

## O 44: Poster Session II (Semiconductors; Oxides and Insulators: Adsorption, Clean Surfaces, Epitaxy and Growth; Surface Chemical Reactions and Heterogeneous Catalysis; Surface or Interface Magnetism; Solid-Liquid Interfaces; Organic, Polymeric, Biomolecular Films; Particles and Clusters; Methods: Atomic and Electronic Structure; Time-resolved Spectroscopies)

Time: Wednesday 17:00–19:30

Location: Poster C

O 44.1 Wed 17:00 Poster C

**A Novel Approach to Measure the Step Line Tension and the Step Dipole Moment on Vicinal Au(001) Electrodes** — ●GUILLERMO BELTRAMO, HARALD IBACH, and MARGRET GIESEN — Forschungszentrum Jülich, Institut für Bio- und Nanosysteme IBN 4, D 52425 Jülich, Germany

The step line tension plays a crucial role in the electrochemical deposition and dissolution of metals, and in particular, in the creation of nanostructures and their dynamical properties. In the present work, we introduce a new method to measure the step line tension on metal electrodes, using a theoretical model proposed by Ibach and Schmickler [1]. Vicinal Au(11n) and Au(001) electrodes were investigated by impedance spectroscopy in weakly adsorbing electrolytes. Within the limits of error the shift in the potential of zero charge is proportional to the step density of the electrode surfaces and we determine a dipole moment per step atom of about  $6 \cdot 10^{-3}$  eÅ for all electrolytes. The line tension of the steps is then calculated from the difference between the surface tension of the stepped and the step free surfaces. In accordance with [1], the step line tension decreases (roughly linear) with the electrode potential in absence of specifically adsorbed ions. Furthermore we are able to give an estimation of the step capacity. The results will be discussed with respect to a recent theoretical model [2].

- [1] H. Ibach and W. Schmickler, *Physical Rev. Lett.* 91 (2003) 016106.  
[2] H. Ibach et al., *J. Electroanal. Chem.* 544 (2003) 13.

O 44.2 Wed 17:00 Poster C

**Electron Induced Desorption of Water on Ruthenium(0001)** — ●FRANZISKA TRAEGER, DELER LANGENBERG, YOUKUN GAO, and CHRISTOF WÖLL — Physikalische Chemie 1, Ruhr-Universität Bochum, Universitätsstr. 150, 44801 Bochum

When electrons impinge on adsorbed water molecules, desorption, dissociation or structural phase transitions may occur. The system water/Ru has been found to be particularly sensitive, as structures with varying coverage and similar energies have been observed, some of them stabilized by dissociation products (OH and H). In this work the influence of electrons on the adsorbate D<sub>2</sub>O/Ru has been investigated by the diffraction of a neutral He atom beam. Without electron impact a high order commensurate structure with 27.3 Å periodicity is found, in contrast to LEED experiments. These results can be explained in terms of a bilayer with slightly larger lattice constant than the bulk ice and which is rotated by 4.7° with respect to the substrate [1]. In further experiments electrons were accelerated with 1000-1200 V onto the surface. The observed changes in the specular He signal and in the He diffraction pattern strongly indicate, that at larger coverages desorption is the dominant mechanism. A quantitative analysis of the He intensity gives a desorption probability of about 0.7 % per electron. Several models for the analysis and their errors are presented. Finally, the results are discussed in comparison with electron induced desorption from the multilayer D<sub>2</sub>O/Ru and from ice surfaces.

- [1] F. Traeger, D. Langenberg, Y.K. Gao and Ch. Wöll, submitted to *Phys. Rev. Lett.*

O 44.3 Wed 17:00 Poster C

**Controlled immobilization of "device" molecules: self-assembled monolayers of ferrocene-substituted biphenyl ethynyl thiols** — ANDREY SHAPORENKO<sup>1</sup>, KATRIN RÖSSLER<sup>2</sup>, HEINRICH LANG<sup>2</sup>, and ●MICHAEL ZHARNIKOV<sup>1</sup> — <sup>1</sup>Angewandte Physikalische Chemie, Universität Heidelberg, 69120 Heidelberg, Germany — <sup>2</sup>Lehrstuhl für Anorganische Chemie, Technische Universität Chemnitz, 09111 Chemnitz, Germany

Homogeneous and mixed (with biphenylthiol: BPT) self-assembled monolayers (SAMs) of ferrocene-substituted biphenyl ethynyl thiols (Fc) were prepared on Au(111) substrates and characterized by several complementary spectroscopic techniques. The mixed films were fabricated either by subsequent immersion of the substrates into the BPT and Fc solutions or by immersion of the substrate into a mixed solution of BPT and Fc. The first procedure resulted in the prepara-

tion of high-quality mixed SAMs, in which the Fc molecules were stochastically distributed in the BPT matrix and well separated from each other. The portion of these molecules in such films could be precisely varied from ca. 7 to 42% by selection of the immersion time in the BPT solution. The films prepared from the mixed solution exhibited a phase separation between the Fc and BPT constituents. These films contained mostly the Fc molecules, showing, thus, a significant deviation from the relative content of the target molecules in the primary solution. This means that the Fc molecules, when competing with BPT, preferably adsorb onto Au(111) substrate, suggesting a significant impact of the ferrocene groups onto the structure-building interactions.

O 44.4 Wed 17:00 Poster C

**Surface kinetics and structure of thin polymer films** — ●CHRISTIAN VREE and S. G. MAYR — I. Physikalisches Institut, Georg-August-Universität Göttingen, Friedrich-Hund-Platz 1, D-37077 Göttingen

Structure formation at surfaces during thin film deposition is of great scientific interest due to the demand for smooth or regularly structured surfaces and interfaces for miniaturized functional films in science and technology. The deposition processes which govern morphology evolution during vapour deposition of polymer films are still poorly understood and need closer investigation.

In the present work this is achieved by a combined experimental - simulation study:

While the kinetics of single chains on polymer surfaces was investigated with MD simulations, experimentally Poly (Bisphenol A carbonate) (BPAPC) thin films were evaporated in a vacuum chamber. Surface morphologies were investigated using scanning force (SFM) and scanning electron microscopy (SEM). Fourier transform infrared spectroscopy (FTIR) and size exclusion chromatography (SEC) were performed for a detailed chemical characterization. It is found, that the rms roughness decreases rapidly, once closed surfaces are obtained at thicknesses as high as 30 nm.

This work was supported by the DFG SFB 602 (TP B3), as well as the GIF No. 1428-303.1/2004.

O 44.5 Wed 17:00 Poster C

**In-situ synthesis and reactivity of adsorbed iron(II) and cobalt(II) tetraphenylporphyrins** — ●YUN BAI, SVEN SCHÖFFEL, KEN FLECHTNER, LIAM BRADSHAW, HANS-PETER STEINRÜCK, and J. MICHAEL GOTTFRIED — Universität Erlangen-Nürnberg, Lehrstuhl für Physikalische Chemie II, Egerlandstr. 3, 91058 Erlangen, Germany

In biological systems, Fe and Co porphyrins play an important role as the active centers of enzymes. Our approach to studying their reactivity is based on well ordered monolayers of these planar metal complexes at a Ag(111) surface. Their reactions with biologically relevant molecules such as O<sub>2</sub> and NO were studied under ultrahigh vacuum conditions with photoelectron spectroscopy and related techniques. Experimental difficulties arise from the extreme oxidation sensitivity of the Fe(II)-porphyrins. Therefore, the commonly employed ex-situ synthesis of the metalloporphyrin and subsequent vacuum deposition was ruled out as a way to prepare Fe(II)-porphyrin monolayers. Instead, we used an approach recently developed for the in-situ synthesis of adsorbed Co(II)-tetraphenylporphyrin [1] and succeeded to metalate monolayers of tetraphenylporphyrin with stoichiometric amounts of vapor-deposited Fe atoms. Supported by the Deutsche Forschungsgemeinschaft through SFB 583.

- [1] Gottfried et al., *J. Am. Chem. Soc.* 2006, 128, 5644.

O 44.6 Wed 17:00 Poster C

**STM Investigations on the ordered layers of a Tricarbonyl-(triphenylene)chromium-complex on Ag(111) and Ag(100)** — ●CHRISTOPH SCHMITZ<sup>1</sup>, IORDAN KOSSEV<sup>1</sup>, CAROLA RANG<sup>2</sup>, KARL HEINZ DÖTZ, and MORITZ SOKOLOWSKI<sup>1</sup> — <sup>1</sup>Institut für Physikalische und Theoretische Chemie, Universität Bonn, Wegelerstr. 12, 53115 Bonn, Germany — <sup>2</sup>Kekulé-Institut für Organische Chemie und Bio-

chemie, Universität Bonn, Gerhard-Domagk-Strasse 1, 53121 Bonn, Germany

Metal-organic complexes of chromium are interesting as catalysts and also in the role of molecular switches [1]. The switching, i.e., the reversible haptotropic migration of the chromium, has been extensively studied in solution [2]. However, possible technical applications require that the switching process occurs, when the substance is bonded on a surface or in the solid state. Here we show first STM investigations of a monolayer of such metal-organic complex on the Ag(111) and Ag(100) surfaces in ultra-high vacuum. The deposition of the substance was done by sublimation from a home build Knudsen cell. STM measurements at room temperature and low temperatures (80-100 K) reveal long-range ordered structures. Based on the unit cell geometry, the tunneling contrast, and DFT calculations we draw conclusions about the ordering of the molecules in the unit cell. The DFT calculations were kindly provided by Y. Su and F. Neese. This work is supported by DFG, SFB 624. [1] B. L. Feringa, (Ed.), *Molecular Switches*, Wiley-VCH, Weinheim (2001). [2] H. C. Jahr, M. Nieger and K. H. Dötz, *Chemical Communications* (2003) 2866.

O 44.7 Wed 17:00 Poster C

**SPA-LEED and NIXSW investigations of PTCDA on Ag(100)** — ●JULIAN IKONOMOV<sup>1</sup>, OLIVER BAUER<sup>1</sup>, SERGUEI SOUBATCH<sup>2</sup>, ADAM LASSISE<sup>2</sup>, STEFAN TAUTZ<sup>2</sup>, and MORITZ SOKOLOWSKI<sup>1</sup> — <sup>1</sup>Institut für Physikalische und Theoretische Chemie der Universität Bonn, Wegelerstr. 12, 53115 Bonn, Germany — <sup>2</sup>International University Bremen, School of Engineering and Science, P.O. Box 750 561, 28725 Bremen, Germany

We report studies of vacuum deposited PTCDA films on Ag(100). The SPA-LEED (Spot Profile Analysis Low Energy Electron Diffraction) measurements show two ordered structures on Ag(100). Up to one monolayer coverage, PTCDA forms a commensurate  $c(4 \times 4)$  structure with two molecules, perpendicularly oriented to each other in the unit cell. The ordered structure is stable up to a sample temperature of 690 K, at which a phase transition to a disordered phase occurs. Cooling the sample back to room temperature recovers the ordered structure. At a coverage above one monolayer the second layer orders in a different structure on top of the  $c(4 \times 4)$ -ordered first layer. Herein the molecules are arranged in a herring-bone pattern, and the unit cell is very similar to that of the (102) plane of the PTCDA bulk crystal. NIXSW (Normal Incidence X-Ray Standing Wave) experiments were performed on the monolayer in order to determine the vertical adsorption height and to compare it with values determined earlier for PTCDA on Ag(111) [1]. Supported by SFB 624.

[1] A. Hauschild et al., *Physical Review Letters* 94 (2005) 036106.

O 44.8 Wed 17:00 Poster C

**Looking for optimal Parameters for the self-assembly of linear organic Thiophenes** — ●FRANK SPERKA<sup>1</sup>, OTHMAR MARTI<sup>1</sup>, and ELENA MENA-OSTERITZ<sup>2</sup> — <sup>1</sup>Ulm University, Institute of Experimental Physics — <sup>2</sup>Ulm University, Institute of Organic Chemistry II

Macrocyclic Thiophenes are interesting substances to produce organic semiconductors. The self-assembly-behaviour of various types of macrocycles Cycloterthiophene-diene was studied in the last few years by means of STM. In order to gain a deeper insight into these mechanisms one also has to investigate how the assembly of linear Thiophene-Molecules on a substrate works. In order to do this, we investigated the R,R- and S,S-type of linear molecule Dihexyl-EDOT (EDOT=EthylenDioyThiophene) on mica and graphite with an AFM in tapping mode. At the beginning it was found that our measurements were inconsistent. In this poster we will describe the influences of several environmental parameters like temperature, humidity and time on the quality of the films. Additionally it was found that the films degrade quite rapidly after formation.

O 44.9 Wed 17:00 Poster C

**Interaction of Acetic Acid with Solid Water: A Study with IR Reflection-Absorption Spectroscopy (RAIRS) and Electron Spectroscopies (MIES; UPS)** — ●STEPHAN BAHR and VOLKER KEMPTER — Institut für Physik und Physikalische Technologien, Technische Universität Clausthal, 38678 Clausthal-Zellerfeld, Germany

The interaction of cyclic dimers of acetic acid,  $\text{CH}_3\text{COOH}$ , with solid water ( $\text{D}_2\text{O}$ ) at 120K on polycrystalline Ag was investigated. Metastable Impact Electron Spectroscopy (MIES) and Ultraviolet Photoelectron Spectroscopy UPS(HeII) were utilized to obtain information on the electronic structure of the outermost surface. Infrared

Reflection-Absorption spectroscopy (RAIRS) allowed for the identification of the AA species, and provides information on their hydration and the water-induced fragmentation.

The AA species quickly saturate the water OD dangling bonds at the ice surface, even before the first AA layer becomes saturated. For less than 0.3ML coverage the cyclic dimers break up into monomers and linear dimers under the influence of their interaction with the  $\text{D}_2\text{O}$  molecules. For coverages  $>0.3\text{ML}$  strong lateral interaction between AA monomers increases the linear dimer fraction. The second and following adlayers formed at 120K consist of cyclic dimers, mainly. The results will be compared to theoretical predictions [1,2].

[1] Picaud, S.; Hoang, P.; Peybernès, N.; Le Calvé, S.; Mirabel, P. *J. Chem. Phys.* **2005**, *122*, 194707. [2] Allouche, A.; Bahr, S. *J. Phys. Chem. B* **2006**, *110*, 8640.

O 44.10 Wed 17:00 Poster C

**Coverage and temperature dependence of ordered thin pentacene films on Ag(111) investigated with SPA-LEED** — ●ANNEGRET HAUSCHILD and MORITZ SOKOLOWSKI — Universität Bonn, Institut für Physikalische und Theoretische Chemie, Wegeler Str. 12, 53115 Bonn

Ultra thin films (1-15 monolayers) of the organic molecule pentacene (C<sub>22</sub>H<sub>14</sub>) were deposited with organic molecular beam epitaxy (OMBE) on the Ag(111) surface. Depending on coverage and deposition temperature, different highly ordered structures were found by spot profile low energy electron diffraction (SPA-LEED). For the sub-monolayer, no long range order has been observed. At low temperatures (LT), different to the well known room temperature (RT) phase [1], two further highly ordered structures could be observed in the monolayer. However, by growing multilayers at low temperatures, no change in the LEED patterns was recorded. The LEED spots become only more diffuse, this indicates a cluster growth in the Stranski-Krastanov mode. These LT phases are meta stable. By warming up the sample to room temperature, a phase transition to the RT phase occurs.

[1] M. Eremitchenko et al., *Phys. Rev. B* 72, 1 (2005)

O 44.11 Wed 17:00 Poster C

**Charge transfer dynamics in self-assembled monolayers** — ●STEFAN NEPPL<sup>1</sup>, ULRICH BAUER<sup>1</sup>, PETER FEULNER<sup>1</sup>, ANDREY SHAPORENKO<sup>2</sup>, MICHAEL ZHARNIKOV<sup>2</sup>, and DAVE ALLARA<sup>3</sup> — <sup>1</sup>Physikdepartment E20, TU-München, Germany — <sup>2</sup>Angewandte Physikalische Chemie, Universität Heidelberg, Germany — <sup>3</sup>Chemistry and Materials Science, Pennsylvania State University, USA

Charge transfer dynamics is a key quantity for the use of self-assembled monolayer as functional interfaces. Utilizing the core hole clock method, we study the endgroup to substrate electron transfer dynamics for cyanide terminated aliphatic thiolates on Au substrates. For aliphatic backbones consisting of 16 methylene groups, we observe pure autoionization spectra for pi-resonant N1s and C1s excitation of the CN endgroup. For resonant CN excitation of short chains of only 2 methylene groups, a mixture of resonant and non-resonant decay indicates endgroup to substrate charge transfer during the lifetime of the core holes. Quantitative results are obtained from the ratios of these contributions. Supported by the DFG (Fe 346/1-3) and the BMBF (05 KS4VHA/4 and 05 ES3XBA/5).

O 44.12 Wed 17:00 Poster C

**BINAP's on Au(111) - Electronic interface properties** — ●BENGT JAECKEL and BRUCE PARKINSON — Colorado State University; Department of Chemistry; 200 West Lake Street; Fort Collins, CO-80523/USA

Substituted binaphthyl-ligands (BINAPs) are important ligands for chiral selective homogeneous catalysis. We are attempting to prepare chiral selective surface by using organic MBE to prepare thin films of various racemic mixtures and enantiomerically pure BINAPs on freshly prepared Au(111)-surfaces. The interface properties were studied by X-Ray- and ultraviolet- photoelectron spectroscopy. Binaphthol, the simplest and lightest molecule only forms a sub-monolayer coverage on Au(111) at room temperature. Substituted BINAPs (e. g. with two additional Br-atoms or two substitutional  $\text{PC}_{12}\text{H}_{10}$ -groups) show a higher sticking probability and provide interesting insight into the important parameters responsible for the interface formation. By varying the substitution of the basis molecule one can investigate the influence on the physical and chemical interactions with the substrate. Scanning tunneling microscopy studies will be carried out to determine

the chiral properties of the molecules on the Au(111)-surface and if it possible to prepare enantiomeric pure surface which can be used for catalysis or sensing applications.

O 44.13 Wed 17:00 Poster C

**Subphase dependent (2D) ordering in monolayers of amphiphile molecules** — ●SASKIA SCHMACKE<sup>1</sup>, BERND STRUTH<sup>2</sup>, LUTZ WIEGART<sup>3</sup>, HENRI GLEYZOLLE<sup>3</sup>, and METIN TOLAN<sup>1</sup> — <sup>1</sup>Experimentelle Physik E1a, Universität Dortmund, Otto-Hahn-Str. 4, D-44221 Dortmund — <sup>2</sup>Deutsches Elektronen-Synchrotron DESY, Notkestr. 85, D-22607 Hamburg — <sup>3</sup>ESRF, 6 rue Jules Horowitz, BP 220, F-38043 Grenoble Cedex

Layers of amphiphile molecules on liquid subphases show a different phase behaviour depending on environmental parameters like temperature, surface pressure and subphase. Gaseous, liquid and solid phases are observable. In this work the influence of different subphases on the crystal structure of the Phospholipid monolayers DPPA (dipalmitoyl-phosphatidic acid) and DPPC (dipalmitoyl-glycerophosphocholine) was investigated. The crystal structure was determined by using Grating Incidence X-Ray Diffraction technique (GID) at the beamline ID10b, ESRF. The obtained diffraction patterns are analysed in two steps: First the information about the 2D unit cell of the crystalline phase, e.g. lattice spacings, lattice type (2D Bravais lattice) and the deformation of the lattice was determined. Secondly the intensity dependence on wave vector transfers perpendicular to the surface was analysed leading to information about the scatterer itself, like chain length, diameter, tilt angle and orientation within the lattice of the molecules forming the monolayer. The calculation of the differential cross section using a cylinder model for the lipid molecules shows very good agreement with the experiment for all subphases.

O 44.14 Wed 17:00 Poster C

**Complex Structures in Multilayer Polymer-Blends on Glass Substrates** — ●HUBERTUS MARBACH, FLORIAN MAIER, and HANSPETER STEINRÜCK — Universität Erlangen-Nürnberg, Lehrstuhl für Physikalische Chemie II, Egerlandstraße 3, D-91058 Erlangen, Germany

Recently, multicomponent polymer systems have attracted attention due to their capability to form a wealth of structures in thin films on various substrates. The three-dimensional morphology of these structures depends on the phase separation processes of the polymers involved, and on the corresponding experimental parameters and procedures, such as the polymer mixture, the spin coating parameters, thermal treatments, etc.. In the present paper we focus on layer systems of a mixture of polymethylmethacrylate and polystyrene (PMMA/PS) on glass slides. The polymer-blend films were prepared by a spin-coating technique and interjacent thermal treatments. The resulting rich variety of complex structures was characterized by means of atomic force microscopy under ambient conditions. In addition, the exposure of the PMMA/PS films to cyclohexane leads to the selective dissolution of PS. This enables the identification of the features attributed to PS (or PMMA) and serves as the starting point for the generation of even more complex structures. The main findings of systematic measurements will be presented and the underlying mechanisms will be discussed.

O 44.15 Wed 17:00 Poster C

**Site selective growth of organic molecules** — WENCHONG WANG<sup>1</sup>, DINGYONG ZHONG<sup>1</sup>, JIA ZHU<sup>1</sup>, FELIX KALISCHEWSKI<sup>2</sup>, ●CHUAN DU<sup>1</sup>, ANDREAS HEUER<sup>2</sup>, HARALD FUCHS<sup>1</sup>, and LIFENG CHI<sup>1</sup> — <sup>1</sup>Physikalisches Institut and Center for Nanotechnology (CeNTech), Universität Münster, 48149 Münster, Germany — <sup>2</sup>Institut für Physikalische Chemie, Universität Münster, 48149 Münster, Germany

Devices with active organic layers are of great interest recently due to their less energy consumable process and potential low cost. However, the future success of these interesting materials in applications will strongly depend on fabrication processes that include patterning. We present a general method to pattern organic molecules by template-directed nucleation control using organic molecular beam deposition. Fully sites selective growth of organic molecules can be controlled at optimized conditions. We use simple Lennard-Jones (LJ) pair potentials to mimic the molecular interactions. The simulation results have good agreements with experimental data. This technique can be applied to fabricate large area uniform organic devices.

O 44.16 Wed 17:00 Poster C

**Molecules can climb : Islands formation during organic**

**molecular beam epitaxy** — DINGYONG ZHONG<sup>1,2</sup>, ●RUIFEN DOU<sup>2</sup>, WENCHONG WANG<sup>2</sup>, HARALD FUCHS<sup>1,2</sup>, and LIFENG CHI<sup>2</sup> — <sup>1</sup>Institut für Nanotechnologie, Forschungszentrum Karlsruhe, 76021 Karlsruhe, Germany — <sup>2</sup>Physikalisches Institut and Center for Nanotechnology, Universität Münster, Wilhelm-Klemm-str. 10, 48149 Münster, Germany

The epitaxial growth of organic thin film has been studied. Islands with sharp edge, flat top and nearly uniform height are formed on metal crystalline substrate at certain range of growth temperatures. To understand the mechanism of the islands formation, a model is proposed in which the binding energy of molecules at the step edge is various at different terraces due to the lattice mismatching of the first monolayer and the three-dimensional island beyond the first monolayer. Both the ascending and descending interlayer transport processes are considered. The numerical simulations of the rate equations based on this model are consistent well with the experimental results.

O 44.17 Wed 17:00 Poster C

**Molecular flexibility as a factor affecting the surface ordering of organic adsorbates on metal substrates** — ●S. SOUBATCH, R. TEMIROV, and F. S. TAUTZ — International University Bremen (Jacobs University Bremen as of spring 2007), Bremen, Germany

The effect of molecular flexibility on the surface ordering of complex organic adsorbates is explored by mean of LEED and STM, using DH4T and mixed DH4T-tetracene phases on Ag(111) as model systems. Above 273 K, DH4T forms a nematic liquid crystalline phase. At 273 K, a reversible phase transition to a long-range ordered, point-on-line coincident phase is observed. However, this ordered state is still affected substantially by the flexible nature of DH4T, which materializes in a large number of local structural defects. If traces of DH4T are co-evaporated with tetracene, inclusions of a 1:1 stoichiometric DH4T-tetracene phase are found in a tetracene/Ag(111) matrix. In this mixed phase, tetracene and the two surface enantiomers of DH4T arrange in a complex stripe structure. The mixed phase shows a higher degree of order than present at the pure DH4T/Ag(111) interface, which also lacks chiral organization. The addition of tetracene molecules as structural templates stabilizes certain conformations of DH4T and thus, by balancing its structural flexibility, allows the surface-induced chirality of DH4T to become a decisive factor in determining the structure of the mixed phase.

O 44.18 Wed 17:00 Poster C

**STM Observation of Molecular Chains consisting of Mn<sub>6</sub>Cr Single Molecule Magnets on Highly Ordered Pyrolytic Graphite (HOPG)** — ●AARON GRYZIA<sup>1</sup>, ARMIN BRECHLING<sup>1</sup>, WIEBKE HACHMANN<sup>1</sup>, MARC DAVID SACHER<sup>1</sup>, ULRICH HEINZMANN<sup>1</sup>, MAIK HEIDEMEIER<sup>2</sup>, and THORSTEN GLASER<sup>2</sup> — <sup>1</sup>Faculty of Physics — <sup>2</sup>Faculty of Chemistry, University of Bielefeld, D-33615 Bielefeld

We report on the preparation and characterization of Mn<sub>6</sub>Cr-Single Molecule Magnets<sup>1</sup> on a HOPG(0001) surface.

The Mn<sub>6</sub>Cr-molecules showed 1D molecular arrangements with many interesting features, such as the occurrence of discrete kink angles in the molecular chains of 30°, only two different molecular orientations, the orientation of the chains along the main crystal axis of HOPG and a much larger molecule-molecule distance than expected from the van der Waals radii of the molecules. The orientation of single Mn<sub>6</sub>Cr-molecules in the chain and the orientation of the chain, in respect to the main crystal axis of the HOPG substrate, shows a clear dependence. Segments of the chain with the same orientation of the Mn<sub>6</sub>Cr-molecules are parallel to the main crystal axis and parts with an alternating molecular orientation are tilted by 30° in respect to this axis, which is a clear evidence for molecular-substrate interactions.

The observed structures appear to be a very promising model system to study the competition between molecule-molecule interactions and substrate-molecule interactions.

<sup>1</sup> T. Glaser et al., *Angew. Chem.*, **118**, 6179-6183 (2006).

O 44.19 Wed 17:00 Poster C

**Valence electronic structure of the PTCDA/Au(111) interface** — ●JOHANNES ZIROFF, SIMON HAME, FRANK FORSTER, AZZEDINE BENDOUNAN, and FRIEDRICH REINERT — University of Würzburg, Experimental Physics II, Am Hubland, 97074 Würzburg, Germany

We present angular and energy resolved UPS spectra of PTCDA (3,4,9,10-perylene-tetracarboxylic-dianhydride) on the Au (111) surface from the sub-monolayer range to thick films. Using the Shockley state as a probe, one can investigate the substrate-adsorbate interac-

tion of the first monolayer. We will show and discuss changes of binding energy and Rashba term upon adsorption. The valence features of the adsorbed PTCDA molecule, as well as their coverage dependent changes in intensity and binding energy will be addressed. Examples for the use of the surface state as an indicator for the type of thin film growth will also be presented.

O 44.20 Wed 17:00 Poster C

**Inelastic electron tunnelling spectroscopy of the ordered PTCDA/Ag(111) interface** — ●R. TEMIROV and F.S. TAUTZ — International University Bremen, Bremen, Germany (Jacobs University Bremen as of spring 2007)

Understanding complex adsorption phenomena is an issue of rising importance. Recently it has been shown that the STM-based Inelastic Electron Tunnelling Spectroscopy (IETS) is a powerful technique for the analysis of adsorption on a single molecular level. Nevertheless the interpretation of the IETS data was shown in general to be far from straightforward. In this contribution we use the well studied case of PTCDA/Ag(111) adsorption as a model system to which the IETS is applied. The results of IETS are compared with HREELS data and theoretically calculated spectra of a free molecule. On the basis of a simple symmetry analysis two vibrational modes are identified. Remarkably, slight variations of the adsorption conditions are found to enhance IETS signal by an order of magnitude. The origin of this enhancement is discussed.

O 44.21 Wed 17:00 Poster C

**High-Resolution Photoemission Spectra of Cytosine, Thymine and Uracil** — ●ANDREA HAUG, MARIA-BENEDETTA CASU, HEIKO PEISERT, and THOMAS CHASSÉ — Institut für Physikalische und Theoretische Chemie, Auf der Morgenstelle 8, D-72076 Tübingen

In the last decade, significant progress has been made in the use of DNA bases as molecules for electronic applications such as bioorganic field effect transistors and molecular nanowires. Questions arise to which extent they could improve the present status of molecular electronics. These questions can be answered by the investigation of their electronic structure, of their interfaces with metals, and of their growth modes as thin films. In this work we present our investigations on the electronic and molecular structure of the DNA and RNA bases cytosine, thymine and uracil by X-ray photoemission spectroscopy (XPS) and ultraviolet photoemission spectroscopy (UPS). The films were grown by organic molecular beam deposition on polycrystalline gold with different film thickness (between 0.2 and 10 nm and above 20 nm). After each step the sample surface was characterized in situ by monochromatized XPS (Al-K $\alpha$  1486.6 eV) and UPS (He I, 22.2 eV) under UHV conditions. We have investigated the stability of the bases upon evaporation, the growth mode, and the interface properties.

O 44.22 Wed 17:00 Poster C

**Electron spectroscopy on functionalized lignin-like materials** — ●LOTHAR KLARHÖFER<sup>1</sup>, BURKHARD ROOS<sup>1</sup>, WOLFGANG MAUS-FRIEDRICHS<sup>1</sup>, VOLKER KEMPTER<sup>1</sup>, and WOLFGANG VIÖL<sup>2</sup> — <sup>1</sup>Institut für Physik und Physikalische Technologien, Leibnizstraße 4, D-38678 Clausthal-Zellerfeld, Germany — <sup>2</sup>Hochschule für angewandte Wissenschaft und Kunst, Fakultät Naturwissenschaften und Technik, Von-Ossietzky-Str. 99, D-37085 Göttingen, Germany

XPS is a common technique for characterizing lignin-like materials, such as pulp and paper or wood surfaces. We combine valence band XPS with MIES (Metastable Impact Electron Spectroscopy) UPS (HeI) (Ultraviolet Photoelectron Spectroscopy) in order to identify functionalities which are difficult to detect with core level XPS due to the small chemical shift. With MIES / UPS it is possible to identify different functional groups of the surfaces, allowing to control surface - modification techniques applied to lignin - like materials, such as the optimization of the plasma treatment of wooden surfaces. Lignin surfaces were characterized by XPS, MIES and UPS. In order to understand the results, additional fingerprint spectra were recorded using the lignin precursors (coniferyl alcohol and sinapyl alcohol), cinnamyl alcohol, phenol and benzene. The comparison with the MIES and UPS spectra of these molecules allows the identification of the contributions of the hydroxyl, methoxy and phenol groups the the lignin spectra.

O 44.23 Wed 17:00 Poster C

**Characterisation of multi-wall carbon nanotubes functionalised with carboxyl groups** — ●MARCEL HIMMERLICH, UWE RITTER, HENRY ROMANUS, JUERGEN A. SCHAEFER, PETER SCHARFF, and STEFAN KRISCHOK — Institut für Physik und Institut für Mikro- und

Nanotechnologien, TU Ilmenau, P.O. Box 100565, 98684 Ilmenau, Germany

The impact of nitric acid (HNO<sub>3</sub>) treatment on the structure, surface composition and surface electronic structure of multi-wall carbon nanotubes (MWCNTs) is investigated employing scanning electron microscopy (SEM) and transmission electron microscopy (TEM) as well as X-ray and ultraviolet photoelectron spectroscopy (XPS, UPS) together with electron energy loss spectroscopy (EELS). The investigated MWCNTs have been synthesised at 900°C by spray pyrolysis using benzene and 1% ferrocene in an Argon flow. After subsequent purification the samples were functionalised by a treatment with nitric acid at 100°C for 2 h. The valence band structures of functionalised and unfunctionalised samples are compared to reference measurements on formic acid (HCOOH) and polyacrylic acid. The analysis of the C1s and O1s core levels together with the observed differences in the valence band structure reveals the formation of carboxyl (-COOH) groups on the nanotubes. TEM measurements indicate that the main reaction takes place at the end of the nanotubes resulting in a cracking of the MWCNT end caps.

O 44.24 Wed 17:00 Poster C

**X-ray absorption of spin crossover complexes** — ●MATTHIAS BERNIEN<sup>1</sup>, MARTEN PIANTEK<sup>1</sup>, JORGE MIGUEL<sup>1</sup>, RADU ABRUDAN<sup>1</sup>, HEIKO WENDE<sup>1,2</sup>, WOLFGANG KUCH<sup>1</sup>, MARCO HARYONO<sup>3</sup>, HOLGER KÄMPF<sup>3</sup>, and ANDREAS GROHMANN<sup>3</sup> — <sup>1</sup>Freie Universität Berlin, Fachbereich Physik, Arnimalle 14, D-14195 Berlin, Germany — <sup>2</sup>Universität Duisburg-Essen, Fachbereich Physik, Lotharstr. 1, D-47048 Duisburg, Germany — <sup>3</sup>Technische Universität Berlin, Institut für Chemie, Straße des 17. Juni 135, D-10623 Berlin, Germany

Spin crossover (SCO) molecular complexes consist of a central metal ion surrounded by organic ligands. Depending on temperature, pressure, or optical excitation, these complexes can switch between two magnetic states, for which the electrons of the d-orbitals align such that their spins add up (high spin) or compensate partly (low spin) [1].

We report on X-ray absorption (XAS) measurements of thin layers of Fe(II) bispyrazolylpyridine SCO complexes deposited from solution on gold metal surfaces. By means of angle-dependent XAS at the C- and N-K edges we determine the alignment of the molecules on the surface, whereas their spin state is determined by comparing the Fe-L<sub>3,2</sub> spectra to measurements on bulk samples. We find that the interaction with the surface plays an important role on the switching phenomenon.

[1] O. Kahn and C.J. Martinez, Science 279, 44 (1998)

O 44.25 Wed 17:00 Poster C

**Geometric and electronic structure of azobenzene - alkanethiols on gold** — ●DANIEL BRETE<sup>1,2</sup>, ROLAND SCHMIDT<sup>1,2</sup>, SANJA KORIKÄ<sup>1</sup>, CORNELIUS GAHL<sup>1</sup>, and MARTIN WEINELT<sup>1,2</sup> — <sup>1</sup>Max-Born-Institut, Max-Born-Str. 2A, 12489 Berlin — <sup>2</sup>Freie Universität Berlin, Fachbereich Physik, Arnimallee 14, 14195 Berlin

Azobenzene is a conformational photo-switch. Upon optical excitation at 350 nm and 430 nm geometric changes of the chromophore occur on a sub-picosecond to picosecond timescale. This ultrafast dynamics suggests that switching may even occur when azobenzene is bound to a surface, where charge transfer into the substrate efficiently quenches electronic excitations. Associated with the geometric change of the azobenzene molecule from trans to cis conformation is a shift of the optical  $\pi$  to  $\pi^*$  transition.

We have investigated self-assembled monolayer of azobenzene - alkanethiols adsorbed on gold and their potential as a molecular switch by X-ray absorption as well as by X-ray and VUV photoemission spectroscopy. The molecules are well oriented at 100 K and the azobenzene entity is sufficiently decoupled from the substrate by the alkane chain. The occupied frontier orbitals of non-bonding  $n$  and of  $\pi$  character are identified by angle-resolved photoemission and autoionization spectroscopy at the N1s and C1s absorption edges. Their energetics and oscillator strengths are substantially modified by substituents attached to the azobenzene entity. Resultant implications for the switching efficiency will be discussed.

O 44.26 Wed 17:00 Poster C

**Molecular distortion upon adsorption: The case of NTCDA/Ag(111)** — ●CHRISTIAN KUMPF, CHRISTOPH STADLER, INGO KRÖGER, MICHAEL SCHEUERMANN, and EBERHARD UMBACH — Univ. Würzburg, Experimentelle Physik II, Am Hubland, 97074 Würzburg

The properties of many functional materials and electronic devices based on (multi-)layer systems and thin films are dominantly defined by their surfaces and interfaces. This is particularly true for organic thin films and adsorbate systems, the properties of which largely depend on their interaction with the underlying substrate. Therefore a detailed investigation of this interaction is extremely important in order to obtain a comprehensive understanding of these materials.

In this contribution recent results for one of the most important model systems for molecular adsorption on surfaces is presented: 1,4,5,8-naphthalene-tetracarboxylicacid-dianhydride (NTCDA) on Ag(111). Using the techniques x-ray standing waves (XSW) and quantitative low energy electron diffraction (LEED-IV) a significant bending of the molecules was found upon adsorption. The results demonstrate the chemisorptive character of the adsorption.

Furthermore, a novel method for the interpretation of PES- and Auger-based XSW data is presented. The correction of non-dipolar effects in photoemission as well as electron-induced effects in Auger-electron emission was lively discussed within the last years. Using the example NTCDA/Ag(111) we demonstrate how the results from these different detection channels can be reconciled in a self-consistent iterative correction-method.

O 44.27 Wed 17:00 Poster C

**Laser-tailoring of the size and shape of gold nanoparticles in solution** — ●FLORIAN VOGEL, FRANK HUBENTHAL, and FRANK TRÄGER — Institut für Physik and Center for Interdisciplinary Nanostructure Science and Technology – CINSaT, Universität Kassel, Heinrich-Plett-Strasse 40, 34132 Kassel, Germany

Tailoring of metal nanoparticles with laser light has been a well known technique since several years. Although selective tailoring of certain shapes or sizes of supported metal nanoparticles has been demonstrated with ns-pulsed laser light, tailoring of nanoparticles in solution has remained a challenge.

In this contribution, we present recent studies on tailoring colloidal gold particles prepared by wet chemical reduction of HAuCl<sub>4</sub> with trisodium citrate. In general, this method produces elongated particles with relatively broad shape and size distributions. Post-synthesis irradiation with ns-pulsed laser light with photon energies of 1.9 eV and a laser fluence of  $(52 \pm 4)$  mJ/cm<sup>2</sup> permits reshaping to spherical particles. This is accompanied by a clear reduction of the half width of the plasmon resonance, while the size of the particles remains nearly constant at approximately  $R = 25$  nm. In contrast, if a photon energy of 1.4 eV and a comparable fluence is used, particles with axial ratios of about 0.3 are selectively heated and form colloids with radii up to 70 nm by coagulation.

O 44.28 Wed 17:00 Poster C

**DFT-Investigations of Coalescence Behaviour of Small Magic Si Clusters on Surfaces** — ●WOLFRAM QUESTER and PETER NIELABA — Fachbereich Physik, Universität Konstanz, 78457 Konstanz

Experimental results indicate that small magic Si clusters do not form islands of bulk Si on weakly interacting surfaces (HOPG). For Si<sub>4</sub> this was confirmed in earlier calculations [1]. This leads to the question if these clusters are suited as building blocks for new cluster materials.

These investigations were extended to Si<sub>7</sub>. Potential energy curves of two approaching Si<sub>7</sub> clusters were calculated for different reaction channels using Density Functional Theory implemented in the CPMD code available at [2]. It could be shown that the cluster-cluster interaction is either repulsive or there are fusion barriers higher than room temperature.

Since the influence of the surface is important, the next step was to include the graphite surface in the simulations. Also the influence of defects was to be studied.

[1 ] M. Grass, D. Fischer, M. Mathes, G. Ganteför and P. Nielaba, *Appl. Phys. Lett.*, **81**, 3810 (2002)

[2 ] www.cpmid.org

O 44.29 Wed 17:00 Poster C

**Kinetics of Ir-cluster lattice formation on a moiré of graphene with Ir(111)** — ●TIM PLASA<sup>1</sup>, ALPHA T. NDIAYE<sup>1</sup>, JOSEF MYSLIVEČEK<sup>2</sup>, and THOMAS MICHELY<sup>3</sup> — <sup>1</sup>I. Physikalisches Institut, RWTH Aachen — <sup>2</sup>Institut für Bio- und Nanosysteme IBN-3, Forschungszentrum Jülich — <sup>3</sup>II. Physikalisches Institut, Universität Köln

Highly ordered arrays of Ir clusters can be obtained by depositing Ir

on Ir(111) surface covered with a graphene monolayer. The periodicity of these arrays is determined by the moiré pattern of graphene on Ir(111) [N'Diaye et al., Phys. Rev. Lett. 97, 215501, 2006]. In order to uncover the mechanisms of Ir-cluster lattice formation on a moiré of graphene with Ir(111) we investigated the average cluster size and the occupation probability of moiré cells as a function of coverage, temperature and annealing time. We used a simple kinetic Monte Carlo simulation to derive atomistic parameters of adatom and cluster motion during the lattice formation. Assuming monomer and dimer mobility only, the data for temperatures up to 400 K may be reproduced fairly well, while at higher temperatures or longer annealing time the effect of the mobility of larger clusters become noticeable.

O 44.30 Wed 17:00 Poster C

**W<sub>n</sub>S<sub>m</sub>: Possible material for new fullerene structures** — ●WILKO WESTHÄUSER<sup>1</sup>, TIM FISCHER<sup>1</sup>, TOBIAS MANGLER<sup>1</sup>, SIBYLLE GEMMING<sup>2</sup>, GOTTHARD SEIFERT<sup>2</sup>, and GERD GANTEFÖR<sup>1</sup> — <sup>1</sup>AG Ganteför, FB Physik, University of Konstanz, Germany — <sup>2</sup>Institut für Physikalische Chemie und Elektrochemie, University of Dresden, Germany

As the layered semiconductor material WS<sub>2</sub> in bulk is similar to graphite, it is of interest to find out whether this material might form small stable cage-like fullerene structures. In combination with density functional theory calculation and gas phase mass and photoelectron spectroscopy [1,2], certain magic clusters were deposited in soft-landing mode on Ag- and Si-substrates. In gas phase theoretically predicted 2-dimensional triangular shaped platelets of W<sub>n</sub>S<sub>m</sub>-clusters with  $n > 5$  were detected and similar structures of Mo<sub>n</sub>S<sub>m</sub> were studied [3]. For first measurements deposited W<sub>1</sub>S<sub>3</sub>-, W<sub>2</sub>S<sub>6</sub>- and W<sub>5</sub>S<sub>6</sub>-clusters known as particularly stable in gas phase experiments were investigated via HREELS and XPS. These data were compared to WS<sub>2</sub> bulk material, additionally.

[1] N. Bertram, Y.D. Kim, G. Ganteför, Q. Sun, P. Jena, J. Tamuliene and G. Seifert, Chem. Phys. Lett. 396 (2004), 341

[2] S. Gemming, J. Tamuliene, G. Seifert, N. Bertram, Y.D. Kim and G. Ganteför, Appl. Phys. 82 (2006), 162

[3] B. Bertram, J. Cordes, Y.D. Kim, G. Ganteför, S. Gemming and G. Seifert, Chem. Phys. Lett. 418 (2006), 36

O 44.31 Wed 17:00 Poster C

**Ag cluster growth on biaxially oriented PET** — ●GÜNTHER WEIDLINGER, LIDONG SUN, JOSÉ MANUEL FLORES-CAMACHO, MICHAEL HOHAGE, and PETER ZEPPEFELD — Institut für Experimentalphysik, Johannes Kepler Universität Linz, Linz, Austria

Metallic clusters show new and interesting properties different from bulk material, e.g. catalytic effects as well as optical effects. We report our in-situ optical characterization of metal clusters during growth with Reflectance Difference Spectroscopy (RDS). Ag was deposited on biaxially oriented Polyethylene terephthalate (PET) at a constant rate of about 0.1nm/min in Ultra High Vacuum (UHV). Since Ag does not wet the PET surface, the Ag atoms form clusters on the surface and in the surface-near region. Cluster layers with a nominal thickness from 0.1nm to 5nm were investigated. A strong anisotropy of the particle plasmon induced by the biaxially oriented substrate has been observed. Furthermore, this anisotropy shows a strong dependence on the nominal thickness of the silver layer. The relation between the observed optical properties and the size as well as the spacial distribution of the clusters will be discussed.

O 44.32 Wed 17:00 Poster C

**CO oxidation and partial oxidation of light alkanes over TiO<sub>2</sub> supported gold catalysts in microreactors** — ●GUIDO WALTHER<sup>1</sup>, SEBASTIAN HORCH<sup>1</sup>, ULRICH QUADE<sup>2</sup>, IB CHORKENDORFF<sup>2</sup>, SØREN JENSEN<sup>3</sup>, and OLE HANSEN<sup>3</sup> — <sup>1</sup>CAMD, Department of Physics, DTU, DK-2800 Kgs. Lyngby, Denmark — <sup>2</sup>CINF, Department of Physics, DTU, DK-2800 Kgs Lyngby, Denmark — <sup>3</sup>MIC, Department of Micro and Nanotechnology, DTU, DK-2800 Kgs Lyngby, Denmark

In a new setup, based on microfabricated silicon reactors, oxidation reaction over TiO<sub>2</sub> supported gold catalysts have been studied. In a first experiment size selected gold nanoclusters have been deposited into the microreactor using a cluster source. Here single charge gold clusters were mass selected by a QMS. The cluster beam was focused on the reactor bed using an einzel lens. Hence CO and oxygen were applied at a total flow rate of 0.1 ml min<sup>-1</sup>, the amount of produced CO<sub>2</sub> was still below the detection limit of the used gas chromatograph. An increased amount of catalyst has been realized in a second experiment. Here a powder catalyst, based on TiO<sub>2</sub> supported 3.5 nm Au

particles, was used. Appropriate measurements to CO oxidation gave rise to study partial oxidation of light alkanes over those catalysts. To investigate the reaction products the microreactor was interfaced to a gas chromatograph and a mass spectrometer, as well. Since methane reacts with oxygen in a stoichiometric ratio 1:2, water will be detected associated with CO<sub>2</sub>. A significant increase in hydrogen signal marks the onset of the partial oxidation of methane.

O 44.33 Wed 17:00 Poster C

**Dynamics of Metal Nanodroplets** — ANJA HABENICHT<sup>1</sup>, PAUL LEIDERER<sup>1</sup>, JOHANNES BONEBERG<sup>1</sup>, MORITZ TRAUTVETTER<sup>2</sup>, DANIEL TOLD<sup>2</sup>, CHRISTIAN PFAHLER<sup>2</sup>, ALFRED PLETTL<sup>2</sup>, PAUL ZIEMANN<sup>2</sup>, MICHAEL KINYANJUI<sup>3</sup>, and UTE KAISER<sup>3</sup> — <sup>1</sup>Universität Konstanz, Fachbereich Physik, 78457 Konstanz — <sup>2</sup>Universität Ulm, Institut für Festkörperphysik, 89069 Ulm — <sup>3</sup>Universität Ulm, Zentrale Einrichtung Elektronenmikroskopie, 89069 Ulm

Liquid metal nanodroplets are generated by a dewetting-induced detachment process: flat metal nanostructures evaporated onto a substrate through colloidal masks or structured by e-beam lithography are illuminated with an intensive ns laser pulse. If heated above the melting point, the liquid structures reduce their surface energy by reforming to spheres. For the small aspect ratios used here this involves a vertical movement of the center of mass and due to inertia the droplets leave the surface. The velocities of the detached nanodroplets are measured with a light barrier technique and compared with the velocity deduced from simple estimations for the dewetting process. Results are shown for different materials, intermediate layers and multilayers. Further we present first results of impact experiments, where the droplets are landed on another substrate. The particles cool down during the flight due to thermal radiation and solidify on the substrate. By catching at different distances, the landing temperature can be varied. Snapshots of different stages of droplet impact are shown. For the latter case, the focused ion beam technique was applied to cut directly through differently formed droplets.

O 44.34 Wed 17:00 Poster C

**Electronic structure of iron oxide nanoparticles** — ALADIN ULLRICH, DANIEL GYASI-ANTWI, MARCUS PREISINGER, MICHAEL KRISPIN, and SIEGFRIED HORN — Lehrstuhl für Experimentalphysik II, Universität Augsburg, D-86135 Augsburg

We have investigated the electronic structure of nanosized iron oxide and its precursor material apo-ferritin by scanning tunnelling microscopy (STM) and spectroscopy (STS) as well as conductive atomic force microscopy (CAFM). The remineralization of apo-ferritin molecules resulted in core sizes varying from 3 – 7 nm depending on the filling quantity of iron. Iron oxide nanoparticles were produced by thermal treatment of remineralized apo-ferritin molecules in air. Depending on the thermal treatment we were able to prepare different phases of nanosized iron oxide resembling  $\alpha$ -Fe<sub>2</sub>O<sub>3</sub>,  $\gamma$ -Fe<sub>2</sub>O<sub>3</sub> and mixtures thereof. The electronic structure of remineralized apo-ferritin and iron oxide nanoparticles has been investigated under ambient conditions and will be compared with previous measurements performed in UHV. We show that the band gap can differ from bulk material and is dominated by surface effects.

O 44.35 Wed 17:00 Poster C

**Fabrication and Characterization of Gold Nanocrystals on NaCl(001)-Surfaces** — ANDREAS WINTER, JAWAD SLIEH, ARMIN BRECHLING, WIEBKE HACHMANN, ULF KLEINEBERG, and ULRICH HEINZMANN — University of Bielefeld, Faculty of Physics, D-33615 Bielefeld

We report on the fabrication of dispersive gold nanocrystals using a vacuum evaporation technique. Gold has been evaporated under ultra high vacuum conditions on a freshly cleaved NaCl(001) surface. The substrate temperature, the averaged thickness and the potential of the sample were studied systematically. After preparation, the gold nanocrystals have been characterized by means of different techniques such as Atomic Force Microscopy (AFM), Transmission Electron Microscopy (TEM), X-Ray Diffraction (XRD) and Laue Diffraction. Depending on the preparation parameters, the gold grows in clusters with lateral and vertical sizes between 10 nm and 25 nm. XRD-measurements revealed a crystal growth with a preferred orientation of the Au(001)-axis parallel to the NaCl(001)-axis. A second Au(111) orientation, parallel to the NaCl surface normal was observed at a substrate potential between 200 V and 400 V and a substrate temperature of ca. 300°C, only. Estimations of the cluster size, measured by AFM, and the crystal size, measured by XRD exhibit comparable results,

which indicate a high amount of single gold crystals. TEM-images, made after dissolving the gold-crystals in an aqueous CHAPS-solution support these results.

O 44.36 Wed 17:00 Poster C

**Herstellung und Vermessung von Kobalt-Clustern** — MATTHIAS GRUBE, MATTHIAS BÜNFELD, FRANK SCHMIDL und PAUL SEIDEL — Institut für Festkörperphysik, Friedrich-Schiller-Universität Jena, Germany

Kobalt-Cluster sind wichtige Katalysatoren für Kohlenstoff-Nanoröhren, wobei deren Größe mitbestimmend für den Durchmesser der Röhren ist.

Um die Cluster herzustellen, haben wir durch thermisches Verdampfen eine geschlossenen Kobaltschicht erzeugt, die anschließend getempert wurde. Der Temperprozess erfolgte sowohl an Luftatmosphäre als auch unter Vakuum. Es wurden Clustergrößen in Abhängigkeit von der Temperatur und den Dicken der geschlossenen Schichten untersucht. Als Substrat verwendeten wir Silizium mit und ohne einer zusätzlich gesputterten SiO<sub>2</sub>-Schicht.

O 44.37 Wed 17:00 Poster C

**Ag islands on C<sub>60</sub> functionalized Au(111) compared to deposited Ag clusters** — TORSTEN RICHTER<sup>1</sup>, STEFANIE DUFFE<sup>1</sup>, THOMAS IRAWAN<sup>1</sup>, BENEDIKT SIEBEN<sup>1</sup>, HEINZ HÖVEL<sup>1</sup>, CHUNRONG YIN<sup>2</sup>, and BERND VON ISSENDORFF<sup>2</sup> — <sup>1</sup>Universität Dortmund, Experimentelle Physik I, 44221 Dortmund, Germany — <sup>2</sup>Universität Freiburg, Fakultät für Physik, 79104 Freiburg, Germany

We are interested in the electronic structure of clusters in contact with a surface. In addition to experiments with mass selected Ag clusters we grew Ag islands by evaporation of Ag atoms on a C<sub>60</sub> functionalized Au(111) surface at a temperature below 50 K. The investigation of the silver islands with a low temperature scanning tunnelling microscope shows quite broad height distributions. Tempering the cluster/surface system up to different temperatures leads to a higher mobility of the silver islands and more and more coalescence. We observed a strong coalescence at temperatures above 150 K. These experiments can be compared with experiments of mass selected geometrically magic clusters deposited on C<sub>60</sub>/Au(111) at room temperature. Here we observed very narrow height distributions. We also studied the position of the clusters relative to the C<sub>60</sub> molecules. We found out that the size selected clusters are on top of a C<sub>60</sub> molecule and the grown islands at a position between two C<sub>60</sub> molecules.

O 44.38 Wed 17:00 Poster C

**GISAXS studies of micellar supported Au nanoparticles on TiO<sub>2</sub>** — NICOLE JEUTTER<sup>1</sup>, DIDIER WERMEILLE<sup>1</sup>, JOACHIM BANSMANN<sup>2</sup>, STEFAN KIELBASSA<sup>2</sup>, CHRISTINE FIX<sup>2</sup>, ULF WIEDWALD<sup>3</sup>, HANS-GERD BOYEN<sup>3</sup>, and PAUL ZIEMANN<sup>3</sup> — <sup>1</sup>E.S.R.F., 6 Rue Jules Horowitz, 38000 Grenoble, France — <sup>2</sup>Institute for Surface Chemistry and Catalysis, Ulm University, D- 89069 Ulm — <sup>3</sup>Institute of Solid State Physics, Ulm University, D- 89069 Ulm

Metal oxide supported gold catalysts have attracted considerable attention because of their surprising activity in a number of reactions such as low temperature CO oxidation [1]. The activity of catalysts might be closely related to the morphology and shape changes of the catalysts under different gas environments. Grazing Incidence Small Angle Scattering (GISAXS) experiments can monitor the morphology evolution in-situ and provide the possibility to determine the reaction parameter when shape changes occur.

Au nanoparticles of a nominate thickness of 12 nm have been deposited on a fully oxidized TiO<sub>2</sub> (110) substrate by micellar technique. The characterization of the average size and shape of the catalysts in air before and after annealing to 400°C has been carried out with GISAXS.

First results show that, before the annealing treatment, the average particle to particle distance can be clearly seen in GISAXS. After the annealing procedure the correlation maxima in the GISAXS pattern are broader and weaker than before.

[1] M.Haruta et al, J.Cat.144 (1993) 175

O 44.39 Wed 17:00 Poster C

**Tunneling through single atoms** — MARTYNA POLOK, DMITRY FEDOROV, MICHAEL CZERNER, and INGRID MERTIG — Martin Luther University Halle-Wittenberg, Department of Physics, Institute of Theoretical Physics, 06099 Halle (Saale), Germany

Scanning tunneling microscopy (STM) is of great importance nowa-

days, since it allows for probing electronic and magnetic properties of surfaces.

In this study we concentrate on the theoretical description of a Cu tip interacting with a Co adatom adsorbed on the Cu (100) surface. The ground state electronic structure of the system was determined by means of density functional theory (DFT) combined with the screened Korrington-Kohn-Rostoker (KKR) Green's function method. It was shown that with the varying tip-surface distance  $d$  the geometry of the system undergoes complex structural relaxation[1].

We use Kubo linear response theory in Baranger-Stone formulation to find the conductance of the system for different  $d$ . The attention is focused on the value of the tunneling current as a function of  $d$ . Additionally we want to determine precisely the tip-surface distance  $d_0$  for which the conductance changes from the tunneling to the contact mode. Results pertaining to tunneling regime will be presented.

[1] R. Z. Huang et al., Phys. Rev. B 12, 8169 (2006)

O 44.40 Wed 17:00 Poster C

**Experimental band structure of  $V_2O_5$  by angle resolved photoelectron spectroscopy** — •TORSTEN STEMMLER, MAXIMILIAN KAUERT, HELMUT DWELK, and RECARDO MANZKE — Institut für Physik, Humboldt-Universität zu Berlin, Newtonstr. 15, 12489 Berlin

Due to the manifold of catalytic applications, the vanadium oxides, and among them  $V_2O_5$ , came into the scientific focus. For a basic understanding a detailed knowledge of the electronic structure is important. In particular because the experimental data base on the electronic valence band structure on  $V_2O_5$ (010) single crystals is very scarce. Here we present high-resolution angle-resolved photoemission experiments carried out with synchrotron radiation and with the light of a HeI resonance lamp. The results will be compared with theoretical calculations, e.g. from J.C.Parker et al.[1] and A.Chakrabarti et al.[2]. Furthermore the problem of degradation of the surface due to the high reactivity will be discussed.

[1] J.C.Parker, D.J.Lam, Y.-N.Xu and W.Y.Ching, Phys. Rev. B42, 5289 (1990)

[2] A.Chakrabarti, K.Hermann, R.Druzinic, M.Witko, M.Petersen and F.Wagner, Phys. Rev. B59, 10583 (1999)

O 44.41 Wed 17:00 Poster C

**Fermi surface map of metallic  $MoTe_2$**  — •THORSTEN ZANDT, ROBERT HEIMBURGER, CHRISTOPH JANOWITZ, and RECARDO MANZKE — Institut für Physik, Humboldt-Universität zu Berlin, Newtonstraße 15, 12489 Berlin

$MoTe_2$  undergoes a phase transition at about 1125 K from a low-temperature semiconducting  $\alpha$ -phase (hexagonal, isostructural with  $MoS_2$ ) to a high-temperature metallic  $\beta$ -phase (monoclinic, distorted  $CdI_2$ ). Upon further cooling an additional phase transition is observed at 250 K for monoclinic  $\beta$ - $MoTe_2$ . This transition is accompanied by a discontinuous structural change, i.e. the monoclinic angle  $\beta$  of  $93^\circ 55''$  changes to  $90^\circ$  [1] resulting in an orthorhombic  $Td$ - $MoTe_2$  structure, which is isostructural with  $WTe_2$ .

Angular resolved photoemission was performed on  $\beta$ - and  $Td$ - $MoTe_2$  with HeI radiation and in the photon energy range  $50eV < h\nu < 100eV$  at the U125-2 SGM monochromator at BESSY II. Fermi surface images were obtained by scanning the polar emission angle as well as the photon energy while monitoring the photoemission intensity at the Fermi level. The experimental results will be compared with additional tight-binding band structure calculations.

[1] R. Clarke, E. Marseglia and H.P. Hughes, Phil. Mag. B38 121 (1978)

O 44.42 Wed 17:00 Poster C

**Spin- and momentum-resolved (inverse) photoemission for *in situ* investigation of the electronic structure of magnetic thin films** — •MICHAEL BUDKE, TOBIAS ALLMERS, and MARKUS DONATH — Physikalisches Institut, Wilhelm-Klemm-Str. 10, 48149 Münster

We present a combined experimental set-up for spin- and momentum-resolved photoemission (PE) and inverse photoemission (IPE). This unique combination allows the investigation of the electronic structure below and above the Fermi level  $E_F$  of magnetic materials in one chamber on the same sample preparation. The system for PE is commercially available and consists of a gas discharge lamp and an electron analyzer equipped with a SPLEED detector for spin-resolved measurements. Our spin-resolved IPE system is home-made and consists of a spin polarized electron gun and a Geiger-Müller tube filled with acetone vapour for photon detection. The main advantage of our IPE system is its superior energy resolution of 165 meV (FWHM).

This is a factor of two better than other state-of-the-art set-ups for IPE and enables us to resolve narrow spectral features not seen before, especially close to  $E_F$ . First results will be shown, which demonstrate the improved energy resolution in IPE on the Cu(001) image-potential states. The angular resolution is demonstrated on the surface state of Cu(111). In addition, the advantage of the in situ investigation of the electronic structure below and above  $E_F$  will be shown on the system Cr(001) which has been discussed intensely due to a peak right at  $E_F$ , previously interpreted as an orbital Kondo resonance [1]. [1] Kolesnychenko *et al.*, Nature 415, 507 (2002)

O 44.43 Wed 17:00 Poster C

**Excited states of matter probed with soft X-rays** — •MARTIN BEYE<sup>1</sup>, MARTIN DEPPE<sup>1</sup>, ALEXANDER FÖHLISCH<sup>1</sup>, FRANZ HENNIES<sup>2</sup>, MITSURU NAGASONO<sup>1</sup>, EDLIRA SULJOTI<sup>1</sup>, and WILFRIED WURTH<sup>1</sup> — <sup>1</sup>Institut für Experimentalphysik, Universität Hamburg, Luruper Chaussee 149, D-22761 Hamburg, Germany — <sup>2</sup>MAX-lab, Lund University, Ole Römers väg 1, SE-22100 Lund, Sweden

Resonant soft X-ray spectroscopy allows to determine local electronic structure and binding properties of matter in all aggregate states. Here we present an investigation on crystalline silicon between room temperature and the melting point.

We measured the temperature dependence of the onset of absorption at the silicon  $L_3$  edge in fluorescence yield. We find a shift to lower photon energies with increasing temperature that we attribute to electron-phonon interactions, lattice expansion effects and a change in the electronic screening of the final state.

In RIXS (resonant inelastic X-ray scattering) at low temperatures scattering is coherent and crystal-momentum conserving and shows features related to specific points in the bandstructure. Raising the temperature, coherence is disturbed due to electron-phonon scattering. This leads to bandstructure-integrated spectra showing the density of states. Similar effects can be observed by detuning the incident photon energy relative to the resonance which changes the duration of the scattering process. Shorter scattering duration times suppress electron-phonon scattering channels, thus restoring the k-conservation rule and enhancing bandmapping features.

O 44.44 Wed 17:00 Poster C

**Matrix-Element Effects in Valence-Band Photoemission of  $Fe_xTiS_2$  using Circularly Polarized Light** — •MARTIN MARCZYNSKI-BÜHLOW<sup>1</sup>, SABRINA LANG<sup>1</sup>, JENS BUCK<sup>1</sup>, KAI ROSSNAGEL<sup>1</sup>, LUTZ KIPP<sup>1</sup>, NATHANIEL JANKE-GILMAN<sup>2</sup>, ANDREW WALTER<sup>2</sup>, and JOHN RILEY<sup>2</sup> — <sup>1</sup>Institut für Experimentelle und Angewandte Physik, Universität Kiel, D-24098, Germany — <sup>2</sup>Physics Department, La Trobe University, Melbourne, Australia

The effect of iron intercalation on the structural, magnetic and electronic properties of the layered transition metal dichalcogenide  $TiS_2$  is an interesting and extensively studied question.

We investigated the valence band structure of  $Fe_xTiS_2$  ( $x = 0; 0.1; 0.33$ ) by angle-resolved photoemission taking advantage of a second generation toroidal electron spectrometer with fast data acquisition. Particularly, we have studied whether and to what extent Fe intercalation leads to modifications of the host valence band structure, such as increased band filling, hybridization between the Fe 3d orbitals and the host Ti 3d and S 3p orbitals, or new Fe 3d-derived electronic states below the Fermi energy.

Our main aim in this work was to reveal possible spin polarization effects at the Fermi energy by using fully circularly polarized light from beamline U56/2-PGM1 ( $h\nu = 89$  to  $1328$  eV) at BESSY. Although we were not able to answer the question concerning spin polarization, interesting matrix-element effects were observed for the iron intercalated as well as for the pristine  $TiS_2$  compound.

This work is supported by the DFG Forschergruppe 353.

O 44.45 Wed 17:00 Poster C

**Spatially resolved photoemission measurements using reflective photon sieves** — •MATTHIAS KALLÄNE, TIM RIEDEL, DIRK RAHN, SÖNKE HARM, KAI ROSSNAGEL, JENS BUCK, MARTIN MARCZYNSKI-BÜHLOW, CLAAS THEDE, and LUTZ KIPP — Institut für Experimentelle und Angewandte Physik, Universität Kiel, D-24098, Germany

A new angle and spatially resolved photoemission experiment is being set up, which exploits a SPECS PHOIBOS 150 analyzer with a 2-dimensional CCD detector, and a grazing incidence photon sieve — a new type of diffraction optics for focusing synchrotron radiation with suppressed side lobes and reduced background [1]. In order to test the

setup before its planned use at the VUV-FEL monochromator beamline at HASYLAB, we carried out experiments at beamline BW3 of the storage ring DORIS III at HASYLAB with a photon energy of 100 eV. The photoemission measurements were done on the transition-metal dichalcogenide misfit compound  $(\text{PbS})_{1.13}\text{TaS}_2$  which consists of layers of cubic PbS and hexagonal 2H-TaS<sub>2</sub> subsystems. After cleavage in UHV the surface typically shows islands of both subsystems with sizes in the  $\mu\text{m}$  regime. The spatially resolved core level measurements are compared to spatially resolved spectra taken at the photoelectron microscope beamline BL31 at MAX-lab in Lund.

This work is supported by Innovationsfond des Landes Schleswig-Holstein.

[1] L. Kipp, M. Skibowski, R.L. Johnson, R. Berndt, R. Adelung, S. Harm and R. Seemann, *Nature* **414**, 184 (2001).

O 44.46 Wed 17:00 Poster C

**Spin-Orbit Induced Valence-Band Splitting in Mg Thin Films Grown on W(110) and Mo(110)** — ●ALEXANDER GOTTBORG, ALEXANDER HELMKE, VICTOR SOLTWISCH, GÜNTER KAINDL, and EUGEN WESCHKE — Institut für Experimentalphysik, Freie Universität Berlin, Arnimallee 14, 14195 Berlin, Germany

Due to the comparably long penetration depth of its wave function into the bulk [1], the Shockley-like Mg(0001) surface state is strongly influenced in thin films by the substrate. The surface-state band is known to interact with an interface resonance formed at the substrate. This interaction gives rise to a parity-induced energy splitting that depends on the Mg film thickness [2].

Using high resolution angle-resolved photoelectron spectroscopy a second, thickness-independent splitting is observed in Mg/W(110) that is absent in case of Mg/Mo(110). This comparison supports the interpretation of this additional splitting in terms of a Rashba-like spin-orbit effect induced by the W substrate. Since spin-orbit effects scale with the atomic number, this splitting is supposed to be weak in case of Mo, which is in agreement with the experiment.

[1] T. K. Kim *et. al.* *Phys. Rev. B* **72**, 075422 (2005)

[2] F. Schiller *et. al.* *Phys. Rev. B* **95**, 126402 (2005)

O 44.47 Wed 17:00 Poster C

**Dependence of ultrafast charge transfer on orbital overlap** — ●MARTIN DEPPE<sup>1</sup>, ALEXANDER FÖHLISCH<sup>1</sup>, FRANZ HENNIES<sup>2</sup>, MITSURU NAGASONO<sup>1</sup>, MARTIN BEYE<sup>1</sup>, and WILFRIED WURTH<sup>1</sup> — <sup>1</sup>Institut für Experimentalphysik, Universität Hamburg, Luruper Chaussee 149, D-22761 Hamburg, Germany — <sup>2</sup>MAX-lab, Lund University, Ole Römers väg 1, SE-22100 Lund, Sweden

We have determined the dependence of the charge transfer time  $\tau_{CT}$  on orbital overlap for a chemisorbed S monolayer on a Ru(0001) single crystal substrate by core hole clock spectroscopy. By changing the polarization of the synchrotron light relative to the surface plane S 3p orbitals with different spatial orientations can be selected.

We show that the process is much faster for orbitals with their main symmetry axis perpendicular to the substrate surface (out-of-plane) than for those oriented parallel to the surface plane (in-plane). In both cases the transfer occurs on a timescale faster than 1 fs; in out-of-plane geometry we find  $\tau_{CT} = 0.18 \pm 0.04$  fs, while the in-plane case yields  $\tau_{CT} = 0.84 \pm 0.36$  fs, both for photon energies directly above the autoionization resonance. This is the direct consequence of the fact that charge transfer is governed by the orbital overlap at the different atomic sites. To achieve the necessary temporal resolution, ultrafast Coster-Kronig autoionization decays are used as internal reference clocks.

O 44.48 Wed 17:00 Poster C

**Unbuckling dimers at the Silicon(100) surface** — ●CHRISTIAN EICKHOFF<sup>1,2</sup>, CORNELIUS GAHL<sup>1</sup>, TANJA GIESSEL<sup>1</sup>, JENS KOPPRASCH<sup>1,2</sup>, IRINA OSTAPENKO<sup>1</sup>, HELENA PRIMA GARCIA<sup>1</sup>, ROLAND SCHMIDT<sup>1,2</sup>, and MARTIN WEINELT<sup>1,2</sup> — <sup>1</sup>Max-Born-Institut, Max-Born-Straße 2A, 12489 Berlin — <sup>2</sup>Freie Universität Berlin, Arnimallee 14, 14195 Berlin

Electronic structure and electron dynamics at the Si(100) surface have been studied by means of time-resolved photoemission spectroscopy. For low IR pump-laser intensity, i.e. in the limit of single-electron dynamics, electrons excited to the  $D_{down}$  dangling-bond band decay exponentially with a lifetime of  $\simeq 200$  ps. At larger excitation densities the decay rate scales quadratically with the population which indicates an effective phonon- and/or defect-assisted surface recombination between the occupied and unoccupied  $D_{up}$  and  $D_{down}$  dangling-bond

bands. Having established significant depletion of the  $D_{up}$  and corresponding population of the  $D_{down}$ -bands, we observe spectroscopic signatures of atomic motion of the buckled dimers at the Si(100) surface. Time-dependent density functional theory predicts this electronically driven motion to occur on a femtosecond time-scale and to effectively lift the ground-state Peierls distortion of the buckled silicon dimers [1].

[1] J. van Heys, M. Lindenblatt, and E. Pehlke, *Phase Transitions* **78**, Nos. 9-11 (Sept.-Nov. 2005), 773-786

O 44.49 Wed 17:00 Poster C

**Pretreatment of Steel Surfaces** — ●CHRISTIAN HOLZHEU, MATTHIAS LASKE, and OTHMAR MARTI — Institute of Experimental Physics, University of Ulm, 89069 Ulm, Germany

Steel is used for many purposes in several industrial fields. To improve the material properties several pretreating methods were tested. Especially laser treating was investigated. The characterization of the effected changes was done by performing different surface measurements. XPS (x-ray photoelectron spectroscopy) and Auger method were used to define the chemical structure, XRD (x-ray diffraction) to characterize the crystalline device. The Roughness was investigated by AFM (atomic force microscope).

O 44.50 Wed 17:00 Poster C

**Microscopic picture of adsorption and desorption of D2O processed Au nanoparticles onto amino-terminated SiO2 surface studied by in situ ATR-SEIRA spectroscopy** — ●TADAAKI NAGAO<sup>1,2</sup>, DOMINIK ENDERS<sup>1,2</sup>, and TOMONOBU NAKAYAMA<sup>1,2</sup> — <sup>1</sup>National Institute for Materials Science (NIMS), Tsukuba — <sup>2</sup>ICORP-JST

By use of ATR-SEIRA spectroscopy, we revealed the microscopic mechanism of the adsorption and the desorption process of Au nanoparticles onto amino-terminated SiO<sub>2</sub> surface. In order to avoid overlapping the faint C-H peak with the strong O-H peak, we used Au nanoparticles produced in D<sub>2</sub>O solution instead of those processed in normal H<sub>2</sub>O solution. In this way, we could sensitively detect the C-H signal of the ligand citric molecules directly covering the Au nanoparticles as well as the O-D peaks of the D<sub>2</sub>O near the nanoparticles. By combining the in situ ATR-SEIRA spectroscopy and the ex situ SEM observations, we successfully explain the reason of the observed Langmuir kinetics of the nanoparticle adsorption, and further we correlate the surface number density of the particles and their morphology (uniform distribution vs. aggregates) to the status of the ligand citrate molecules. When the adsorbed nanoparticles are exposed to the solution of aminoethanethiol (AET: small thiol molecule terminated with amino group), the nanoparticles desorb via two-step substitutional adsorption of the molecules, and are removed completely from the SiO<sub>2</sub> substrate.

O 44.51 Wed 17:00 Poster C

**Atomic Force Microscopy studies on** — ●JÖRN WOCHNOWSKI<sup>1</sup>, THIMO GÖLLNITZ<sup>2</sup>, GERMAR HOFFMANN<sup>2</sup>, JÜRGEN HECK<sup>1</sup>, and ROLAND WIESENDANGER<sup>2</sup> — <sup>1</sup>Institute of Inorganic and Applied Chemistry, University of Hamburg — <sup>2</sup>Institute of Applied Physics, University of Hamburg

The coating of temperature-sensitive substrates, e.g. vitreous substrates in the microtechnology with high melting point materials, is challenging. Organometallic chemical vapour deposition of volatile compounds is one solution. We have developed<sup>1</sup> an experimental setup for the deposition of elements (metals), element oxides and other functional composites in a glass microreactor (diameter: 70  $\mu\text{m}$  or lower) and in mesoporous material. In a preliminary study numerous organometallic compounds as precursors have been tested as catalytic materials. The catalytic system ( $\text{CrO}_x/\text{SiO}_2$ ) was successfully deposited in a glass microreactor by OMCVD of  $\text{Cr}(\text{CO})_6$  as precursor for the catalyst and tetraethoxysilane as precursor for the SiO<sub>2</sub> support. The deposited layers were investigated by REM and EDX. To study the surface morphology on the nanometer scale we employed Atomic Force Microscopy (AFM). Here, we will present our AFM investigations for surfaces prepared by organometallic chemical vapour deposition. We will discuss the preparation and the analysis of the surfaces with the focus to tailor material properties.

<sup>1</sup> J. Heck, S. Kneip, A. Knöchel, M. Haller, F. Moritz, (FZ Karlsruhe GmbH), DE 19852722, EP 1001050 A2 (2000).

O 44.52 Wed 17:00 Poster C



**CO oxidation on modified Pt surfaces** — ●REGINE STREBER, BARBARA TRÄNKENSCHUH, MICHAEL LORENZ, CHRISTIAN PAPP, REINHARD DENECKE, and HANS-PETER STEINRÜCK — Lehrstuhl für Physikalische Chemie II, Universität Erlangen-Nürnberg, Egerlandstr. 3, 91058 Erlangen

In order to get closer to realistic systems, we studied the CO oxidation reaction not only on Pt(111) [1] but also on stepped Pt surfaces. We investigated the reaction between adsorbed atomic oxygen and CO on Pt(355) and Pt(322), which both have (111) oriented terraces with a width of five atomic rows but different step orientations, (111) vs. (100), respectively. Time-dependent in situ XP spectra in the O 1s and C 1s binding energy region showed that the reaction rate is increased on the stepped surfaces and depends on the step orientation. The preadsorbed atomic oxygen occupies different adsorption sites on both surfaces with different saturation coverages, leading to interesting temperature-dependent phenomena. In order to obtain a more detailed insight, we modified the system by deposition of Ag, which grows in rows along the lower step edges [2]. In this way the oxygen distribution can be modified. However, since higher CO coverages move Ag atoms away from the step edges to form islands on the terraces, the influence of Ag rows can only be studied for the initial period of the oxidation reaction.

The work was supported by the DFG (Ste 620/4-3).

[1] Kinne et al., J. Chem. Phys. 120 (2004) 7113.

[2] Gambardella et al., Phys. Rev. B 61 (2000) 2254.

O 44.53 Wed 17:00 Poster C

**Photoinduced catalytic reactions on mars analogous surfaces** — ●DOMINIK SCHWENDT, BURKHARD ROOS, and WOLFGANG MAUS-FRIEDRICH — Institut für Physik und Physikalische Technologien, TU Clausthal, 38678 Clausthal-Zellerfeld, Germany

Many environmental facts about mars are known through NASA missions. Recently, traces of methane as well as formaldehyde in the marsian atmosphere have been found.

The purpose of this work was to find non-biological explanations for the presence of these gases on mars. Thus we tried to find ways to produce methane and formaldehyde on mars-like surfaces under marsian atmospheric conditions. We used Quadrupole Mass Spectroscopy to detect the gases and X-ray Photoelectron Spectroscopy to analyze the substrate. Our research has shown that formaldehyde emerges on watery hematite in a 6 mbar carbon dioxide atmosphere at temperatures around 260 K. Methane forms as well, if ultraviolet irradiation on the hematite is added to the named conditions.

Consequently with this work we present another possible source for the methane and formaldehyde traces in the marsian atmosphere.

O 44.54 Wed 17:00 Poster C

**The influence of surface oxygen and oxide layers on adsorption systems on Ni(111)** — ●MICHAEL PETER ANDREAS LORENZ, REGINE STREBER, FABIAN BEBENSEE, REINHARD DENECKE, and HANS-PETER STEINRÜCK — Lehrstuhl für Physikalische Chemie II, Universität Erlangen-Nürnberg, Egerlandstraße 3, 91058 Erlangen

During many surface reactions, especially under realistic conditions, oxygen layers and even surface oxides form. We have studied the influence of such surface modifications at Ni(111) on the adsorption of small molecules, such as CO<sub>2</sub> and CH<sub>4</sub>. Using in-situ x-ray photoelectron spectroscopy at BESSY II we characterized these oxygen layers by means of O 1s and Ni 2p core levels. In order to facilitate dissociative methane adsorption, we provided molecules with a well-defined kinetic energy (up to 0.8 eV) using a supersonic molecular beam. Interestingly, both the saturated oxygen adlayers as well as a surface Nickel oxide completely prevent dissociative methane adsorption for all energies studied. On the other hand, the physisorption regime seems to be shifted to higher temperatures as compared to clean Ni(111). The same seems to be true for CO<sub>2</sub>, which also shows enhanced physisorption in the presence of oxygen.

O 44.55 Wed 17:00 Poster C

**Multiple charge states of Ag atoms on ultrathin NaCl films** — ●JASCHA REPP<sup>1,2</sup>, GERHARD MEYER<sup>1</sup>, FREDRIK OLSSON<sup>3</sup>, SAMI PAAVILAINEN<sup>4</sup>, and MATS PERSSON<sup>5</sup> — <sup>1</sup>IBM Research, Zurich Research Laboratory, 8803 Rueschlikon, Switzerland — <sup>2</sup>Institute of Experimental and Applied Physics, University Regensburg, 93053 Regensburg, Germany — <sup>3</sup>Department of Applied Physics, Chalmers University of Technology, 41296 Goteborg, Sweden — <sup>4</sup>Institute of Physics, Tampere University of Technology, 33720 Tampere, Finland — <sup>5</sup>Surface Science Research Centre and Department of Chemistry,

The University of Liverpool, Liverpool L69 3BX, UK

So far the observation and manipulation by means of scanning tunneling microscopy (STM) of different charge states of adsorbed atoms have been limited to Au atoms on NaCl films supported by a Cu substrate.

On our poster, we show from a combined STM and density functional calculations study that Ag atoms adsorbed on NaCl bilayers on Cu(111) exhibit charge tristability and can be switched reversibly between the neutral adatom state and the negatively or the positively charged adatom state. Thus, the charge multistability of adatoms is not at all unique for Au adatoms and it is even possible to have more than two different charge states of an adatom. Furthermore, based on a simple model, we identify and discuss the key adatom, film and substrate parameters for the stabilization of multiple charge states. This model can be used as a guide to find other systems of interest.

O 44.56 Wed 17:00 Poster C

**Controlling molecular adsorption through domain-patterned lithium niobate** — ●ALEXANDER HAUSSMANN, MARC TOBIAS WENZEL, STEFAN GRAFSTRÖM, THOMAS HÄRTLING, CHRISTIAN LOPPACHER, and LUKAS ENG — Institut für Angewandte Photophysik, Technische Universität Dresden, D-01062 Dresden

Recent progress in engineering ferroelectric domains has led to the possibility of creating domain patterns on the submicron scale. Because the domain arrangement corresponds to a pattern of opposite surface charges, such structured ferroelectric materials promise interesting applications as templates for the structured adsorption of charged molecules on surfaces. Recent work has reported on the adsorption of noble-metal nanoparticles [1] to such surfaces. Here, we report on the adsorption of λ-DNA to LiNbO<sub>3</sub> single-crystal surfaces. The DNA molecules of some 10 μm in length were marked with the fluorescent dye yoyo-1 to facilitate optical tracking of their distribution on the surface. We found that λ-DNA preferentially adsorbs to c<sup>+</sup> domains. The recently discovered reduction of the coercive field of LiNbO<sub>3</sub> under UV illumination [2] offers a promising way for writing arbitrary domain patterns on the micrometer scale. Here, we will report first results on the switching and adsorption behavior observed in a setup in which the sample is mounted in a liquid cell and a focused He-Cd laser beam (at λ = 325 nm) is used for UV patterning.

[1] J. L. Giocondi and G. S. Rohrer, Chem. Mater. **13**, 241 (2001)

[2] M. Müller, E. Soergel, K. Buse, Appl. Phys. Lett. **83**, 1824 (2003)

O 44.57 Wed 17:00 Poster C

**Interaction of different SrTiO<sub>3</sub> surfaces with reactive gases** — ●FLORIAN VOIGTS<sup>1</sup>, DOMINIK SCHWENDT<sup>1</sup>, MARTIN FRERICHS<sup>2</sup>, CHRISTOS ARGIRIS<sup>2</sup>, GÜNTER BORCHARDT<sup>2</sup>, and WOLFGANG MAUS-FRIEDRICH<sup>1</sup> — <sup>1</sup>Institut für Physik und Physikalische Technologien, TU Clausthal, Leibnizstrasse 4, 38678 Clausthal-Zellerfeld, Germany — <sup>2</sup>Institut für Metallurgie, TU Clausthal, Robert-Koch-Strasse 42, 38678 Clausthal-Zellerfeld, Germany

Donor doped SrTiO<sub>3</sub> is well known for its capability as resistive high temperature oxygen sensor. An interesting application of this sensor would be the analysis of automobile exhaust, as it would allow the optimisation of fuel injection and of catalytic oxidation of toxic exhaust, thus reducing fuel consumption and pollution of the environment. Before this application can be implemented, preliminary studies aiming at the interaction of SrTiO<sub>3</sub> with reactive gases must demonstrate the stability of the material in this environment. Also, the influence of these gases on the interaction with oxygen must be clarified.

We use Metastable Impact Electron Spectroscopy and Ultraviolet Photoelectron Spectroscopy to analyse the valence band structure of SrTiO<sub>3</sub> and its adsorbates. X-ray Photoelectron Spectroscopy is used to check the stoichiometry of the samples. Our results for the interaction of SrTiO<sub>3</sub> with CO, CO<sub>2</sub>, H<sub>2</sub>O, CH<sub>4</sub> and other reactive gases being part of automobile exhaust are presented in this poster. We use SrTiO<sub>3</sub>(100) as model substance and compare our results with experiments on polycrystalline SrTiO<sub>3</sub> produced via a sol-gel route.

O 44.58 Wed 17:00 Poster C

**Surface properties of indium oxide and its interaction with ozone for the use as gas sensor** — ●MARCEL HIMMERLICH, CHUNYU WANG, VOLKER CIMALLA, JUERGEN A. SCHAEFER, OLIVER AMBACHER, and STEFAN KRISCHOK — Institut für Mikro- und Nanotechnologien, TU Ilmenau, P.O. Box 100565, 98684 Ilmenau, Germany

Polycrystalline indium oxide thin films have great potential for low

cost and low energy consumption environmental sensors, e.g. for the detection of ozone. We have examined the surface properties of indium oxide films prepared by metal organic chemical vapour deposition using X-ray and ultraviolet photoelectron spectroscopy (XPS, UPS). The influence of the growth temperature on stoichiometry as well as the surface electronic structure is presented. Especially for low temperature (200°C) grown samples strong emission from an up to date unidentified state below the valence band maximum is observed. In order to identify the photoreduction and oxidation mechanisms related to the ozone sensor principle, we have investigated the interaction of indium oxide with ozone and UV radiation. For the interaction with ozone, two adsorbate related states at 6.1 eV and 11.3 eV appear in the valence band together with an increase in the work function and a change in the surface band bending. A model will be proposed to explain the interaction of ozone with the indium oxide surface with respect to the observed drastic changes in resistivity of the samples.

O 44.59 Wed 17:00 Poster C

**Stability of Fe<sub>3</sub>O<sub>4</sub>(001) in a humid environment** — ●NARASIMHAM MULAKALURI<sup>1</sup>, ROSSITZA PENTCHEVA<sup>1</sup>, and MATTHIAS SCHEFFLER<sup>2</sup> — <sup>1</sup>Section Crystallography, Dept. for Earth and Environmental Sciences, University of Munich — <sup>2</sup>Fritz-Haber-Institut der MPG, Berlin

The interaction of water with a mineral surface is a fundamental process both in nature and technology. We study the influence of water adsorption on the energetics and properties of the Fe<sub>3</sub>O<sub>4</sub>(001) surface using density functional theory (DFT)-calculations with the FP-LAPW method in the WIEN2k implementation. The surface stability of different terminations as a function of the O<sub>2</sub> and H<sub>2</sub>O pressure is compared in the framework of ab initio thermodynamics. On the clean surface a bulk termination containing oxygen and octahedral iron is stabilized through a Jahn-Teller distortion [1]. For this so called modified B-layer as well as the half occupied A-layer termination we vary the degree of hydroxylation of the surface. At water rich conditions where the surface is completely covered by hydroxyl groups a B-layer is found to be favored compared to other models. We investigate also the role of water adsorption on surface reconstruction and find a tendency towards outward relaxation of the surface atoms covered by hydroxyl groups. For the hydroxylated surfaces we obtain metallic behavior compared to the half-metallic bulk, however, the surface states in the majority band gap have a different character compared to the clean surface.

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

O 44.60 Wed 17:00 Poster C

**α-Fe<sub>2</sub>O<sub>3</sub> (0001) surface structure analysis by LEED** — ●MAIKE LÜBBE and WOLFGANG MORITZ — LMU, Department für Geo- und Umweltwissenschaften, Theresienstr. 41, D-80333 München

Despite the importance of the haematite, α-Fe<sub>2</sub>O<sub>3</sub>, surface in chemical and technological applications its structure has not been determined unambiguously up to now although being subject to both theoretical [1, 2] and experimental [3, 4] investigations.

We therefore analysed the (1×1) (0001) surface structure of a bulk α-Fe<sub>2</sub>O<sub>3</sub> crystal by low energy electron diffraction.

The polished crystal was installed in an UHV chamber with a base pressure of  $2 \cdot 10^{-10}$  mbar and annealed at 500°C in an O<sub>2</sub> atmosphere,  $p_{O_2} \approx 3 \cdot 10^{-8}$  mbar, for several hours. The diffraction spots were sharp although a somewhat elevated diffuse background was observed. An *I-V*-curve data set of 10 symmetrically independent diffraction spots was measured at room temperature in the energy range  $E \approx 150 \dots 500$  eV. Measurements at lower electron energies were not possible due to charging effects of the insulating crystal.

Our analysis indicates that the α-Fe<sub>2</sub>O<sub>3</sub> (0001) surface is terminated by iron partially occupying two bulk sites when prepared at low oxygen pressure. Relaxation effects along *c*-axis are quite large and involve several iron double layers.

[1] A. Rohrbach et al., Phys. Rev. B **70**, 125426 (2004) [1] W. Bergmayer, H. Schweiger, Phys. Rev. B **69**, 195409 (2004) [3] G. Ketteler et al., Surf. Rev. Lett. **8**, 661 (2001) [4] S. Chambers, S. Yi, Surf. Sci. Lett. **439**, L785 (1999)

O 44.61 Wed 17:00 Poster C

**Temperature dependent femtosecond two-photon photoemission from ultrathin MgO films** — ●TOBIAS GLEITSMANN, MIHAI E. VAIDA, and THORSTEN M. BERNHARDT — Institut für Oberflächenchemie und Katalyse, Universität Ulm, 89069 Ulm, Germany

Due to their chemical and electronic properties, ultra-thin Magnesia

films represent an ideal substrate system in order to investigate small deposited metal clusters. Especially the band gap of these isolating films in principle enables the observation of the cluster electronic states near the Fermi level independently from the substrate states whereas avoiding charging effects. The electronic structure of these ultra-thin magnesia films supported on a Mo(100) single crystal surface is investigated as a function of the post-deposition annealing temperature via femtosecond two photon photoemission spectroscopy and electron energy loss spectroscopy. Additionally, the film composition and crystal structure is analyzed by temperature programmed desorption mass spectrometry, Auger electron spectroscopy, and low energy electron diffraction, respectively. Strong evidence is found for the formation of an optical resonance at 4.6 eV with increasing annealing temperature accompanied by a change in the surface work function.

O 44.62 Wed 17:00 Poster C

**Surface morphology and surface stress of CaF<sub>2</sub> films on Si(111)** — ●MARKUS NEUBERT, PETER KURY, FRIEDRICH KLASING, and MICHAEL HORN VON HOEGEN — University of Duisburg-Essen, Institut of Experimental Physics

Thin CaF<sub>2</sub> films with low defect density could be grown epitaxially on Si(111) due to the small lattice mismatch between CaF<sub>2</sub> and Si. Due to the large thermal expansion coefficient ( $\alpha_{CaF_2} \approx 19 \cdot 10^{-6} K^{-1}$ ) of CaF<sub>2</sub> the lattice mismatch increases strongly with temperature ( $\alpha_{Si} \approx 2.6 \cdot 10^{-6} K^{-1}$ ). As a consequence the vertical lattice parameter of thin CaF<sub>2</sub> films increases by tetragonal distortion due to the build-up of compressive stress. We have grown CaF<sub>2</sub> films at temperatures between 600K and 1100K by Molecular Beam Epitaxy (MBE). The resulting surface stress was measured in-situ during deposition by Surface Stress Induced Optical Deflection (SSIOD). The film morphology was investigated by ex-situ non-contact AFM. The thickness of the films was independently calibrated by X-Ray Reflection (XRR) measurements.

O 44.63 Wed 17:00 Poster C

**Improvement of the thermal stability of the HfO<sub>2</sub>/Si(100) system using a diffusion barrier** — ●D. WEIER<sup>1</sup>, A. DESIEVRO<sup>2,3</sup>, M. SCHÜRMAN<sup>1</sup>, C. FLÜCHTER<sup>1</sup>, M. CARAZZOLNE<sup>3</sup>, A. PANCOTTI<sup>3</sup>, R. LANDERS<sup>2,3</sup>, G. KLEIMAN<sup>3</sup>, and C. WESTPHAL<sup>1</sup> — <sup>1</sup>Experimentelle Physik 1 - Universität Dortmund, Otto-Hahn-Str. 4, D 44221 Dortmund, Germany — <sup>2</sup>Laboratório Nacional de Luz Síncrotron, C.P. 6192, 13084-971 Campinas, SP, Brazil — <sup>3</sup>Instituto de Física - Universidade Estadual de Campinas, C.P. 6165, 13083-970 Campinas, SP, Brazil

The ongoing miniaturisation of transistor devices requires a new gate dielectric to replace silicon oxide (SiO<sub>2</sub>) that has been used for the last decades. The possible substitutes have to fulfill several requirements like band gap alignment to the silicon, a good interface quality, and a thermal stability. HfO<sub>2</sub> meets most of the requirements, but it is shown in many studies that its thermal stability is one of the main problems of the system HfO<sub>2</sub>/Si(100) due to silicide formation at high temperature annealing. In this work a film of silicon nitride was deposited on the silicon substrate via sputtering and annealing. The silicon nitride (Si<sub>3</sub>N<sub>4</sub>) is stable when a high temperature annealing up to approximately 1100 °C is applied. Thus, it can be used as a diffusion barrier for the HfO<sub>2</sub> in the high temperature range. We will show several heating cycles for different diffusion barrier thicknesses and we compare them with similar cycles for HfO<sub>2</sub>/Si(100) films without a diffusion barrier. It will be shown that it is possible to increase the thermal stability of HfO<sub>2</sub> with a Si<sub>3</sub>N<sub>4</sub> layer.

O 44.64 Wed 17:00 Poster C

**Cerium oxide films on TiO<sub>x</sub> coated Pt(111)-single crystals** — ●THORSTEN STAUDT and KLAUS SCHIERBAUM — : Institut für Experimentelle Physik der kondensierten Materie, Abteilung für Materialwissenschaft, HHU Düsseldorf, 40225 Düsseldorf

The epitaxial growth of thin and continuous CeO<sub>2</sub>(111) films on metal surfaces suffers from the preferential formation of a 3 D-like morphology, even though epitaxial relationships exist with the substrate lattices. This holds for films prepared by reactive evaporation of Ce in O<sub>2</sub> on Pd(111) and Rh(111)[1], or by oxidation of an ordered surface alloy Pt<sub>5</sub>Ce/Pt(111)[2]. One may expect a decreased lattice mismatch if metal surfaces are used that are coated with ultra thin and ordered oxide-based buffer layers. As a candidate we have chosen the "wagon wheel" phase of TiO<sub>x</sub> grown on a Pt(111) surface which reveal a hexagonal symmetry and an interatomic spacing of 3.26 Å. This value is closed to the lattice constant of 3.86 Å for CeO<sub>2</sub>(111).[3] The film is

1.2 ML thick and shows a continuous morphology in STM.

CeO<sub>x</sub> films are subsequently grown by thermal evaporation of cerium in O<sub>2</sub> at RT. The films were analysed by LEED and XPS to determine the geometric structure, chemical composition and stoichiometry. First measurements reveal a change in the stoichiometry of the TiO<sub>x</sub> film that is discussed in terms of an interface reaction. Additional information on the initial stages of growth is obtained from STM.

- [1]: S. Eck et al., Surf. Sc. 520 (2002), 173-185 and reference therein  
 [2]: U. Berner and K. Schierbaum, Phys. Rev. B 65 (2002), 235404  
 [3]: F. Sedona et al., J. Phys. Chem. B 109 (2005), 24411-24426

O 44.65 Wed 17:00 Poster C

**EELS investigations of surface color centers in BaO, SrO and lattice matched Ba<sub>0.7</sub>Sr<sub>0.3</sub>O on Si(001)** — ●DIRK MÜLLER-SAJAK and HERBERT PFNÜR — Leibniz-Universität Hannover, Institut für Festkörperphysik, Appelstr. 2, 30167 Hannover, Germany

We investigated the generation of color centers in ultrathin films of BaO and SrO on Si(001) by electron bombardment both as a function of electron energy and of exposure. Both materials grow nanocrystalline on this surface. In a second stage, lattice matched and crystalline layers of Ba<sub>0.7</sub>Sr<sub>0.3</sub>O on the same surface are investigated. Electron energy loss spectroscopy was used to identify the color centers formed. These color centers will finally be used as nucleation centers for metal wires and dots.

The dependence of cross sections in the energy range 30-100eV for color center generation on electron energy is compatible with a Knotek-Feibelman generation mechanism. Apart from energetic positions, decay processes and rate dependent behavior were investigated. By controlled oxygen exposure and their extinction as a function of exposure, these defects were clearly identified as oxygen vacancies. Two peaks with characteristic losses at 0.75 and 1.39 eV in the EELS spectra of electron bombarded BaO films decay with the same time constant. They were assigned to surface color centers. A third loss peak at 2.15 eV coincides with that bulk color centers. Correlations with structural properties of the films are discussed.

O 44.66 Wed 17:00 Poster C

**In situ STM study of the adsorption and oxidation of sulfide on the Au(100) surface** — ●CHRISTIAN SCHLAUP, DANIEL FRIEBEL, PETER BROEKMANN, and KLAUS WANDELT — Institut für Physikalische und Theoretische Chemie, Wegelerstr. 12, D-53115 Bonn

In contrast to the well described adsorption behavior of sulfide on the Au(111) surface, the adsorption of sulfide on the Au(100) surface has not yet been part of extensive investigation. In 0.01 M NaOH / 0.5 mM Na<sub>2</sub>S electrolyte, the formation of different ordered sulfide adsorbate layers could be detected. Depending on the applied electrochemical potential a simple p(2 × 2) (Θ<sub>S</sub> = 0.25 ML), a more complex c(2 × 6) (Θ<sub>S</sub> = 0.33 ML) or a c(2 × 2) (Θ<sub>S</sub> = 0.5 ML) overlayer is formed. The well-known Au(100)-(hex) reconstruction, which could be observed at cathodic potentials, is lifted during the initial stages of sulfide adsorption leading to the formation of small, well oriented gold islands. By increasing the S coverage from initially Θ<sub>S</sub> = 0.25 ML, the shape of these islands changes significantly to a serrated form. Thereby a complex bi-layer phase, coexisting with the c(2 × 6) S adlayer, is formed. Upon further oxidation, the characteristic ring-like structure appears, which has already been observed on the S-covered Au(111) surface at high potentials (EC) and high S coverage (UHV), respectively.

O 44.67 Wed 17:00 Poster C

**Surface science approach to study surface and interface properties of room temperature ionic liquids** — ●OLIVER HÖFFT<sup>1</sup>, STEPHAN BAHR<sup>1</sup>, VOLKER KEMPTER<sup>1</sup>, MARCEL HIMMERLICH<sup>2</sup>, STEFAN KRISCHOK<sup>2</sup>, MAXIM EREMTCHENKO<sup>2</sup>, YONGHE LIU<sup>2</sup>, ROLF ÖTTKING<sup>2</sup>, ANITA NEUMANN<sup>2</sup>, JENS UHLIG<sup>2</sup>, PIERRE LORENZ<sup>2</sup>, IMAD AHMED<sup>2</sup>, and JÜRGEN SCHAEFER<sup>2</sup> — <sup>1</sup>Institut für Physik und Physikalische Technologien, TU Clausthal, 38678 Clausthal-Zellerfeld, Germany — <sup>2</sup>Institut für Physik und Institut für Mikro- und Nanotechnologien, TU Ilmenau, 98684 Ilmenau, Germany

Despite the immense importance of the surface and interface properties of ambient temperature ionic liquids for technical applications, only a few surface sensitive investigations have been performed to date. Therefore, we have chosen the latter approach under well defined ultra high vacuum conditions in order to get some first insight into different surface and interface related properties of liquids like [EMIM]Tf<sub>2</sub>N. We used ultraviolet and X-ray radiation (20 eV up to 1500 eV), metastable helium atoms and primary electrons by applying a number of techniques like UPS, MIES, XPS, HREELS. The emitted photoelectrons

and the elastically and/or inelastically scattered electrons give some first detailed information about the elemental composition, the electronic and vibronic structure and about its radiation induced changes. Some of the experimental results are compared with first principle calculations (DFT-LSDA). Our present status of understanding will be discussed in detail at the conference.

O 44.68 Wed 17:00 Poster C

**Corrosion Inhibition by Diphenylviologen on Cu(100)** — ●KNUD GENTZ, PETER BROEKMANN, SIMONE KOSSMANN, BARBARA KIRCHNER, and KLAUS WANDELT — Institut für Physikalische und Theoretische Chemie, Universität Bonn

The effect of preadsorbed Diphenylviologen (DPV) on the corrosion of a bromide-modified Cu(100) surface in 5mM sulfuric acid has been studied by cyclic voltammetry (CV) and in-situ STM measurements, conducted with a home-built electrochemical STM [3]. In the anodic sweep, the oxidative dissolution of Cu(100) under the given conditions is shifted about 100 mV to more positive potentials with respect to the same surface in the absence of the viologen. Certain structural elements of DPV on the surface lead to the proposal of a tentative model of the mechanism of the corrosion inhibition, that has been developed on basis of DFT calculations of the structure of the viologen. The halide-modification generates a high surface mobility of the copper, leading to ordered step-edges aligned with the <010> directions of the halide lattice. These ordered step-edges induce a structure of the viologen near the edge, which is different from the structures on the terraces. The compact arrangement of this structure effectively blocks the step-edges as reactive sites for the copper corrosion.

- [1] Wilms et al., *Rev. Sci. Instr.*, **70** 7 (1999) 473

O 44.69 Wed 17:00 Poster C

**STM results on Electrochemical Surface Electron Transfer Reactions** — ●DUC THANH PHAM, KNUD GENTZ, CAROLIN ZÖRLEIN, PETER BROEKMANN, and KLAUS WANDELT — Institut für Physikalische und Theoretische Chemie, Universität Bonn

The structural characterization of 1,1'-dibenzyl-4,4' bipyridinium molecules (dibenzyl-viologen, DBV), adsorbed on a chloride modified Cu(100) electrode is studied by means of Cyclic Voltammetry (CV) and in-situ Scanning Tunneling Microscopy (STM), showing the formation of laterally well-ordered 2D-array of different supramolecular ensembles. By reducing the pre-existing di-cationic *DBV*<sup>2+</sup> species to the corresponding radical mono-cation *DBV*<sup>•+</sup>, a quasi-reversible phase transition is initiated from a cavitand phase to a stripe pattern. These structural motifs are widely independent on the electronic and structural substrate properties. While each cavitand consists of 4 individual *DBV*<sup>2+</sup> sub-units arranged in a circular manner making this supramolecular cavitands chiral, the *DBV*<sup>•+</sup> in the stripe pattern are adsorbed with their main molecular axis parallel to the surface in a side-on adsorption geometry. However, by exchanging the pure supporting electrolyte for the viologen-containing solution in the potential regime where this phase transition takes place, it reveals two further metastable phases, which can be irreversibly transformed into the stripe pattern or the cavitand phase. In addition, chloride desorption through the viologen film is discussed as reason for an order-disorder transition within the viologen film at even more negative potentials.

O 44.70 Wed 17:00 Poster C

**Potential dependent structures of adsorbed viologens on Cu(100)** — ●KNUD GENTZ, PETER BROEKMANN, SIMONE KOSSMANN, BARBARA KIRCHNER, and KLAUS WANDELT — Institut für Physikalische und Theoretische Chemie, Uni Bonn

The structures of two different viologens (1,1'-disubstituted 4,4'-Bipyridins) adsorbed on a bromide-modified Cu(100) surface in an electrochemical environment have been studied by cyclic voltammetry (CV) and Scanning Tunneling Microscope (STM) studies. Upon adsorption, both viologens arrange in characteristic structures, dependent on the potential of the electrochemical cell. Via potential variation various structures are accessible and have been characterized. The phase transition are completely reversible between the *DBV*<sup>2+</sup> dication and the *DBV*<sup>•+</sup> radical cation of Dibenzylviologen and the *DPV*<sup>2+</sup> and *DPV*<sup>•+</sup> of the Diphenylviologen respectively. For the DPV molecule, this phase transition proceeds in two steps. First, the bulk phase is oxidized through the adsorbed layer of the *DPV*<sup>•+</sup> radical cation. Only at a significantly higher potential the adsorbed viologen is oxidized. In the cathodic sweep a corresponding surface reduction peak can be observed in the cv at higher potential than the bulk reduction peak. The reduction to the neutral DBV and DPV

molecules occurs only at low potentials beyond the onset of the hydrogen evolution reaction. Based on DFT calculations of the structure of individual and groups of Viologen molecules, models for the observed structures are proposed.

O 44.71 Wed 17:00 Poster C

**Electric field effects at the ice/SiO<sub>2</sub> interface** — ●HEIKO SCHRÖDER<sup>1</sup>, SEBASTIAN SCHÖDER<sup>1,2</sup>, MARKUS MEZGER<sup>1</sup>, HARALD REICHERT<sup>2</sup>, VEIJO HONKIMÄKI<sup>2</sup>, JÖRG BILGRAM<sup>3</sup>, and HELMUT DOSCH<sup>1</sup> — <sup>1</sup>Max-Planck-Institut für Metallforschung, Heisenbergstr. 3, D-70569 Stuttgart, Germany — <sup>2</sup>ESRF, 6 rue Jules Horowitz, F-38000 Grenoble, France — <sup>3</sup>ETH Zürich, Schafmattstr. 16, CH-8093 Zürich, Switzerland

Since the water molecule has a dipole moment, electric fields are expected to have a strong influence on the water/ice phase transition [1]. A deeper knowledge of the underlying mechanisms could improve our understanding of atmospheric cloud chemistry. To achieve this, we investigate electric field effects at the ice/SiO<sub>2</sub> interface by employing high energy x-ray reflectivity. In earlier experiments, we have studied pre-melting phenomena of ice extensively [2], leading to both a fully established sample preparation technique and a robust experimental setup at a 3rd generation synchrotron source (ESRF, ID15A). Our ice samples are sandwiched between smooth Si(100) substrates to guarantee the application of homogeneous electric fields across the two interfaces. The setup allows voltages up to 40 kV with switchable direction. We show polarization dependent electric field effects leading to structural changes at the ice/SiO<sub>2</sub> interface. Furthermore, our data suggests an influence of substrate preparation on the pre-melting behaviour of buried ice interfaces.

[1] Choi *et al.*, PRL **95** 085701 (2005)

[2] Engemann *et al.*, PRL **92**, 200401 (2004)

O 44.72 Wed 17:00 Poster C

**A x-ray reflectivity study of the structural arrangement of ionic liquids at solid interfaces** — ●MARKUS MEZGER<sup>1</sup>, HARALD REICHERT<sup>1</sup>, MOSHE DEUTSCH<sup>2</sup>, BENJAMIN OCKO<sup>3</sup>, HEIKO SCHRÖDER<sup>1</sup>, JOHN OKASINSKI<sup>1</sup>, SEBASTIAN SCHÖDER<sup>1,4</sup>, LILACH TAMAM<sup>2</sup>, HELMUT DOSCH<sup>1</sup>, and VEIJO HONKIMÄKI<sup>4</sup> — <sup>1</sup>Max-Planck-Institut für Metallforschung, Heisenbergstr. 3, D-70569 Stuttgart — <sup>2</sup>Bar-Ilan University, Dept. of Physics, Ramat-Gan 52900, Israel — <sup>3</sup>Brookhaven National Laboratory, Upton, NY 11973, USA — <sup>4</sup>European Synchrotron Radiation Facility, F-38043 Grenoble, France

Room temperature ionic liquids (IL) are promising candidates for a variety of new technological processes, ranging from applications as special solvents in green chemistry to catalytic reactions in biotechnology. Although crucial for the understanding of solvent properties, only little is known about the structural rearrangement of anions and cations at solid interfaces. To get access to these deeply buried interfaces, high energy x-ray reflectivity ( $\sim 70$  keV) is an ideal tool. In our systematic study, we observed differently ordered structures, caused by changes in composition, water content, and temperature. By choosing different combinations of anion and cation, we can tune the ion-ion and ion-substrate interaction. Trace amounts of water dissolved in the ILs can interact with the solid surface or the ions, and therefore alter the interfacial properties significantly. By varying the temperature, we can change the ratio between entropy, and interfacial energy, favoring a disordered liquid, or interfacial layering respectively.

O 44.73 Wed 17:00 Poster C

**High-resolution in-situ x-ray study of the hydrophobic gap at the water-OTS interface** — ●MARKUS MEZGER, HARALD REICHERT, HEIKO SCHRÖDER, JOHN OKASINSKI, SEBASTIAN SCHÖDER, and HELMUT DOSCH — Max-Planck-Institut für Metallforschung, Heisenbergstr. 3, D-70569 Stuttgart

The detailed knowledge of the microscopic structure of water at hydrophobic interfaces is essential for the understanding of key interfacial phenomena in biology, drug design and technology. In order to access such hydrophobic interfaces and extract the microscopic details of the local interfacial structure of water with highest resolution we have applied x-ray reflectivity using high energy x-ray microbeams. The experiments have been carried out with the new HEMD (High Energy Micro Diffraction) setup, which has recently been installed at beamline ID15A (ESRF, Grenoble). We have studied in great detail atomically smooth silicon substrates covered by a native oxide layer which have been functionalized by a densely packed self-assembled monolayer of Octadecyl-Trichloro-Silane (OTS). We have obtained high quality scat-

tering data up to  $q_z = 0.8 \text{ \AA}^{-1}$  from which structural information on a sub-nanometer length scale can be extracted. The experimental data provide clear evidence for the existence of a hydrophobic gap on the molecular scale with an integrated density deficit  $\rho d = 1.1 \text{ \AA g cm}^{-3}$  at the solid-water interface. In addition, measurements on the influence of gases (Ar, Xe, Kr, N<sub>2</sub>, O<sub>2</sub>, CO, CO<sub>2</sub>), dissolved in the water, have been performed. No effect on the hydrophobic water gap was found. [1] M. Mezger *et al.*, PNAS **103**, 18401-18404 (2006).

O 44.74 Wed 17:00 Poster C

**Adsorption of Au on Rutile TiO<sub>2</sub>(011)-(2x1) and (110) films grown on Rhenium Host Surfaces** — ●SUSANNE ROTH, WILHELMINE KÜDERNATSCHE, DIRK ROSENTHAL, and KLAUS CHRISTMANN — Institut für Chemie und Biochemie, FU-Berlin, Germany

In order to bridge the materials gap in heterogeneous catalysis and to mimic catalyst supports with increasing complexity, we have studied the epitaxy and chemical properties of titanium dioxide films grown with different surface termination on Re(10 $\bar{1}$ 0) and Re(0001) host surfaces, respectively. Titania films with a defined stoichiometry and long-range order were prepared by co-deposition of Ti vapor in an O<sub>2</sub> atmosphere at elevated temperatures ( $T \geq 830$  K). Thus, a unique  $pg(2 \times 2)$  LEED phase with a characteristic glide mirror plane is formed on Re(10 $\bar{1}$ 0), with intermediate faceting. XRD and LEED reveal that the films consist of rutile terminated by a (2x1)-reconstructed (011) phase. On Re(0001), deposition of TiO<sub>2</sub> leads to hexagonal LEED patterns indicating the growth of three domains of rutile(110) rotated by 120° against each other. In a finite coverage range, faceting is observed (as with the Re(10 $\bar{1}$ 0) surface) pointing to a Stranski-Krastanov type of growth for both Re surfaces. Model catalyst systems were then prepared by vapor deposition of Au onto the rutile films. Results on the growth and properties of the Au crystallites on TiO<sub>2</sub>(110)/Re(0001) using LEIS, XPS and TPD will be presented. Furthermore, we will compare the adsorption of CO, CO<sub>2</sub> and H<sub>2</sub>O on the Au-titania surfaces with the respective adsorption on the bare TiO<sub>2</sub>(011)-(2x1) films.

O 44.75 Wed 17:00 Poster C

**Experimental identification of the “active site” on a nano catalyst:** — THOMAS JARAMILLO<sup>1</sup>, KRISTINA JØRGENSEN<sup>1</sup>, JACOB BONDE<sup>1</sup>, JANE NIELSEN<sup>1</sup>, ●SEBASTIAN HORCH<sup>2</sup>, and IB CHORKENDORFF<sup>1</sup> — <sup>1</sup>Center for Individual Nanoparticle Functionality (CINF), NanoDTU, Department of Physics, Technical University of Denmark, DK-2800 Lyngby, Denmark — <sup>2</sup>Center for Atomic-scale Materials Design (CAMD), NanoDTU, Department of Physics, Technical University of Denmark, DK-2800 Lyngby, Denmark

One of the most important problems in heterogeneous catalysis is the identification of the “active site”. Only when this site and its relative abundance are known, it is possible to determine turnover-rates per active site (cf. our contribution on CO dissociation on Ni(111)).

We have determined the active site of a well-known model system: single-layered MoS<sub>2</sub> nanoparticles as catalyst for hydrogen evolution. MoS<sub>2</sub> nanoparticles were grown on Au(111) under UHV. Particle sizes were tuned by controlled sintering. Morphological details of the model systems were revealed with STM under UHV. The same samples were subsequently characterized in an electrochemical cell under ambient conditions, where it was found that the electrocatalytic hydrogen evolution scales linearly with the number of *edge sites* of the nanoparticles — and not the *area* of the exposed basal plane — regardless of particle size. These findings are in excellent agreement with theoretical predictions for hydrogen evolution catalysts.

O 44.76 Wed 17:00 Poster C

**Thermal and Redox Stability of PdZn Catalysts in Vacuum and During Methanol Adsorption Studied by In-Situ XPS** — ●KARIFALA DUMBUYA, REINHARD DENECKE, and HANS-PETER STEINRÜCK — Lehrstuhl für Physikalische Chemie II, Universität Erlangen-Nürnberg, Egerlandstr. 3, 91058 Erlangen

We have investigated the thermal and redox behaviour of the technically important methanol steam reforming PdZn catalysts between 300-700 K in UHV and during MeOH dosage at 300 K for pressures up to 0.1 mbar. We compare samples from a washcoating process<sup>1</sup> before and after the reduction to PdZn. In both cases, we observed significant structural changes upon heating in the Zn 2p, Pd 3d and O 1s regions, respectively, in agreement with studies on Pd(111)<sup>2</sup>. However, annealing both samples to 700 K led to a significant drop in intensity of the Zn 2p signals, indicating alloy destruction in UHV, accompanied by the emergence of large Mg peaks, which are further enhanced by H<sub>2</sub>

exposure of the surfaces at this temperature.

The resulting surface was exposed to MeOH background pressures ( $1.2 \cdot 10^{-6}$ -0.1 mbar) at 300 K and C 1s, Pd 3d and Zn 2p spectra were collected. A comparison with similar results on fully intact catalysts<sup>3</sup> show slightly different adsorption behaviour of MeOH. This is relevant, because Mg is known to affect the oxidative methanol steam reforming on Pd/ZnO catalysts.

[1] Pfeifer et al., Appl. Cat. A: 270 (2004) 165. [2] Bayer et al., Surf. Sci. 600 (2006) 78. [3] Pantförder, PhD thesis, Universität Erlangen-Nürnberg, 2004.

O 44.77 Wed 17:00 Poster C

**CO oxidation measurements on Au/TiO<sub>2</sub> model catalysts** — ●STEFAN KIELBASSA, JOACHIM BANSMANN, and JÜRGEN BEHM — Institute of Surface Chemistry and Catalysis, Ulm University

Au nanoparticles on metal oxide supports exhibit a high catalytic activity for numerous reactions, e.g., the low temperature CO oxidation. It was found, that the activity is not only very sensitive to the size and the shape of the Au particles, but also to the chemical composition of the support. Especially reducible metal oxides, like TiO<sub>2</sub>, are known to increase the catalytic activity and thus, they are not only passive spectators.

Planar model catalysts are ideally suited to investigate the influence of structural properties on the catalytic activity by varying the numbers of defects, steps and kinks on the substrate surface. Therefore, different types of planar titania surfaces, from well-ordered single crystal via epitaxially ordered to polycrystalline films, have been prepared and their influence on the CO oxidation activity of Au/TiO<sub>2</sub> model catalysts was studied using a micro-flow reactor attached to the UHV preparation chamber. We found, that significant differences in the catalytic activity can be observed with respect to the surface structure of the support. The results will be discussed with respect to activity data on model catalysts presented previously.

O 44.78 Wed 17:00 Poster C

**Enhanced sensitivity and long-term stability for surface stress measurements** — ●FRIEDRICH KLASING, PETER KURY, and MICHAEL HORN-VON HOEGEN — University of Duisburg-Essen, Institute for Experimental Physics

Surface stress is one of the most important physical quantities determining the surface structure and morphology due to its large contribution to the total energy. Unfortunately, a direct measurement of surface stress is not possible, but it can be determined via the elastic response of a thin substrate as utilized in bending sample techniques like surface stress induced optical deflection (SSIOD) [1]. A sensitivity of the order of  $0.5 \text{ Nm}^{-1}$  can easily be achieved, to some extent even with commercially available tools [2].

A strongly enhanced sensitivity down to  $0.005 \text{ Nm}^{-1}$  (corresponding to stress effects induced by less than a percent of an adsorbate monolayer) together with a long-term stability on a time scale of one hour is only possible with extensive modifications. Still, long-term measurements over several hours suffer under drift effects caused by laser instabilities, ambient air motion and even minor detector nonlinearities. The influence of these effects on the surface stress signal drift is discussed and modifications are presented to reduce the typical drift to below  $0.1 \text{ Nm}^{-1} \text{ hour}^{-1}$ .

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

[2]: <http://www.k-space.com/HTML/Products/mos/>

[3]: P. Kury et al., Rev. Sci. Instrum., 76(2), 023903 (2005)

O 44.79 Wed 17:00 Poster C

**Depth profiling of thin film solar cell components by synchrotron excited Soft X-Ray Emission Spectroscopy (SXES)** — ●HARRY MÖNIC<sup>1</sup>, MARKUS BÄR<sup>3</sup>, CHRISTIAN CAMUS<sup>2</sup>, AHMED

ENNAOUI<sup>2</sup>, ALEXANDER GRIMM<sup>1</sup>, CHRISTIAN JUNG<sup>4</sup>, CHRISTIAN KAUFMANN<sup>2</sup>, PAUL KÖRBER<sup>2</sup>, TIMO KROPP<sup>2</sup>, IVER LAUERMANN<sup>2</sup>, SEBASTIAN LEHMANN<sup>2</sup>, MARTHA LUX-STEINER<sup>1,2</sup>, TIM MÜNCHENBERG<sup>2</sup>, PAUL PISTOR<sup>2</sup>, STEFAN PUTTNINS<sup>2</sup>, RODRIGO SAEZ-ARAOZ<sup>1</sup>, HANS-WERNER SCHOCK<sup>2</sup>, STEFAN SOKOLL<sup>2</sup>, and CHRISTIAN-HERBERT FISCHER<sup>1,2</sup> — <sup>1</sup>Freie Universität Berlin — <sup>2</sup>Hahn-Meitner-Institut Berlin — <sup>3</sup>University of Las Vegas — <sup>4</sup>BESSY GmbH Berlin

Depending on the elemental composition of a material, SXES provides an information depth of 50-1000 nm. For studies of thin multilayer structures tuning of this parameter is highly desirable. One possibility is the variation of the excitation energy, which is accompanied by variation of photoionisation cross sections. Alternatively, we performed angle resolved SXES on the solar cell absorber material Cu(In,Ga)Se<sub>2</sub> covered by CdS or Zn(S,O) buffer layers (10-50 nm). Due to our setup geometry, the emission spectra clearly display increased surface sensitivity at small (grazing exit) and large (grazing incidence) exit angles. A model based on Beer-Lamberts law and setup geometry is in reasonable agreement with our experimental data. The presented results show that angle resolved SXES measurements yield depth-dependent information on multilayer structures. The increased surface sensitivity at grazing exit and grazing incidence angles allows the detection of extremely thin cover layers at reasonable recording times.

O 44.80 Wed 17:00 Poster C

**Using a scanning tunnelling microscope for pressure measurement** — ●THOMAS MADENA and ACHIM KITTEL — Energy and Semiconductor Research Laboratory, Institute of Physics, University of Oldenburg

Changes in mechanical stress distorts the scanning tunnelling microscope (STM) operation during the scanning of the high information. This effect is the starting point of the idea to use the STM-principle for pressure measurements. A simple tunnelling microscope without xy-scanning stage measures the bending of a membrane due to an applied pressure. The voltage applied to the high control is now the dependent quantity of the pressure on the rear side of the membrane. The high resolution of the STM makes it possible to see displacement on the nanometer scale. The thickness and the choice of material of the membrane are free parameter to alter the steepness of the pressure sensor. Results of the measurements of the different sensor features are discussed, like the linearity of the characteristics and sensitivity of the sensor. A possible procedure to calibrate the sensor is proposed. Furthermore, the unwanted influence of different interfering quantities was investigated and solutions to reduce their influence are given. For example the influence of a temperature drift can be reduced by the right choice of the used materials.

O 44.81 Wed 17:00 Poster C

**PGM-Beamline at the Undulator U55 at DELTA** — ●ULF BERGES<sup>1,2</sup>, SVEN DÖRING<sup>1,2</sup>, and CARSTEN WESTPHAL<sup>1,2</sup> — <sup>1</sup>DELTA, University of Dortmund, Maria-Goeppert-Mayer Str. 2, 44221 Dortmund, Germany — <sup>2</sup>Fachbereich Physik, University of Dortmund, Otto-Hahn-Str. 4, 44221 Dortmund, Germany

A VUV-beamline for linearly polarized synchrotron radiation from a permanent magnet undulator is operated at DELTA, a synchrotron radiation facility at the university of Dortmund, Germany.

The energy range of this PGM-type beamline is 55 to 1500 eV, the calculated focus spot size  $70 \text{ μm}$  (h)  $\times$   $30 \text{ μm}$  (v). The measured photon flux is about  $10^{12}$  photons/s/100 mA at 400 eV and 200 μm exit slit size and cff-value of 2. The beamline can also be operated in a high resolution mode with an expected energy resolution up to 30000. Various measurements concerning energy resolution, flux and beam stability leading towards a characterization of this beamline will be presented. The instrumentation of the beamline will be discussed, too.