 Berlin, Germany

One of the basic questions in solid state physics is to understand why a material behaves like an insulator or a metal. Systems with a half-filled band are usually expected to be metallic, however, may undergo a metal-to-insulator transition at low temperatures due to Peierls instabilities (charge density wave (CDW) formation) or electron correlations (Mott insulator). We use femtosecond time- and angle-resolved photoelectron spectroscopy (trARPES) to optically excite and probe two

model systems, namely the Mott insulator 1T-TaS<sub>2</sub> and the CDW compound TbTe<sub>3</sub>, to investigate the dynamics of such insulator-to-metal transitions directly in the time domain. In TaS<sub>2</sub> photoexcitation by an intense laser pulse leads to an ultrafast transition towards a gapless phase which is accompanied by periodic oscillations of the electronic states. The qualitative difference between the oscillatory dynamics of the CDW, the quasi-instantaneous collapse of the electronic gap and the monotonic recovery of the electronic gap proves that 1T-TaS<sub>2</sub> is indeed a Mott insulator. Moreover it is in clear contrast with the retarded (>100fs) response which we observe for the transient melting of the CDW phase in TbTe<sub>3</sub>. Using trARPES we are able to identify the role of collective vibrations in the transition and to document the highly anisotropic dynamics of the electronic system in real time.