

## O 36: Poster Session II (Metals; Nanostructures at surfaces; Surface or interface magnetism; Spin-Orbit Interaction at Surfaces; Electron and spin dynamics; Surface dynamics; Methods; Theory and computation of electronic structure)

Time: Tuesday 18:30–22:00

Location: P4

O 36.1 Tue 18:30 P4

**Electron pair emission from a Cu(111) surface** — RAJENDRA S. DHAKA, ●FRANK O. SCHUMANN, GRANT A. VAN RIESSEN, ZHENG WEI, and JÜRGEN KIRSCHNER — Max-Planck-Institut für Mikrostrukturphysik, Weinberg 2, D-06120 Halle, Germany

We aim to explore the validity of an important assumption of the theoretical description of the (e,2e) process, namely an effective single electron description of the electronic properties of the sample. If affirmative the orbital character of the valence state can be identified and it would be of interest to find conditions where the emission is dominated by a particular valence state. In order to test the conjecture we selected a Cu(111) surface as sample which has a well-known electronic structure. We varied the primary energy in the range 19-65 eV. The sum energy spectra reveal features which can be directly related to the effective single particle band structure of the sample. This proves that for Cu an effective single particle picture is an adequate description within a (e,2e) experiment. The relative pair emission intensity from the surface state and 3d states is observed to vary dramatically with the primary energy. At low excitation energies the spectrum is dominated by the contribution from the Shockley surface state. We propose a simplified model based on the diffraction of pairs to explain this observation.

O 36.2 Tue 18:30 P4

**Oxidation of Ruthenium Surfaces** — ●MARIUS ERNST<sup>1,2</sup>, THANH-NAM NGUYEN<sup>1</sup>, SINA GUSENLEITNER<sup>1,2</sup>, DIRK EHM<sup>2</sup>, and FRIEDRICH REINERT<sup>1,3</sup> — <sup>1</sup>University of Würzburg, Experimental Physics VII, Am Hubland, 97074 Würzburg, Germany — <sup>2</sup>Carl Zeiss SMT GmbH, Rudolf-Eber-Strasse 2, Oberkochen, Germany — <sup>3</sup>Karlsruhe Institute of Technology, Gemeinschafts Labor für Nano-Analytik, Germany

Multilayer mirrors for extreme ultraviolet (EUV) Lithography applications are threatened by various deterioration processes of the surface. During exposure, the dominating contamination processes are carbonization and oxidation due to adsorption of hydrocarbons and oxygen and their reaction with the mirror surface, reducing the mirror lifetime. One possibility to extend the lifetime is to coat the mirror with a dedicated capping material, such as Si, Ti, Mo, Pd, Ru, or their oxides. To study the influence of oxidative species (O<sub>2</sub> and H<sub>2</sub>O), in this work Ru single crystals were used as model systems for real mirror capping layers. The (0001) surface of a Ru single crystal was exposed to oxidative environments with a total pressure ranging from 10<sup>-9</sup> mbar to 10<sup>-4</sup> mbar and analyzed with low energy electron diffraction (LEED), X-ray photoelectron spectroscopy (XPS) and ultra-violet photoelectron spectroscopy (UPS). Depending on pressure and exposure, different surface reconstructions could be found. At oxygen partial pressures higher than 10<sup>-4</sup> mbar and sufficiently long oxygen exposure, bulk oxide formed, the thickness of which was analyzed with ellipsometry. The oxidation behaviour of single crystalline surfaces was compared with the oxidation of thin evaporated Ru layers.

O 36.3 Tue 18:30 P4

**Scanning tunneling microscopy study of asymmetric Pd pincer complexes on a Cu(111) Surface** — ●SHIH-HSIN CHANG<sup>1,4</sup>, ALESSANDRO SCARFATO<sup>2,3</sup>, CHRISTIAN CHRISTIAN KLEEGER<sup>3</sup>, MARTIN BRÖRING<sup>3</sup>, GERMAR HOFFMANN<sup>1</sup>, and ROLAND WIESENDANGER<sup>1</sup> — <sup>1</sup>Institute of Applied Physics and Microstructure Research Center Hamburg, University of Hamburg, Germany — <sup>2</sup>Dipartimento di Fisica E.R. Caianiello, Università degli Studi di Salerno, Italy — <sup>3</sup>Fachbereich Chemie, Philipps-Universität Marburg, Germany — <sup>4</sup>Research Center for Applied Sciences, Academia Sinica, Taipei, Taiwan

The adsorption of asymmetric Pd pincer complexes on a Cu(111) surface was investigated by means of ultra-high vacuum scanning tunneling microscopy. The structural asymmetry is manifested in the observation of two chiral enantiomers. To enable an unambiguous identification of individual constituents, three closely related complexes with small modifications are investigated in parallel. Thereby, methyl substituents determine attractive molecule-molecule interaction. Depending on their distribution, dimerization and tetramerization can be

observed.

O 36.4 Tue 18:30 P4

**Self-Assembled Monolayers of Dimethylselenide on Au(111)** — ●LYDIA EL-KAREH, AXEL BEIMBORN, PATRICK MEHRING, and CARSTEN WESTPHAL — Experimentelle Physik I, TU Dortmund, Otto-Hahn-Str. 4, 44221 Dortmund, Germany

Self-assembled monolayers (SAMs) attract considerable attention due to their large potential in applications such as molecular electronics, tailoring of metallic surface properties and biological sensors. In recent years many studies of sulfur based SAMs have been performed. As the Se-Au bond is stronger than the S-Au bond selenium based SAMs are very interesting. In this study the structural formation of Dimethylselenide (DMDSe) monolayers on a Au(111) surface was investigated by scanning tunneling microscopy. SAMs were prepared by immersing the gold substrate in ethanolic solution of DMDSe. We report on the formation of a striped DMDSe phase at the surface and its thermal evolution upon heating. After annealing at 90°C the striped phase disappeared due to reorganization of molecules on the surface.

O 36.5 Tue 18:30 P4

**Specific protein patterning in protein-repelling monomolecular matrix by UV promoted exchange reaction** — ●JEYACHANDRAN YEKKONI<sup>1</sup>, ANDREAS TERFORT<sup>2</sup>, and MICHAEL ZHARNIKOV<sup>1</sup> — <sup>1</sup>Angewandte Physikalische Chemie, Universität Heidelberg, 69120 Heidelberg, Germany. — <sup>2</sup>Institut für Anorganische und Analytische Chemie, Universität Frankfurt, Max-von-Laue-Straße 7, 60438 Frankfurt, Germany.

Oligo(ethylene glycol) (OEG) self assembled monolayers, well known for their protein resistance behaviour, could be used to produce protein patterns upon introduction of specific receptor groups by exchange reaction enabled by controlled degradation. We investigated the degradation of OEG monolayers using UV irradiation at 254, 312, and 366 nm to achieve well-controlled exchange reaction and protein patterning. OEG molecules with different lengths of the alkyl and OEG stems as well as with different tail groups (OCH<sub>3</sub> or OH) were used to prepare monolayers on Au surface and biotinylated alkanethiol was used as a receptor for avidin or streptavidin. Experiments at zero dose showed that the OH terminated OEG monolayers with a sufficiently long alkyl linker and the EG chain (minimum 5 units) are stable towards non-specific receptor exchange reaction for at least 5 min. incubation. At 254 nm irradiation the degradation kinetics of the OEG chains was very fast that produced complete degradation (direct patterning) at dose below 8 J/cm<sup>2</sup>. However, 312 and 366 nm irradiation provided the possibility to control the degradation (defects formation) at low doses followed by direct patterning at doses greater than 103 J/cm<sup>2</sup>.

O 36.6 Tue 18:30 P4

**Comparing CuPc and H<sub>2</sub>Pc sub-monolayer films on Ag(111): A NIXSW and SPA-LEED study** — ●INGO KRÖGER<sup>1</sup>, PATRICK BAYERSDORFER<sup>2</sup>, BENJAMIN STADTMÜLLER<sup>1</sup>, CHRISTOPH KLEIMANN<sup>1</sup>, GIUSEPPE MERCURIO<sup>1</sup>, FRIEDRICH REINERT<sup>2</sup>, and CHRISTIAN KUMPF<sup>1</sup> — <sup>1</sup>Peter Grünberg Institut (PGI-3), Forschungszentrum Jülich, 52425 Jülich, Germany and JARA-Fundamentals of Future Information Technology — <sup>2</sup>Experimentelle Physik 7, Universität Würzburg, 97074 Würzburg

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 - a continuous series of phases with point-on-line coincidence with the substrate [1,2]. The latter is caused by repulsive intermolecular interaction. In order to clarify the role of the central metal atom for this repulsion, we compare SPA-LEED and NIXSW data of the metal free H<sub>2</sub>Pc/Ag(111) with CuPc/Ag(111). The similarity of the phase diagrams leads to the conclusion that in principle the intermolecular repulsion does not depend on the metal atom. For H<sub>2</sub>Pc the adsorption heights show a significant bending of the nitrogen atoms toward the surface. This "N-down" configuration leads to a stronger and more localized bonding to the surface, and therefore stabilizes the commensurate phase

in a wider coverage regime and at higher temperature compared to CuPc/Ag(111). [1] Kröger et al., *New Journal of Physics* 12, 083038 (2010) [2] Stadler et al., *Nature Physics* 5, 153 (2009)

O 36.7 Tue 18:30 P4

**DFT studies on the adsorption of thiols at transition metal surfaces** — ●PORNTIP SEEMA, JÖRG BEHLER, and DOMINIK MARX — Lehrstuhl für Theoretische Chemie, Ruhr-Universität Bochum, D-44780 Bochum

The interaction of sulfur-containing molecules with transition metal surfaces plays an important role for example in the poisoning of heterogeneous catalysts and the formation of self-assembled monolayers. A large number of theoretical and experimental studies has been carried out in recent years, but still several questions on the structures of these systems remain open. We present density-functional theory (DFT) calculations for the adsorption of several sulfur-containing species (e.g. S atoms, H<sub>2</sub>S, CH<sub>3</sub>SH) on Cu(111) and Ag(111) surfaces. Calculations have been carried out for a variety of adsorbate coverages, binding sites and surface models (slabs and clusters). We find that the order of the binding energies is S > SH > SCH<sub>3</sub>, with an increased binding energy at surface defects. In general, the sulfur-metal interaction is stronger for Cu(111) than for Ag(111).

O 36.8 Tue 18:30 P4

**Structural formation of thiophene-2-thiol on gold** — LYDIA EL-KAREH<sup>1</sup>, ●AXEL BEIMBORN<sup>1</sup>, PATRICK MEHRING<sup>1</sup>, DOMINIQUE HANDSCHAK<sup>1</sup>, and CARSTEN WESTPHAL<sup>1,2</sup> — <sup>1</sup>Experimentelle Physik 1 - TU Dortmund, Otto-Hahn-Str.4, D 44221 Dortmund, Germany — <sup>2</sup>DELTA -TU Dortmund, Maria-Goeppert-Mayer-Str. 2, D 44227 Dortmund, Germany

In recent years self assembled monolayers (SAMs) have been extensively studied because of their well-defined structures resulting from simple dipping preparation. An ideal system for the understanding of self-organisation processes are alkanethiols that were widely examined during the last decades. These molecules can be prepared with different head groups leading to different applications in molecular electronics, nanotechnology, bio-sensing, and corrosion inhibition. One possible head group is thiophene. The orientation of thiophene-2-thiol adsorbed on Au(111) has been investigated by scanning tunneling microscopy (STM). Thiophene-2-thiol molecules are found forming highly ordered adlayers. High-resolution STM reveals well ordered molecular stripes of different length. On the gold surface the stripes arrange displaced with respect to the substrate lattice forming a two-dimensional molecular network.

O 36.9 Tue 18:30 P4

**Configurational and Electronic Switching of Single Azopyridine-Substituted Porphyrin Molecules** — ●FRANCESCA MATINO<sup>1</sup>, GUILLAUME SCHULL<sup>2</sup>, UMASISH JANA<sup>3</sup>, FELIX KÖHLER<sup>4</sup>, RAINER HERGES<sup>4</sup>, and RICHARD BERNDT<sup>1</sup> — <sup>1</sup>Institut für Experimentelle und Angewandte Physik, Christian-Albrechts-Universität zu Kiel, 24098 Kiel, Germany — <sup>2</sup>Institut de Physique et Chimie des Matériaux de Strasbourg, UMR 7504 (CNRS, Université de Strasbourg), 67034 Strasbourg, France — <sup>3</sup>Department of Chemistry, Jadavpur University, Kolkata-700032, India — <sup>4</sup>Institut für Organische Chemie, Christian-Albrechts-Universität zu Kiel, 24098 Kiel, Germany

Switching is an elementary step in many sophisticated functions, such as directed motion, pumping, information storage and processing, in the macroscopic world as well as at the molecular scale. For nanoscale applications of such functions, molecules have to be immobilized on solid supports in a well defined geometry and orientation, in order to achieve advanced and reproducible dynamic functions. Here we report on a new azopyridine functionalized porphyrin synthesized as a model switch for deposition on surfaces. The porphyrin platform provides bonding to the surface, some electronic decoupling and a defined orientation of the azopyridine unit. Two geometrically and electronically different states of single molecules on Au(111) were found and analyzed by Scanning Tunneling Microscopy and Spectroscopy. Switching between two conformational states occurs upon tunneling of electrons through LUMO orbitals.

O 36.10 Tue 18:30 P4

**Structural and electronic properties of thin organic heterointerfaces SnPc/PTCDA/Ag(111)** — MARK HÄMING<sup>1</sup>, ●CHRISTOPH SAUER<sup>1</sup>, MICHAEL GREIF<sup>1</sup>, ACHIM SCHÖLL<sup>1</sup>, and FRIEDRICH REINERT<sup>1,2</sup> — <sup>1</sup>Universität Würzburg, Experimentelle Physik VII, D-97074 Würzburg — <sup>2</sup>KIT, Gemeinschaftslabor für Nanoanalytik,

D-76021 Karlsruhe

Knowledge about the structural and electronic properties of organic heterointerfaces is of vital importance for electronic devices based on organic semiconductors. Yet information about these systems is still scarce due to difficulties in preparing well defined interfaces. With tinphthalocyanine (SnPc) deposited on a Ag(111) surface precovered by perylene-tetracarboxylic acid dianhydride (PTCDA) we present a well suited model system to gain insight into such heterointerfaces. Photoelectron spectroscopy (XPS and UPS) as well as near edge X-ray absorption fine structure (NEXAFS) studies are applied in order to gain both structural and electronic information. Distinct features in core-level and valence spectra allow us to unambiguously distinguish between both molecules. We show clear evidence that SnPc forms a flat lying wetting layer on top of PTCDA with a mainly physisorptive character. Moreover a rigid level shift of all spectroscopic SnPc features with respect to the homomolecular SnPc films is observed, similar to what is known for Schottky contacts, which corresponds to a change in work function. We demonstrate that the built-in electric field at the interface can be explained by the formation of an interface dipole, which extends over several adsorbate monolayers.

O 36.11 Tue 18:30 P4

**First STM measurements on a new class of nanowheels** — ●ANJA WADEWITZ<sup>1</sup>, JÖRG MEYER<sup>1</sup>, FRANCESCA MORESCO<sup>1</sup>, GWÉNAËL RAPENNE<sup>2</sup>, HENRI-PIERRE JACQUOT<sup>2</sup>, CHRISTIAN JOACHIM<sup>2</sup>, and GIANAURELIO CUNIBERTI<sup>1</sup> — <sup>1</sup>Institute for Materials Science and Max Bergmann Center of Biomaterials, Dresden University of Technology, 01062 Dresden, Germany — <sup>2</sup>CEMES-CNRS, Toulouse, France

Manipulation of single molecules with a scanning tunneling microscope (STM) tip is a well established technique to study the adsorption of molecules and their mechanical properties on a surface. Recent progress in molecular manipulation has stimulated the design and synthesis of molecules that mimic macroscopic machinery, transposing mechanical functions to the scale of a single molecule. Here, we present the first low temperature STM measurements of a new class of nanowheels on Au(111). A nanowheel consists of two subphthalocyanine molecules connected by a carbon axis. The phthalocyanine fragments are nitrogen-tagged. Due to the tagging it should be possible to follow the rolling motion of the wheel just by imaging the molecule. A fast dissociation of the molecules with temperatures and light intensity is expected. Therefore, the evaporation temperature was kept as low as possible and after evaporation the sample was transferred immediately into the STM to minimize temperature and light effects. Nanowheels on Au(111) were imaged by STM, showing intact molecules as well as fragments. These first results show that the nanowheels can be deposited intact on a metal surface and that it is therefore possible to manipulate them with the STM tip.

O 36.12 Tue 18:30 P4

**Electronic structure of novel air-stable n-type organic semiconductors: A comparison of different bay-substituted perylene-bisimide dyes** — ●MARKUS SCHOLZ<sup>1</sup>, RÜDIGER SCHMIDT<sup>2</sup>, SEBASTIAN FIEDLER<sup>1</sup>, ACHIM SCHÖLL<sup>1</sup>, FRANK WÜRTHNER<sup>2</sup>, and FRIEDRICH REINERT<sup>1,3</sup> — <sup>1</sup>Universität Würzburg, Experimentelle Physik VII, 97074 Würzburg — <sup>2</sup>Universität Würzburg, Institut für Organische Chemie, 97074 — <sup>3</sup>Gemeinschaftslabor für Nanoanalytik, Karlsruher Institut für Technologie, 76021 Karlsruhe

The development of air stable n-conducting organic semiconductors are one of the current bottle necks in organic electronic. We present a comparative analysis of the electronic structure of various bay-substituted perylene bisimide (PBI) dyes, which have already demonstrated very high mobilities in thin film devices. The occupied and unoccupied valence levels were investigated by UPS and IPES, which allows determining the transport gap. Interestingly, the transport gap does not differ substantially between the different compounds. If the contact properties to a Ag(111) metal substrate are investigated, work function measurements reveal strong interface dipoles. In case of PBIs with fluoro alkyl chains the interface dipole is about 0.7 eV, which can be related to the C<sub>4</sub>F<sub>7</sub>-chains oriented out of the film surface. For Films of PBIs with isopropylphenyl-groups the magnitude and the direction of the interface dipole depend strongly on the film preparation and provide a possible route for a tailoring of the interfacial electronic structure.

O 36.13 Tue 18:30 P4

**Surface-confined reaction of porphyrins with Cu atoms: An**

**X-ray photoelectron spectroscopy study** — •MIN CHEN, MARTIN SCHMID, JIE XIAO, HANS-PETER STEINRÜCK, and J. MICHAEL GOTTFRIED — Universität Erlangen-Nürnberg, Lehrstuhl für Physikalische Chemie II, Erlangen, Germany

Porphyrin derivatives are wide-spread in nature and of considerable technological importance as candidates for the construction of functional devices. Examples are the usage of metalloporphyrins and similar macrocycles as organic semiconductors or for the functionalization of surfaces in catalysis or sensor applications. As shown previously, free-base porphyrins readily form ordered monolayers on single-crystalline substrates and represent redox-active ligand precursors, which can oxidize and coordinate adsorbed metal atoms. In this study, we focus on the reactivity of various porphyrin derivatives towards adsorbed Cu atoms. As a first model system, we studied the reaction of tetrapyrrolylporphyrin (2HTPyP) with Cu atoms on Au(111). The co-adsorbed reactants form an intermediate at 300 K, which reacts further to Cu(II) tetrapyrrolylporphyrin at higher temperatures. If 2HTPyP is deposited on a Cu/Au(111) subsurface alloy, the metalation reaction leads to a segregation of Cu due to the strong Cu-porphyrin bond. Related experiments with tetraphenylporphyrin and phthalocyanine will be discussed. In addition, the above results for Cu atoms on Au(111) will be compared with reactions of porphyrins on Cu(111). Support by the Deutsche Forschungsgemeinschaft through SFB 583 and by the Alexander von Humboldt Foundation is acknowledged.

O 36.14 Tue 18:30 P4

**Electrospray Ion Beam Deposition for Scanning Tunneling Microscopy Studies in Ultrahigh Vacuum** — •GORDON RINKE<sup>1</sup>, STEPHAN RAUSCHENBACH<sup>1</sup>, NICHIA THONTASEN<sup>1</sup>, ZHITAO DENG<sup>1</sup>, NICOLA MALINOWSKI<sup>1</sup>, and KLAUS KERN<sup>1,2</sup> — <sup>1</sup>Max Planck Institute for Solid State Research, Heisenbergstrasse 1, 70569 Stuttgart, Germany — <sup>2</sup>Institut de Physique de la Matière Condensée, Ecole Polytechnique Fédérale de Lausanne, 1015 Lausanne, Switzerland

The deposition of complex molecules in vacuum is an important technological step towards applications. In recent years, electrospray ion beam deposition (ES-IBD) was developed in our laboratory as a technique for the deposition of molecular layers of nonvolatile molecules on well defined surfaces in ultrahigh vacuum.[1,2] Thereby the key mechanism is the creation of molecular ions or clusters, which deposited on surfaces result in the growth of molecular nanostructures or films.

Here we show that this technique has now matured into a ready tool for surface scientists to prepare a great variety of surface coatings with unprecedented control. By employing state of the art ion optics, ES-IBD offers mass-selection, deposition energy control and coverage monitoring as features that are intrinsic to the process. We demonstrate the versatility of the deposition method by showing surface coatings of highest quality from molecular magnets (Mn<sub>12</sub>), proteins, host-guest compounds, dye molecules and membrane like layers.[2,3]

[1] Small 2 (2006), pg. 540

[2] ACS Nano 3 (2009), pg. 2901

[3] J. Phys. Chem. C 114 (2010), pg. 17768

O 36.15 Tue 18:30 P4

**Substrate- and temperature-dependent adsorption studies of spiropyran molecules** — •ALEX KRÜGER<sup>1</sup>, MARTEN PIANTER<sup>1</sup>, CH. FELIX HERMANN<sup>1</sup>, JORGE MIGUEL<sup>1</sup>, MATTHIAS BERNIEN<sup>1</sup>, KLAUS HERMANN<sup>2</sup>, and WOLFGANG KUCH<sup>1</sup> — <sup>1</sup>Freie Universität Berlin, Institut für Experimentalphysik — <sup>2</sup>Theory Department, Fritz-Haber- Institut der Max-Planck-Gesellschaft

The adsorption of trimethyl-6-nitrospiropyran, a photoswitch that can be optically switched between its spiropyran (SP) and merocyanine (MC) isomer forms, on Au(111) and Bi(110) single-crystal surfaces was studied as a function of coverage and substrate temperature by near-edge x-ray absorption fine structure (NEXAFS) and X-ray photoelectron spectroscopy (XPS). For one monolayer on Au(111) at 150 K and room temperature (RT), we find that the molecules are physisorbed in their SP conformation. After annealing the sample to 330 K, the angle dependence and intensity of the N  $\pi^*$ -resonances changed, and a chemical shift of the N 1s XPS signal was observed and interpreted as a thermally induced ring-opening reaction of molecules from the SP into the MC form. On Bi(110) the adsorption behavior is similar but the nitro group experiences a chemical modification. Based on a peak assignment derived from DFT simulations of the NEXAFS spectra, this species is interpreted as the ring-opened MC conformer. The ability for conformational switching of the adsorbed molecules was studied by illuminating the sample with UV and visible light. The N K edge NEXAFS spectra showed a significant change after illumination

with UV as well as with visible light.

O 36.16 Tue 18:30 P4

**Cobalt phthalocyanine molecules adsorbed on Ag(111): Examination of interfacial interactions** — •MARTIN SCHMID, ANDRE KAPTAN, MIN CHEN, JIE XIAO, HANS-PETER STEINRÜCK, and J. MICHAEL GOTTFRIED — Universität Erlangen-Nürnberg, Lehrstuhl für Physikalische Chemie II

The modification of interfacial properties by adsorbates is a fundamental aspect in catalysis and molecular electronics. As a model system for metal/organic interfaces, we studied the adsorption of Co(II)-phthalocyanine (CoPc) on Ag(111). In general, metallophthalocyanines form well ordered layers on metallic substrates. To obtain a deeper insight into the CoPc/Ag interaction, we examined submonolayers, monolayers, and multilayers of CoPc with photoelectron spectroscopy (XPS/UPS) and low-energy ion scattering (LEIS). Up to one monolayer, the adsorption of CoPc induces two new electronic states in the vicinity of the Fermi edge and a negative work-function shift. XPS shows a strong modification of the Co 2p<sub>3/2</sub> and 2p<sub>1/2</sub> core level states due to the CoPc-Ag(111) interaction. These levels exhibit a binding energy  $\sim 2$  eV lower than in molecules without a direct contact to the metal interface. This finding can be interpreted by a charge transfer from the Ag(111) substrate into the molecules. Furthermore, the binding energy differences between the 2p<sub>1/2</sub> and 2p<sub>3/2</sub> levels are altered by the contact to the single crystal surface. This observation suggests a change in the electronic state of the central Co ion. Support by the DFG through SFB 583 is gratefully acknowledged.

O 36.17 Tue 18:30 P4

**Spatially resolved electron-vibration coupling in an organic charge transfer salt on Au(111)** — •ISABEL FERNANDEZ-TORRENTE, KATHARINA J. FRANKE, and JOSE IGNACIO PASCUAL — Institut für Experimentalphysik, Freie Universität Berlin

Understanding the process of vibrational excitations in molecules is a subject of fundamental importance in potential organic-based device application due to the crucial influence vibrations have in the electronic transport properties. We have measured the vibrational properties of the acceptor molecule TCNQ embedded in a self-assembled layer with TTF, a charge donor. We find that TCNQ hosts, upon charge transfer, an unpaired spin in its Lowest Unoccupied Molecular Orbital (LUMO). This state is demonstrated by the observation of a Kondo resonance. Besides Kondo, this spin is coupled to vibrational modes of the TCNQ that induce a splitting of the Kondo resonance in vibrational sidebands, each one consisting on a peak and a step. While the steps correspond to a pure inelastic process, the peaks have an elastic character (i.e. vibrations excited through the resonant Kondo channel), demonstrated by the quenching of intensity of the central Kondo peak with increasing number of excited vibrations. The vibrations are spatially localized in particular regions of the molecule. The analysis of the STS elastic peaks and STS maps taken on individual TCNQ molecules allow us to resolve with submolecular precision the strength of the electron-phonon coupling and its specific location.

O 36.18 Tue 18:30 P4

**Local anchoring and functionalization of tetraphenylporphyrins on composite surfaces: A Scanning Tunneling Microscopy Study** — •MICHAEL STARK, STEFANIE GLÄSSEL, FLORIAN BUCHNER, ELISABETH ZILLNER, MICHAEL RÖCKERT, HANS-PETER STEINRÜCK, and HUBERTUS MARBACH — Lehrstuhl für Physikalische Chemie II and Interdisciplinary Center for Molecular Materials (ICMM), Universität Erlangen-Nürnberg, Egerlandstr. 3, D-91058

The understanding of the adsorption behavior of large organic molecules on surfaces is a prerequisite to utilize their functional properties either in single molecule devices or in self-assembled supramolecular architectures.

Herein, we investigate to which extent composite surfaces can act as a template to engineer the adsorption of different tetraphenylporphyrins (TPP). In particular, we investigate the dynamics and assembly of different TPPs on Cu(111) covered with monoatomic thick Ni or oxygen islands via scanning tunneling microscopy (STM) in ultra-high vacuum (UHV), mainly at room temperature (RT). On Ni precovered Cu(111) we find, e.g., that TPP molecules are immobilized selectively on the Ni-islands at RT. Furthermore, we demonstrate the possibility of local anchoring and/or functionalization of the porphyrins on prestructured Cu(111) surfaces.

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

O 36.19 Tue 18:30 P4

**Tuning the energy level alignment at the SnPc/Ag(111) interface using an STM tip** — ●MARIUS TOADER and MICHAEL HETSCHOLD — Chemnitz University of Technology, Institute of Physics, Solid Surfaces Analysis Group, D-09107 Chemnitz, Germany

The tip influence on the energy level alignment at the SnPc/Ag(111) interface has been addressed via the Scanning Tunneling Spectroscopy (STS). A collective effect characteristic for both molecular conformations up and down is reported to shift the corresponding first filled (HOMO) and empty (LUMO) levels towards the Fermi energy via a tip-sample distance decrease. The importance of the tin ion coupling to the metal electrodes is emphasized for the newly reported cross-bending (cross-shifting) effect. The observation is proven to be driven by the bistable donor/acceptor character of the SnPc molecules. Distinct types of coupling to the metal surface have been found for the two molecular conformations. However, a similar adsorption geometry of the molecular plane is emphasized by the same energy position of the HOMO level. Moreover, the crucial importance of the HOMO-1 (found using DFT to show strong contribution from the Sn ion) for a conformational change is proven via a controllable and irreversible tip-induced single-molecule switching and nano-writing within densely packed molecular arrays.

O 36.20 Tue 18:30 P4

**SnPc on Ag(111) investigated by STM** — ●CHRISTOPH KLEIMANN, INGO KRÖGER, CHRISTIAN WEISS, CHRISTA ELSAESSER, BENJAMIN STADTMÜLLER, and CHRISTIAN KUMPF — Peter Grünberg Institut (PGI-3), Forschungszentrum Jülich, 52425 Jülich, Germany and JARA-Fundamentals of Future Information Technology

Tin(II)-phthalocyanine (SnPc) is a large, non-planar, organic molecule which shows a number of different structural phases when adsorbed on Ag(111). While at low coverages a gas-like phase was observed, larger coverages result in a series of ordered, incommensurate structures at room temperature, a behavior that indicates intermolecular repulsion. At low temperature the formation of commensurate SnPc islands was found within a certain range of coverage. These different phases have already been studied intensively in our group by SPA-LEED, XSW and other techniques [1]. Two different adsorption geometries have been identified using scanning tunneling microscopy (STM) in some of these structures: The central Sn atom can either be oriented towards (Sn down) or away from the surface (Sn up). Here we show STM measurements for different coverages at room temperature and low temperature. The results confirm and complement our previous findings and demonstrate that the fine interplay of molecule-molecule and molecule-substrate interactions is crucial for the structure formation in this system.

[1] Stadler et al, Nat.Phys. 5, pp 153-158 (2009)

O 36.21 Tue 18:30 P4

**Multi-Technique Investigation of the Interface of Perfluoropentacene on Ag(111)** — ●CHRISTIAN SCHMIDT, MANUEL MARKS, JAN GÖTZEN, CHRISTIAN H. SCHWALB, GERSON METTE, ULRICH HÖFER, and GREGOR WITTE — Fachbereich Physik und WZMW, Philipps-Universität Marburg, D-35032 Marburg

The performance of organic electronic devices is to a large extent determined by the interaction at the electrodes which affects the charge carrier injection and also the morphology of the organic semiconductor films. Since a common understanding of such interfaces properties is still lacking, a detailed characterization is required for every new available organic material. Here we have studied the structure and electron dynamics of the interface between Perfluoropentacene (PF-PEN) and a Ag(111) surface by combining STM, LEED, XPS, NEXAFS and 2PPE. While a recent study revealed the formation of a commensurate PF-PEN monolayer at 90 K [1], we observed reversible phase transition between this low temperature phase and a gas phase behavior at room temperature. While multilayer films can be selectively desorbed by gentle heating thus allowing the preparation of monolayer films the molecules reveal a cracking for temperatures above 400K. Further on 2PPE enables us to study the interface electron dynamics directly in the time domain. While no predominant contributions due to molecular states were observed in the time resolved 2PPE spectra, a series of surprisingly strongly bound image-potential related interface states occur that mainly determine the interfacial electron dynamics.

[1] S.L. Wong et al. *J.Phys.Chem. C* **114**, 9356 (2010).

O 36.22 Tue 18:30 P4

**Adsorption of metal-free phthalocyanine molecules on Pd(110) and Au/Pd(110)** — ●DANIEL DÜCK<sup>1</sup>, TOBIAS PERTRAM<sup>1</sup>, and KLAUS WANDEL<sup>1,2,3</sup> — <sup>1</sup>Institute of Physical and Theoretical Chemistry, University of Bonn, Germany — <sup>2</sup>Institute of Experimental Physics, University of Wrocław, Poland — <sup>3</sup>Department of Physics, University of Rome Tor Vergata, Italy

The {110} surfaces of fcc metals show an intrinsic anisotropy due to the rectangular surface unit cell. This anisotropy is even more pronounced in case of the (1 × 2) missing row reconstruction. The clean Pd(110) surface does not show the tendency to reconstruct. But under the influence of hydrogen we find missing row reconstruction. 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 (1 × 2) reconstruction, which still remains pseudomorphic to Pd(110) [2]. We have used these reconstructed surfaces as a substrate for the ordered ("templated") deposition of phthalocyanine molecules.

Phthalocyanines have attracted considerable attention owing to their promising application in optical and electronic devices. Especially the adsorption behaviour and film growth have been investigated.

STM investigations under UHV reveal a specific adsorption behaviour of the metal-free phthalocyanine molecules, which are oriented along rows of the reconstructed surfaces, and detailed structure models are discussed.

O 36.23 Tue 18:30 P4

**Two photon photo-emission study of doped and undoped Pentacene thin films on Cu(111)** — ●MARTIN LAUX, INDRANIL SARKAR, ANDREAS RUFFING, and MARTIN AESCHLIMANN — Department of Physics and Research Center OPTIMAS, University of Kaiserslautern

Organic-metal interfaces plays a very important role in the performance of opto-electronic devices based on organic semiconductors, as the interface strongly affects the carrier injection in these devices. So, it is of utmost importance to understand the energy level alignment and corresponding energetics at organo-metallic interfaces [1]. Among various organic semiconductors, Pentacene ( $C_{22}H_{14}$ ) forms a very important organic compound for organic devices due its intrinsically high carrier mobility and controllable electronic properties by doping [2]. Here we report, one-photon photoemission (1PPE) and two-photon photoemission (2PPE) measurements on pentacene thin films on Cu(111). Our results show presence of highly dispersive HOMO band, with effective mass of  $0.35 m_e$ . For very low thickness of pentacene an unoccupied interface state appears. We also present time resolved 2PPE measurements on Cs doped pentacene thin films. Our results, indicate strong Cs induced modification of surface, bringing out the possibility of tuning the organic metal interface state using dopants.

[1] T. S. Kuhlman et. al. *J. Am. Chem. Soc.* **132**, 3431 (2010)

[2] A. Scheybal et. al. *Phys. Rev. B* **79**, 115406 (2009).

O 36.24 Tue 18:30 P4

**Infrared Reflection Absorption Spectroscopy (IRRAS) of Ethene ( $C_2H_4$ ) Chemisorbed on the Bare and Roughened Cu(110) and Cu(111) Surfaces** — ●JAN PISCHEL, OLAF SKIBBE, and ANNEMARIE PUCCI — Kirchhoff-Institut für Physik, Im Neuenheimer Feld 227, D-69120 Heidelberg

As a model for an organic-metal interface, the chemisorption systems  $C_2H_4/Cu(111)$  and  $C_2H_4/Cu(110)$  have attracted attention because of their remarkable absorption properties in infrared (IR) spectroscopy [1-4]. Not only were two gas phase Raman active modes observed that are expected to be IR forbidden by the Raman-IR exclusion principle for centrosymmetric molecules, but also the only IR active mode allowed by the metal surface selection rule seemed to disappear at higher coverages on Cu(110). No final conclusion concerning these findings has been drawn so far. This brought us to reinvestigate the system  $C_2H_4/Cu(110)$  by means of IRRAS. Additionally the influence of small amounts of cold-evaporated copper in the submonolayer region has been studied. The results are compared to those of ethene adsorbed on Cu(111) [4]: While the spectra obtained on the bare surfaces are found to differ strongly, the absorption properties become similar with increasing surface roughness.

[1] C. J. Jenks et al. *Surf. Sci. Lett.*, **277**:L89-L94, 1992.

[2] J. Kubota et al. *Phys. Chem.*, **98**:7653-7656, 1994.

[3] R. Raval. *Surf. Sci.*, **331-333**:1-10, 1995.

[4] O. Skibbe et al. *J. Chem. Phys.*, 128:194703-1 - 194703-6, 2008.

O 36.25 Tue 18:30 P4

**Ballistic hole transport through PTCDA molecules** — ●ALEXANDER BERNHART, MARK KASPERS, CHRISTIAN BOBISCH, and ROLF MÖLLER — Faculty of Physics, Center for Nanointegration Duisburg-Essen, University of Duisburg-Essen, Lotharstr. 1, 47048 Duisburg, Germany

Ballistic Electron Emission Microscopy (BEEM) not only represents an ideal technique to study the electronic transmission at the Schottky-interface between a metal and a semiconductor, but moreover it offers capabilities to analyze the ballistic transport through adsorbates on top of a metal. By using a 6 nm Bi film on a p-doped Si(001) substrate it is possible to analyze the ballistic transport of holes through the occupied states of organic adsorbates. For the perylene derivate PTCDA the ballistic current varies between alternating rows of molecules. The comparison to the bare Bi surface reveals that the total BEEM current is reduced by the molecular layer.

O 36.26 Tue 18:30 P4

**Monolayer formation and electronic structure of tetracyanoethylene on Ag(111) and Ag(100) studied by scanning tunneling microscopy** — ●HASMİK HARUTYUNYAN, TATJANA WALTH, TOBIAS ALLMERS, and DANIEL WEGNER — Physikalisches Institut and CeNTech, WWU Münster, Germany

Tetracyanoethylene [TCNE, (CN)<sub>2</sub>C=C(CN)<sub>2</sub>] is a very strong  $\pi$ -electron acceptor that easily forms metal-organic charge-transfer complexes. Particular interest exists for TCNE-based complexes involving transition-metal atoms because they are promising candidates for molecular magnets [1]. Recent studies showed that TCNE adsorbs quite differently on various noble metal surfaces due to a varying ratio of molecule-molecule vs. molecule-substrate interaction [2]. Here we present new results of the growth of TCNE on Ag(100) and Ag(111) studied by low-temperature STM and STS. We show that, different from previous results, TCNE can form closed-packed monolayer patterns on both surfaces. In case of Ag(100), we find local order in shifted rows that form zig-zag patterns with  $(3 \times 5n)$  unit cells ( $n = 1 \dots 4$ ). On Ag(111), TCNE forms an ordered porous network with a  $(\sqrt{67} \times \sqrt{67})$ -R12.1° unit cell containing six molecules. The arrangement of the molecules leads to chirality. STS reveals molecular orbitals as well as vibrations whose dependence on molecule-molecule and molecule-substrate interaction will be discussed.

[1] D. Wegner et al., *PRL* 103, 087205 (2009).

[2] D. Wegner et al., *Nano Lett.* 8, 131 (2008).

O 36.27 Tue 18:30 P4

**Investigations of Aza-Bodipy adsorbed on metallic surfaces** — ●LOKA MANI, CORMAC TOHER, JÖRG MEYER, ANJA WADEWITZ, FRANCESCA MORESCO, and GIANAURELIO CUNIBERTI — Institute for Materials Science and Max Bergmann Center of Biomaterials, Dresden University of Technology, 01062 Dresden, Germany.

Bodipy dyes (difluoroboradiazas-indacene) are notable for their high quantum yield, intense fluorescence, strong chemical stability and highly tuneable, sharp absorption wavelength with uniquely small Stokes shift. Aza-Bodipy dyes, resulting from the replacement of the methene carbon atom in the bodipy core with a nitrogen atom, additionally show sizable red-shift of the absorption wavelengths. Electron donor materials for organic photovoltaics has recently emerged as promising application of Aza-Bodipy, due to its strong infra-red absorption. Here we present the results of a combined theoretical and experimental investigation of the adsorption characteristics, electronic structure and bonding geometry of single Aza-Bodipy molecules on Au(111) and Ag(110) surfaces. Density functional theory calculations of the density of states (DOS) and adsorption geometry were found to be in qualitative agreement with local DOS and scanning tunneling spectroscopy measurements with a low-temperature scanning tunneling microscope (STM). The strength of the bonding interaction to the substrate was also calculated, and the mobility of the molecule on the surface was investigated by calculating the energy barrier for translations and rotations which were compared with data obtained from STM manipulations.

O 36.28 Tue 18:30 P4

**Site-specific polarization screening in organic thin films: Tetracene on Ag(111)** — TOMOKI SUEYOSHI<sup>1,2</sup>, CHRISTIAN WEISS<sup>1</sup>, AXEL DELHEY<sup>1</sup>, MARKUS ESCHBACH<sup>1</sup>, ●SERGEY SUBACH<sup>1</sup>, and STEFAN TAUTZ<sup>1</sup> — <sup>1</sup>Peter Grünberg Institut (PGI-3),

Forschungszentrum Jülich, 52425 Jülich, Germany and JARA-Fundamentals of Future Information Technology — <sup>2</sup>Graduate School of Advanced Integration Science, Chiba University Yayoi-cho, Inage-ku, Chiba 263-8522, Japan

Organic semiconductors attract considerable attention due to their relevance for electronic devices. The electronic properties of molecules on metals have been studied in particular. For example, it has been shown that the chemical bonding to a metal surface may change both the electronic levels and geometric structure of organic molecules profoundly. Upon charge transport, the electronic states of a molecular material may also be influenced by polarization screening, i.e., the stabilization of a locally injected charge through the polarization of the surrounding molecular environment. Another aspect we report on, namely, the site specificity of the polarization energy in complex unit cells and at surfaces of organic materials can thus have a significant influence on transport properties. Scanning tunneling spectroscopy and ultraviolet photoelectron spectroscopy of tetracene films reveal strong energy level shifts by up to 1 eV from molecule to molecule. This effect can be traced back to the site specificity of polarization energy caused by a combination of different molecular environments, the intrinsic anisotropy of molecular polarizability, and the influence of the substrate.

O 36.29 Tue 18:30 P4

**Long range ordered monolayers and lifting of the Au(111) reconstruction by sulfur containing organic donor molecules** — ●BENJAMIN FIEDLER<sup>1</sup>, ELENA ROJO-WIECHEL<sup>1</sup>, JOHANN CLASSEN<sup>1</sup>, JULIA SIMON<sup>2</sup>, JOHANNES BECK<sup>2</sup>, and MORITZ SOKOLOWSKI<sup>1</sup> — <sup>1</sup>Institut für Physikalische und Theoretische Chemie der Universität Bonn — <sup>2</sup>Institut für Anorganische Chemie der Universität Bonn

We have studied the adsorption and monolayer formation on Au(111) of the well-known donor molecule TTT (Tetrathiotetracene) and the novel donor molecules TBTA (Tetrabenzothianthrene) by high resolution LEED. TTT forms a commensurate monolayer, whereas the submonolayer is disordered, which we interpret to be related to repulsive intermolecular interactions. Interestingly, the  $(\sqrt{3} \times 22)$  herringbone reconstruction of the Au(111) surface is lifted already for small coverages. Quite differently the reconstruction is preserved for adsorption of TBTA, which also forms a highly ordered monolayer, which is incommensurate. With respect to the molecule in the bulk, the surface bonded molecule is planarized. We discuss these findings in the relation to the electron donating character of the molecules and the chemical bonding to the surface.

This work was supported by the DFG under SFB 813.

O 36.30 Tue 18:30 P4

**Investigation of Interface Dipole Formation of Dithiocarbamate Molecules on Gold by Density Functional Theory and Photoelectron Spectroscopy** — ●TOBIAS SCHÄFER<sup>1</sup>, PHILIP SCHULZ<sup>1</sup>, DOMINIK MEYER<sup>1</sup>, RICCARDO MAZZARELLO<sup>2</sup>, and MATTHIAS WUTTIG<sup>1</sup> — <sup>1</sup>I. Physikalisches Institut (IA), RWTH Aachen University — <sup>2</sup>Institut für Theoretische Physik C, RWTH Aachen University

One of the main challenges in constructing organic optoelectronic devices is to control the charge carrier injection between the active organic material and metal contact electrodes. The insertion of a self assembled monolayer (SAM) between the organic/inorganic interface depicts an advantageous way to align the metal work function to the frontier molecular orbitals of adjacent organic species.

In this study Dithiocarbamate terminated molecules (DTC) on gold have been investigated as a potential SAM building block. Photoelectron Spectroscopy reveals a strong lowering of the metal work function upon adsorption of DTC molecules. Hence, calculations employing density functional theory (DFT) have been conducted in order to correlate this effect to the formation of a layer of permanent as well as induced dipoles.

O 36.31 Tue 18:30 P4

**Stability and Structure of Benzenethiol, Pentafluorobenzenethiol and mixed SAMs on Pd(111) prepared by immersion** — ●HEIKO HEIM, CHRISTIAN SCHMIDT, and GREGOR WITTE — AG Molekulare Festkörperphysik, Philipps-Universität Marburg, D-35032 Marburg

Self assembled monolayers of (partly) fluorinated aromatic organothioles have been successfully employed to modify metal-organic interfaces such as gold electrodes in order to improve the properties of

organic electronic devices [1,2]. Recent studies have further shown that apart from gold also palladium constitutes a promising electrode material for such devices [3,4]. However, compared to the case of gold the thiol/palladium interface is by far less extensively investigated. In this study we have characterized the structure and thermal stability of benzenethiol- (BT) and pentafluorobenzenethiol-SAMs (PFBT) on Pd(111) by means of XPS, NEXAFS and TDS. Moreover, since perfluorination causes an inversion of the quadrupole moment of the phenyl rings which may lead to an additional stabilization between fluorinated and non-fluorinated molecules also SAMs of different stoichiometric mixtures of BT and PFBT have been studied.

[1] D.J. Gundlach et al., *Nature Materials*, **7**, 216 (2008)

[2] N. V. Venkataraman et al., *J. Phys. Chem.*, **113**, 5620 (2009)

[3] J. Love et al., *J. A. Chem. Soc.*, **105**, 1171 (2005)

[4] C. Bock et al., *Physica E*, **40**, 2107 (2008)

O 36.32 Tue 18:30 P4

**Shape and dynamics of 2D hierarchic bicomponent networks** — ●WOLFGANG KRENNER<sup>1</sup>, FLORIAN KLAPPENBERGER<sup>1</sup>, YOUNES MAKOUDI<sup>1</sup>, NENAD KEPČIJA<sup>1</sup>, DIRK KÜHNE<sup>1</sup>, SVETLANA KLYATSKAYA<sup>2</sup>, MARIO RUBEN<sup>2,3</sup>, and JOHANNES V BARTH<sup>1</sup> — <sup>1</sup>Physik Department E20, TU München, München, Germany — <sup>2</sup>Institute of Nanotechnology, Karlsruhe Institute of Technology, Karlsruhe, Germany — <sup>3</sup>IPCMS-CNRS UMR 7504, Université de Strasbourg, Strasbourg, France

Towards the construction of molecular networks driven by hierarchic principles, the combination of tailored molecular building blocks has proven to be an essential tool. We present an UHV, low-temperature scanning tunneling microscopy study employing a hierarchic growth scenario to realize bicomponent, self-assembled molecular networks. The molecular templates constructed in this fashion display two types of bonding schemes.

The two building blocks, namely dicarbonitrile sexiphenyl and N,N'-diphenyl oxalic amide, arrange in a variety of molecular networks. By tuning the stoichiometry, the formation of a predominant type of the long range networks found on the Ag(111) surface, can be steered. With this approach it is possible to construct open-porous networks with variable pore size and geometry.

Moreover, thermally induced molecular motion is found to occur in the networks with the largest pore size. A migration of sexiphenyl, acting as weaker bound spacers in these networks, along the chain direction of the bi-molecular template is encountered.

O 36.33 Tue 18:30 P4

**Structural transformation of the PTCDA/Ag(110) interface induced by potassium adsorption** — ●MARTIN WILLENBOCKEL<sup>1</sup>, GIUSEPPE MERCURIO<sup>1</sup>, OLIVER BAUER<sup>2</sup>, BENJAMIN FIEDLER<sup>2</sup>, CHRISTIAN WEISS<sup>1</sup>, RUSLAN TEMIROV<sup>1</sup>, SERGEY SUBACH<sup>1</sup>, MORITZ SOKOLOWSKI<sup>2</sup>, and STEFAN TAUTZ<sup>1</sup> — <sup>1</sup>Peter Grünberg Institut (PGI-3), Forschungszentrum Jülich, 52425 Jülich, Germany and JARA - Fundamentals of Future Information Technology — <sup>2</sup>Institut für Physikalische und Theoretische Chemie, Universität Bonn, Wegelerstr. 12, 53115 Bonn, Germany

Using X-ray photoemission spectroscopy, scanning tunneling microscopy and low energy electron diffraction, the transformation of PTCDA/Ag(110) after deposition of potassium and subsequent annealing is studied. The initially planar molecule/metal interface undergoes significant structural modification: upon annealing, potassium atoms intercalate under the molecular layer partially unbinding PTCDA molecules from silver. This induces significant reorganization of the top-most silver layer resulting in the formation of silver terrace trains with K<sup>+</sup>PTCDA chains on top.

O 36.34 Tue 18:30 P4

**Bisterpyridine adlayers on metal surfaces as 2D model systems - A STM study** — ●THOMAS WALDMANN<sup>1</sup>, HARRY E. HOSTER<sup>1,2</sup>, and R. JÜRGEN BEHM<sup>1</sup> — <sup>1</sup>Ulm University, Institute of Surface Chemistry and Catalysis, 89069 Ulm, Germany — <sup>2</sup>Current address: Technische Universität München, Centre for Electromobility, 50 Nanyang Drive, Singapore 637553

Adlayers of the bisterpyridine derivative 2,4'-BTP on Au(111), Ag(111) and Ag(100) are used as two-dimensional (2D) model systems for studying self-assembly and for direct observation of (reaction)dynamics by scanning tunneling microscopy (STM). (i) At low coverages, we find a preference for a step-crossing behavior of 2,4'-BTP that can be explained by the intramolecular building blocks of the adsorbate. The self-organization on terraces is influenced by (N...metal)-type molecule-

substrate interactions, producing 12 preferred azimuthal orientations of the adsorbates with respect to the close packed surface directions in both, ordered and disordered areas [1]. (ii) Domains of freely rotating molecules, which are stabilized significantly by rotational entropy resulting from the large moment of inertia of 2,4'-BTP [2] exist in a dynamic equilibrium with non-rotating molecules at 300 K. We compare the stabilization by rotational entropy with that for other typical small and large adsorbates. (iii) Ordered monolayers of 2,4'-BTP on Ag(111) are used as a model system for direct STM observation of the reaction between the adlayer and oxygen to a N-oxide network.

[1] T.Waldmann et al., *ChemPhysChem* **11**, 1513 (2010).

[2] M.Roos et al., *PCCP* **12**, 812 (2010).

O 36.35 Tue 18:30 P4

**Intermolecular vs. molecule-substrate interactions - a STM study** — ●MICHAEL ROOS<sup>1</sup>, DANIELA KÜNZEL<sup>2</sup>, HARRY E. HOSTER<sup>1,3</sup>, AXEL GROSS<sup>2</sup>, and R. JÜRGEN BEHM<sup>1</sup> — <sup>1</sup>Ulm University, Institute of Surface Chemistry and Catalysis, 89069 Ulm, Germany — <sup>2</sup>Ulm University, Institute of Theoretical Chemistry, 89069 Ulm, Germany — <sup>3</sup>Current address: Technische Universität München, Centre for Electromobility, 50 Nanyang Drive, Singapore 637553

The formation of 2D molecular networks is governed by a competition between intermolecular interactions and the lateral variation in molecule-substrate interactions. In this contribution we study the effect of varying the location of the heteroatoms (N atoms) in planar organic adsorbates by using two Bis(terpyridine) derivatives (BTP) as model systems. On smooth surfaces the resulting structures are dominated by weak C-H...N-type hydrogen bonds. We will compare the ordering behavior with the network formation on graphene monolayers supported by Ru(0001). The moiré pattern of these surfaces has a periodicity of 3 nm, i.e., in the order of the BTP dimensions. Submolecularly resolved STM images show that the BTP molecules are confined to the valleys of the graphene ripple structure. We will discuss the template effect quantitatively by means of force field calculations and supporting thermal desorption experiments.

O 36.36 Tue 18:30 P4

**Interactions of the biomolecules L-cysteine and adenine with metals investigated by STM** — ●SYBILLE FISCHER, ANTHOULA PAPAGEORGIOU, MATTHIAS MARSCHALL, JOACHIM REICHERT, and JOHANNES V. BARTH — Physik Department E20, TU München, James-Frank-Straße, D-85748 Garching

Understanding the interactions between biomolecules like amino acids and nucleobases as building blocks of the DNA and metal binding sites of proteins are important for the comprehension of many neurodegenerative diseases. Metal-organic coordination networks can act as model systems to investigate these interactions and represent at the same time robust, room temperature stable bio-interfaces which might be useful for enantio-selective catalysis. Here we present a scanning tunneling microscopy (STM) study of L-cysteine and adenine with and without metal adatoms on noble metal surfaces to visualize the self-assembly of these molecules at varying temperatures.

O 36.37 Tue 18:30 P4

**Self-Assembly of Individually Addressable Complexes of C60 and Phthalocyanines on a Metal Surface: Structural and Electronic Investigations** — TOMAS SAMUELY<sup>1</sup>, SHI-XIA LIU<sup>2</sup>, MARCO HAAS<sup>2</sup>, SILVIO DECURTINS<sup>2</sup>, THOMAS JUNG<sup>3</sup>, and ●MEIKE STÖHR<sup>4</sup> — <sup>1</sup>University of Basel, Switzerland — <sup>2</sup>University of Bern, Switzerland — <sup>3</sup>Paul-Scherrer-Institute, Switzerland — <sup>4</sup>University of Groningen, Netherlands

A complex phase behavior was found for a specific phthalocyanine (Pc) derivative adsorbed on either Au(111) or Ag(111). The Pc molecule is symmetrically substituted with eight peripheral di-(tert-butyl)phenoxy (DTPO) groups. The pronounced ability of the DTPO groups to rotate, allows the molecule to adopt different conformations and hence to arrange itself in different ordered patterns. In particular, when all DTPO substituents are arranged above the plane of the Pc core (a bowl-like structure is formed), the interaction of the Pc core with the metal substrate is enabled. Moreover, for such an assembly the hosting properties for the adsorption of C60 were investigated. The C60 molecules adsorb at two clearly distinguishable positions on the pre-deposited Pc layer: they are in contact either with the metal substrate in between two adjacent Pc molecules or with the Pc core. For the latter case, the C60 is located directly above the pi-conjugated Pc core. Hence, the presented system combines the three following features: (i) the direct electronic interaction between donor and acceptor moieties,

(ii) the formation by self-assembly, and (iii) thermal stability. Thereby, the direct investigation of a single donor-acceptor complex is enabled.

O 36.38 Tue 18:30 P4

**A local structure determination of Uracil on Cu(110) by energy scanned photoelectron diffraction** — DAVID DUNCAN<sup>1</sup>, •WERNER UNTERBERGER<sup>2</sup>, TSENOLO LEROTHOLI<sup>1</sup>, DAGMAR KREIKEMEYER-LORENZO<sup>2</sup>, and PHIL WOODRUFF<sup>1</sup> — <sup>1</sup>University of Warwick — <sup>2</sup>Fritz-Haber-Institut

While there is growing interest in investigations of biologically-related molecules on surfaces, very few such studies involve quantitative determination of the local adsorption geometries. The technique of photoelectron diffraction (PhD) is particularly well-suited to this problem because it allows one to determine the local adsorption site of the molecule's atoms. Here we report the results of a new study, namely of the nucleobase molecule uracil (a six-membered ring comprising CH<sub>2</sub>CH<sub>2</sub>CO.NH.CO.NH) on Cu(110). The results for uracil, as one might expect, are closely similar to those reported previously for thymine [1]. Analysis of the O 1s and N 1s PhD spectra shows that the molecular plane is essentially perpendicular to the surface, and the molecule bonds to the surface through the two O atoms and the deprotonated N atom that lies between them. All three of these bonding atoms occupy near-atop sites on the Cu(110) surface, with the molecular plane twisted 11+/-5° off of the <1-10> plane.

[1] F. Allegretti, M. Polcik, D.P. Woodruff, Surf. Sci. 601 (2007) 3611

O 36.39 Tue 18:30 P4

**New ordered structures of  $\omega$ -(4'-methyl-biphenyl-4-yl)alkanethiols Bp4 evaporated under UHV conditions on Au(111) surfaces** — •MIRKO MÜLLER<sup>1,2</sup> and GERHARD PIRUG<sup>1,2</sup> — <sup>1</sup>Peter Grünberg Institut (PGI-3), Forschungszentrum Jülich, 52425 Jülich, Germany — <sup>2</sup>JARA-Fundamentals of Future Information Technology

Depending on the evaporation conditions we observed under UHV two new structures for  $\omega$ -(4'-methyl-biphenyl-4-yl)alkanethiols (Bp4) molecules adsorbed on Au(111) surfaces using a Micro-Channel-Plate (MCP)-LEED system. The resulting patterns could be identified assuming a

$\begin{pmatrix} 1 & 2 \\ 12 & 1 \end{pmatrix} ((\sqrt{3} \times \sqrt{133}) \angle 85.7^\circ)$  and a  $\begin{pmatrix} 14 & 7 \\ 0 & 7 \end{pmatrix} ((7\sqrt{3} \times 7) \angle 90^\circ)$  unit cell. Possible surface structures will be discussed on the basis of a detailed interpretation of these LEED patterns. Apart from the corresponding sharp spots of the  $(\sqrt{3} \times \sqrt{133}) \angle 85.7^\circ$  structure the first pattern contains streaks lining up at positions which would be expected for additional spots from a  $\begin{pmatrix} 2 & 4 \\ 12 & 1 \end{pmatrix} ((2\sqrt{3} \times \sqrt{133}) \angle 85.7^\circ)$  structure. These streaks result from characteristic domain shapes and boundaries. Missing spots in the  $(7\sqrt{3} \times 7) \angle 90^\circ$  pattern can be explained by a pgg symmetry group with two perpendicular glide mirror planes. Consequences on the packing within such selfassembled layer of Bp4 molecules will be discussed.

O 36.40 Tue 18:30 P4

**Surface-enhanced and tip-enhanced Raman spectroscopy of biological molecules on nanostructured metallic surfaces** — •LAURA E. HENNEMANN<sup>1</sup>, ANDREAS KOLLOCH<sup>2</sup>, JOSIP MIHALJEVIC<sup>1</sup>, KAI BRAUN<sup>1</sup>, ALFRED J. MEIXNER<sup>1</sup>, and DAI ZHANG<sup>1</sup> — <sup>1</sup>Institute of Physical and Theoretical Chemistry, University of Tübingen, Auf der Morgenstelle 8, 72076 Tübingen, Germany — <sup>2</sup>Department of Physics, University of Konstanz, Universitätsstrasse 10, 78457 Konstanz, Germany

We use a custom built apertureless scanning near-field optical microscope (SNOM) to investigate several kinds of biological molecules. The setup is an extended parabolic mirror based confocal microscope working with higher order laser modes in order to tune the polarization of the light in its focus. We detected the presence of a (sub)monolayer of biological molecules ranging from DNA bases to double stranded DNA by collecting their unique Raman fingerprint spectrum.

In order to detect such small amounts of molecules, we performed surface-enhanced Raman scattering (SERS) or tip-enhanced Raman scattering (TERS). For SERS, either the irregular rough edges of evaporated noble metal grids or regular arrays of gold nano triangles served as enhancing substrates. We compared the plasmonic properties of gold triangles of different aspect ratios and on different substrates to optimize the electromagnetic enhancement for the 632.8 nm laser excitation. The obtained optical patterns were compared to those com-

puted in simulations.

In the case of TERS, an electrochemically etched sharp gold tip (approx. 20 nm tip apex diameter) was approached to the surface, thus acting simultaneously as a scanning probe microscopy tip for topographic measurements and as a near-field antenna collecting optical information. We collected TERS spectra of single calf thymus DNA molecules immobilized on smooth Au (111) surfaces. Strongly enhanced spectra were obtained both in the SERS and in the TERS measurements.

References: [1] "Parabolic mirror-assisted tip-enhanced spectroscopic imaging for non-transparent materials" D. Zhang, X. Wang, K. Braun, H.-J. Egelhaaf, M. Fleischer, L. Hennemann, H. Hintz, C. Stanciu, C.J. Brabec, D.P. Kern, A.J. Meixner, Journal of Raman Spectroscopy 40 (2009) 1371-1376. [2] "Surface- and Tip-Enhanced Raman Spectroscopy of DNA" L.E. Hennemann, A.J. Meixner, D. Zhang, Spectroscopy Biomedical Applications 24 (2010) 119-124.

O 36.41 Tue 18:30 P4

**Structures of metal electrodes at the solid-liquid interface studied by density functional theory** — •XIAOHANG LIN and AXEL GROSS — Institute of Theoretical Chemistry, Ulm University, D-89069 Ulm, Germany

Recently, the operation of an electrochemical atomic-scale quantum conductance switch has been demonstrated, which is controlled by an external electrochemical voltage applied to an independent third gate electrode [1]. However, the microscopic processes underlying this atomic switch are still unclear. Using density functional theory (DFT) calculations, we have addressed the structure of Ag and Pb metal surfaces which are both used as electrode materials for the switch. We have considered the presence of water layers and the self-diffusion on flat and stepped metal surfaces in order to contribute to the understanding of electrodeposition. We find that the substantial difference in the lattice constants between Ag and Pb leads to significant changes, as far as the stable water structure at the metal-water interface is concerned. With respect to the metal diffusion, the DFT results indicate that exchange processes can have considerably lower barriers than hopping processes.

[1] F.-Q. Xie *et al.*, Phys. Rev. Lett. **93**, 128303 (2004).

O 36.42 Tue 18:30 P4

**Surface Structure and Morphology of Cu-free and Cu-covered Au(100) and Au(111) Electrodes in Alkaline Solution** — •CHRISTIAN SCHLAUP<sup>1</sup>, DANIEL FRIEBEL<sup>2</sup>, and KLAUS WANDEL<sup>3</sup> — <sup>1</sup>Technical University of Denmark, Department of Physics, Fysikvej, DK-2800 Kongens Lyngby, Denmark — <sup>2</sup>Stanford Synchrotron Radiation Lightsource, SLAC National Accelerator Laboratory, 2575 Sand Hill Rd, Menlo Park, CA 94025, USA — <sup>3</sup>University of Bonn, Institute for Physical and Theoretical Chemistry, Wegelerstr. 12, D-53115 Bonn, Germany

For both Cu-free Au-electrodes three different phases were observed as a function of the applied electrode potential. While at low potentials the onset of surface reconstruction points towards an apparently adsorbate free surface and, thus, a weak interaction with species from the electrolyte, a Au-hydroxide and a Au-oxide phase are formed subsequently during potential increase.

A similar phase behavior was also found for Cu-covered Au-electrodes, while at low potentials an apparently adsorbate free Cu layer is observed, a Cu-hydroxide coadsorbate phase and a Cu-oxide phase are formed under increased potential conditions. In addition the apparently adsorbate free Cu-film tends to form a Cu-Au alloy phase while keeping the electrode for a sufficient long time at low potential conditions.

O 36.43 Tue 18:30 P4

**Equilibrium Step Fluctuations on Stepped Au(001) in Electrolyte** — •MOHAMMAD ALSHAKRAN<sup>1</sup>, GUILLERMO BELTRAMO<sup>1</sup>, HARALD IBACH<sup>2</sup>, and MARGRET GIESEN<sup>1</sup> — <sup>1</sup>Institut für Komplexe Systeme Biomechanik ICS-7, Forschungszentrum Jülich GmbH — <sup>2</sup>Peter Grünberg Institut PGI-3, Forschungszentrum Jülich GmbH

Equilibrium step fluctuations on stepped Au(001) with Miller indices (1 1 17) and (1 1 29) in electrolyte were studied by electrochemical scanning tunneling microscopy. Measuring the step-step correlation function we determine the time dependence of the fluctuations. From the time dependence one can deduce the dominant mass transport involved in the fluctuations as a function of the electrode potential. For both samples we find an exponent close to 1/4. Unexpectedly, the fluctuations depend also on the step-step distance with an exponent

3/2. The strong dependence on the step-step distance indicates a mass transport mechanism not considered yet theoretically. We furthermore obtained kink energies as a function of electrode potential. From that potential dependence we obtain a kink dipole moment in the order of  $2.2 \pm 0.6$  e pm.

O 36.44 Tue 18:30 P4

**AIMD simulations of adsorption processes of water on metal surfaces** — ●ANJA KOBEL and AXEL GROSS — Institute for Theoretical Chemistry, Ulm University, D-89069 Ulm, Germany

Studying surface adsorption processes, ab initio molecular dynamics (AIMD) simulations have proven a useful tool for obtaining statistically meaningful results with respect to kinetic quantities such as sticking coefficients. There have been various investigations considering surface adsorption of diatomic molecules, hydrogen in particular, employing AIMD [1]. We focus in our study on the quantitative modelling of the interaction of water on a platinum(111) surface, evaluating an ensemble of AIMD trajectories. This will provide insight into reaction probabilities and distributions of molecules beyond diatomics and give important trend understanding for more complex molecules. Besides the adsorption of single molecules on clean metal surfaces, we also consider the adsorption of water molecules on water-precovered metal surfaces in order to address the first steps of the formation of a water layer on a metal surface.

[1] A. Groß, *ChemPhysChem* **11**, 1374 (2010).

O 36.45 Tue 18:30 P4

**Laterally resolved dependence of the surface-state band edge on Ag islands on Nb (110)** — ●TIHOMIR TOMANIC<sup>1</sup>, CHRISTOPH SÜRGER<sup>1</sup>, DOMINIK STÖFFLER<sup>1</sup>, and HILBERT V. LÖHNEYSSEN<sup>1,2</sup> — <sup>1</sup>Karlsruher Institut für Technologie, Physikalisches Institut, 76131 Karlsruhe — <sup>2</sup>Karlsruher Institut für Technologie, Institut für Festkörperphysik, 76021 Karlsruhe

We investigate the growth of Ag on Nb (110) by in-situ STM at low temperatures ( $T_{\min} = 3$  K). The surface of a Nb (110)-oriented single crystal is prepared by repeated cycles of flashing up to 2300 °C and subsequent Ar<sup>+</sup> sputtering. At a substrate temperature  $T_S = 573$  K, evaporation of nominal 5 nm Ag on Nb (110) leads to the formation of large, flat, and well separated islands. On top of these islands the band edge of electronic surface state in the  $\Gamma$ -L bandgap is resolved by local tunnelling spectroscopy. This state is shifted by 70 - 100 meV towards the unoccupied band - when compared to homoepitaxially grown Ag on Ag (111) - due to large tensile strains originating from the difference in thermal expansion of Ag and Nb between 573 and 3 K. This allows a laterally resolved investigation of the strain distribution in these Ag islands on the nanometer scale.

Work supported by the Kompetenznetz Funktionale Nanostrukturen der Baden-Württemberg Stiftung and by the DFG Center for Functional Nanostructures.

O 36.46 Tue 18:30 P4

**Structural Phases and Magnetism of the Co Monolayer on W(001)** — ●ARNE KÖHLER, RENÉ SCHMIDT, ALEXANDER SCHWARZ, and ROLAND WIESENDANGER — Institute of Applied Physics, University of Hamburg, Jungiusstraße 11, 20355 Hamburg

Theory predicts an antiferromagnetic ground state for a monolayer (ML) of Fe or Co grown pseudomorphically on W(001) [1]. Spin-polarized scanning tunneling microscopy (SP-STM) could detect the characteristic  $c(2 \times 2)$  checkerboard pattern for the Fe ML [2], but not for the Co ML. An alternative approach to map spin-structures with atomic resolution is magnetic exchange force microscopy (MExFM) [3], a novel atomic force microscopy (AFM) based technique, which has been successfully applied to the Fe ML on W(001) [4].

With STM we could detect three phases in the Co ML: a pseudomorphic  $p(1 \times 1)$  phase, a reconstructed  $(2 \times 1)$  phase and a third unidentified phase. Temperature dependent measurements indicate that the  $(2 \times 1)$  phase is more densely packed than the  $p(1 \times 1)$  phase. Employing AFM the  $p(1 \times 1)$  phase could be also imaged with atomic resolution. Moreover, AFM data revealed the arrangement of atoms within the  $(2 \times 1)$  phase, because the positions of atoms are not masked by peculiarities in the local density of states like with STM. First MExFM experiments have been performed as well.

[1] P. Ferriani *et al.*, *PRB* **71**, 024452 (2005).

[2] A. Kubetzka *et al.*, *PRL* **94**, 087204 (2005).

[3] U. Kaiser *et al.*, *Nature* **446**, 522 (2007).

[4] R. Schmidt *et al.*, *Nano Lett.* **9**, 200 (2009).

O 36.47 Tue 18:30 P4

**Role of closed compact island during submonolayer pulsed deposition** — MARTIN MAŠIN and ●MIROSLAV KOTRLA — Institute of Physics, ASCR, Na Slovance 2, Prague, Czech Republic

We study temperature dependence of island densities during Pulsed Laser Deposition (PLD) in submonolayer regime. We employ full diffusion kinetic Monte Carlo simulation. Attachment of monomers to islands is irreversible at low temperatures while it becomes reversible at higher temperatures. Our model allows us to study processes on different time scales with parameters for typical PLD experiments: fast deposition (on scale order of  $10^{-5}$  s), and relaxation between pulses (on scale of order of 0.1 s).

In this contribution, we further explore recently observed anomalous behavior of temperature dependence of island density [EPL 90 (2010) 18006] which is due to interplay between the cluster decay time and the interval between pulses. The anomalous behavior is caused by the temperature limited stability of *closed-compact* clusters. We investigate temperature dependent distribution of the closed-compact island for different material and deposition parameters. In particular, we study the dependence on range and strength of the binding interaction (we include interactions to second and third neighbors) and on frequency of pulses. We compare island density of small islands for two modes: PLD and continuous Molecular Beam Epitaxy (MBE) growth. Furthermore, by varying interactions energies, diffusion barrier and parameters of deposition, we compare results of simulations with the PLD experiment for Fe/Mo system.

O 36.48 Tue 18:30 P4

**Rational design of two-dimensional metal-organic frameworks for functional catalysis** — ●CHRISTOPHER KLEY<sup>1</sup>, JAN CECHAL<sup>1</sup>, TAKASHI KUMAGAI<sup>1</sup>, FRANK SCHRAMM<sup>2</sup>, SEBASTIAN STEPANOW<sup>1</sup>, MARIO RUBEN<sup>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>Karlsruhe Institute of Technology, Hermann-von-Helmholtz-Platz 1, 76344 Eggenstein-Leopoldshafen, Germany — <sup>3</sup>École Polytechnique Fédérale de Lausanne, Institut de Physique de la Matière Condensée, 1015 Lausanne, Switzerland

The prospect of tailored metal-organic frameworks (MOF) by rational design makes them attractive candidates for functional structures. Here, we perform surface-confined bimetallic coordination with organic ligands to build-up two-dimensional MOFs with metal rich nanopores for heterogenous catalysts. We study the self-assembly and metal coordination of a rod-like organic ligand with transition metal atoms on Cu and Ag surfaces. The ligand comprises carboxylic and alkynyl functionalities for the selective binding of metal centers. By means of variable temperature scanning tunneling microscopy we observed substrate induced conformational changes of the organic molecule with strong molecular relaxations on the Cu(100) surface. Regular and open metal-coordination networks have been obtained with Fe centers coordinating preferably to the carboxylate oxygen atoms, while Ni atoms tend to bind to the alkynyl groups. This allows for the rational design of bimetallic coordination networks comprising different metal atoms for the structural and catalytic properties at surfaces.

O 36.49 Tue 18:30 P4

**Epitaxial growth of hexagonal boron nitride monolayers by a three-step boration-oxidation-nitration process** — ●FRANK MÜLLER<sup>1</sup>, STEFAN HÜFNER<sup>1</sup>, SAMUEL GRANDTHYLL<sup>1</sup>, HERMANN SACHDEV<sup>2</sup>, STEFAN GSELL<sup>3</sup>, and MATTHIAS SCHRECK<sup>3</sup> — <sup>1</sup>Department of Experimental Physics, Saarland University, D-66041 Saarbrücken, Germany — <sup>2</sup>Inorganic Chemistry, Saarland University, D-66041 Saarbrücken, Germany — <sup>3</sup>Institute of Physics, University of Augsburg, 86135 Augsburg, Germany

The formation of well-ordered monolayers of hexagonal boron nitride on the surface of a Rh/YSZ/Si(111) multilayer substrate via a three-step boration-oxidation-nitration process was investigated by X-ray photoelectron spectroscopy (XPS), X-ray photoelectron diffraction (XPD) and low-energy electron diffraction (LEED). The chemical vapor deposition (CVD) of trimethylborate (BOCH<sub>3</sub>)<sub>3</sub> results in a selective decomposition of the precursor leading to a dilute distribution of boron within the interstitials of the Rh lattice. After oxidation, the layer of a boron oxygen species of about 1 nm thickness can be transformed into a hexagonal monolayer of BN by annealing in an appropriate NH<sub>3</sub> atmosphere. The results of the present study clearly show that the formation of BN monolayers is also possible when boron and nitrogen are provided successively from separate sources. This procedure

represents an alternative routine for the preparation of well-ordered BN monolayers, which benefits from a strong reduction of hazardous potential and economic costs compared to the use of borazine as the current standard precursor. *Phys. Rev. B* 82, 075405 (2010)

O 36.50 Tue 18:30 P4

**Epitaxial growth of hexagonal boron nitride on Ag(111)** — ●FRANK MÜLLER<sup>1</sup>, STEFAN HÜFNER<sup>1</sup>, HERMANN SACHDEV<sup>2</sup>, ROBERT LASKOWSKI<sup>3</sup>, PETER BLAHA<sup>3</sup>, and KARLHEINZ SCHWARZ<sup>3</sup> — <sup>1</sup>Department of Experimental Physics, Saarland University, D-66041 Saarbrücken, Germany — <sup>2</sup>Inorganic Chemistry, Saarland University, 66041 Saarbrücken, Germany — <sup>3</sup>Institute of Materials Chemistry, Vienna University of Technology, A-1060 Vienna, Austria

The epitaxial growth of hexagonal boron nitride on a Ag(111) surface by chemical vapor deposition of borazine (HBNH)<sub>3</sub> and trichloroborazine (ClBNH)<sub>3</sub> is investigated by X-ray photoelectron spectroscopy (XPS) and low-energy electron diffraction (LEED). In contrast to other transition-metal surfaces of hexagonal symmetry, such as Ni(111), Rh(111), or Ru(0001), the hexagonal BN layers form domains of arbitrary orientation, independent on the precursor. This indicates that - with respect to the Ag(111) lattice - there is no preferred direction for the growth of BN. These results are in accordance with recent ab initio calculations that predict vanishing or at least very weak bonding energies for BN on (111) surfaces of noble metals. *Phys. Rev. B* 82, 113406 (2010)

O 36.51 Tue 18:30 P4

**Surface Phases and Structure Determination of Thin Gold Films Grown on a Re(10 $\bar{1}0$ ) Surface** — ●LYRIA MESSAHEL, CHRISTIAN PAULS, and KLAUS CHRISTMANN — Institut für Chemie und Biochemie, FU-Berlin

Gold atoms deposited onto a clean Re(10 $\bar{1}0$ ) surface form, as a function of surface concentration, various submonolayer phases leading to (1 × n) LEED structures (n = 3, 4, 5, 6), the final one being a (1 × 1) phase associated with a pseudomorphic Au bilayer and a coverage of two monolayers ( $\Theta = 2$ ) [1].

The first well-ordered Au overlayer structure is a (1 × 3) phase [1]. If we relate its coverage to the surface concentration of the full bilayer ( $\Theta = 2$ ) we end up with a coverage  $\Theta_{1 \times 3} = \frac{4}{3}$ . LEED calculations have been performed for various Au surface geometries based on this coverage. However, a plausible ball model suggests an additional Au atom in the (1 × 3) unit cell, and a LEED I,V calculation has also been carried out for  $\Theta_{1 \times 3} = \frac{5}{3}$ . We will present the calculated I,V curves for both coverages and compare their structural parameters (geometrical displacements and thermal vibration amplitudes). An additional analysis of the Au(1 × 4) phase's experimental data will also be presented as a support to the assumption  $\Theta_{1 \times 3} = \frac{5}{3}$ .

[1] C. Pauls and K. Christmann, *J. Physics: Condens. Matter* 21 (2009) 134012

O 36.52 Tue 18:30 P4

**Analysis of electrochemically inserted Lithium in metal electrodes** — ●PHILIPP BACH, ANDREAS SEEMAYER, and FRANK UWE RENNER — Max-Planck-Institut für Eisenforschung, Max-Planck-Straße 1, 40237 Düsseldorf

Due to the very negative potential of Li, Li-ion batteries supply a high voltage and high energy density. Lithium ion batteries will continue to be the most important power source for mobile applications in the near future. For achieving longer lifetime and even higher capacity a more detailed knowledge of the basic processes is required. Li alloys with Si, Sn, or Ag provide anodes with higher capacities than the actually used graphite. We focus on the investigation of the electrochemical insertion process of Lithium into simple model anodes like polycrystalline discs or thin films. As electrolyte we use the ionic liquid 1-Butyl-1-methylpyrrolidinium bis(trifluoromethanesulfonyl)imide (PYR14TFSI) with 0.3M LiTFSI. The electrochemical processes, i.e. alloying and dealloying of the anode material, are characterised by Cyclic Voltammetry (CV). The chemical characterisation of the produced alloys is performed ex-situ by the means of Atom Probe Tomography (APT) and Secondary Ion Mass Spectrometry (SIMS). First in-situ measurements using a droplet cell for x-ray diffraction (XRD) experiments using synchrotron radiation are presented.

O 36.53 Tue 18:30 P4

**Aufbau einer Magnetronsputteranlage zur Untersuchung dünner Schichten mit PAES, STM und XPS** — ●ELISABETH LACHNER and CHRISTOPH HUGENSMIDT — FRM II, TU München

In der vorliegenden Arbeit werden Oberflächenprozesse wie Bildung von Oberflächenlegierungen und Segregation untersucht. Neben Scanning Tunneling Microscopy (STM) und X-ray Photoelectron Spectroscopy (XPS) soll die extrem oberflächensensitive Positron-annihilation induced Auger-Electron Spectroscopy (PAES) zum Studium der Oberflächenprozesse genutzt werden. Mittels PAES ließ sich bereits die Segregation von Cu in Pd eindrucksvoll beobachten [*Phys. Rev. Lett.* 105, 207401 (2010), Mayer et al.].

Zur Herstellung von atomaren Schichten im Submonolagenbereich wird eine UHV-Probenpräparationskammer aufgebaut. Diese arbeitet mit drei Magnetronsputterkanonen, einem heizbaren Probenhalter, einem Pyrometer und einem Schichtdickencontroller. Im Rahmen dieses Beitrags soll das gesamte Spektrometer samt Erweiterungen wie eine drehbare Ausführung des Probenhalters für größere Gleichmäßigkeit der Materialdeposition vorgestellt werden.

O 36.54 Tue 18:30 P4

**Vibrational properties of copper on Cu(111)** — HEINER MASLOSZ, ●OLAF SKIBBE, and ANNEMARIE PUCCI — Kirchhoff-Institut für Physik, Im Neuenheimer Feld 227, D-69120 Heidelberg

In the context of understanding the properties of rough and defect-rich surfaces it is useful to be able to characterize the surfaces roughness. By the use of electron energy loss spectroscopy (HREELS) we examined the vibrational features of small amounts of copper on Cu(111) evaporated at liquid nitrogen temperature. We found after annealing to  $\sim 160$  K a vibration with an energy of 44 meV polarized perpendicular to the surface. This is an extraordinary high energy compared to the bulk phonon band. Upon annealing to temperatures above 200 K the peak disappears. The attribution of the vibration features to morphological changes upon annealing is ongoing work.

O 36.55 Tue 18:30 P4

**Investigating metal phthalocyanine molecules on Cu(100)** — ●SARAH FAHRENDORF<sup>1</sup>, CHRISTIAN HAHN<sup>1</sup>, FRANK MATTHES<sup>1</sup>, CLAIRE BESSON<sup>1</sup>, PAUL KÖGERLER<sup>1,2</sup>, CLAUD M. SCHNEIDER<sup>1</sup>, and DANIEL E. BÜRGLER<sup>1</sup> — <sup>1</sup>Peter Grünberg Institut (PGI-6), Forschungszentrum Jülich — <sup>2</sup>Institut für Anorganische Chemie, RWTH Aachen

Magnetic molecules play an important role for the further evolution of spintronics to nanospintronics. Organic molecules, such as metal phthalocyanines, show promising properties for the field of nanospintronics due to (i) their electronic tunability e. g. by adding magnetic atoms to the centre or combining two or three single phthalocyanines, (ii) the high thermal stability and (iii) possible self-organization. For envisaged applications it is important to understand the interaction between the substrate and the molecules and its influence on the electronic and magnetic properties.

Here we study the electronic structure of single metal phthalocyanine molecules deposited on Cu(100) surfaces. We chose two different magnetic atoms and molecule configurations, namely iron phthalocyanine (FePc) and neodymium doubledecker phthalocyanine (NdPc2), to investigate the influence of the substrate on molecules with 3d and 4f like centres and different ligand environments of the central atoms. The molecules were sublimated from a Knudsen cell and in-situ characterized by surface science techniques. First results from scanning tunneling microscopy and spectroscopy are shown.

O 36.56 Tue 18:30 P4

**Struktur und Dynamik von Metallclustern auf dielektrischen Substraten** — ●BERNHARD FABER und PAUL-GERHARD REINHARD — Institut für Theoretische Physik 2, Staudtstr. 7, 91058 Erlangen, Germany

Es wird die Deposition von kleinen Natriumclustern auf einer Ar(001)-Schicht, die auf einer Metallunterlage aufliegt, simuliert. Dabei wird ein hierarchisches Modell aus zeitabhängiger DFT und Molekulardynamik verwendet. Die Valenzelektronen der Natriumatome werden im Kohn-Sham Schema mit Selbstwechselwirkungskorrektur behandelt. Die Wechselwirkung zwischen den Edelgasteilchen und den Natriumionen wird durch Atom-Atom-Potentiale beschrieben und die Ankopplung an die quantenmechanischen Elektronen durch lokale Pseudopotentiale. Ein entscheidender Bestandteil des Modells ist die dynamische Polarisierbarkeit der Edelgasatome. Die optionale Metallunterlage wird durch die Methode der Bildladungen berücksichtigt.

Wir untersuchen den Einfluss der Bildladungskräfte der Metallunterlage und der Schichtdicke der Ar-Schicht auf Struktur, optischen Response und Depositionsdynamik von Na<sub>6</sub> und Na<sub>8</sub>. Die Struktur der Cluster wird kaum beeinflusst; es gibt lediglich geringfügige Ver-

schiebung des Abstands von Cluster zu Oberfläche. In der optischen Absorption bleibt die Position der Mie-Resonanz robust, wohingegen die Details der spektralen Fragmentierung sehr empfindlich auf jede Veränderung reagieren. Bei der Deposition der Cluster spielt die Bildladungskraft der Metallunterlage nur eine untergeordnete Rolle wohingegen die Dicke der Ar-Schicht die Dissipation stark beeinflusst.

O 36.57 Tue 18:30 P4

**RHEED Study of grown AuSi Nanoparticles on Si(111) and deposited Cu Clusters** — ●STEPHAN BARTLING, HANNES HARTMANN, VLADIMIR POPOK, INGO BARKE, KRISTIAN SELL, STEFAN POLEI, VIOLA VON OEYNSHAUSEN, and KARL-HEINZ MEIWES-BROER — Institut für Physik, Universität Rostock, 18051 Rostock, Germany

The contribution focuses on *in situ* reflection high energy electron diffraction (RHEED) of grown AuSi nanoparticles on Si(111) and deposited Cu clusters. After Au deposition of >1ML on vicinal Si(111) three-dimensional gold-rich AuSi nanoparticles are formed via Stranski-Krastanov growth. A mean particle height of 5.8nm has been determined from large-scale STM images for  $\approx$  3ML Au. The RHEED diffraction pattern can be modeled by a quasi close-packed structure with rhombohedral unit cell [1]. We do not observe flat top facets reported for similar preparation conditions [2]. This is in agreement with the crystal orientation determined by RHEED.

First experimental results of RHEED investigations on deposited Cu clusters produced by a magnetron sputtering source are presented. The evolution of diffraction features for different sample treatments (heating, oxygen exposure) is discussed. The analysis is supported by ex-situ AFM measurements.

[1] S. Bartling et al., submitted to Eur. Phys. J. D

[2] E. Moyan et al., Appl. Phys. Lett. 94, 233101 (2009)

O 36.58 Tue 18:30 P4

**Ultra-High Vacuum Cluster Deposition for in-situ RHEED Studies** — ●HANNES HARTMANN, VLADIMIR POPOK, STEPHAN BARTLING, INGO BARKE, and KARL-HEINZ MEIWES-BROER — Institut für Physik, Universität Rostock, 18051 Rostock, Germany

Clusters and nanoparticles deposited on surfaces are of significant interest for applications in electronics, data storage, spintronics, plasmonics, and catalysis. Among a variety of methods for particle production the cluster-beam technique in connection with size selection offers several advantages. Particularly magnetron sputtering is nowadays a well established technique widely used for the production of continuous cluster beams of various species. The design and construction of a compact and flexible cluster-deposition setup is presented. Key elements are a commercial magnetron-sputtering cluster source, a five-stage differential pumping scheme, online flux measurement, and simple ion guiding. It is optimized for deposition of size-selected metal clusters ranging from a few atoms to more than 20 nm in diameter on atomically clean substrates in ultra-high vacuum. Characterization is done by flux measurement and ex-situ microscopy (AFM, TEM). First results of in-situ RHEED investigations of deposited copper nanoparticles on atomically clean surfaces are presented.

O 36.59 Tue 18:30 P4

**Synthesis of vanadium oxide nanoparticles and characterization by TEM** — ●CHRISTINA KUNZMANN, ALADIN ULLRICH, MATTHIAS KLEMM, MICHAEL KRISPIN und SIEGFRIED HORN — Lehrstuhl für Experimentalphysik II, Universität Augsburg, D-86135 Augsburg

We have synthesized vanadium oxide nanoparticles by thermal decomposition of vanadylacetylacetonate ( $\text{VO}(\text{acac})_2$ ) on a highly oriented pyrolytic graphite substrate under  $\text{Ar}/\text{H}_2$  atmosphere. Particles were analyzed by high resolution transmission electron microscopy (HR-TEM) and atomic force microscopy (AFM). Chemical composition of the particles was confirmed by TEM energy dispersive x-ray analysis (EDX). Our analysis shows that the degree of crystallinity as well as the morphology depends on the reaction parameters, e.g. temperature and concentration. For low concentrations of  $\text{VO}(\text{acac})_2$  the particle size varies between 9 and 17 nm. With increasing concentration of  $\text{VO}(\text{acac})_2$  the particle size increases and particle size distribution broadens. Particles with cubic section exhibit lattice spacing in agreement with  $\text{V}_2\text{O}_3$ . In addition, for high concentration samples, rod-like particles are found, which show a different crystalline vanadium oxide phase.

O 36.60 Tue 18:30 P4

**Controlled coupling of interface quantum well states** — ●WILLI AUWÄRTER<sup>1</sup>, KNUD SEUFERT<sup>1</sup>, DAVID ECJJA<sup>1</sup>, NIVEDITHA

SAMUDRALA<sup>1</sup>, SARANYAN VIJAYARAGHAVAN<sup>1</sup>, SUSHOBHAN JOSHI<sup>1</sup>, F. JAVIER GARCIA DE ABAJO<sup>2</sup>, and JOHANNES V. BARTH<sup>1</sup> — <sup>1</sup>Physik Department E20, Technische Universität München, 85748 Garching, Germany — <sup>2</sup>Instituto de Optica, CSIC, 28006 Madrid, Spain

The confinement of surface state electrons in artificial nanostructures permits exploring and visualizing fundamental aspects of quantum mechanics. Here, we introduce a new approach to engineer quantum wells by combining a scanning tunneling microscope manipulation technique with recipes for molecular self-assembly on surface-state-supporting surfaces. Following this procedure, we can not only fabricate resonators of varying size, but also build specific arrangements of quantum wells, such as dimers or one-dimensional chains. The electronic structure of such coupled systems, representing artificial molecules, is studied by local scanning tunneling spectroscopy. Hereby, the scattering characteristics of the potential walls enclosing the wells are determined by the molecules employed as barriers. In particular, we compare quantum well states in free-base and metalated porphyrin arrays on Ag(111). The experimental data on the electron confinement and the coupling of quantum wells are corroborated by boundary element method calculations. These simulations might also be used to design structures with specific electronic properties.

O 36.61 Tue 18:30 P4

**Template-Assisted Growth of Regular Arrays of One-Dimensional Nanostructures using Anodic Aluminum Oxide Membranes** — ●HUAPING ZHAO<sup>1,2</sup>, FABIAN GROTE<sup>1,2</sup>, FENG XU<sup>1,2</sup>, SHIKUAN YANG<sup>1,2</sup>, and YONG LEI<sup>1,2</sup> — <sup>1</sup>Institute of Materials Physics, University of Muenster — <sup>2</sup>Center for Nanotechnology, Muenster 48149

Organic one-dimensional (1D) nanostructures represent attractive building blocks for nano-scale optoelectronic devices because they behave in a unique way that differentiates them from the isolated molecule or the bulk. The synthesis of such organic nanostructures with good control of both size and morphology is still a challenge due to the weak intermolecular interactions in organic molecules compared with those in inorganic materials. Anodic aluminum oxide (AAO) membranes are excellent templates for fabricating organic 1D nanostructures with high arrangement regularity, variable length and diameter. The highly ordered nano-sized channels of the AAO templates force the organic molecules to assemble within a well-defined space. Moreover, the AAO templates are thermal and mechanical stable as well as resistant to organic solvents. By using a combination of solvent saturation and low temperature solvent annealing process, crystalline organic semiconductor nanowires were fabricated with AAO as template. Besides the organic nanostructures, ordered 1D nanostructure arrays of other materials were also synthesized in our group, including different semiconductors and metals.

O 36.62 Tue 18:30 P4

**Cutting Carbon Nanotubes and Graphene** — ●CORNELIUS THIELE and RALPH KRUPKE — Institut für Nanotechnologie, Karlsruhe Institut für Technologie (KIT), Hermann-von-Helmholtz-Platz 1, 76344 Eggenstein-Leopoldshafen

A new technique to locally oxidize carbon-based materials at the nanometer scale is presented. In an oxygen atmosphere, an electron beam is scanned across the material. Secondary electrons ionize the oxygen and induce oxidation around the focal point. Here the formation of trenches in graphene sheets and cuts across carbon nanotubes is shown. These gaps could provide means to contact single molecules. In-situ electrical measurements are used to characterize the cutting process.

O 36.63 Tue 18:30 P4

**Contacting of individual InAs nanowires without photoresist** — ●KILIAN FLÖHR<sup>1,3</sup>, MARCUS LIEBMANN<sup>1,3</sup>, KAMIL SLADEK<sup>2,3</sup>, HILDE HARDTDEGEN<sup>2,3</sup>, THOMAS SCHÄPERS<sup>2,3</sup>, DETLEV GRÜTZMÄCHER<sup>2,3</sup> und MARKUS MORGENSTERN<sup>1,3</sup> — <sup>1</sup>II. Institute of Physics, RWTH-Aachen University, 52074 Aachen — <sup>2</sup>Institut für Bio- und Nanosysteme (IBN-1), Forschungszentrum Jülich, 52425 Jülich — <sup>3</sup>Jülich Aachen Research Alliance (JARA)

We investigated methods to spacially control InAs nanowires on a substrate using micromanipulators attached to an optical microscope with the goal of producing InAs tips for scanning tunneling microscopy. The wires, which were grown by metalorganic vapor phase epitaxy (MOVPE) on a GaAs wafer without catalysts, could be picked up individually using a sharp indium tip exploiting adhesion forces. Later,

the wires were placed onto a desired position somewhere on or at the edge of a double cleaved wafer. Contacting the wires was accomplished using indium microsoldering [1] or electron beam induced deposition [2], since standard lithographic methods are not possible close to the wafer edge due to non-uniform photoresist thickness. Several variations of contacting the wires and optimizing the InAs/metal interface were tested and ohmic contacts could be realized.

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

[2] S. Bauerdick and C. Hierold, *J. Vac. Sci. Technol. B* 24, 3144 (2006).

O 36.64 Tue 18:30 P4

**The resistance of single atomic steps in ultrathin Pb nanowires on Si(557)** — JAN RÖNSPIES, ●LISA KÜHNEMUND, SVEND WIESEL, and HERBERT PFNÜR — Leibniz-Universität Hannover, Inst. f. Festkörperphysik

We studied the local electronic transport properties of a monolayer thick Pb wire by local potentiometry with the tip of a tunneling microscope. 50-nm-wide wires on bare Si(557) were generated by direct writing with an electron beam in an ultrathin film of SiO<sub>2</sub> using the process of electron-beam-induced selective stimulated thermal desorption of oxygen (EBSTD) in combination with a shadow mask technique and macroscopic TiSi<sub>2</sub> contacts. The resistivity of this wire agrees well with expectations derived from anisotropic monolayer thick Pb films on Si(557). Although small Pb clusters nucleated during annealing and desorption of excess Pb, they had a negligible effect on the local resistive properties of the wire. Steps in the substrate of atomic height apparently do not interrupt the conducting path, but due to local scattering at step edge states increase the local resistivity by more than one order of magnitude. Furthermore, a systematic study of the resistance as a function of the lateral width of the wires revealed an effective conducting width, which is about 3 nm smaller on both sides than the geometrically determined width. In addition, we found deviations from Ohm's law at widths below 20 nm.

O 36.65 Tue 18:30 P4

**Na adsorption on In/Si(111)-(4x1) nanowires: electron transport and structural properties** — ●MARTIN BABILON, CHRISTIAN THIERFELDER, STEFAN WIPPERMANN, and WOLF GERO SCHMIDT — Theoretische Physik, Universität Paderborn, 33098 Paderborn, Germany

Quasi one-dimensional structures, such as artificial atomic-scale wires, have attracted considerable attention recently [1,2]. They do not only show fascinating physical properties, but also have a large technological potential, e.g., as atomic-scale interconnects. Highly anisotropic surface superstructures are suitable model systems to explore atomic-scale wires both experimentally and computationally. The In/Si(111)-(4x1) surface [3] is probably the most intensively investigated system in this context. Here we present first-principles calculations on the adsorption geometries and the influence of Na adatoms on the Landauer conductance of these In nanowires. Our findings with regard to structural properties confirm the results by Kleinman et al. [4]. Additionally, we discuss the implications of the Na adatoms on the temperature induced (4x1) → (8x2) phase transition [5].

[1] N. Nilus, T. M. Wallis and W. Ho, *Science* 297, 1853 (2002).

[2] A. Calzolari et al., *Phys. Rev. Lett.* 93, 096404 (2004).

[3] O. Bunk et al., *Phys. Rev. B* 59, 12228 (1999).

[4] J.-H. Cho et al., *Phys. Rev. B* 66, 075423 (2002).

[5] H. Morikawa et al., *Phys. Rev. B* 81, 075401(2010).

O 36.66 Tue 18:30 P4

**Temperature-Dependent Ordering in Au-induced Chains on Ge(001)** — CHRISTIAN BLUMENSTEIN<sup>1</sup>, ●SEBASTIAN MIETKE<sup>2</sup>, JÖRG SCHÄFER<sup>1</sup>, SEBASTIAN MEYER<sup>1</sup>, MICHAEL LOCHNER<sup>2</sup>, RENÉ MATZDORF<sup>2</sup>, and RALPH CLAESSEN<sup>1</sup> — <sup>1</sup>Physikalisches Institut, Universität Würzburg — <sup>2</sup>Institut für Physik, Universität Kassel

Atomic nanowires may be formed by self-organization on a semiconductor surface. Their structure and the resulting quasi-one-dimensional character is determined by the choice of metal adatom and the substrate material. It is commonly believed that many of these systems will undergo a Peierls instability upon cooling. Here we scrutinize nanowires realized by Au chains on Ge(001) to investigate the potential occurrence of lattice instabilities. In combining scanning tunneling microscopy with electron diffraction, we find a phase transition, notably occurring at elevated temperature. It is of second order, and leads to a complex ordering with transversal elongations in addition to the c(8 × 2) reconstruction. However, since it lacks the electronic prerequisites, such as a nesting condition or an energy gap, this excludes

a Peierls scenario. Instead, this transition points at cooperative interactions of charge and lattice including the substrate. As important consequence, these chains remain metallic even at low temperature.

O 36.67 Tue 18:30 P4

**Investigation of a Single Chiral Nano-Structure** — ●PAWEŁ WOŹNIAK<sup>1,2</sup>, PETER BANZER<sup>1,2</sup>, KATJA HÖFLICH<sup>3,4</sup>, SILKE CHRISTIANSEN<sup>1,3</sup>, and GERD LEUCHS<sup>1,2</sup> — <sup>1</sup>Max Planck Institute for the Science of Light, Günther-Scharowsky-Str. 1, D-91058 Erlangen, Germany — <sup>2</sup>Institute of Optics, Information and Photonics, University Erlangen-Nuremberg, Staudtstr. 7/B2, D-91052 Erlangen, Germany — <sup>3</sup>Institute of Photonic Technology, Albert-Einstein-Str. 9, D-07745 Jena, Germany — <sup>4</sup>Max Planck Institute of Microstructure Physics, Weinberg 2, D-06120 Halle, Germany

It was shown just recently that polarization tailored light beams can be used as a versatile tool for investigating the resonance behavior and the optical properties of single nano-structures in detail [1]. We now apply this technique to investigate the properties of single three-dimensional chiral nano-particles namely nanoscopic spirals experimentally. The use of polarization tailored light beams allows for the realization of different coupling scenarios. Due to their chirality the single nanospirals show for instance different response to left- and right-handed circularly polarized light. Experimental results for different excitation schemes and structure designs are presented.

[1] Peter Banzer, Ulf Peschel, Susanne Quabis, and Gerd Leuchs, "On the experimental investigation of the electric and magnetic response of a single nano-structure," *Optics Express* 18, 10905-10923 (2010)

O 36.68 Tue 18:30 P4

**template fabrication of highly ordered arrays of organic semiconductor nanowires** — ●CHRISTIAN HECKEL, STEFAN OSTENDORP, YONG LEI, and GERHARD WILDE — Institut fuer Materialphysik, Wilhelm - Klemm - Str. 10, 48149 Muenster

Porous alumina membrane (PAM) is a widely used template for the fabrication of highly ordered arrays of one-dimensional (1D) nanostructures. The structural parameters of the PAMs are adjustable, including the pore diameter and spacing, and the thickness of the membranes. And thus the structures of the 1D nanomaterials prepared using PAMs can be controlled.

On the other hand, the investigation of organic semiconductors opens a new field of applications in computer technology like twistable displays or printing integrated circuits.

In the current work, these two technologies are combined by depositing organic n-type semiconductors into the pores of PAMs using different synthesizing processes such as molecular evaporation and solution-phase self-assembly. As a result, highly ordered arrays of organic semiconducting wires are obtained within the pores with a diameter of about 50 nm, which indicates that it is possible to fill the pores with organic materials. The properties of these "filled" membranes are characterized by measuring the electrical properties of several nanowires pooled together and also of single nanowires by AFM-based methods.

[1] Y. Lei, W. Cai, G. Wilde, *Prog. Mater. Sci.*, 52, 465 (2007).

[2] J. Puigdollers, *Thin Solid Films*, 517, 6271 (2009).

[3] A. L. Briseno, *Nano Lett.*, 7, 2847 (2007).

O 36.69 Tue 18:30 P4

**Fabrication of tungsten oxide nanotube arrays in porous alumina membranes by a sol-gel-process** — ●STEFAN BARTELS<sup>1,2</sup>, HUI SUN<sup>1,2</sup>, YONG LEI<sup>1,2</sup>, and GERHARD WILDE<sup>1,2</sup> — <sup>1</sup>Institut für Materialphysik, WWU Münster — <sup>2</sup>Center for NanoTechnology, Münster

Tungsten oxide (WO<sub>3</sub>) is a suitable material for gas sensing applications relying on the change of conductivity by adsorbed molecules. Regular arrays of nanotubes provide a large surface area and promise very high sensitivity. This work presents the production of such nanotube arrays with the potential of tuning the surface area by sol-gel-deposition of WO<sub>3</sub> in porous alumina membranes (PAM) from the precursors tungsten hexachloride (WCl<sub>6</sub>) and acetylacetone (C<sub>5</sub>H<sub>8</sub>O<sub>2</sub>). Dimensions and composition of the nanotubes are characterized by SEM and EDX, their sensing properties for CO and NO<sub>2</sub> will be investigated.

O 36.70 Tue 18:30 P4

**Selective Growth of Si Nanorods on Si Surfaces** — L. KÜHNEMUND<sup>1</sup>, ●K. MEYER AUF DER HEIDE<sup>1</sup>, C. TEGENKAMP<sup>1</sup>, H. PFNÜR<sup>1</sup>, R. BRENDEL<sup>2</sup>, and J. SCHMIDT<sup>2</sup> — <sup>1</sup>Leibniz Universität

Hannover, Institut für Festkörperphysik, Appelstraße 2, 30167 Hannover — <sup>2</sup>Institut für Solarenergieforschung Hameln, Am Ohrberg 1, 31860 Emmerthal

The growth of silicon nanorods and in particular of highly ordered arrays of nanorods on surfaces are promising concepts for improving further the efficiency of photovoltaic devices. From a fundamental point of view such antenna structures in combination with ultra-thin metallic films or quantum wires are interesting assemblies for the study of opto-electrical conversion in low dimensional systems. However, the transition between the surface and the vertically grown rods is decisive.

In this study the morphology, the chemical composition of the rods and its vicinity as well as the transport properties of single rods have been investigated by means of a combined SEM-STM system. The Si-rods were grown via the VLS mechanism using metallic clusters (Au, Al) as catalyzer and silane as CVD precursor gas. Selective growth single rod structure was realized using electron beam lithography. It was found that after growth of the rods with diameters in between 100 nm and 1  $\mu$ m, the area around the rod (1-2  $\mu$ m) is contaminated with Au. As such effects limit the lifetimes of electron-hole pairs in photovoltaic cells other VLS catalyst materials such as Al, which forms only shallow acceptor states in Si, have been studied as well.

O 36.71 Tue 18:30 P4

**Conservation of hexagonal order during photochemical particle growth and its application to SiO<sub>2</sub> nanostructuring** — ●AXEL SEIDENSTÜCKER, BURCIN ÖZDEMİR, ALFRED PLETTL, and PAUL ZIEMANN — Universität Ulm, Institut für Festkörperphysik, 89069 Ulm (Germany)

Recently, we reported on a photochemically controlled growth of metallic nanoparticles which initially formed hexagonally ordered arrays [1]. During the growth process, however, some of the particles are displaced from their original position. In this contribution we will report on how the hexagonal order can be conserved and the particle enlargement extended up to 50 nm. It turned out that coating the Au seed particles by a thin layer of OTMS their hexagonal order is practically conserved during each photochemical growth step. The resulting ordered and size controlled particle arrays were used as a starting point for subsequent nanostructuring SiO<sub>2</sub> surfaces by reactive ion etching (RIE). In this way, well defined nanoscaled pillars and pores are obtained.

T. Härtling, A. Seidenstücker, P. Olk, A. Plettl, P. Ziemann and L. M. Eng, *Nanotechnology* 21, 145309 (2010)

O 36.72 Tue 18:30 P4

**A combination of pulsed laser interference and block copolymer micelle lithography** — ●FABIAN ENDERLE<sup>1</sup>, ALFRED PLETTL<sup>1</sup>, PAUL ZIEMANN<sup>1</sup>, STEPHEN RIEDEL<sup>2</sup>, JOHANNES BONEBERG<sup>2</sup>, PAUL LEIDERER<sup>2</sup>, and ELKE SCHEER<sup>2</sup> — <sup>1</sup>Institut für Festkörperphysik, Universität Ulm, D-89069 Ulm — <sup>2</sup>Fachbereich Physik, Universität Konstanz, D-78457 Konstanz

A basic goal of surface nanopatterning is to provide possibilities to "write" lateral patterns decorated with e.g. metallic nanoparticles (NPs) as opposed to homogeneously decorated surfaces. The latter type of NP coating can be accomplished by exploiting the self-organization of precursor loaded diblock-copolymers forming reverse spherical micelles in apolar solvents. After optimized dip-coating a surface and removing the polymer matrix by oxygen/hydrogen plasma treatments, one finally obtains homogeneous hexagonally ordered arrays of metallic NPs. To add lateral patterning, one may try to influence the wetting behavior of the micelle containing solution. For this end, first an OTS-SAM (octadecyltrichlorosilane) is prepared on the surface and exposed to a nanosecond pulsed laser interference pattern. Above a certain energy density of the laser, the related temperature pattern will remove SAM molecules in the high temperature regions by thermal desorption. It will be demonstrated that upon dip-coating the micellar solution on top of such a laser pre-patterned surface a corresponding deposition contrast of metal NPs can be achieved.

O 36.73 Tue 18:30 P4

**Gold nanoparticle arrays generated by modified Electron Beam Lithography and their applicability to plasmonic sensors** — ●SUSAN DERENKO<sup>1</sup>, JOCHEN GREBING<sup>2</sup>, and THOMAS HÄRTLING<sup>1</sup> — <sup>1</sup>Fraunhofer Institute for Non-Destructive Testing, Dresden — <sup>2</sup>Helmholtz-Zentrum Dresden-Rossendorf, Dresden

Gold nanoparticle arrays manufactured by a modified Electron Beam

Lithography method are presented. The method allows to write highly ordered dot structures with a dot size of 50 nm and total area of 4 x 4 mm in a reasonable time.

The arrays are evaluated with respect to the desired application as plasmonic sensors. Therefore the uniformity of the particles created by the modified method is investigated. Using far-field optical spectroscopy the spectral position and FWHM of the surface plasmon resonance (SPR) of the arrays are determined. Influences of plasmonic coupling effects on the SPR properties of closely packed array structures are elucidated by comparing the results to single particle SPR spectra. The experiments are conducted on arrays with different interparticle spacings.

O 36.74 Tue 18:30 P4

**Accommodation of molecular guests in adaptive 2D nanoporous metal-organic networks** — ●DAVID ECIJA<sup>1</sup>, SARANYAN VIJAYARAGHAVAN<sup>1</sup>, WILLI AUWÄRTER<sup>1</sup>, SUSHOBHAN JOSHI<sup>1</sup>, KNUD SEUFERT<sup>1</sup>, CLAUDIA AURISICCHIO<sup>2</sup>, DAVIDE BONIFAZI<sup>2</sup>, KENTARO TASHIRO<sup>3</sup>, and JOHANNES V. BARTH<sup>1</sup> — <sup>1</sup>Physik Department E20, Technische Universität München, D-85748 Garching, Germany — <sup>2</sup>Department of Chemistry, University of Namur, B-5000 Namur, Belgium — <sup>3</sup>National Institute for Materials Science, Tsukuba 305-0044, Japan

Flexibility in host frameworks is a key issue regarding their molecular recognition capabilities. The impact of guest species on the host structure ranges from conformational variation to pronounced structural changes. Here we report the usage of a glassy supramolecular porous network on Cu(111) to spatially organize and control CO and Ce(TPP)<sub>2</sub> guest molecules, the latter representing molecular rotors. For the assembly of the host lattice a de novo synthesized molecule with three-fold symmetry was employed, featuring three terminal pyridyl groups. By STM experiments we show the flexibility of the realized open network where a local variation of the pore shapes can be induced. In order to assess the host-guest adaptability, we dose molecular species of different size. We study the selective accommodation of the guests in pores of different shape and geometry. Whereas the host network behaves as a rigid entity in the uptake and removal of CO, preliminary results signal that the dosing of Ce(TPP)<sub>2</sub> species entails an adaptive response of the porous network towards the guest species.

O 36.75 Tue 18:30 P4

**Selforganized periodic 2D-Nanotemplates in Surfactant Mediated Epitaxy of Ge on Si(111)** — ●CLAUDIUS KLEIN, MARTIN KAMMLER, and MICHAEL HORN-VON HOEGEN — Department of Physics & Center for Nanointegration Duisburg Essen (CeNIDE), University Duisburg-Essen, D-47057 Duisburg, Germany

Surfactant mediated growth of epitaxial Ge heterofilms on Si(111) is utilized to create selforganized 2-dim. ordered nano templates. Using Sb as surfactant a honeycomb pattern like reconstruction of 4 x 4 nm size is formed between 1 - 2 bilayer Ge coverage. Employing the spot width in SPA-LEED the degree of order in the honeycomb pattern has been optimized at a growth temperature of 700°C. STM studies confirm the increase of periodicity with growth temperature. Relaxed Ge films were grown using Bi as surfactant at 450°C. For coverages above 4 bilayers of Ge the lattice mismatch of 4.2% is then accommodated by the formation of a 2-dim. ordered hexagonal dislocation array confined to the hetero interface. Each dislocation is surrounded by a strain field causing a lateral and vertical distortion of the film. The vertical displacement field causes a height undulation of about 1 Å of the surface which becomes apparent in LEED by spot splitting. The lateral displacement fields have been explored in STM and their amplitude determined by highly sophisticated image analysis. Above an interfacial dislocation line the lattice parameter of the Ge film is expanded by more than 10% with respect to the bulk value. In between two dislocation lines the Ge is still compressed to the Si lattice parameter.

O 36.76 Tue 18:30 P4

**DFT study of Mn-oxide nanostructures on vicinal Pd surfaces** — CESARE FRANCHINI<sup>1</sup> and ●RAIMUND PODLOUCKY<sup>2</sup> — <sup>1</sup>Faculty of Physics, Univ. Vienna — <sup>2</sup>Faculty of Chemistry, Univ. Vienna

The research of oxide-metal hybrid structures with reduced dimensionality is of interest for nanotechnology. By means of density functional theory (DFT) we study the formation and the physical characterization of MnO<sub>x</sub> nanostructures on the Pd (1 1 17), (1 1 19) and (1 1 21) vicinal surfaces[1]. Experimentally it is found that the deposition of 0.1 ML of Mn atoms followed by oxidation, results in a regular deco-

ration of the Pd step edges by mono-atomic rows of  $\text{MnO}_x$  structures which coexist with an oxygen-induced  $p(2 \times 2)$  reconstruction on the flat terraces. The complete coverage of the  $(1\ 1\ 17)$  and  $(1\ 1\ 19)$  vicinal surfaces by Mn-oxide (0.75 ML) leads to the formation of a well ordered  $c(4 \times 2)\text{-Mn}_3\text{O}_4$  superstructure accompanied by a substrate-refaceting towards a  $(1\ 1\ 21)$  surface. On the basis of the calculated surface phase diagram and STM simulations the full structural and compositional details as well as the electronic properties of the Mn-oxide nanostructures are resolved and interpreted at low (Mn-oxide nanowires) and high ( $c(4 \times 2)\text{-Mn}_3\text{O}_4$ ) coverage.

[1] F. Li, F. Allegretti, S. Surnev and F. P. Netzer, *Surf. Sci.* **604**, 143-147 (2010).

O 36.77 Tue 18:30 P4

**Production and electrical properties of nano and micro structures on graphite surfaces** — ●LUKAS PATRYARCHA<sup>1</sup>, KARL BAUER<sup>1</sup>, SVEN BAUERDICK<sup>2</sup>, LARS BRUCHHAUS<sup>2</sup>, and HEINZ HÖVEL<sup>1</sup> — <sup>1</sup>TU Dortmund, Experimentelle Physik I — <sup>2</sup>Raith GmbH, Dortmund

Nano structures on HOPG surfaces were produced by using focused  $\text{Ga}^+$  ion beams (FIB, 10nm beam width). Nano structures were produced either using high doses by a direct milling process with a structure depth up to 300nm or after a low dose exposure by an additional oxidation process with  $\text{Ar}/\text{O}_2$  (2%  $\text{O}_2$ ) at 770K for 3h where the structure depth abruptly increases at a critical ion dose of  $15\text{-}20\mu\text{As}/\text{cm}^2$  to values between 50-70nm dependent on the acceleration voltage. Structuring on thin ( $0.1\mu\text{m}$ ) but large ( $2.5\text{mm}^2$ ) HOPG films on an insulating mica slice create structures without electrical contact to the rest of the HOPG sample. The purpose of the project is to control the production process of these structures and to measure their physical properties using AFM and four-point measurements for nano and micro scaled structures.

O 36.78 Tue 18:30 P4

**Electron Beam Induced Surface Activation Lithography on Silicon Oxide, Silicon Nitride and Titanium Oxide** — ●MARIE-MADELEINE WALZ, FLORIAN VOLLNHALS, FLORIAN RIETZLER, MICHAEL SCHIRMER, HUBERTUS MARBACH, and HANS-PETER STEINRÜCK — Lehrstuhl für Physikalische Chemie II and Interdisciplinary Center for Molecular Materials (ICMM), Friedrich-Alexander-University Erlangen-Nuremberg, Egerlandstr. 3, 91058 Erlangen

Recently, we were able to demonstrate that a focused electron beam can be used to locally activate  $\text{SiO}_x$  to allow for a new kind of nanoscale lithography. In contrast to the established direct write technique electron beam induced deposition (EBID), where a precursor gas adsorbs on a substrate and is decomposed locally by a focused electron beam, in electron beam induced surface activation (EBISA) the e-beam is used to locally activate the surface. In a second step a precursor gas is introduced and may decompose at the activated areas. In combination with a precursor that exhibits autocatalytic growth effects, like  $\text{Fe}(\text{CO})_5$ , this can be used to fabricate nanostructures on surfaces [1].

In the present work we expand the EBISA concept to other substrates, i.e. ultrathin  $\text{Si}_3\text{N}_4$  membranes and a  $\text{TiO}_2$  single crystal. The basic principle of EBISA and the corresponding experimental results will be presented and discussed.

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

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

O 36.79 Tue 18:30 P4

**Growth of nanostructures for multi-tip STM investigations** — ●MARCUS BLAB, VASILY CHEREPANOV, and BERT VOIGTLÄNDER — Peter Grünberg Institut (PGI-3), Forschungszentrum Jülich, 52425 Jülich, Germany, and JARA-Fundamentals of Future Information Technology

The main field of research of a multi-tip STM is the investigation of self assembled conducting nanostructures. The study of silicide nanostructures is often a benchmark test for a multi-tip STM. Therefore, we searched for the ideal parameters to grow MnSi-nanowires on a  $\text{Si}(111)\text{-}7 \times 7$  surface.  $2\mu\text{m}$  long MnSi-nanowires occur at a sample-temperature of  $590^\circ\text{C}$  and a low deposition rate of 0.13 ML/min. These nanowires with typical diameters and height of  $\sim 20\text{\AA}$  are ideal to contact and investigate their electrical properties by a multi-tip STM.

Small defects in epitaxial layers can be used to search for the Landauer conductivity dipole. Defects which occur by depositing Bi on  $\text{Si}(111)\text{-}7 \times 7$  at RT, are of the size between 10-100 nm. To reduce the defect-size we deposit small Si-cluster on a flat Bi-layer, which change the surface state. These defects can be explored by scanning tunneling

potentiometry using a multi-tip STM.

O 36.80 Tue 18:30 P4

**Probe-based thermomechanical direct-writing** — ●FELIX HOLZNER, PHILIP PAUL, CYRILL KUEMIN, MICHEL DESPONT, HEIKO WOLF, ARMIN KNOLL, and URS DUERIG — IBM Research GmbH, Rueschlikon, Switzerland

A probe-based patterning method is presented. The presence of a hot tip leads to a local material desorption from specific organic resists. Structures with a half-pitch of 8 nm have been fabricated. Moreover, 3D patterns can be written by controlling the amount of material removal at each pixel. The method can reach patterning speeds comparable to electron beam lithography (so far a pixel rate of 400kHz).

The poster shows the principle of the patterning process as well as studies of the kinetics of the material evaporation.

Furthermore it is shown how the written 3D structures can be used as traps to catch and align gold nanorods ( $25 \times 75\text{ nm}$ ) using Capillary Assembly.

O 36.81 Tue 18:30 P4

**Manipulation of Rashba-split surface states in  $\text{PbAg}_2/\text{Ag}(111)$  by rare-gas and alkali metal adsorption** — ●ARNE BUCHTER<sup>1</sup>, HENDRIK BENTMANN<sup>1</sup>, and FRIEDRICH REINERT<sup>1,2</sup> — <sup>1</sup>Universität Würzburg, Experimentelle Physik VII, Am Hubland, D-97074 Würzburg, Germany — <sup>2</sup>Karlsruhe Institute of Technology, Gemeinschaftslabor für Nanoanalytik, D-76021 Karlsruhe, Germany

Surface alloys like  $\text{BiAg}_2$  or  $\text{PbAg}_2$  show a huge Rashba-splitting in their 2D electronic structure. But unlike in the  $\text{BiAg}_2$ -case the exact size of the splitting for the  $\text{PbAg}_2$ -alloy is not yet clearly determined since in the latter case the spin-split bands are not fully occupied. Using angle-resolved photoelectron spectroscopy we studied the  $\text{PbAg}_2$  surface alloy after Xe adsorption and evaporation of alkali metals. Xe adsorbes in a  $9 \times 9$  reconstruction [1] and backfolding of the electronic bands is clearly visible. Electron doping via adsorption of alkali metals (K, Cs) allows for a continuous band-shift towards higher binding energies [2]. The aim of our study is to gain further insight into the actual size of the splitting, the character of these electronic states and to tune the spin topology at the Fermi level.

O 36.82 Tue 18:30 P4

**Growth mode and evolution of electronic properties for  $\text{Bi}_{1-x}\text{Sb}_x$  alloys on  $\text{W}(110)$**  — ●THOMAS EELBO, MIKE GYAMFI, MARTA WAŚNIEWSKA, and ROLAND WIESENDANGER — Institute of Applied Physics, University of Hamburg, Jungiusstr. 11a, D-20355 Hamburg

Recent experiments show that the alloy of bismuth and antimony is a prominent example for topological insulators[1]. In order to systematically study the properties of  $\text{Bi}_{1-x}\text{Sb}_x$  alloys on  $\text{W}(110)$ , we firstly report on the early stage of Bi and Sb growth on  $\text{W}(110)$ . The LEED and STM measurements reveal that Bi and Sb grow ordered in the pseudocubic (001) orientation. The growth mode was found to vary with thickness and temperature of the deposition for both films. For Bi thick films we observe prominent peaks in  $dI/dU$  spectra at  $-0.35\text{ eV}$ ,  $+0.4\text{ eV}$ ,  $+0.7\text{ eV}$ . However, for thick films of antimony a characteristic peak is observed at  $+0.6\text{ eV}$ . Furthermore we studied the growth mode and evolution of electronic properties of  $\text{Bi}_{1-x}\text{Sb}_x$  alloys. The LEED images for different alloys exhibit hexagonal patterns, indicating (111) surfaces and STM topographies show a two-dimensional growth mode. STS measurements performed on the  $\text{Bi}_{1-x}\text{Sb}_x$  alloy films on  $\text{W}(110)$  are consistent with the electronic structure obtained on the single crystal surface[1].

[1] P. Roushan et al., *Nature* **460**, 1106 (2009)

O 36.83 Tue 18:30 P4

**Geometric spin-Hall effect of light in highly focused vector beams** — ●MARTIN NEUGEBAUER<sup>1,2</sup>, PETER BANZER<sup>1,2</sup>, THOMAS BAUER<sup>1,2</sup>, ANDREA AIELLO<sup>1,2</sup>, NORBERT LINDLEIN<sup>2</sup>, and GERD LEUCHS<sup>1,2</sup> — <sup>1</sup>Max Planck Institute for the Science of Light, Günther-Scharowsky-Str. 1, D-91058 Erlangen, Germany — <sup>2</sup>Institute of Optics, Information and Photonics, University Erlangen-Nuremberg, Staudtstr. 7/B2, D-91052 Erlangen, Germany

Optical angular momentum plays a key role in many fundamental and applied research areas. One example for its appearance is the spin Hall-effect of light (SHEL). The SHEL amounts to the split of a linearly polarized light beam at an interface into its two right- and left-handed

circularly polarized components.

In a recent paper [1] it has been shown that in a beam observed from a tilted reference frame a polarization dependent intensity shift of the Barycenter is found. This can be interpreted as a purely geometric effect (gSHEL).

We investigate this gSHEL in highly focused vector beams. The highly focused beam consists of left-handed and right-handed circularly polarized light generated by a split aperture. We use a sub-wavelength nano-particle for probing the focal field distribution experimentally. First results of these measurements are shown and compared to analytical calculations.

[1] A. Aiello et al., PRL 103, 100401 (2009)

O 36.84 Tue 18:30 P4

**Standing-wave excited hard x-ray phototomission studies on a Au-sandwiched Fe/MgO interface** — SVEN DÖRING<sup>1</sup>, ●CHRISTOPH KEUTNER<sup>1</sup>, FRANK SCHÖNBOHM<sup>1</sup>, ULF BERGES<sup>1</sup>, DANIEL E. BÜRGLER<sup>2</sup>, MIHAELA GORGOS<sup>3</sup>, FRANZ SCHÄPFERS<sup>3</sup>, CLAUD M. SCHNEIDER<sup>2</sup>, and CARSTEN WESTPHAL<sup>1</sup> — <sup>1</sup>DELTA/Experimentelle Physik I, TU Dortmund, Otto-Hahn-Str. 4, 44221 Dortmund — <sup>2</sup>IFF-9, Forschungszentrum Jülich, 52425 Jülich — <sup>3</sup>Helmholtzzentrum Berlin für Materialien und Energie, Albert Einstein Str. 15, 12489 Berlin

Magnetic tunnel junctions (MTJs) consisting of a thin layer-stack of Fe/MgO/Fe show a high tunnel-magneto resistance (TMR) ratio at room temperature. The strength of this effect is mainly driven by the interface and thus the Fe/MgO interface has been subject of many studies during the last years. Quite recently, calculations predicted an even higher TMR ratio for modified interfaces [1]. In that work it was proposed that a monolayer of Au at the interface prevents the oxidation of the Fe-layer, and thus an increase of the TMR effect is expected. Up to now there is no experimental evidence that a well-defined Au monolayer can be prepared with the objective of preventing the Fe oxidation at the interface. In this work we studied a Au-modified interface with standing-wave excited hard x-ray photoemission. The goal of this study was the determination of the effective roughness of the Au layer. Our data-analysis shows that Au does not grow as a protective monolayer nor any hint of FeO formation was found.

[1] J. Mathon and A. Umerski, Phys. Rev. B **71**, 220402 (2005)

O 36.85 Tue 18:30 P4

**Coordination defects at the Si/SiO<sub>2</sub> interface investigated via ab initio g-tensor calculations** — ●MARTIN ROHRMÜLLER, UWE GERSTMANN, and WOLF GERO SCHMIDT — Theoretische Physik, Universität Paderborn, 33098 Paderborn, Germany

The interface between silicon and SiO<sub>2</sub> and its defects such as the P<sub>b</sub> centers are technologically highly relevant and intensively investigated. Electron paramagnetic resonance (EPR) gives a magnetic fingerprint of the centers including the electronic *g*-tensor and the hyperfine splittings.

The so-called P<sub>b1</sub> center at the Si(100) surface is characterized by a strongly anisotropic *g*-tensor. Interestingly, the angular average coincides exactly with the EPR-resonance found in hydrogenated  $\mu c$ -Si:H. In order to clarify if this coincidence is simply by chance, we calculate the elements of the electronic *g*-tensor for surface states and several oxidation stages from first principles, using the gauge-including projector augmented plane wave (GI-PAW) approach in the framework of density functional theory.

We find that (1) hydrogen adsorption at the Si(100) surface influences the magnetic signature of the material dramatically, whereby a large variety of *g*-tensors is obtained. (2) After oxidation, however, the *g*-tensors do not change considerably. The *g*-tensors resemble those of hydrogenated Si surfaces if the surface atoms are coordinated in the same way. This holds for all investigated surface states and the complete EPR fingerprint suggesting this technique to probe sensitively the crystalline part of the interface structures.

O 36.86 Tue 18:30 P4

**A novel electron spectrometer for surface magnon scattering** — ●RAJESWARI JAYARAMAN, LUTZ BAUMGARTEN, BERND KÜPPER, HARALD IBACH, and CLAUD MICHAEL SCHNEIDER — Peter Grünberg Institut, Forschungszentrum Jülich, 52425 Jülich, Germany

Technical improvements in electron energy loss spectroscopy have enabled studies on the dispersion of spin waves (magnons) [1]. The previously designed spectrometer for surface magnon scattering featured a 90°/180° monochromator section and had the spin orientation perpendicular to the scattering plane and parallel to the surface [2].

Based on a calculation of the electron optical properties [3] we have designed a new electron spectrometer with spin orientation longitudinal to the electron beam and have implemented this spectrometer into an experimental set-up for studies on magnetic thin films. In agreement with theoretical calculations, a current of 3nA in direct beam has been achieved at 11meV resolution which is 6 times larger than for the previous instrument. First experimental results obtained with a new spectrometer will be reported.

[1] R. Vollmer et al., Phys. Rev. Lett. 91 (2003) 147201.

[2] H. Ibach et al., Rev. Sci. Instrum. 74 (2003) 4089.

[3] H. Ibach et al., Surface and Interface Analysis 38 (2006) 1615.

O 36.87 Tue 18:30 P4

**Magnetic Fe-porphyrin on superconducting Pb (111)** — ●LUKAS Z. BRAUN, BENJAMIN W. HEINRICH, JOSE I. PASCUAL, and KATHARINA J. FRANKE — Institut für Experimentalphysik, Freie Universität Berlin, Germany

The temperature dependent Fermi-Dirac broadening of electronic states is a physical limit of the energy resolution for Scanning Tunneling Spectroscopy on metal surfaces. A higher energy resolution can be achieved in a superconducting system due to tunneling through the well defined BCS states. Here, we studied Fe(III)-Octaethylporphyrin-Chloride adsorbed on Pb(111) at 4.8 K. At submonolayer coverage, we observed on molecular islands a magnetic fingerprint with submolecular spatial resolution.

O 36.88 Tue 18:30 P4

**Structure and magnetism of Mn-tetrapyrrolyl porphyrin molecules on Ag(111)** — TOBIAS R. UMBACH<sup>1</sup>, ●CHRISTIAN FELIX HERMANN<sup>1</sup>, ALEX KRÜGER<sup>1</sup>, ZECHAO YANG<sup>1</sup>, ISABEL FERNÁNDEZ-TORRENTE<sup>1</sup>, NILS KRANE<sup>1</sup>, MATTHIAS BERNIEN<sup>1</sup>, CONSTANTIN CZEKELIUS<sup>2</sup>, KATHARINA J. FRANKE<sup>1</sup>, JOSE I. PASCUAL<sup>1</sup>, and WOLFGANG KUCH<sup>1</sup> — <sup>1</sup>Institut für Experimentalphysik, Freie Universität Berlin, Germany — <sup>2</sup>Institut für Chemie und Biochemie - Organische Chemie, Freie Universität Berlin, Germany

Deposition of metal porphyrines on metallic surfaces can lead to the modification of the magnetic moment of the metal ion. We investigated a submonolayer 5,10,15,20-Tetrakis-(4-pyridyl)-porphyrin-Mn(III)-chloride (TPyP-Mn(III)-Cl) on a Ag(111) surface by Low Temperature Scanning Tunneling Microscopy (LT-STM) and X-Ray Magnetic Circular Dichroism (XMCD). Our measurements reveal that T4PyP-Mn(III)-Cl forms a self-assembled ordered phase with a small fraction of ordered second-layer molecules even for submonolayer coverage after annealing to 370 K. The first monolayer consists of domains with alternating molecular rows. The second layer forms a square lattice on top of the first monolayer. By Low Temperature Scanning Tunneling Spectroscopy (LT-STS) we identify similar resonances of the metallic ion of TPyP-Mn(III)-Cl molecules in the first and second monolayer, indicating no strong interactions with the metallic surface underneath. XMCD measurements on the same system show that the TPyP-Mn(III)-Cl molecules keep a magnetic moment upon adsorption with an easy axis along the surface normal.

O 36.89 Tue 18:30 P4

**The magnetic properties of Ni on modified Cu(110) surfaces** — ●MICHAEL HOHAGE, MARIELLA DENK, DANIEL QUETESCHNER, RICHARD DENK, and PETER ZEPPENFELD — Institut für Experimentalphysik, Johannes Kepler Universität Linz, A-4040 Linz, Austria

The magnetism and morphology of thin Ni films deposited on Cu(110) surfaces reconstructed by exposure to oxygen and nitrogen has been studied. Both, oxygen and nitrogen act as a surfactant for the Ni growth, leading to smoother films. Scanning Tunneling Microscopy (STM), as well as Reflectance Difference Spectroscopy (RDS) is used to characterize the sample properties. The sensitivity of the RDS to the polar Magneto-Optic Kerr Effect has been exploited (RD-MOKE). Contrary to the growth on pristine Cu(110), thin Ni films on oxygen covered Cu(110)-(2x1)O show a spin reorientation transition (SRT) from in-plane to out-of-plane magnetization at 9 ML Ni coverage [1], [2]. Increasing the oxygen pre-coverage to form the Cu(110)-c(6x2)O reconstruction leads to a shift of the SRT to thicker Ni-films. However, Ni films grown on the Cu-CuO stripephase at lower oxygen pre-coverage only exhibit an SRT after post-growth exposure to oxygen. Ni films evaporated on the Cu(110)-(2x3)N do not show an SRT as long as no coadsorption of oxygen is permitted. The origin of the magnetic properties of these systems will be discussed and in particular the crucial role of the oxygen will be addressed.

[1] Th. Herrmann et al., Phys. Rev. B **73**, 134408 (2006).

[2] R. Denk et al., Phys. Rev. B 79, 073407 (2009).

O 36.90 Tue 18:30 P4

**Depth Resolved Photoelectron Microscopy of Nanostructures via Soft X-Ray Standing Wave Excitation** — ●FLORIAN KRONAST<sup>1</sup>, ALEXANDER GRAY<sup>2</sup>, CHRISTIAN PAPP<sup>3</sup>, SEE-HUN YANG<sup>4</sup>, ALEXANDER KAISER<sup>4</sup>, FARHAD SALMASSI<sup>6</sup>, ERIC M. GULLIKSON<sup>6</sup>, DAWN L. HILKEN<sup>6</sup>, ERIK H. ANDERSON<sup>6</sup>, HERMANN A. DÜRR<sup>1</sup>, CLAUS M. SCHNEIDER<sup>5</sup> und CHARLES S. FADLEY<sup>2</sup> — <sup>1</sup>Helmholtz-Zentrum Berlin - BESSY II, Berlin, Germany — <sup>2</sup>Department of Physics, University of California, Davis, CA, USA — <sup>3</sup>Physical Chemistry II, University of Erlangen, Germany — <sup>4</sup>IBM Almaden Research Center, San Jose, CA, USA — <sup>5</sup>Juelich Research Center, Jülich, Germany — <sup>6</sup>Center for X-Ray Optics, Lawrence Berkeley National Laboratory, Berkeley, CA, USA

We demonstrate the addition of depth resolution to the usual two-dimensional images in photoelectron emission microscopy (PEEM), with application to a square array of circular magnetic Co microdots. The method is based on excitation with soft x-ray standing-wave (SW) generated by Bragg reflection from a multilayer mirror substrate. The standing wave is moved vertically through the sample simply by varying the photon energy around the Bragg condition. Photoemission intensities as functions of photon energy were compared to x-ray optical theoretical calculations in order to quantitatively derive the depth-resolved film structure of the sample. This SW approach thus provides complementary information to the usual lateral information provided by the PEEM, and should have wide applicability to studies of magnetic nanostructures in the future.

O 36.91 Tue 18:30 P4

**Investigation of magnetic properties in a multiferroic layer system** — ●MARTIN WELKE<sup>1</sup>, REMYA KUNJUVETIL GOVIND<sup>2</sup>, MARTIN TRAUTMANN<sup>2</sup>, VASILI HARI BABU<sup>1</sup>, KARL-MICHAEL SCHINDLER<sup>2</sup>, and REINHARD DENECKE<sup>1</sup> — <sup>1</sup>Wilhelm-Ostwald-Institut für Physikal. und Theoret. Chemie, Universität Leipzig, Linnestr. 2, 04103 Leipzig, Germany — <sup>2</sup>Institut für Physik, Martin-Luther-Universität Halle-Wittenberg, Von-Danckelmann-Platz 3, 06120 Halle, Germany

Systems with multiferroic properties are of interest for research since the 1960s. In the beginning single phase multiferroics were in the focus of research, whereas nowadays layer systems with a ferroelectric and a ferromagnetic component are investigated. The work presented covers the system Cobalt on Bariumtitanate (001) within SFB 762. In particular, XAS measurements of 3, 6, 9, 12, and 21 monolayer thick Co films prepared by e-beam evaporation are taken into account.

Magnetic properties are determined by X-ray magnetic circular dichroism (XMCD) at the Co L edge. The films show in-plane magnetization starting from 6 ML. It is possible to calculate the magnetic moments using the sum rule formalism. The calculated values correspond to those for Co (hcp) bulk reported in literature [1,2].

Changes to the BaTiO<sub>3</sub> substrate by heating in vacuum up to 600 °C prior to Co deposition, resulting in O vacancies and increased conductivity, do not yield significant differences for the magnetic moments. Work supported by the DFG through SFB 762.

[1] Eriksson et al., Phys. Rev. B 42 (1990) 2707

[2] Guo et al., Phys. Rev. B 50 (1994) 3861

O 36.92 Tue 18:30 P4

**Two Photon Photoemission Studies of FeO-films on ZnO(0001)** — ●STEPHAN HILGENFELDT and MICHAEL BAUER — Institut für Experimentelle und Angewandte Physik, Universität Kiel, 24098 Kiel, Germany

We investigated FeO films prepared on a ZnO(0001) substrate by two photon photoemission (2PPE). The FeO was produced by epitaxial growth of Fe on ZnO in ultra high vacuum and a subsequent annealing of the films to 670K. In the 2PPE-data we were able to identify a distinct spectral feature of FeO from an unoccupied state at a binding energy of  $E - E_F = +2.5$  eV exhibiting a clear parabolic dispersion in  $k_{\parallel}$ . The nature and the properties of this electronic band will be discussed under consideration of additional time resolved 2PPE data.

O 36.93 Tue 18:30 P4

**The Formation of Shockley derived Interface States at Metal-Organic Interfaces studied with 2PPE** — ●MANUEL MARKS<sup>1</sup>, CHRISTIAN H. SCHWALB<sup>1</sup>, SÖNKE SACHS<sup>2</sup>, BENJAMIN SCHMIDT<sup>1</sup>, ACHIM SCHÖLL<sup>2</sup>, FRIEDRICH REINERT<sup>2</sup>, EBERHARD UMBACH<sup>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>Universität Würzburg, Experimentelle Physik II, D-97074 Würzburg

The charge carrier injection across a metal-organic interface into the active regions of a functional device is one major influence on the efficiency of organic electronics. New electronic states that emerge at such interfaces can alter these dynamical processes substantially. We applied time- and angle-resolved 2-photon photoemission (2PPE) to study the electron dynamics at structurally well characterized interfaces directly in the time domain. With adsorption of monolayer films of PTCDA and NTCDA on a Ag(111) surface strongly dispersing interface states (IS) form above the Fermi Level  $E_F$ . For PTCDA the inelastic electron lifetime of 54 fs indicates a significant overlap with the metal substrate and the state mainly originates from an upshifted Shockley state [1]. For NTCDA films the IS has comparable properties though lying closer to  $E_F$ . In the stronger chemisorbed disordered precursor phase of the PTCDA monolayer [2] an interface state emerges at  $E - E_F = 0.45$  eV. The lifetime of 63 fs and its non-dispersing behavior raise the question whether this state has more molecular character.

[1] C. H. Schwalb *et al.*, Phys. Rev. Lett. **101**, 146801 (2008)

[2] L. Kilian *et al.*, Phys. Rev. Lett. **100**, 136103 (2008)

O 36.94 Tue 18:30 P4

**Two-photon photoelectron spectroscopy of graphene on SiC(0001)** — ●DIETER GUGEL<sup>1</sup>, DANIEL NIESNER<sup>1</sup>, FLORIAN SPECK<sup>2</sup>, THOMAS SEYLLER<sup>2</sup>, and THOMAS FAUSTER<sup>1</sup> — <sup>1</sup>Lehrstuhl für Festkörperphysik, Universität Erlangen-Nürnberg, Staudtstr. 7, 91058 Erlangen, Germany — <sup>2</sup>Lehrstuhl für Technische Physik, Erwin-Rommel-Straße 1, 91058 Erlangen, Germany

A monolayer of graphene grown epitaxially on the silicon face of silicon carbide was investigated using angle- and time-resolved two-photon photoelectron spectroscopy. In this measurement, the surface electrons were excited by a UV pump laser with a photon energy of 4.66 eV and a pulse duration of 58 fs. Using an IR probe pulse with an energy of 1.55 eV and a pulse width of 33 fs, we determined the energy dispersion and lifetime of the lowest unoccupied image potential state. The lifetime of this state was observed to be 50 fs. Moreover, we measured the work function of the surface, which amounts to 4.5 eV.

O 36.95 Tue 18:30 P4

**Time-resolved ARPES studies with high-order harmonic radiation** — ROBERT CARLEY<sup>1</sup>, KRISTIAN DÖBRICH<sup>1</sup>, ●BJÖRN FRIETSCH<sup>1,2</sup>, CORNELIUS GAHL<sup>1</sup>, MARTIN TEICHMANN<sup>1</sup>, KAI GODEHUSEN<sup>3</sup>, OLAF SCHWARZKOPF<sup>3</sup>, PHILIPPE WERNET<sup>3</sup>, FRANK NOACK<sup>1</sup>, and MARTIN WEINELT<sup>1,2</sup> — <sup>1</sup>Max-Born-Institut, Berlin — <sup>2</sup>Fachbereich Physik, Freie Universität, Berlin — <sup>3</sup>Helmholtz-Zentrum für Materialien und Energie (BESSY II), Berlin

We present characterization results of our newly developed high-order harmonics XUV source and beamline. The scope of this new setup is to provide XUV photons between 20-65 eV, at an energy resolution of a few 100 meV and a pulse duration  $\geq 100$  fs for time-resolved photoelectron spectroscopy studies of metal and semi-conductor surfaces as well as gas-phase experiments.

40-fs pulses from a commercial amplified Ti:Sapphire laser system running at 10 kHz repetition rate are focused into an argon-filled gas cell to create harmonics, currently up to the 25th order (=38.4 eV). We select the XUV wavelength and energy resolution using a toroidal grating monochromator. Our current resolution is 170 meV and the time resolution is 140 fs (both FWHM) at a reasonable harmonic yield. We performed first pump-probe experiments on the lanthanide metals Gadolinium and Terbium.

O 36.96 Tue 18:30 P4

**Hot phonons in the relaxation dynamics at the Si(001) surface** — ●THI UYEN-KHANH DANG<sup>1</sup>, CHRISTIAN EICKHOFF<sup>2,3</sup>, MARTIN WEINELT<sup>2,3</sup>, ANDREAS KNORR<sup>1</sup>, and CARSTEN WEBER<sup>1</sup> — <sup>1</sup>Institut für Theoretische Physik, Technische Universität Berlin, Germany — <sup>2</sup>Max-Born-Institut für Nichtlineare Optik und Kurzzeitspektroskopie, Berlin, Germany — <sup>3</sup>Freie Universität Berlin, Fachbereich Physik, Berlin, Germany

We investigate the relaxation dynamics of photo-excited carriers at the Si(001) surface. Relaxation occurs mainly from the bulk conduction band into the surface state  $D_{\text{down}}$ . We present time-resolved experimental results on the relaxation dynamics obtained via two-photon photoemission measurements. The results are compared to theoretical calculations based on the Bloch-Boltzmann-Peierls approach, where the influences of electron-phonon and electron-electron scattering are analyzed. We find that the electronic temperature remains well above

the equilibrium lattice temperature for times much longer than the typical scattering times of the system (even after 10 ps). This is found to be due to strong heating of LO phonon modes due to electron relaxation in the bulk via LO phonon emission. The different contributions of the scattering channels as well as phonon bottleneck effects are discussed.

O 36.97 Tue 18:30 P4

**A time-of-flight electron spectrometer for angle- and time-resolved 2PPE** — ●ANDREAS DAMM<sup>1</sup>, ANNE SPENDE<sup>1</sup>, JENS GÜDDE<sup>1</sup>, ACHIM CZASCH<sup>2</sup>, OTTMAR JAGUTZKI<sup>2</sup>, HORST SCHMIDT-BÖCKING<sup>2</sup>, and ULRICH HÖFER<sup>1</sup> — <sup>1</sup>Fachbereich Physik, Philipps-Universität, D-35032 Marburg — <sup>2</sup>Institut für Kernphysik, Goethe-Universität, D-60438 Frankfurt am Main und RoentDek Handels GmbH, D-65779 Kelkheim

Many studies on surface electron dynamics employing two-photon photoemission (2PPE) would benefit from the ability to map the full two-dimensional surface bandstructure in a single time-resolved experiment. Examples include the study of quasi-elastic electron scattering within electronic surface bands or the extension of 2PPE for the generation of coherently excited electrical currents at surfaces.

Thus, we have developed a position-sensitive time-of-flight spectrometer capable of measuring the kinetic energy as well as the full parallel momentum  $\vec{k}_{||}$  of low-energy electrons photoemitted from a surface with a maximum rate of few MHz. Its main components are a field-free drift tube and a delay-line detector for a position-sensitive detection. A variable drift length allows to enhance either the acceptance angle or the energy- and momentum-resolution. The energy resolution for low kinetic energy electrons as typical for 2PPE experiments is better than 10 meV even at the maximum acceptance angle of  $\pm 25^\circ$ .

Investigations on the momentum-dependence of the decay of image-potential electrons on Cu(100) will be presented underlining the capabilities of this instrument.

O 36.98 Tue 18:30 P4

**Time resolved desorption of atomic hydrogen from graphite induced by femtosecond laser pulses** — ●ROBERT FRIGGE<sup>1</sup>, TIM HÖGER<sup>1</sup>, HENRIK WITTE<sup>1</sup>, THOMAS OLSEN<sup>2</sup>, JAKOB SCHIOTZ<sup>2</sup>, and HELMUT ZACHARIAS<sup>1</sup> — <sup>1</sup>Physikalisches Institut, Universität Münster, Germany — <sup>2</sup>CINF, Technical University of Denmark, Denmark

The desorption of hydrogen from graphite (HOPG) is an important issue in the understanding of molecular hydrogen formation on dust particles upon irradiation. The velocity distribution of atomic hydrogen from HOPG is examined after surface excitation with fs-laser pulses at  $\lambda = 400$  nm. Desorbed neutral H atoms are ionized using (2+1) REMPI via the  $2s \leftarrow 1s$  transition, and are detected with a time-of-flight mass spectrometer. As a result the velocity distribution reveals a structure consisting of different maxima for fast, medium and very slow desorbed hydrogen atoms. Electron scattering calculations have been performed employing a repulsive electronic excited state and H-graphite adsorption potentials corresponding to different adsorption sites [1]. Via populating different vibrationally excited intermediate states by multiple scattering events velocity distributions for desorption out of different adsorption sites are obtained. A good agreement with the experimentally observed velocities is obtained. A nonlinear fluence dependence for the fast electrons, allow two pulse-correlation experiments and as a result we derive a pulse-delay dependent yield with a FWHM of about 700 fs. This correlation time indicates short lifetimes of the excited electrons and supports a calculation in the DIMET model. [1]R. Frigge et al., *Phy. Rev. Lett.*, 104, 256102 (2010)

O 36.99 Tue 18:30 P4

**Photo-induced melting of a Pb overlayer on Cu(111) observed with time- and angle-resolved XUV photoemission** — ●ANDREAS RUFFING<sup>1</sup>, STEFFEN EICH<sup>1</sup>, ADRA V. CARR<sup>2</sup>, DANIEL STEIL<sup>1</sup>, ALEXANDER HASSDENTEUFEL<sup>1</sup>, MARGARET M. MURNANE<sup>2</sup>, HENRY C. KAPTEYN<sup>2</sup>, MICHAEL BAUER<sup>3</sup>, STEFAN MATHIAS<sup>1,2</sup>, and MARTIN AESCHLIMANN<sup>1</sup> — <sup>1</sup>Department of Physics and Research Center OPTIMAS, University of Kaiserslautern, 67663 Kaiserslautern, Germany — <sup>2</sup>JILA, University of Colorado and NIST, Colorado 80309 0440, USA — <sup>3</sup>Institut für Experimentelle und Angewandte Physik, Christian-Albrechts-Universität zu Kiel, 24908 Kiel, Germany

The electronic structure during a thermally induced melting transition was investigated by Baumberger et al. in 2004 [1]. Baumberger et al. found that the liquid film of Pb/Cu(111) shows electronic features as the persistence of a Fermi surface, the filling of band gaps, and the localization of the electron wave functions upon melting. In our ex-

periment, we use intense femtosecond infrared pulses to photo-induce this melting transition of the Pb overlayer on Cu(111). We monitor the dynamical changes in the electronic structure as a function of time by using time- and angle-resolved XUV photoemission spectroscopy. XUV pulses are generated from high-harmonic upconversion, and are needed to access the Brillouin zone boundary, where the melting transition can be followed by a transient change of the electronic band structure.

[1] Baumberger et al., *Science* 306 (2004), 2221-2224

O 36.100 Tue 18:30 P4

**2PPE-measurement on Cu(1 1 1) with an angle-resolving time-of-flight spectrometer** — ●THOMAS KUNZE<sup>1,2</sup>, JENS KOPPRASCH<sup>1</sup>, MARTIN TEICHMANN<sup>1</sup>, THORSTEN U. KAMPEN<sup>2</sup>, and MARTIN WEINELT<sup>1</sup> — <sup>1</sup>Max Born Institut, Berlin, Germany — <sup>2</sup>SPECS GmbH, Berlin, Germany

We present two-photon photoemission measurements with the angle-resolved time-of-flight spectrometer THEMIS. The spectrometer allows us to measure the kinetic energy and wave vector parallel to the surface of the photo emitted electrons. Due to the maximum angle acceptance of  $\pm 15^\circ$  and the usable energy range of up to more than 20 % of the passenergy, it is possible to measure a remarkable part of the band structure concurrently.

We present measurements of the image-potential states (IPS) on Cu(111) and Cu(1 1 1), a vicinal surface with (001)-terraces. For both measurements we calculated the effective mass and the binding energy of the electrons. The dispersion relations correspond to other measurements (M. Roth). Furthermore we measured the Umklapp band and the lifetime differences of the IPS depending on the parallel momentum of the photo emitted electrons of Cu(1 1 1).

O 36.101 Tue 18:30 P4

**Collective electron excitations on potassium-covered Be(0001)** — ●MARTIN JAHN and JÖRG KRÖGER — Institut für Physik, TU Ilmenau, PF 100565, DE-98684 Ilmenau, Germany

Electron-energy-loss spectroscopy (EELS) of clean Be(0001) demonstrated the existence of acoustic surface plasmons in agreement with ab initio calculations [1]. The origin of these low-energy collective excitations with a soundlike dispersion relation is the dynamical screening of surface state electrons by bulk electrons. Calculations and photoemission experiments showed that on potassium-covered Be(0001) the interaction of quantum well states with bulk electrons results in coverage-dependent acoustic surface plasmons [2]. We report on EELS measurements on potassium-covered Be(0001). The dispersion relation of the acoustic surface plasmon depending on the potassium coverage is presented. Furthermore, the influence of potassium adsorption on the ordinary surface plasmon and on the phonons of Be(0001) is investigated.

[1] B. Diaconescu et al., *Nature* 448, 57 (2007).

[2] J. Algdal et al., *Phys. Rev. B* 78, 085102 (2008).

O 36.102 Tue 18:30 P4

**Adsorption of Hydrazine (N<sub>2</sub>H<sub>4</sub>) on Hexagonal Ice(0001): First-Principles Investigations on the Mechanism of Chirality Changes** — ●PAWEŁ RODZIEWICZ and BERND MEYER — Interdisciplinary Center for Molecular Materials ICMM and Computer-Chemistry-Center CCC, University of Erlangen-Nürnberg, Germany

Surfaces can have a pronounced effect on the chiral properties of adsorbed molecules. For example, it has been observed that chiral molecules spontaneously separate into domains with different chirality or that enantiopure adsorbates are transformed into racemate mixtures by lowering of the activation barrier for chirality flips. We have used hydrazine as a simple model of a chiral molecule to study possible binding sites and flips of chirality on ice(0001) surfaces. The chemical properties of hydrazine are similar to those of water. Due to the presence of electron lone pairs and N-H groups hydrazine is simultaneously a proton acceptor and a proton donor. Density functional theory (DFT) calculations and Car-Parrinello molecular dynamics (CP-MD) simulations were used to investigate the interplay between molecule-molecule and molecule-substrate interactions. Hydrazine monomers and different enantiomers of its dimers were adsorbed on the hexagonal ice (0001) surface. The adsorbed aggregates were analyzed in terms of their coordination to the surface, with special focus on identifying hydrogen bonds. Finally, the process of chirality flips was studied using coordination constrained CP-MD simulations in order to obtain free energy barriers for rearrangements of enantiomers with Gauche A into Gauche B.

O 36.103 Tue 18:30 P4

**Towards time- and angle-resolved photoemission at a free-electron laser with an angle-resolving ToF spectrometer** — CHRISTIAN SOHRT<sup>1</sup>, •KERSTIN HANFF<sup>1</sup>, STEFAN HELLMANN<sup>1</sup>, MICHAEL BAUER<sup>1</sup>, WILFRIED WURTH<sup>2</sup>, LUTZ KIPP<sup>1</sup>, and KAI ROSSNAGEL<sup>1</sup> — <sup>1</sup>Institut für Experimentelle und Angewandte Physik, Kiel, Germany — <sup>2</sup>Institut für Experimentalphysik and Center for Free-Electron Laser Science, Hamburg, Germany

The Free-Electron Laser (FEL) in Hamburg (FLASH) generates highly brilliant, ultrashort pulsed radiation with pulse durations down to 50 fs and photon energies up to 1000 eV. This enables unique experiments, as for example time-resolved core-level photoelectron spectroscopy. However, to establish photoelectron spectroscopy as a completely viable technique at an FEL, one has to develop a detection scheme with maximum efficiency, because the pulse repetition rates of FELs are notoriously low and the available beam time is extremely scarce. Our proposed solution is a photoelectron spectroscopy experiment based on a novel angle-resolved time-of-flight spectrometer. Compared to traditional detection schemes the instrument is expected to enhance the detection efficiency by a factor of about 200—due to the larger acceptance angle—and the temporal resolution by a factor of seven to about 100 fs—due to single-pulse detection. Thus, it will become possible to correlate core-level dynamics which is sensitive to changes in the charge distribution around specific atomic sites, with the dynamics of electrons at the Fermi surface in a single experiment. This work is supported by the BMBF (FSP 301 FLASH).

O 36.104 Tue 18:30 P4

**Coupling of Pb adsorbate vibrations to Si(111) substrate studied by molecular dynamics** — SUNG SAKONG, •PETER KRATZER, SIMONE MÖLLENBECK, ANNIKA KALUS, ANJA HANISCH-BLICHARSKI, MARTIN KAMMLER, and MICHAEL HORN-VON HOEGEN — Fakultät für Physik and Center for Nanointegration (CeNIDE), Universität Duisburg-Essen, Duisburg, Germany

The decay of low-lying vibrational modes of heavy adsorbates is best studied in the time domain. Time-resolved electron diffraction (RHEED) experiments provide evidence for a long (several ns) and a short (100 ps) time scale in the dissipation of vibrational energy of a Pb monolayer following pulsed laser irradiation. We perform density functional (DFT) calculations of a Pb/Si(111) ( $\sqrt{3} \times \sqrt{3}$ ) surface to obtain the vibrational modes. To study the vibrational dynamics on the ns time scale, we use classical molecular dynamics with a Pb-Si interaction potential that matches the DFT data. The lattice dynamics at  $T = 100\text{K}$  is simulated using a large super cell with 12 nm in depth, and the lower part of the Si slab is coupled to a thermostat. As initial condition, we assume that the energy deposited by the laser has already been converted to kinetic energy of the Pb atoms. We watch how this extra kinetic energy is dissipated into the Si substrate. After averaging over many trajectories, the relaxation dynamics monitored by the mean-square displacements of the Pb adatoms can be compared to the experimental data. In conclusion, we assign the experimentally observed short time scale to the decay of the "optical" Pb-Si mode, i.e., the Pb vibration relative to the top-most Si layer.

O 36.105 Tue 18:30 P4

**Dynamics of the  $\beta(\sqrt{3} \times \sqrt{3}) \leftrightarrow (3 \times 3)$ -Pb/Si(111) phase transition on the ps-timescale** — •JÖRG REIMANN, TIM FRIGGE, SIMONE MÖLLENBECK, FRIEDRICH KLASING, MARTIN KAMMLER, and MICHAEL HORN-VON HOEGEN — Department of Physics and Center for Nanointegration Duisburg-Essen (CeNIDE), University of Duisburg-Essen, D-47057 Duisburg, Germany

The structural dynamics of strongly driven phase transitions on surfaces take place on a picosecond timescale. Ultrafast time resolved electron diffraction in a RHEED (reflection high energy electron diffraction)-geometry is an excellent technique to study such processes after excitation by a fs laser pulse [1]. In a metallic adsorbate system absorption of the photons results in an excitation of the electron system. Electron-phonon coupling causes heating of the adsorbate layer and may trigger the phase transition. In order to study the dynamics of an order-disorder phase transition far away from thermal equilibrium we performed time resolved measurements on the  $\beta(\sqrt{3} \times \sqrt{3}) \leftrightarrow (3 \times 3)$ -Pb/Si(111) phase transition with  $T_c = 84^\circ\text{C}$ . The Pb adlayer is excited by a 50 fs laser pulse with 800 nm at a sample temperature of 25 K. After excitation the  $\beta(\sqrt{3} \times \sqrt{3})$ -diffraction spot intensity drops instantaneously due to the Debye Waller effect but is followed by a sharp increase which is delayed by 30 ps. While the intensity decrease

is explained by thermal heating of the adsorbate layer up to 125 K, we attribute the increase of intensity to a delayed structural phase transition triggered by the temperature rise.

[1] A. Janzen et al., Surf. Sci. 600, 4094 (2006)

O 36.106 Tue 18:30 P4

**Generation, characterization and compression of pJ white-light-continuum pulses for ultrafast spectroscopy** — •DANIEL WEGKAMP<sup>1</sup>, SIMON WALL<sup>1</sup>, DANIELE BRIDA<sup>2</sup>, STEFANO BONORA<sup>2</sup>, GIULIO CERULLO<sup>2</sup>, JULIA STÄHLER<sup>1</sup>, and MARTIN WOLF<sup>1</sup> — <sup>1</sup>Fritz-Haber-Institute of the MPG, Dep. of Physical Chemistry, Berlin, Germany — <sup>2</sup>Politecnico di Milano, Dipartimento di Fisica, Milan, Italy

Broadband white-light-continuum pulses are widely used as a probe for optical spectroscopies, providing a probing bandwidth of several hundred nanometers in the UV, visible and IR. However, their use in ultrafast spectroscopy is limited due to the long duration of the pulses. In addition, pulse diagnostics are difficult because of their low power. We report the measurement of the group-delay of such white-light pulses with sub-nJ pulse energy. Furthermore we describe the setup and application of a deformable mirror-based compressor resulting in optimized temporal shapes of the pulses. White-light pulses are generated by self-phase modulation due to focusing of 40 fs laser pulses (800nm, provided by a 300 kHz Ti:Sa regenerative amplifier system) into a YAG crystal. The resulting pulses have durations of several hundred femtoseconds and contain spectral components ranging from near-UV to the IR. These are characterized by spectrally resolved measurement of the transient reflectivity. Compression of the pulses is achieved by adjustment of the extracted group delays [1] using the deformable mirror.

[1] Parmigiani et al. Appl. Phys. Lett. 96 (2010) 021102

O 36.107 Tue 18:30 P4

**NanoESCA, a new nanospectroscopy tool with synchrotron radiation** — •MARTEN PATT<sup>1</sup>, CARSTEN WIEMANN<sup>1</sup>, INGO KRUG<sup>1</sup>, MATTHIAS ESCHER<sup>2</sup>, NILS WEBER<sup>2</sup>, MICHAEL MERKEL<sup>2</sup>, and CLAUDIUS MICHAEL SCHNEIDER<sup>1</sup> — <sup>1</sup>PGI-6, Forschungszentrum Jülich GmbH, Jülich, Germany — <sup>2</sup>Focus GmbH, Hünstetten, Germany

Nanotechnology and nanoscience are developing more and more to smaller length scales. We face the need for the characterization of surface electronic and magnetic states in these reduced dimensions with a new energy-filtered photoelectron emission microscope (PEEM), which we have recently installed at the ELETTRA synchrotron facility (Italy)[1]. The instrument features a novel electrostatic lens system with 30 kV extraction voltage, enabling spatially resolved photoelectron imaging with a lateral resolution smaller than 100 nm and combines it with a double-hemispherical energy filter [2], a single-event counting detector unit and a liquid helium cooled sample manipulator with five degrees of freedom. A second operation mode provides the mapping of the angular distribution (k-space microscopy) of the photoelectrons. We discuss the capabilities and the performance of the instrument with respect to its lateral and energy resolution, sensitivity and signal-to-noise-ratio.

[1] <http://www.elettra.trieste.it/beamlines/NASP>

[2] M. Escher et al., J. Electron Spectr. Rel. Phen., 144-147 (2005) 1179

O 36.108 Tue 18:30 P4

**Observation of the topological state and a two-dimensional electron gas in Bi<sub>2</sub>Se<sub>3</sub> by multidimensional photoemission spectroscopy** — •LUPULESCU C.<sup>1,2</sup>, OVSYANNIKOV R.<sup>2</sup>, RIENKS E.D.L.<sup>2</sup>, FINK J.<sup>2</sup>, KING P.D.C.<sup>3</sup>, BAUMBERGER F.<sup>3</sup>, HATCH R.C.<sup>4</sup>, HOFMANN P.<sup>4</sup>, MI J.<sup>4</sup>, IVERSEN B.B.<sup>4</sup>, LINDBLAD A.<sup>5</sup>, SVENSSON S.<sup>5,6</sup>, and EBERHARDT W.<sup>1,2</sup> — <sup>1</sup>Technische Universität Berlin, Berlin, Germany — <sup>2</sup>Helmholtz Zentrum Berlin, Berlin, Germany — <sup>3</sup>University of St Andrews, St Andrews, UK — <sup>4</sup>Aarhus University, Aarhus, Denmark — <sup>5</sup>MAX-lab, Lund, Sweden — <sup>6</sup>Uppsala University, Uppsala, Sweden

The electronic structure of Bi<sub>2</sub>Se<sub>3</sub> (0001) was investigated using a new time-of-flight angle-resolved electron spectrometer (VG Scienta, ARTOF 10k). Measurements were taken at the 10m NIM beamline of BESSY II, operating in single-bunch mode. Both the topological surface state and a two-dimensional electron gas near the surface were observed. The main advantage of using this type of electron analyzer is the simultaneous mapping of both kinetic energy and angular distribution in two dimensions, ruling out various artefacts induced by sample misalignment, temperature-induced drifts, etc. Moreover, the collection of such data sets is rather fast, so that the temporal evolu-

tion of the electronic structure can be studied. Utilizing this, we study the time-dependence of band bending at the surface of  $\text{Bi}_2\text{Se}_3$ , which leads to the emergence of a two-dimensional electron gas.

O 36.109 Tue 18:30 P4

**Development of a thin film spin filter optics for PEEM** — ●DANIEL PANZER<sup>1,2</sup>, JAN DAVID KUTTIG<sup>1</sup>, and GERD SCHÖNHENSE<sup>1</sup> — <sup>1</sup>Institut für Physik, Johannes-Gutenberg Universität Mainz — <sup>2</sup>Max-Planck Institut für Polymerforschung, Mainz

Analyzing the spin polarization of electrons is a vital aspect of many experiments in nuclear, molecular, surface and solid-state physics, and of fundamental importance for investigations of ferromagnetic materials. However, combining spin detection with a laterally resolved method like PhotoEmission Electron Microscopy (PEEM) is quite demanding. One possibility is the use of low energy electron diffraction for spinfiltering of an image or a momentum distribution [1].

Here we test a new method that takes advantage of the spin dependence of the mean free path of electrons in magnetized ferromagnet. We use a tandem lens to extract electrons from a sample and project the magnified electron image onto a thin metal film that acts as a spin filter at low kinetic energies. On the opposite side the spinfiltered image is then picked up and further magnified by a regular PEEM optics.

We have successfully tested the electron optics at low magnification with a calibration sample and confirmed transmission through nm-thick layers of metals and semiconductors with a thermal emitter as electron source. The next challenge is combining photoemission, electron optics and transmission in a way that provides sufficient intensity so PEEM images can be acquired fast enough for regular use.

Funded by DFG(SCHO341/7-1); [1] Tusche et al., this conference

O 36.110 Tue 18:30 P4

**High-Efficiency Multichannel-Spindetector** — ●MICHAELA HAHN, BERND PETEREIT, HANS-JOACHIM ELMERS, and GERD SCHÖNHENSE — Institut für Physik, Staudinger Weg 7, 55128 Mainz

The spinpolarisation analysis of electrons is a central demand in surface and solid state physics, especially for investigations of ferromagnetic materials. All state-of-the-art spindetectors work in a single-channel mode, i.e. monoenergetic and with only one detection angle. This leads to a very low efficiency in comparison with modern, parallel-detecting intensity analysers. We present a new type of spindetector with strongly improved efficiency by implementing a strategy for parallel multichannel detection.

The spinresolved photoelectron spectrometer comprises a hemispherical analyzer (Leybold EA10) and a helium discharge lamp ( $h\nu=21.23\text{eV}$ ). Spindependent scattering at  $W(100)$  (asymmetry function  $S=0.45$ ) yields a spinfiltered image of the analyzer exit plane, detected using a delayline detector (Surface Concept GmbH). A high-resolution spinfiltered image requires an acquisition time of minutes, whereas the same distribution with a state-of-the-art single channel detector would take several hours measuring time. A similar approach is used for the detection of spinfiltered momentum distributions [1].

Funded by Stiftung Rheinland-Pfalz für Innovation (project 886) and DFG (Scho 341/9-1)

Patent DE 10 2005 045 622 B4

[1] Ch. Tusche et al., this conference

O 36.111 Tue 18:30 P4

**The High Resolution Diffraction Beamline at PETRA III - First Experiments** — ●CARSTEN DEITER, FLORIAN BERTRAM, KATHRIN PFLAUM, and OLIVER H. SEECK — DESY, Notkestr. 85, 22607 Hamburg

Since 2009 the new synchrotron radiation source PETRA III is operational. At the High Resolution Diffraction Beamline (P08) the equipment and the beam parameters are highly suited for surface and interface studies. Different sample cells with heating and cooling capability and the possibility of vacuum and gas atmosphere up to 1bar are available. These cells can be installed in the six circle diffractometer (Kohzu) for extreme angular resolution and will be supported by an UHV infrastructure with MBE preparation, structural (LEED) and chemical (AES) analysis operational in late summer 2011. The first regular user experiments have been performed and some results will be presented which show the benefits of the PETRA III beam parameters.

O 36.112 Tue 18:30 P4

**NMR of buried interfaces** — ●ANUSCHKA SCHMITT, MATTHIAS BUSCHMANN, RICHARD KASTELIK, ALEXANDER POTZUWEIT, and

HEINZ JÄNSCH — Fachbereich Physik, Philipps-Universität Marburg, D-35032 Marburg

We employ Xe-NMR to investigate surface phenomena by adsorbing hyperpolarized  $^{129}\text{Xe}$  onto a helium-cooled single crystal and studying the electronic interactions of substrate and adsorbate. The high nuclear spin polarization of the adsorbed Xe-film could be transferred to buried interfaces within the substrate (which then would be accessible for further NMR experiments) via dipolar distant-field transfer. Such a transfer can be achieved by applying two rf-frequencies at the same time using a double resonant probe, integrated into an UHV system. Furthermore, an inhomogeneous magnetic structure of the Xe-film is needed, which could be provided by a geometrically structured sample in the  $\mu\text{m}$  range. Here, we present the development of the double resonant probe and first experiments.

O 36.113 Tue 18:30 P4

**Preparation of highly polarized Xe with variable  $^{129}\text{Xe}$  content** — ●ALEXANDER POTZUWEIT, MATTHIAS BUSCHMANN, RICHARD KASTELIK, ANUSCHKA SCHMITT, and HEINZ JÄNSCH — Fachbereich Physik, Philipps-Universität Marburg, D-35032 Marburg

We employ NMR of hyperpolarized  $^{129}\text{Xe}$  to investigate surface phenomena. Dynamic processes at the bulk surfaces can be monitored by exchange spectroscopy (EXSY) of the bulk and surface atoms ( $\Delta\sigma \approx 100\text{ppm}$ ). The annealing of Xe films can be investigated by line narrowing. To increase the sensitivity towards structurally caused, local inhomogeneities a small line width is favorable. In solid Xe the line width is dominated by dipolar interaction with neighboring nuclear spins. This can be substantially reduced by diluting the NMR-active isotope  $^{129}\text{Xe}$  in the NMR-inactive isotope  $^{132}\text{Xe}$ . With the new, improved experimental setup we will be able to provide mixtures of highly polarized  $^{129}\text{Xe}$  and  $^{132}\text{Xe}$  with adjustable abundances. Here we present the technical development of the apparatus and discuss first results.

O 36.114 Tue 18:30 P4

**Molecule-Surface Scattering with Velocity-Controlled Molecular Beams** — ●FABIAN GRÄTZ<sup>1</sup>, DANIEL ENGELHART<sup>2</sup>, HENRIK HAAK<sup>1</sup>, DANIEL J. AUERBACH<sup>2</sup>, ALEC M. WODTKE<sup>2</sup>, and GERARD MEIJER<sup>1</sup> — <sup>1</sup>Fritz-Haber-Institut der Max-Planck-Gesellschaft, Faradayweg 4-6, D-14195 Berlin — <sup>2</sup>Max-Planck-Institut für biophysikalische Chemie, Am Faßberg 11, D-37077 Göttingen

The production of cold molecular beams with a tunable velocity by means of pulsed electric fields, known as Stark deceleration, is now mature and convenient. At the same time, molecular beam experiments that use traditional ways of velocity manipulation have been commonly used to study different aspects of molecule-surface interactions in the regime of high kinetic energy. We present a new generation of molecule-surface scattering machine, which brings the advantages of Stark decelerated molecular beams to the field of surface physics. Using this machine, CO molecules will be scattered at surfaces, quantum-state selective with respect to both impacting and scattered molecules, while providing a tunable velocity in the range of 1000 to 20 m/s with an exceptional translational energy resolution.

O 36.115 Tue 18:30 P4

**Quasiparticle energies and excitonic effects of alkali-metal fluorides** — ●CHRISTOPH SOMMER, PETER KRÜGER, and JOHANNES POLLMANN — Institut für Festkörpertheorie, Universität Münster, D-48149 Münster, Germany

We present a comparative study of quasiparticle and excitonic properties of the alkali-metal fluorides LiF, NaF and KF. For the calculation of quasiparticle effects within the GW approximation, we use a localized Gaussian basis set.

Excitonic effects are obtained by solving the Bethe-Salpeter equation for an effective two-particle problem.

Furthermore, the applicability of self-interaction corrected DFT-LDA energies and wavefunctions as a substitute for computationally highly demanding quasiparticle energies in the Bethe-Salpeter equation is discussed.

The calculated optical spectra are in accord with experimental and theoretical results available in the literature for these systems.

O 36.116 Tue 18:30 P4

**Methane adsorption on graphene: Influence of dispersion interaction** — ●MATTHIAS WITTE<sup>1</sup>, CHRISTIAN THIERFELDER<sup>1</sup>, STEPHAN BLANKENBURG<sup>1,2</sup>, EVA RAULS<sup>1</sup>, and WOLF GERO

SCHMIDT<sup>1</sup> — <sup>1</sup>Theoretische Physik, Universität Paderborn, 33100 Paderborn, Germany — <sup>2</sup>Eidgenössische Materialprüfungs- und Forschungsanstalt (EMPA), 8600 Dübendorf, Switzerland

Van der Waals interaction is not properly described in density functional theory within commonly used exchange-correlation functionals. Therefore several semi-empirical and ab-initio solutions have been proposed and implemented in widely used program packages. Here we use the methane-graphene interaction as benchmark system to compare the results of semiempirical dispersion correction schemes (DFT-D) [1,2] and an ab initio van der Waals density functional (vdW-DF) ansatz [3]. Møller Plesset perturbation theory (MP2) [4] calculations are used as a reference. The adsorption energy of 0.17 eV and the molecular distance of 3.28 Å obtained from the MP2 calculations are close the experimental data, while the vdW-DF scheme results either in a realistic adsorption energy or a realistic adsorption geometry, depending on the exchange-correlation functional. The present implementation of DFT-D overbinds about as much as bare DFT calculations underbind, but yields a meaningful adsorption height. [1] F. Ortman, W.G. Schmidt and F. Bechstedt, *Phys. Rev. Lett.* 95, 186101 (2005) [2] S. Grimme, *J. Comp. Chem.* 27, 1787 (2006) [3] M. Dion, H. Rydberg, E. Schröder, D.C. Langreth and B.I. Lundqvist, *Phys. Rev. Lett.* 92, 246401 (2004) [4] C. Møller and M.S. Plesset, *Phys. Rev.* 46, 618 (1934)

O 36.117 Tue 18:30 P4

**Adsorption behavior of super-heavy elements ( $Z \geq 100$ ) and their chemical complexes on inert and metal surfaces** — ●JOSEF ANTON and TIMO JACOB — Inst. für Elektrochemie, Uni Ulm

One of the very interesting but on the other site also extremely challenging topics in modern chemistry concerns the properties of super-heavy elements [1]. Due to their very short life times ( $\sim 1$  s) one is limited to experiments on only one atom at a time, which have to be performed before the nucleus decays. Since most standard techniques of 'traditional' chemistry are not applicable, only few experimental setups are available, such as the gas-phase thermochromatography [1, 2]. In this method the volatility of a super-heavy element as well as the adsorption temperature  $T_{\text{ads}}$  of these species on the detector is measured. Adsorption enthalpies,  $\Delta H_{\text{ads}}$ , can then be deduced from  $T_{\text{ads}}$  using statistical thermodynamic models and Monte Carlo simulations. In order to be able to perform accurate calculations one has to describe the motion of the electrons in a fully relativistic manner. We used our four-component DFT code [3] to determine the adoption energies of the super-heavy elements ( $Z \geq 100$ ) and their homologues on different surfaces. After discussing the procedure and the results, we will provide a comparison of some of the obtained trends to recent experimental studies.

[1] M. Schädel, *The Chemistry of Superheavy Elements*, Kluwer Academic Publishers, Dordrecht, 2003.

[2] M. Schädel and A. Türler, *Physik Journal*, 6, 35 (2009).

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

O 36.118 Tue 18:30 P4

**Neural Network Potential-Energy Surfaces for Organic Molecules: First Applications to Tartaric Acid** — ●SINJA KLEES, TOBIAS MORAWIETZ, and JÖRG BEHLER — Lehrstuhl für Theoretische Chemie, Ruhr-Universität Bochum, D-44780 Bochum, Germany

First-principles calculations provide an accurate description of many systems. However, the computational costs severely limit the size of the systems that can be studied. Therefore, the development of efficient interatomic potentials is an important prerequisite for studying complex systems in molecular dynamics simulations. Neural Networks represent a class of flexible functions, which allows to construct accurate potential-energy surfaces (PESs) based on a set of reference points. To date, most Neural Network potentials have been reported for very small molecules or inorganic solids. Here, we investigate the applicability of this method to large organic molecules. Using tartaric acid as a benchmark system we show that a highly accurate PES can be constructed systematically.

O 36.119 Tue 18:30 P4

**Magnetic properties of adatoms and clusters on metal surfaces, the effect of electric field on MAE** — ●TAMENE REGASSA DASA, PAVEL IGNATIEV, and VALERIY STEPANYUK — Max-Planck-Institut für Mikrostrukturphysik, Weinberg 2, 06120 Halle, Germany

Magnetic properties of Co adatoms, chains and mixed Co/Pt chains on Pt surfaces are investigated. This is done by non-collinear density functional theory using the fully relativistic pseudopotentials. Spin-orbit interaction is taken into account. The local magnetization and magnetic anisotropy energies of the studied nanostructures are evaluated and compared with available experimental and theoretical results. Finally, the magnetic effect of electric fields on the magnetic properties is discussed.

O 36.120 Tue 18:30 P4

**polarity-induced oxygen vacancies at LaAlO<sub>3</sub>|SrTiO<sub>3</sub> interfaces** — ●PENGXIANG XU<sup>1</sup>, ZHICHENG ZHONG<sup>2</sup>, and PAUL J. KELLY<sup>2</sup> — <sup>1</sup>Peter Grünberg Institut & Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, 52425 Jülich, Germany — <sup>2</sup>Faculty of Science and Technology and MESA+ Institute for Nanotechnology, University of Twente, P.O. Box 217, 7500 AE Enschede, The Netherlands

Using first-principles density functional theory calculations, we find a strong position and thickness dependence of the formation energy of oxygen vacancies in LaAlO<sub>3</sub>|SrTiO<sub>3</sub> (LAO|STO) multilayers and interpret this with an analytical capacitor model. Oxygen vacancies are preferentially formed at *p*-type SrO|AlO<sub>2</sub> rather than at *n*-type LaO|TiO<sub>2</sub> interfaces; the excess electrons introduced by the oxygen vacancies reduce their energy by moving to the *n*-type interface. This asymmetric behavior makes an important contribution to the conducting (insulating) nature of *n*-type (*p*-type) interfaces while providing a natural explanation for the failure to detect evidence for the polar catastrophe in the form of core level shifts.

O 36.121 Tue 18:30 P4

**Electronic structure calculations on 100,000 atoms** — ●GERALD JORDAN, MARTIJN MARSMAN, and GEORG KRESSE — University of Vienna, Faculty of Physics, and Center for Computational Materials Science, Sensengasse 8/12, A-1090 Wien, Austria

We present an efficient method for tackling electronic structure calculations on the scale of 100,000 atoms, where a full diagonalization of the Kohn-Sham Hamiltonian becomes computationally unfeasible because of cubic scaling with system size. In many applications, however, one is only interested in a few states near the Fermi level. Solving the associated interior eigenvalue problem is numerically difficult and requires a realistic model of the electronic charge density.

Our approach is based on the Jacobi-Davidson method using harmonic Ritz values, which mimics the shift-and-invert strategy to target a specific energy but avoids any explicit inversion. In contrast to the folded spectrum technique, our method easily extends to the generalized eigenvalue problems arising from the use of pseudopotentials. To construct suitable charge densities reproducing the band structure, we fit atomic charge distributions to a self-consistent reference calculation.

O 36.122 Tue 18:30 P4

**Electronic structure and optical spectrum of lonsdaleite** — ●JOHANNES BÜNGELER, STEPHAN BLANKENBURG, and ARNO SCHINDLMAYR — Department Physik, Universität Paderborn, 33095 Paderborn, Germany

Lonsdaleite is a rare but naturally occurring allotrope of carbon. Like in diamond, each carbon atom forms four *sp*<sup>3</sup>-hybridized bonds with a local tetrahedral geometry, but the overall crystal structure is hexagonal, not cubic. First discovered in fragments of the Canyon Diablo meteorite in 1967, it was originally characterized as translucent with a brownish-yellow color and a Mohs hardness of 7–8, whereas recent first-principles calculations predicted a substantially higher indentation strength than that of diamond. If confirmed, this would make lonsdaleite the hardest material known. To resolve the conflicting experimental and theoretical findings, we perform a quantitative study of the quasiparticle band structure, using the *GW* approximation for the nonlocal and dynamic self-energy. Subsequently, the optical absorption spectrum is calculated from time-dependent density-functional theory, including a long-range kernel to account for the electron-hole attraction and the formation of excitons. Our results show unambiguously that pure lonsdaleite crystals are completely transparent in the visible spectral range. This gives strong support to the hypothesis that the analyzed samples were contaminated by impurities and imperfections, which not only influence the color, but also reduce the hardness.

O 36.123 Tue 18:30 P4

**GaN/AlN Structures with Two Dimensional Electron Gas: A**

**Density Functional Theory Study** — JAKUB SOŁTYS<sup>1</sup>, MICHAŁ ŁOPUSZYŃSKI<sup>1</sup>, ●JACEK PIECHOTA<sup>1</sup>, and STANISŁAW KRUKOWSKI<sup>1,2</sup> — <sup>1</sup>Interdisciplinary Centre for Materials Modelling, University of Warsaw, ul. Pawińskiego 5a, 02-106 Warszawa, Poland — <sup>2</sup>Institute of High Pressure Physics, Polish Academy of Sciences, ul. Sokołowska 29/37, 01-142 Warsaw, Poland

GaN is a promising material because of its properties: it can be used in high-temperature, high-frequency and high-power device applications. It has been shown that the GaN/AlN/GaN junction with ultra-thin AlN layer can be prepared and significant improvement in some crucial parameters over GaN/AlGaIn is attained. In our work we present density functional study of the AlN/GaN high electron mobility transistor (HEMT) structure. It was shown that two dimensional electron gas (2DEG) is present at the AlN/GaN interface. Analysis of potential profiles and band structures for different thickness of AlN barrier allow us to assess how the barrier affects 2DEG. It was demonstrated that for too thin AlN barrier 2DEG is not well confined. However, for a thicker AlN barrier, the occupancy of this states is higher, and this result is consistent with the available experimental data [Dabiran et.al., Appl. Phys. Lett. 93 082111 (2008)].

O 36.124 Tue 18:30 P4

**A Density Functional Theory Study of the TMG Adsorption on the GaN Surface** — MARIA PTASIŃSKA<sup>1</sup>, JAKUB SOŁTYS<sup>1</sup>, ●JACEK PIECHOTA<sup>1</sup>, and STANISŁAW KRUKOWSKI<sup>1,2</sup> — <sup>1</sup>Interdisciplinary Centre for Materials Modelling, University of Warsaw, ul. Pawińskiego 5a, 02-106 Warszawa, Poland — <sup>2</sup>Institute of High Pressure Physics, Polish Academy of Sciences, ul. Sokołowska 29/37, 01-142 Warsaw, Poland

TMG (trimetylogallium) and NH<sub>3</sub> (ammonia) are widely used reactants in the metal organic chemical vapor deposition (MOCVD) technique used in the growth of the GaN thin films. We have recently examined theoretically, with the help of the density functional theory (DFT), TMG adsorption on the GaN(0001) surface in order to study formation of bonds between Ga and N. Dangling bonds on the GaN(0001) surface were saturated with the hydrogen atoms. The slab polarization, which is due to the dangling bonds present on the GaN(0001) surface, and energy of the system in the vicinity of TMG was computed for different distances between the surface atoms and TMG. We also studied TMG diffusion on the GaN surface. As a result, the energy path for diffusion from Top N to Hollow was obtained.

O 36.125 Tue 18:30 P4

**Band convergence of all-electron GW calculations: the extreme case of ZnO** — ●CHRISTOPH FRIEDRICH, MATHIAS C. MÜLLER, and STEFAN BLÜGEL — Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, 52425 Jülich, Germany

Recently, Shih *et al.* [1] presented a new one-shot *GW* calculation for the band gap of wurtzite ZnO based on the pseudopotential approach. They showed that a proper convergence with respect to the number of bands used in the construction of the self-energy yields a band gap that is very close to the experimental value of 3.6 eV. This is in contrast to previous all-electron calculations where band gaps in the range 2.12–2.44 eV have been found [2]. In this work we present a *GW* calculation for ZnO that is based on the all-electron full-potential linearized augmented-plane-wave (FLAPW) method [3]. We obtain a band gap that is much larger than that of the previous all-electron calculations, but still smaller than that of Ref. 1. We go beyond their approach in two respects: we neither employ the pseudopotential nor the plasmon-pole approximation. Apart from the band convergence we also discuss the linearization error for high-lying states and how to eliminate it with local orbitals. Our results show that the band

convergence is a very serious issue in the *GW* approach. ZnO is an extreme case in this respect. [1] B.-C. Shih *et al.*, Phys. Rev. Lett. 105, 146401 (2010). [2] M. Usuda *et al.*, Phys. Rev. B 66, 125101 (2002); M. Shishkin and G. Kresse, *ibid.* 75, 235102 (2007); F. Fuchs *et al.*, *ibid.* 76, 115109 (2007). [3] C. Friedrich *et al.*, Phys. Rev. B 81, 125102 (2010).

O 36.126 Tue 18:30 P4

**Time-Dependent Density Functional Theory study of transfer of charge by atomic impact, a case study with C<sub>4</sub>H<sub>10</sub> + Au** — ●GUILLERMO AVENDANO FRANCO, MYRTA GRÜNING, and XAVIER GONZE — Université catholique de Louvain, Louvain-la-Neuve, Belgium

The transfer of charge between metals and organic structures is studied using Time-dependent density functional theory (TDDFT) in a simple case of a molecule of Butane (C<sub>4</sub>H<sub>10</sub>) and an atom of gold (Au).

For a first approach to the problem we studied the transfer of charge in a dynamic dissociation of gold-Butane complex, the range of kinetic energies was between 132 Ha (3.59 keV) and 13 kHa (359 keV). In a second step we studied the effect of a collision of one atom of gold directed to one of the carbon atoms of Butane or bond between carbons.

In both cases we observe the partial or total transfer of one electron from the Butane molecule to the atom of gold, an effect that is dependent on the kinetic energies involved in the process.

O 36.127 Tue 18:30 P4

**Energetics and metastability of the silicon vacancy in cubic SiC** — FABIEN BRUNEVAL and ●GUIDO ROMA — CEA-Service de Recherches de Métallurgie Physique, Saclay, France

The silicon vacancy is a prominent intrinsic defect of cubic SiC (3C-SiC) to which much effort has been devoted so far, experimentally and theoretically. We calculate its properties using the state-of-art *GW* approximation that does not suffer from the band gap problem. The obtained formation and transition energies deviate significantly from the usual density functional theory evaluations and now compare favorably with experiment. A new assignment for the main line of photoluminescence is then proposed. We further perform *GW* calculations for the saddle point of reaction paths. The resulting barrier energies explain the thermal annealing experiments thanks to an original mechanism mediated by a minority charge configuration.

O 36.128 Tue 18:30 P4

**KKRnano, a code for accurate density functional calculations for systems with thousands of atoms** — ●RUDOLF ZELLER, ALEXANDER THIESS, and STEFAN BLÜGEL — Peter-Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich und JARA, D-52425 Jülich

The present state of our newly developed computer code KKRnano will be outlined. The code, which is designed for massively parallel computing, is based on the Korringa-Kohn-Rostoker (KKR) Green function method and can be applied to supercells with arbitrary atomic arrangements. KKRnano uses an iterative solution of the algebraic Dyson equation which describes the interaction between otherwise independent single atomic scattering events. Because of that efficient parallelization and reduced scaling of the computational effort (quadratically instead of cubically with the number of atoms) are easily achieved. For large systems calculations with linear scaling effort are possible if small total energy errors are admitted (less than 1 meV per atom). In particular, it will be explained how a preconditioner for the iterative solution can be constructed so that the calculations are accelerated by about a factor ten for all systems investigated so far which include metallic systems, defect levels in Si, magnetic GaN:Gd with O and N codoping and GeSbTe phase-change materials.