

## O 15 Postersitzung (Adsorption an Oberflächen, Epitaxie und Wachstum, Organische Dünnschichten, Oxide und Isolatoren, Rastersondentechniken, Zeitaufgelöste Spektroskopie, Methoden)

Zeit: Freitag 17:00–20:00

Raum: Poster TU D

O 15.1 Fr 17:00 Poster TU D

**Compression of submonolayer goldfilms by CO adsorption on a Re(10 $\bar{1}0$ ) surface** — ●C. PAULS and K. CHRISTMANN — Inst. f. Chemie, FU Berlin, Takustr. 3, 14195 Berlin

We have studied the adsorption of carbon monoxide on the clean and partially gold-covered Re(10-10) surface by means of LEED, thermal desorption (TPD) and work function change ( $\Delta\Phi$ ) measurements. On the Re(10-10) surface, increasing coverages of Au produce a variety of (1 $\times$ n) LEED superstructures in the submonolayer regime ( $n = 3, 4, 5, 6$ ), until a pseudomorphic (1 $\times$ 1) phase is formed at a complete Au monolayer. This phase has been subjected to a quantitative LEED analysis and clearly reveals a continuation of the Re lattice by a double layer of Au atoms in the 'A' termination of the Re(10-10) surface. Still larger Au coverages lead to a (1 $\times$ 8) LEED phase which is surprisingly stable in the multilayer regime. Interesting effects become apparent, if CO is adsorbed into the submonolayer Au phases: Apparently, CO is able to compress the rows of Au atoms in [0001] direction, i.e., perpendicular to the troughs, since the low-coverage (1 $\times$ 3) and (1 $\times$ 4) Au phases undergo transitions to the (1 $\times$ 4) and (1 $\times$ 5) phases, respectively, in the presence of coadsorbing CO. So far, similar effects have only been reported for coadsorption of oxygen and gold on a ruthenium (10-10) surface [1].

[1] S. Poulston, M. Tikhov, and R.M. Lambert, *Langmuir* 13 (1997) 5356

O 15.2 Fr 17:00 Poster TU D

**Density-functional theory study of oxygen adsorption at vicinal Pd surfaces** — ●YONGSHENG ZHANG, JUTTA ROGAL, and KARSTEN REUTER — Fritz-Haber-Institut, Faradayweg 4-6, D-14195 Berlin

The contact with our O-rich atmosphere can lead to the formation of oxides at transition metal surfaces, and therewith significantly alter the surface properties and functionality. Although atomic steps are generally believed to play a prominent role in this oxide formation process, most of our atomic-scale understanding derives to date from studies concentrating on low-index surfaces. As a first step to explicitly address the effect of atomic steps, we use density-functional theory to investigate the adsorption of oxygen at vicinal Pd(11 $\bar{N}$ ) surfaces ( $N=3,5,7$ ), exhibiting (111) steps and (100) terraces of varying width. Oxygen adsorption close to the steps induces strong changes in the geometric relaxation of the surfaces, that before followed a clear trend with contraction of all surface layers with undercoordinated atoms. Adsorption at the steps is energetically preferred compared to the terrace sites, and we find the geometric, energetic and electronic properties of the center terrace sites at Pd(117) to be already almost indistinguishable from those at a low-index Pd(100) surface.

O 15.3 Fr 17:00 Poster TU D

**Interaction of Formic Acid with Surfaces of Solid Water between 80 and 200K** — ●S. BAHR<sup>1</sup>, O. HÖFFT<sup>1</sup>, A. BORODIN<sup>1</sup>, V. KEMPTER<sup>1</sup>, F. BORGET<sup>2</sup>, T. CHIAVASSA<sup>2</sup>, and A. ALLOUCHE<sup>2</sup> — <sup>1</sup>Institut für Physik und Physikalische Technologien, TU Clausthal, Leibnizstr. 4, D-38678 Clausthal-Zellerfeld — <sup>2</sup>Physique des Interactions Ioniques et Moléculaires, CNRS-UMR6633 Université de Provence, Campus St. Jérôme, Marseille France

The interaction of formic acid (HCOOH) with solid water, deposited on tungsten at 80K, was studied with metastable impact electron spectroscopy (MIES), UPS(HeI and II), IR-Spectroscopy and TPD. In MIES and UPS the emission from the outermost 1b<sub>1</sub>, 3a<sub>1</sub>, 1b<sub>2</sub> MOs of water and the weakest-bonded  $\pi$ - and  $\sigma$ -type MOs of formic acid (FA) were monitored. The results are interpreted with the help of cluster DFT calculations. FA/water interfaces were prepared at 80K, namely FA layers on thin films of solid water and H<sub>2</sub>O adlayers on thin FA films; they were annealed between 80 and 200K. It is concluded that an H-bonded FA-network forms on the solid water surface, suggesting that the lateral interaction between FA species is stronger than that between FA and water. In the entire studied temperature range the FA species remain in the surface layer although a partial solvation takes place above 120K. After the desorption of water (155K TPD peak maximum), weak features of FA can be seen up to about 170K. Under the studied conditions no deprotonation of FA can be detected. Results for the deposition for H<sub>2</sub>O

on FA films at 80K will also be presented.

O 15.4 Fr 17:00 Poster TU D

**Interaction of Cs Halides with the surface of Solid Water between 80 and 200K.** — ●O. HÖFFT, A. BORODIN, S. BAHR, and V. KEMPTER — Institut für Physik und Physikalische Technologien, TU Clausthal, Leibnizstr. 4, D-38678 Clausthal-Zellerfeld

The interaction of the Cs halides (CsX) with X= F, Cl, and I with solid water was investigated with Metastable Impact Electron Spectroscopy (MIES) and UPS(HeI and II) and TPD between 80 and 200K. In MIES and UPS the emission from the outermost H<sub>2</sub>O MOs 1b<sub>1</sub>, 3a<sub>1</sub>, 1b<sub>2</sub> and from the npX-states of X ( $n=2,3,5$  for F, Cl and I, respect.) was monitored. We have prepared CsX/water interfaces, namely CsX layers on thin films of solid water and H<sub>2</sub>O adlayers on thin CsX films; they were annealed between 80 and 200K. At 80K closed CsX layers were obtained on H<sub>2</sub>O and vice versa; no interpenetration of the two components H<sub>2</sub>O and CsX could be observed. However, ionic dissociation of CsX takes place when H<sub>2</sub>O and CsX do interact directly. Above 105K we find that solvation of these ionic species becomes significant. Our results are compatible with a transition of ionic species from a surface site to an energetically favored water-separated site, where the species are solvated. Desorption of the water molecules, not involved in the solvation process, becomes sizeable above 135K. On the other hand, the temperature for desorption of H<sub>2</sub>O molecules interacting with salt ions depends strongly on the particular anion X<sup>-</sup> (120, 140, and 190K for F, Cl and I, respect.).

O 15.5 Fr 17:00 Poster TU D

**Low Temperature STM investigation of pentacene molecule on Cu<sub>3</sub>Au(100)** — ●MICOL ALEMANI, FRANCESCA MORESCO, LEO GROSS, and KARL-HEINZ RIEDER — Inst. für Exp.physik, FU Berlin, Arnimallee 14, D-14195

The adsorption geometry of pentacene molecules on Cu<sub>3</sub>Au(100) is studied by means of a Low-Temperature Scanning Tunneling Microscope. The Cu<sub>3</sub>Au(100) is terminated by the gold-rich plane, as already known and as probed by atomic resolution images. Depending on the substrate geometry the molecules exhibit two different orientations and conformations. Thanks to the stability of the system at low temperature (7 K), it has been possible to perform controlled manipulation of single pentacene molecules. The study of the manipulation of pentacene on Cu<sub>3</sub>Au(100) is presented.

O 15.6 Fr 17:00 Poster TU D

**Neutron Reflectometry from Thin Liquid Layers (Foam Films)** — ●R. KRASSTEV<sup>1,2</sup>, TH. GUTBERLET<sup>3</sup>, N. C. MISHRA<sup>1</sup>, and H. MÖHWALD<sup>1</sup> — <sup>1</sup>Max-Planck Institute of Colloids and Interfaces, 14424 Potsdam, Germany — <sup>2</sup>Hahn-Meitner Institute, Berlin, Glienicker Str. 100, 14109 Berlin, Germany — <sup>3</sup>Paul Scherrer Institute, 5232 Villigen PSI, Switzerland

The properties of liquids confined in small volumes deviate from that of the bulk material. Foam films have been widely used as model system to study interactions between fluid interfaces but they may be also used as a tool to study the properties of liquids in confined volumes. A foam film is formed by two monolayers of surfactant molecules with the hydrophobic parts facing the air and the hydrophilic head groups in contact with a central aqueous core. Film thickness can be tuned by the physicochemical parameters of the bulk solution from which films are formed while their surfaces always stay parallel each other. This way formation of structures with well defined geometry is assured. We used neutron reflectometry to study the composition of the layers which form a foam film. Films were prepared from solutions of surfactants in D<sub>2</sub>O. The layers of surfactant and aqueous core were discriminated due to different scattering length densities (SLD). The SLD of the surfactant layers does not depend on the distance between the film surfaces while that of the film central aqueous layer depends on the film thickness. SLD similar to that of D<sub>2</sub>O was measured in the case of thick films. It decreases when the two surfaces approach each other. The experimental results are shown and future work is discussed.

O 15.7 Fr 17:00 Poster TU D

**Study of the effect of electrolyte ions on the forces between hydrophobic polymer surfaces in aqueous solutions** — ●ASTRID DRECHSLER and KARINA GRUNDKE — Leibniz-Institut für Polymerforschung e.V., Hohe Straße 6, 01069 Dresden

Interfacial phenomena are strongly influenced by adsorption processes. In aqueous environments, even simple electrolyte ions modify the interactions of polymer surfaces. In the present study, the forces between a flat polystyrene surface and a colloidal polystyrene sphere have been measured directly in water and solutions of KCl and KOH using a scanning force microscope. At distances  $> 5...50$  nm, all force-distance curves show an electrostatic repulsion caused by an electrical double-layer of electrolyte ions adsorbed to the surface. The surface potential of the polystyrene surface calculated from the force-distance curves coincides with its zeta potential. The decay length of the electrostatic repulsion diminishes with increasing electrolyte concentration due to the screening of the surface potential by the mobile ion layer. At distances  $< 5...20$  nm, in most of the solutions an attractive force of variable range and strength dominates, the so-called 'hydrophobic force'. We attribute it to the existence of nanoscopic air bubbles on the hydrophobic polymer surfaces. It is not affected by the KCl concentration. In KOH concentrations  $\leq 10^{-4}$  M, this attraction disappears. Instead, a "soft" steric repulsion occurs. The adhesion force decreases steadily with increasing KOH concentration. It is not clear if these phenomena are caused by air nanobubbles or if the nanobubbles are replaced by a strongly adsorbed layer of OH<sup>-</sup> and counterions.

O 15.8 Fr 17:00 Poster TU D

**Particle Size Effects in TPD: Adsorption of CO<sub>2</sub> on Clean and Oxygen-Precovered Au(110)-(1x2)** — ●J.M. GOTTFRIED<sup>1,2</sup> and K. CHRISTMANN<sup>1</sup> — <sup>1</sup>Institut fuer Chemie der Freien Universitaet Berlin, Takustr. 3, D-14195 Berlin — <sup>2</sup>Lehrstuhl fuer Physikalische Chemie II, Universitaet Erlangen-Nuernberg, Egerlandstr. 3, D-91058 Erlangen

Temperature programmed desorption (TPD) spectra of CO<sub>2</sub> on Au(110)-(1x2) exhibit overlapping submonolayer and multilayer peaks, indicating that the intermolecular CO<sub>2</sub>-CO<sub>2</sub> attraction is of similar strength as the CO<sub>2</sub>-gold interaction. Thus, layer-by-layer growth and three-dimensional growth are equally favoured. Accordingly, the TPD spectra show two anomalies: i) A low-temperature and a high-temperature state grow simultaneously, and ii) the second-layer TPD peak appears at a lower temperature than the multilayer peak. This behavior can be explained by three-dimensional growth of the Stranski-Krastanov type. For small CO<sub>2</sub> aggregates, the surface energy contribution to the total energy increases the CO<sub>2</sub> vapour pressure and, hence, the desorption rate (Kelvin effect), whereas larger crystallites inhibit the desorption by excluding a certain fraction of the total coverage from desorption. Semi-quantitative simulations of the TPD spectra, supplemented by UPS and work function measurements, support our growth and interaction model of the CO<sub>2</sub> adsorbate on clean and oxidized gold.

O 15.9 Fr 17:00 Poster TU D

**Adsorption properties of pyridine molecules on TiO<sub>2</sub> surfaces** — ●M. DÜRR, A. YASUDA und G. NELLE — Materials Science Laboratories, Sony Int. (Europe) GmbH, D - 70327 Stuttgart

Photochemical solar cells based on nano-crystalline TiO<sub>2</sub> which is sensitized by organic dye molecules (dye-sensitized solar cells) have been shown to exhibit a strongly increased open circuit voltage and thus improved power conversion efficiency upon the addition of *tert*-butylpyridine to the electrolyte. This improvement of the cell performance was earlier attributed to a suppression of electron transfer between the TiO<sub>2</sub> conduction band and the redox couple in the electrolyte.

For a better understanding of the underlying mechanisms, the adsorption of pyridine molecules on TiO<sub>2</sub> was investigated by means of quartz crystal microbalance techniques and ultraviolet photoemission spectroscopy (UPS). A clear correlation between pyridine adsorption and the increase of open circuit voltage was observed. Moreover, it could be shown that only a small fraction of the total surface area is covered by the pyridine molecules at saturation coverage. The results are interpreted in terms of adsorption at defect sites and are correlated to adsorption-induced changes in the electronic structure as observed by means of UPS.

O 15.10 Fr 17:00 Poster TU D

**Adsorption of Methanol on Pd<sub>3</sub>Sn/Pd(111) Surface- Alloy** — ●CHRISTIAN BREINLICH, THOMAS SCHMIDT, CONRAD BECKER, and KLAUS WANDEL — Institut für Physikalische Chemie, Wegelerstr.12, 53115 Bonn

Over the last decade several experimental UHV- studies have been published, describing the decomposition of methanol, adsorped on Pd(111)-surfaces, into carbon monoxide and hydrogen. We have investigated the adsorption of methanol on a palladium tin surface alloy with a  $p(2 \times 2)$  superstructure. The idea behind this is to reduce the reactivity of the palladium surface by alloying it with a less noble metall. We investigated the geometric and electronic properties of the surface by AES, LEED and UPS. TDS showed a desorption of methanol from the multilayer at 140 K. At 160 K the monolayer desorbs intact. Neither CO nor hydrogen were detected in significant amounts, so that in contrast to the bare Pd surface, methanol does not decompose on this alloy. These results were supported by UPS data and work function measurements. There was no evidence, that carbon monoxide or surface carbon were formed. A Redhead analysis of the TDS data resulted in an adsorption energy of the multilayer of about 0.36 eV, which is similar to that on Pd (111). For the monolayer we found an adsorption energy of about 0.41 eV. These data agree with our studies on the corresponding ( $\sqrt{3} \times \sqrt{3}$ )R30° PdSn<sub>2</sub>/Pd(111) surface alloy.

O 15.11 Fr 17:00 Poster TU D

**Study of conductivity and surface morphology during adsorption of silver atoms on a smooth Ag(111) film** — ●GIRIRAJ JNAWALI, BORIS KRENZER, and M. HORN-VON HOEGEN — Institute for Laser and Plasma Physics, University of Duisburg-Essen, Essen, Germany

The conductivity of ultra-thin metal film has great relevance to technological applications. In contrast to thin metal film, the surface morphology has an enhanced impact on the electronic transport through the film.

In this poster we'll present the results of conductivity measurements along with morphology study of ultra-thin metal films. The conductivity measurements were performed by four-point resistance measurements and the morphology was studied by SPA-LEED.

Ultra-thin Ag(111) films were prepared by depositing silver atoms on Si(100) substrate at 80K and annealed the film carefully until it turned into flat surface. The quality of flatness was checked by SPA-LEED measurements. Subsequently the film was exposed to a low dose silver atoms at different substrate temperatures ranging from 80 to 200K. An increase in resistance due to scattering at adsorbate atoms was observed. The resistance measurements were accompanied by SPA-LEED to determine the surface roughness.

O 15.12 Fr 17:00 Poster TU D

**'Pulse injection': A non-destructive way of depositing large organic molecules under ultrahigh vacuum conditions** — ●INGEBORG STASS, LEONHARD GRILL, FRANCESCA MORESCO, and KARL-HEINZ RIEDER — Institut für Experimentalphysik, Freie Universität Berlin, Arnimallee 14, 14195 Berlin

A fundamental problem in the deposition of molecules from a Knudsen cell is the heating procedure: When the molecules are getting larger the temperature must be increased which results in the dissociation of molecular bonds. We present a low temperature STM study of porphyrin-based molecules on copper surfaces. In order to deposit intact molecules onto the substrate we have used the so-called pulse injection method. Molecules (in solution) are injected by a valve with very short aperture times (few ms). Residual solvent contamination can be desorbed from the surface by heating of the sample, but the chemical structure of the molecules must be maintained. We used various solvents, which differ in their chemical properties, and obtained information on the adsorption and desorption behaviour of the solvents on the metal substrate. The results are compared and discussed by means of the ideal deposition conditions.

O 15.13 Fr 17:00 Poster TU D

**Organische Moleküle auf Oberflächen** — ●ALEXANDER BARTH, MANFRED ALBRECHT, GÜNTER SCHATZ, and FRANK TREUBEL — Universität Konstanz, Fachbereich Physik, 78457 Konstanz

Zur Nanostrukturierung von van der Waals-Oberflächen wurden organische Moleküle durch Organic-MBE-Technik in einem UHV-System aufgebracht. Diese weisen eine langreichweitige selbstorganisierte Ord-

nung auf. Als Materialien wurden Moleküle wie TMA, TPA und TDA verwendet, die alle aus einem Grundgerüst aus Benzolringen bestehen, an denen Carboxylgruppen chemisch gebunden sind. Über Wasserstoffbrückenbindungen zwischen den Molekülen bildet sich dann die selbstorganisierte Ordnung aus. Als Substrate dienten HOPG und Schichthalbleiter, wie Wolframdiselenid, aber auch Cu(111)-Keimschichten auf  $\text{Al}_2\text{O}_3(0001)$ -Substraten. Ziel dieser Arbeit ist es geordnete Ensembles von magnetischen Nanostrukturen zu erzeugen, indem die organischen Moleküle als Monolage eine selbstorganisierte Aufdampfmaske zur Nanostrukturierung bilden. Zur strukturellen Untersuchung wurden AFM und STM benutzt. Aber auch die Selbstorganisation dicker Filme wurde mittels RHEED untersucht.

O 15.14 Fr 17:00 Poster TU D

**Investigation of thin hexane films using coherent X-rays** — ●ROBERT FENDT<sup>1</sup>, SIMONE STREIT<sup>1</sup>, MICHAEL SPRUNG<sup>2,1</sup>, CHRISTIAN GUTT<sup>3,1</sup>, ANDERS MADSEN<sup>4</sup>, and METIN TOLAN<sup>1</sup> — <sup>1</sup>Experimentelle Physik 1, Universität Dortmund; Otto-Hahn-Str. 4, 44227 Dortmund, Germany — <sup>2</sup>ID/IMMY-XOR-CAT, APS/ANL, Argonne, IL, 60439, USA — <sup>3</sup>Department of Physics 0350, University of California, San Diego, 9500 Gilman Drive, La Jolla, CA 92093-0350, USA — <sup>4</sup>ID10A, ESRF, B.P. 220, F-38043 Grenoble, France

Very thin hexane films were prepared on a silicon substrate via condensation from a vapour phase. Using this method, it is possible to produce thin films of different thickness (about 20-200 angstroms) by changing the sample temperature. The films were first investigated by means of X-ray photon correlation spectroscopy to measure the spectrum of the capillary waves which were expected on the liquid surface. However, all XPCS measurements showed no dynamics at all on the investigated length and time scales (i.e., a few  $\mu\text{m}$  and  $10^{-6}$  to 1000s). As a consequence, static diffuse scattering scans of the surface were made, revealing pronounced speckle structures. These speckles were proven to be stable at least on time scales of up to 20 minutes. The pattern changes slightly when changing the film thickness slowly, and very drastically after quick thickness changes. We believe that this corresponds to different growth modes of the sample on the substrate.

O 15.15 Fr 17:00 Poster TU D

**Coverage dependent details of benzene adsorption on Ni (111) studied by XPS** — ●PAPP C., FUHRMANN T., TRÄNKENSCHUH B., STEINRÜCK H.-P., and DENECKE R. — Lehrstuhl für Physikalische Chemie II, Universität Erlangen-Nürnberg, Egerlandstr. 3, 91058 Erlangen.

We studied the adsorption of benzene and fully deuterated benzene on Ni(111) by in-situ XPS at the synchrotron radiation facilities BESSY II, Berlin and MAX II, Lund. The spectra show some significant differences occurring during the adsorption process, which are observed for the first time, due to the high energy resolution achieved. To determine the nature of the spectral features giving rise to these differences, we also studied the adsorption of substituted benzenes (e.g. chlorobenzene) and benzene coadsorbed with CO and NO. Based on a quantitative analysis of the spectra and their features, models are proposed, which can explain the observed differences. The aim of these models is to distinguish between conformational and electronic effects. Supported by the DFG (STE 620/4-2) and a European Community ARI program (HPRI-CT-2001-00135).

O 15.16 Fr 17:00 Poster TU D

**Engineering the Adsorption of Latex Spheres on Charged Surfaces II: Switching the Surface Charge by Adsorption of Layered Double Hydroxides on Mica** — ●D. RAPP<sup>1</sup>, H. GLIEMANN<sup>2</sup>, P.G. WEIDLER<sup>1</sup>, R. NÜESCH<sup>1</sup>, TH. SCHIMMEL<sup>2,3</sup>, Y. MEI<sup>4</sup>, A. WITTEMANN<sup>4</sup>, G. SHARMA<sup>4</sup>, and M. BALLAUFF<sup>4</sup> — <sup>1</sup>ITC-WGT, Forschungszentrum Karlsruhe, 76021 Karlsruhe — <sup>2</sup>INT, Forschungszentrum Karlsruhe, 76021 Karlsruhe — <sup>3</sup>Institut für Angewandte Physik, Universität Karlsruhe, 76128 Karlsruhe — <sup>4</sup>Institut für Physikalische Chemie I, Universität Bayreuth, 95447 Bayreuth

Layered Double Hydroxides (LDH) are rare in nature but easy to synthesize in the laboratory. Because of their positive layer charge LDH can be used to modify negatively charged surfaces or to adsorb negatively charged particles (e.g. polymer particles). The applications of polymer nanoparticles (like coatings or paints) are based on the adsorption of the particles on organic or inorganic surfaces. Therefore the investigation of the adsorption behavior of spherical core-shell polymer particles with negatively charged chains (anionic SPB) on different charged inor-

ganic surfaces was aim of this work. As negatively charged substrate we used freshly cleaved mica. AFM investigations of anionic SPB adsorbed on mica showed the formation of a densely packed particle layer with a two-dimensional long-range order. By the adsorption of LDH on mica the surface charge of the substrate was switched from negative to positive. On this modified surface anionic SPB adsorb as single particles.

O 15.17 Fr 17:00 Poster TU D

**Adsorption and Surface Mobility of Cinchonidine on Pt(111) studied by STM** — ●MARKUS WAHL<sup>1</sup>, MATTHIAS VON ARX<sup>1,2</sup>, THOMAS A. JUNG<sup>1,3</sup>, and ALFONS BAIKER<sup>2</sup> — <sup>1</sup>Institute of Physics University of Basel, Switzerland — <sup>2</sup>Department of Chemistry and Applied Biosciences, ETH Zürich, Switzerland — <sup>3</sup>Paul-Scherrer Institute, Villigen, Switzerland

The investigation of complex organic molecules on metal surfaces by scanning probe microscopies has become a topic of great interest. Most of this research has been focussed on rather unreactive metal surfaces. Here we report [1] on the adsorption of cinchonidine (CD) on Pt(111) in the presence and absence of hydrogen. This investigation is of particular interest due to its relevance to asymmetric heterogeneous catalysis [2].

The time resolved studies revealed that the CD molecules are immobile at low hydrogen pressure, whereas considerable mobility was observed at higher hydrogen pressure. Based on different adsorption geometries and surface mobility different species could be distinguished.

[1] Matthias von Arx et al., Phys. Chem. Chem. Phys., 2005, 7, Advance Article

[2] A. Baiker, H.-U. Blaser in Handbook of Heterogeneous Catalysis, VCH, Weinheim 1997, Vol. 5, 2422.

O 15.18 Fr 17:00 Poster TU D

**Adsorptionsexperimente von Acrylnitril und Allylcyanid auf der Si(001)-2x1 Oberfläche** — ●RALF FUNKE<sup>1</sup>, GUIDO PIASZENSKI<sup>1</sup>, MARTIN KNEPPE<sup>1</sup>, ULRICH KÖHLER<sup>1</sup>, SYLVIE RANGAN<sup>2</sup>, FABRICE BOURNEL<sup>2</sup>, STEFAN KUBSKY<sup>2</sup> und FRANCOIS ROCHET<sup>2</sup> — <sup>1</sup>Experimentalphysik IV / Oberflächenphysik, Ruhr-Universität Bochum, 44780 Bochum — <sup>2</sup>Laboratoire de Chimie Physique Matière et Rayonnement, Université Pierre et Marie Curie, Paris, Frankreich

Das Adsorptionsverhalten zweier organischer Moleküle mit Nitril-Gruppen - Acrylnitril und Allylcyanid - auf der Si(001)-2x1 Oberfläche wurde mit STM, XPS und NEXAFS untersucht. Bei Acrylnitril zeigen für niedrige Bedeckungen ( $< 10^{13}$  Moleküle /  $\text{cm}^2$ ) STM-Aufnahmen nur eine Adsorptionsgeometrie: das Molekül überbrückt den Zwischenraum zweier benachbarter Dimerreihen und bindet an zwei *dangling bonds* des Siliziums. Untersuchungen mit XPS und NEXAFS bei Bedeckungen im Bereich von  $10^{13}$  bis  $10^{14}$  Molekülen /  $\text{cm}^2$  geben Hinweise auf zwei zusätzliche Adsorptionsgeometrien. Im Fall von Allylcyanid erlauben NEXAFS und XPS Spektren die Identifizierung von ebenfalls drei Adsorptionsgeometrien, auch STM zeigt mehrere Bindungsplätze. In allen Fällen werden hier die Adsorptionsplätze auf zwei benachbarten Dimeren einer Reihe gebildet.

O 15.19 Fr 17:00 Poster TU D

**Experimental study of the specific adsorption of DNA on the surface of ferroelectric crystals.** — ●MARC TOBIAS WENZEL — Institute of Applied Photophysics (IAPP), Dresden

At present, many research groups study the metallisation of DNA in order to use it as a conducting nanowire. For the integration into electronic systems, the DNA needs to be bound to contacts or surfaces.

Our intention is to clarify the mechanisms of adsorption of DNA at the surface of ferroelectric barium titanate  $\text{BaTiO}_3$  [100] and to investigate which effects the adsorption has on the properties of the DNA. For this purpose, 16  $\mu\text{m}$  long double-stranded lambda-DNA is deposited on the ferroelectric surface from an aqueous solution. The DNA is labelled by the selective yoyo-1 fluorescence dye for observation. Subsequently, the system is examined by scanning confocal microscopy and scanning force microscopy.

For the investigation of the interaction between the DNA and the charged surface of the ferroelectric, confocal Raman spectroscopy of the DNA is planned in the future.

O 15.20 Fr 17:00 Poster TU D

**Structure of a thin oxide film on Rh(100)** — ●WILHELM HOFER<sup>1</sup>, CHRISTOF KLEIN<sup>1</sup>, MICHAEL SCHMID<sup>1</sup>, PETER VARGA<sup>1</sup>, LUKAS KÖHLER<sup>2</sup>, GEORG KRESSE<sup>2</sup>, JOHAN GUSTAFSON<sup>3</sup>, ANDERS MIKKELSEN<sup>3</sup>, MIKAEL BORG<sup>3</sup>, JESPER ANDERSEN<sup>3</sup>, and EDVIN LUNDGREN<sup>3</sup> — <sup>1</sup>Allgemeine Physik, TU Wien — <sup>2</sup>Materialphysik, Uni Wien — <sup>3</sup>Synchrotron Radiation Research, Lund (Sweden)

We have studied the surface oxide of Rh(100) with different experimental and theoretical methods: STM (scanning tunneling microscopy), LEED (low energy electron diffraction), HRCLS (high resolution core level spectroscopy) and DFT (density functional theory). The HRCLS measurements indicated a trilayer RhO<sub>2</sub> structure with two oxygen layers and one Rh layer in-between. STM and quantitative LEED revealed a close-to-hexagonal surface with a c(8×2) periodicity. In order to coincide with the square Rh(100) substrate, the hexagonal oxide overlayer is slightly distorted, resulting in a c(8×2) structure. The structural details were obtained by quantitative LEED (Pendry R-factor = 0.16) and DFT calculations. It was found that every seventh of the lower O atoms of the trilayer surface oxide resides in on top positions of the Rh(100) substrate. Ab initio DFT calculations give almost perfect agreement with the LEED results in all atomic coordinates. We therefore regard the trilayer surface oxide model as confirmed and thus the oxygen induced c(8×2) structure as solved. [J. Gustafson et al., submitted to Phys.Rev.B]

O 15.21 Fr 17:00 Poster TU D

**Untersuchung atomarer Stapelfolgen und Versetzungen in Co Doppel- und Tripellagen mittels Rastertunnelspektroskopie** — ●MARCO PRATZER und HANS-JOACHIM ELMERS — Institut für Physik, Staudingerweg 7, Universität Mainz, D-55099 Mainz

Die Untersuchung der elektronischen Struktur von ultradünnen ferromagnetischen Filmen, insbesondere der elektronischen Interface-Zustände, ist von entscheidender Bedeutung für zukünftige Spintronik-Anwendungen. Eine wichtige Rolle spielt hierbei die Homogenität der Grenzfläche. Mittels MBE wurde ein System aus Co Doppel- und Tripellageninseln auf einem W(110)-Einkristall präpariert und die elektronische Struktur mittels Rastertunnelspektroskopie (STS) untersucht. Bei einer Präparation bei  $T = 420$  K wachsen die Tripellageninseln dicht gepackt entweder mit hcp- oder fcc-Stapelfolge. Diese lassen sich anhand der unterschiedlichen elektronischen Struktur mit Hilfe von STS leicht unterscheiden. Auch bei der Doppellage können zwei verschiedene Stapelfolgen vorliegen (AB oder AC), die, auch wie die Stapelfolgen ABA und ACA in der Tripellage, elektronisch äquivalent sind. Wachsen während der Präparation zwei Doppellageninseln mit unterschiedlicher Stapelfolge zusammen, so bildet sich eine Versetzungslinie, in deren Bereich die elektronische Struktur leicht geändert ist. Im Spektroskopiebild findet man zwei verschiedene Versetzungstypen, die sowohl in der Doppel- als auch in der Tripellage in Abhängigkeit von der Kristallrichtung auftreten und die mit Hilfe eines Hartkugelmodells erklärt werden können. Mit dieser Information ist es nun möglich, die atomaren Stapelfolgen in den Doppel- und Tripellageninseln zu bestimmen.

O 15.22 Fr 17:00 Poster TU D

**Self-ordering of hexa-peri-hexabenzocoronene and derivatives on Cu(111)** — ●LEO GROSS<sup>1</sup>, FRANCESCA MORESCO<sup>1</sup>, PASCAL RUFFIEUX<sup>2</sup>, ANDRÉ GOURDON<sup>3</sup>, CHRISTIAN JOACHIM<sup>3</sup>, and KARL-HEINZ RIEDER<sup>1</sup> — <sup>1</sup>Institut für Experimentalphysik, Freie Universität Berlin, Arnimallee 14, D-14195 Berlin, Germany — <sup>2</sup>Swiss Federal Laboratories for Materials Testing and Research, Überlandstrasse 129, 8600 Dübendorf, Switzerland — <sup>3</sup>The Nanoscience Group, CEMES-CNRS, 29 rue J. Marvig, P.O. Box 94347, F-31055 Toulouse Cedex, France

An LT-STM study of the submonolayer growth of hexa-peri-hexabenzocoronene (HBC) and three custom designed derivatives on Cu(111) is presented. Thanks to the systematic choice of molecules it was possible to assign properties of adsorbates to specific chemical groups inside the molecule. We find that tert-butyl side groups induce intermolecular attraction, while their influence on the molecule-substrate bonding is negligible. The planar aromatic HBC core is on the other hand strongly bound to the substrate inducing a fixed molecular orientation. Best monolayer ordering has been found for a molecule with tert-butyl side groups and a molecular core that bounds only at the central position, allowing a rotation in the absence of other pinning centres.

O 15.23 Fr 17:00 Poster TU D

**New phases of NaCl monolayers on Ag(100)** — ●HANS-CHRISTOPH PLOIGT, FRANÇOIS PATTHEY, MARINA PIVETTA, and WOLF-DIETER SCHNEIDER — Institut de Physique des Nanostructures, École Polytechnique Fédérale de Lausanne, CH-1015 Lausanne, Switzerland

We used low-temperature scanning tunneling microscopy and scanning tunneling spectroscopy to characterise the growth mode of ultrathin NaCl layers on cold Ag(100) substrates. NaCl was evaporated from a Knudsen cell at substrate temperatures between 0 °C and -120 °C. As a function of decreasing temperature three different atomic arrangements for a NaCl monolayer were found: (i) the square structure of the NaCl(100) plane, (ii) an oblique lattice and (iii) a hexagonal lattice.

O 15.24 Fr 17:00 Poster TU D

**DEPES/DAES investigations of the Pb/Ni(111) adsorption system** — ●ALEKSANDER KRUPSKI<sup>1,2</sup>, MAREK NOWICKI<sup>1</sup>, and STEFAN MRÓZ<sup>1</sup> — <sup>1</sup>Institute of Experimental Physics, University of Wrocław, pl. Maxa Borna 9, PL 50-204 Wrocław, Poland (Permanent address) — <sup>2</sup>Institut für Physikalische und Theoretische Chemie, Universität Bonn, Wegelerstr. 12, D-53115 Bonn, Germany

The crystalline structure of ultrathin Pb layers deposited on the Ni(111) surface in ultrahigh vacuum was investigated with the use of directional elastic peak electron spectroscopy (DEPES) and directional Auger electron spectroscopy (DAES). Experimental DEPES data recorded for the primary electron beam energies in the range 1.0-1.9 keV were compared with theoretical profiles obtained with the use of single scattering cluster (SSC) calculations for clean and covered Ni(111). Similar intensity maxima reflecting the crystalline structure of the Ni(111) sample were observed on experimental and theoretical profiles. Results obtained after deposition of 10 ML of Pb on Ni(111) at the substrate temperature  $T=150$  K exhibit intensity maxima corresponding to two mutually rotated Pb(111) domains. The populations of two possible Pb domains were determined by an R-factor analysis. The growth of one domain was found to be preferred, which can be rationalised by the miscut of the Ni(111) sample and the resulting step orientation.

O 15.25 Fr 17:00 Poster TU D

**Electrospray ion beam deposition in UHV: experimental development and first results** — ●STEPHAN RAUSCHENBACH<sup>1</sup>, FRANK STADTLER<sup>1</sup>, EGENIO LUNEDI<sup>1</sup>, SERGEI KOLTSOV<sup>2</sup>, NICOLA MALINOVSKI<sup>1</sup>, GIOVANNI COSTANTINI<sup>1</sup> und KLAUS KERN<sup>1</sup> — <sup>1</sup>Max-Planck-Institut für Festkörperforschung, D-70569 Stuttgart — <sup>2</sup>Institute for Analytical Instrumentation, Russian Academy of Sciences, 19813 Saint Petersburg

To avoid the intrinsic limitations in vapor deposition of organic molecules a novel ion beam source using Electro Spray Ionization (ESI) was constructed. The single molecular particle beam is formed from charged droplets due to iterative Coulomb explosion. High- and low-pressure radio frequency (RF) quadrupoles and electrostatic ion optics guide the ion beam through four differential pumping stages from ambient pressure to  $10^{-6}$  mbar at the substrate position.

The composition of the ion beam can be adjusted using the quadrupole ion guides as mass filters. Beam properties, particularly kinetic energy, mass and spatial distribution were characterized. The incidence energy could be measured between 5eV and 20eV per charge. A time-of-flight mass spectrometer was integrated.

Particle beams produced by the ESI source were used in a preliminary deposition setup in high vacuum. The samples were analyzed with atomic force microscopy (AFM) under ambient conditions. Organic molecules (Rhodamin  $m=443$  amu) and Albumin (BSA,  $m=66000$  amu) as well as Gold colloids (diameter=3.6-6.5 nm) were deposited on highly ordered pyrolytic graphite (HOPG) or Silicon substrates.

O 15.26 Fr 17:00 Poster TU D

**X-ray Standing Wave Imaging: the Growth of the First Monolayer YBa<sub>2</sub>Cu<sub>3</sub>O<sub>7- $\delta$</sub>  on SrTiO<sub>3</sub>(001)** — ●SEBASTIAN THIESS, TIEN-LIN LEE, BRUCE C.C. COWIE, and JÖRG ZEGENHAGEN — ESRF, Grenoble, France

For structure determination the X-ray Standing Wave (XSW) technique can be used as an element specific Fourier technique, which allows determining amplitude and phase of the Fourier coefficients of atomic distribution functions  $\rho(r)$ . In order to obtain the  $(hkl)^{th}$  Fourier coefficient of  $\rho(r)$ , the photoemission from a sample is recorded while the X-ray

photon energy is simultaneously scanned through the energy range of the (hkl) Bragg reflection. A real space image of  $\rho(r)$  is rendered by back transforming a sufficient number of Fourier coefficients.

We have studied the nucleation of the first monolayer YBCO on the STO(001) surface. 3D Fourier reconstructed images show the crystallographic distribution of all constituent elements of a 1 ML and a 0.5 ML YBCO film grown in situ by pulsed laser deposition. XSW measurements were carried out in UHV at beamline ID32 at the ESRF for 7 different STO(hkl) reflections at photon energies between 2.7 and 5.5 keV.

O 15.27 Fr 17:00 Poster TU D

**STM Untersuchung der Interdiffusion an den Grenzflächen Fe/Nb(110) und Nb/Fe(110)** — ●ISABELLE RAUSCHENBACH, CLAUDIA WOLF und ULRICH KÖHLER — Experimentalphysik IV / Oberflächenphysik, Ruhr-Universität-Bochum, 44780 Bochum

Rastertunnelmikroskopie bei unterschiedlichen Substrattemperaturen (Raumtemperatur bis 900K) wurde angewendet, um das heteroepitaktische Wachstum von Eisenschichten auf Nb(110) und Niobschichten auf Fe(110) zu untersuchen. Bei Raumtemperatur zeigen beide Systeme keine Anzeichen von Interdiffusion, das Vorhandensein einer Schwoebel-Ehrlich-Barriere verhindert jedoch ein glattes Schichtwachstum. Die Relaxation der unterschiedlichen Gitterkonstanten erfolgt ab der dritten Lage durch Ausbildung eines geordneten Versetzungsnetzwerks. Bei dem Wachstum unter erhöhter Proben temperatur verdrängen aufgebraachte Nb-Atome die Fe-Atome aus der ersten Fe(110)-Lage und führen zur Bildung von Eisen-Adinseln. Die Wechselwirkung der in die Oberfläche eingelagerten Nb-Atome führt zu einer linienförmigen Anordnung. Im Falle der Fe auf Nb(110)-Abscheidung äußert sich eine Interdiffusion durch die Koexistenz zweier unterschiedlicher Inseltypen auf der Oberfläche.

O 15.28 Fr 17:00 Poster TU D

**Growth of ultra-thin Fe films on Cu(111)** — ●WERNER RUPP, ALBERT BIEDERMANN, MICHAEL SCHMID, and PETER VARGA — Institut für allgemeine Physik, Technische Universität Wien

Using scanning tunneling microscopy (STM), scanning tunnelling spectroscopy (STS) and low-energy electron diffraction (LEED) we have characterized ultra-thin films of Fe on Cu(111). The films were grown by thermal deposition (TD) at room temperature (RT). Whereas bulk Fe is normally bcc ( $\alpha$ -Fe) at temperatures below 1186 K, fcc Fe ( $\gamma$ -Fe) can be stabilized in ultra thin films on fcc substrates. Analysing these TD-films, we find a pseudomorphic growth at low coverages [1]. With atomically resolved STM images we show the initial formation of strained bcc domains at low coverages (3ML) on flat Fe islands. This strain decreases with the thickness of the film. The bcc domains have Kurdjumov-Sachs orientation in agreement with LEED [2]. With STS measurements we show that the Cu covers the Fe islands decorating the step edges already during the deposition process. Correlated with this Cu coverage is the formation of 1ML high vacancy islands near the step edges of the substrate [3].

[1] J. Shen et al, Phys. Rev. B 56, 11134 [2] P. Ohresser et al, Phys. Rev. B. 59, 3696 [3] A. Brodde et al, Phys. Rev. B 47, 6609

O 15.29 Fr 17:00 Poster TU D

**Schichtwachstum, Grenzflächenreaktion und Elektronische Struktur von ultradünnen 3d-Übergangsmetalloxid/Metall-Schichtsystemen** — ●M. NAGEL, L. ZHANG und T. CHASSÉ — Institut für Physikalische und Theoretische Chemie, Universität Tübingen, Auf der Morgenstelle 8, D-72076 Tübingen

Ultradünne Schichten von Mn auf NiO(100) und Ni auf MnO(100)-Einkristalloberflächen (nominelle Schichtdicken <10nm) wurden in-situ mittels Photoemissionsspektroskopie schichtdickenabhängig charakterisiert. Die Auswertung der O1s-, Mn2p- und Ni2p-Rumpfelektronenspektren ergab Hinweise auf ein Inselwachstum und die partielle Oxidation des Metalls an der Grenzfläche bei den gewählten Präparationsbedingungen. Außerdem wurden ultradünne, pseudomorphe MnO- und NiO-Schichten auf Ag(100)-Einkristalloberflächen präpariert (analog zu [1,2]) und mit XPS sowie LEED in-situ analysiert. Bei der Präparation der MnO-Schichten wurden ergänzend Mn3s-Spektren zur Überprüfung des Oxidationszustandes herangezogen. Nach Aufdampfen einer Deckschicht aus Sb wurden die Proben ex-situ mit XES und XAS in Fluoreszenzdetektion charakterisiert. Die O K $\alpha$ , Mn L $_{2,3}$  und Ni L $_{2,3}$  Röntgenabsorptions- und Fluoreszenzspektren der Schichtsysteme sowie entsprechender Volumen-Referenzproben wurden ausgewertet.

Im direkten Vergleich der ultradünnen Schichten zu den Referenzproben wurden Veränderungen in der elektronischen Struktur durch die verringerte Dimensionalität bzw. das pseudomorphe Wachstum beobachtet.

[1] F. Müller et al., Surf. Sci. 520, 158 (2002)

[2] S.A. Krasnikov et al., Thin Solid Films 428, 201 (2003)

O 15.30 Fr 17:00 Poster TU D

**MOVPE growth analysed by in-situ SPM** — ●RAIMUND KREMWZOW, BERT RÄHMER, MARKUS BREUSING, MARKUS PRISTOVSEK, and WOLFGANG RICHTER — Technische Universität Berlin, IFP, Sekr. PN 6-1 Hardenbergstr. 36, 10623 Berlin

To get insight into the formation of nanostructures, an *in-situ* analysis of the sample morphology during the growth is highly desirable. Especially for the most common technique epitaxial method, (metalorganic vapour phase epitaxy – MOVPE). At present no tool exists which can measure the surface topography in real time and real space with high spatial resolution. We developed a specially designed SPM to deal with the limited space and high temperatures in the MOVPE reactor (caused by the thermal conductivity of the carrier gas). In addition, vibrational disturbances introduced by the pumping system and gas-flow had to be minimized. Another problem arises by the need not to disturb the actual layer growth. Therefore, the tip has to be longer than 2 cm in order to bridge the distance between liner tube and susceptor. The set-up we present, continuously tolerates sample and gas phase temperatures up to 550°C without degradation of the piezo elements.

O 15.31 Fr 17:00 Poster TU D

**Fabrication of well-defined nickel films on self-assembled monolayers** — ●YIAN TAI, ANDREY SHAPORENKO, WOLFGANG ECK, MICHAEL GRUNZE, and MICHAEL ZHARNIKOV — Angewandte Physikalische Chemie, Universität Heidelberg, Im Neuenheimer Feld 253, 69120 Heidelberg, Germany

Self-assembled monolayers (SAMs) suit well as model organic surfaces for metal evaporation experiments. In addition, the fabrication of metal wires on SAM surface is an important issue for future molecular electronics. The major difficulty in fabricating well-defined metallic films on the SAM surface is the penetration of metal atoms into the SAM and to the SAM-substrate interface. Taking nickel as a test adsorbate, we showed that this process can be partly suppressed through the fictionalization of SAMs with a reactive tail group. The full suppression has been achieved by a combination of the SAM fictionalization and electron-induced cross-linking of the molecular layer - a well-defined and stable nickel film on the SAM support could be fabricated. In addition, several interesting effects were observed including a non-homogeneous irradiation-induced cross-linking within a SAM and a drastic decrease in molecular tilt of the SAM constituents at the initial stage of the Ni deposition on thiol-terminated aromatic SAMs. The latter effect was attributed to the formation of Ni-thiol complexes at the SAM-ambient interface.

O 15.32 Fr 17:00 Poster TU D

**Spectroscopy and microscopy studies for the development of lithography with a monomolecular resist** — ●MICHAEL ZHARNIKOV<sup>1</sup>, ANDREY SHAPORENKO<sup>1</sup>, ANNE PAUL<sup>1</sup>, ARMIN GÖLZHÄUSER<sup>2</sup>, and ANDREAS SCHOLL<sup>3</sup> — <sup>1</sup>Angewandte Physikalische Chemie, Universität Heidelberg, Im Neuenheimer Feld 253, 69120 Heidelberg, Germany — <sup>2</sup>Physik Supramolekularer Systeme, Universität Bielefeld, Universitätsstr. 25, 33615 Bielefeld, Germany — <sup>3</sup>Advanced Light Source, Lawrence Berkeley National Laboratory, CA 94720, USA

Soft X-ray absorption microscopy was applied to image and characterize molecular patterns produced by electron irradiation of aliphatic and aromatic thiol-derived self-assembled monolayers (SAMs) on Au substrates. The measurements were performed at all relevant absorption edges. The fabricated patterns could be clearly imaged with a lateral resolution better than 150 nm, which, e.g., allowed to distinguish a fine structure of 1  $\mu$ m features. The X-ray absorption microspectra derived from different areas of the SAM patterns provided specific chemical information on pristine and irradiated areas, and unexpected features in these patterns. The quality of the microspectra is comparable with that of the analogous X-ray absorption spectra acquired with a standard equipment from homogeneous SAMs. In particular, a chemical transformation of the functional tail groups within the irradiated areas of the patterned aromatic SAMs could be directly monitored.

O 15.33 Fr 17:00 Poster TU D

**Ultra-thin hexaphenylene films grown on Au(111) and Au(433)** — ●STEFAN MÜLLEGGGER, AXEL STUPNIK, MANFRED LEISCH, and ADOLF WINKLER — Institute of Solid State Physics, Graz University of Technology, Austria.

The physical properties of ultra-thin films of organic semiconducting materials are to a great extent determined by their structure and morphology. This is important for both fundamental and applied research (e.g. organic thin film transistors, organic light emitting devices). We present experimental investigations on ultra-thin films of para-hexaphenylene (6P) grown by an organic molecular beam epitaxy (OMBE) technique on single crystalline Au(111) and vicinal Au(433) surfaces under ultra-high vacuum conditions. Founded on a variety of surface analytical techniques, e.g. low energy electron diffraction (LEED), thermal desorption spectroscopy (TDS), x-ray photoelectron spectroscopy (XPS) and scanning tunnelling microscopy (STM), several aspects are discussed, concerning the development of a highly regular structure of the first and second 6P monomolecular layer as well as the kinetics of adsorption and growth of several nm thick 6P films. Although 6P is considered chemically rather stable, experimental evidence for a strong dissociative behaviour of 6P adsorbed on the Au(111) surface at elevated temperatures is presented.

O 15.34 Fr 17:00 Poster TU D

**Stereochemistry of 2,3-butanediol adsorbed on Si(001) surfaces from first-principles calculations** — ●KAORI SEINO, WOLF G. SCHMIDT, and FRIEDHELM BECHSTEDT — Institut für Festkörpertheorie und -optik, Friedrich-Schiller-Universität Jena, Max-Wien-Platz 1, 07743 Jena, Germany

The formation of organic thin films on semiconductors allows for adding biological and chemical functionality to microelectronics. Therefore the microscopic details and electronic properties of the interfaces formed by the adsorption of organic molecules on inorganic substrates have become topics of intense research. Here we present results of *first-principles* calculations on the adsorption of 2,3-butanediol on Si(001) surfaces based on density-functional theory in generalized gradient approximation (DFT-GGA). 2,3-butanediol is one of the simplest diol molecules and thus a suitable model system, yet it has found interest in the context of forming chiral surfaces [1]. From our calculations we find that the effects of conformation, well-known to influence the stability of gas-phase molecules, are also important for the interface energetics. The electronic properties for the most relevant bonding configurations are discussed.

[1] J. W. Kim *et al.*, Surf. Sci. **559**, 179 (2004).

O 15.35 Fr 17:00 Poster TU D

**Einfluss des Substrates auf die optischen Eigenschaften von HBC-Moleküllagen** — ROMAN FORKER<sup>1</sup>, ROBERT NITSCHÉ<sup>1</sup>, ●THOMAS DIENEL<sup>1</sup>, KLAUS MÜLLEN<sup>2</sup>, KARL LEO<sup>1</sup> und TORSTEN FRITZ<sup>1</sup> — <sup>1</sup>Institut für Angewandte Photophysik, TU Dresden, Germany — <sup>2</sup>MPI für Polymerforschung, Ackermannweg 10, 55128 Mainz, Germany

Mit Hilfe der Differentiellen Reflexionsspektroskopie (DRS) wurden die optischen Konstanten von Hexa-peri-benzocoronon (HBC) in Abhängigkeit von der Schichtdicke *in situ* auf verschiedenen Substraten ermittelt. Der Messaufbau ermöglicht es, während des Schichtwachstums die Veränderung des optischen Spektrums von typischen Monomerenstrukturen hin zu Kristallstrukturen zu beobachten. Dabei zeigt HBC auf Glimmer für Submonolagen ein ähnliches spektrales Verhalten wie in Lösung, während es auf HOPG und Au(111) stark verbreiterte Monomerspektren aufweist. Frühere STM-Aufnahmen [1] lassen eine Verringerung der Molekülsymmetrie gegenüber dem freien HBC-Molekül vermuten, und es wird der Frage nachgegangen, ob dies zu zusätzlichen Peaks im  $\varepsilon_2$ -Spektrum führt.

[1] T. Schmitz-Hübsch *et al.*, Surf. Sci. **445**, 358 (2000).

O 15.36 Fr 17:00 Poster TU D

**Growth of thin polymer films: Monte Carlo simulations and experiments** — ●CHRISTIAN VREE<sup>1</sup>, JOHANNA RÖDER<sup>2</sup>, HANS-ULRICH KREBS<sup>2</sup>, and S. G. MAYR<sup>1</sup> — <sup>1</sup>I. Physikalisches Institut, Universität Göttingen — <sup>2</sup>Institut für Materialphysik, Universität Göttingen, Friedrich-Hund-Platz 1, 37077 Göttingen

Vapour deposition of thin polymer films was studied by Monte Carlo (MC) simulations and compared with experiments. In the MC simulations single chain molecules are deposited randomly on a lattice, on which they diffuse with the kinetic of the Reptation model. The dependence of roughness and morphology of the surface on film thickness, energy of deposited particles, relaxation time and chain length are investigated. Generally we observe a strong roughening, which starts abruptly at a critical thickness. In the experiment thin PMMA films were produced on a Si substrate using PLD and spin coating at room temperature. The

film surfaces were characterized by atomic force microscopy and scanning electron microscopy.

Differences and similarities of experiment and modelling as well as their possible reasons are discussed.

O 15.37 Fr 17:00 Poster TU D

**Influence of the Molecular Structure on the Interface Formation between Magnesium and Organic Semiconductors** — ●GIANINA GAVRILA<sup>1</sup>, MIHAELA GORGOI<sup>1</sup>, WALTER BRAUN<sup>2</sup>, and DIETRICH R.T. ZAHN<sup>1</sup> — <sup>1</sup>Institut für Physik, Technische Universität Chemnitz, D-09107, Chemnitz, Germany — <sup>2</sup>BESSY GmbH, Albert-Einstein-Straße 15, D-12489 Berlin, Germany

Magnesium is often used in organic devices as a low work function metal contact. On the other hand it is a highly reactive metal. Its reactivity may also depend of the detailed structure of organic molecules involved. Here, 15 nm thick films of perylene derivatives, i.e. 3,4,9,10-perylenetetracarboxylic dianhydride -PTCDA, 3,4,9,10-perylenetetracarboxylic diimide-PTCDI and dimethyl-3,4,9,10-perylenetetracarboxylic diimide-DiMe-PTCDI were deposited onto sulphur passivated GaAs substrates. A detailed study of the interface formation between these materials and Mg using high resolution photoemission spectroscopy is presented. The differences observed in the evolution of C1s, O1s, N1s and Mg2p core levels and valence band spectra as a function of Mg thickness differences are related to the distinct molecular end groups and with the degree to which the metal atoms diffuse into the layer.

O 15.38 Fr 17:00 Poster TU D

**Selbstorganisierte Monolagen durch redox-aktives Bis(diphenyl-phosphan)ferrocen: Untersuchungen mit optischer Frequenzverdopplung** — ●B. KROHN<sup>1</sup>, T. AUCH<sup>2</sup>, T. WEIDNER<sup>1</sup>, U. SIEMELING<sup>2</sup>, and F. TRÄGER<sup>1</sup> — <sup>1</sup>Institut für Physik, Universität Kassel, Heinrich-Plett-Str.40, 34132 Kassel — <sup>2</sup>Institut für Chemie, Universität Kassel, Heinrich-Plett-Str.40, 34132 Kassel

Thiol- und Sulfidderivate sind heute die am besten untersuchten und vielversprechendsten Kandidaten für selbstorganisierte Monolagen auf Goldoberflächen.

Doch auch Phosphane zeigen vielfältige Wechselwirkungen mit Gold. Einer der interessantesten Kandidaten unter ihnen ist das 1,1'-Bis(diphenylphosphan)ferrocen (DPPF). Es spielt wegen seiner katalytischen Eigenschaften in der chemischen Synthese eine übergeordnete Rolle. Während seine vielseitige Komplexchemie im Hinblick auf atomares Gold bereits gründlich untersucht ist, wird das Grenzflächenverhalten von DPPF hier erstmalig beschrieben.

Wir haben die Adsorptionsdynamik auf Gold mit optischer Frequenzverdopplung *in situ* und in Echtzeit verfolgt. Es zeigt sich, dass DPPF einen hervorragenden Baustein zur Präparation redox-aktiver monomolekularer Schichten auf Goldoberflächen darstellt.

O 15.39 Fr 17:00 Poster TU D

**Energy and time resolved coherent x-ray reflectivity from a smooth polymer film** — ●GUDRUN GLEBER, TOBIAS PANZNER, and ULLRICH PIETSCH — Institut für Physik, Universität Potsdam, Am Neuen Palais 10, D-14415 Posdam

Since recent years, x-ray-photon-correlation-spectroscopy is used for the investigation of time depending processes in thin films. Up to now these experiments are performed using single wavelengths.

Recently we have shown that a pink beam provided by the white beam beamline at Bessy II can be exploited for coherence experiments [1]. Here we present, for the first time, time resolved reflectivity measurements from thin polymer films using white synchrotron radiation. The advantage of this approach is the fact, that one can measure simultaneously the time correlation at different values of the momentum transfer.

In particular we have investigated the melting of a polymer film on a silicon substrate as a first example for this new kind of measurements. In detail we will show the extracted autocorrelation functions at temperatures below and above the glass temperature of the polymer film.

[1] W. Leitenberger *et al.* Physica B 2004

O 15.40 Fr 17:00 Poster TU D

**A multi-parameter Ising model for the adsorption of molecules on structured surfaces** — ●CARSTEN OLBRICH<sup>1</sup>, KLAUS MORAWETZ<sup>1</sup>, SIBYLLE GEMMING<sup>1,2</sup>, REINHARD SCHOLZ<sup>1</sup>, MICHAEL SCHREIBER<sup>1</sup>, REGINA ERMICH<sup>2</sup>, and GOTTHARD SEIFERT<sup>2</sup> — <sup>1</sup>Institut für Physik, Technische Universität, D-09107 Chemnitz — <sup>2</sup>Institut für Physikalische Chemie, Technische Universität, D-01062 Dresden

Several modifications of the standard two-parameter Ising model are necessary for the mesoscopic modelling of a realistic adsorbate ensemble on a non-ideal substrate. Depending on the shape of the molecule, the nearest-neighbour coupling exhibits a directionality, and also additional coupling terms with next nearest neighbours are taken into account. Structured or defective surfaces are modelled by local modifications of the magnetisation term. Several sets of coupling parameters were derived from first-principles calculations on PTCDA monomer, dimer, and adsorbate systems. The adsorbate distribution on the surface was investigated by Metropolis-Monte-Carlo simulations and cluster statistics employing the Hoshen-Kopelman cluster recognition algorithm. It was observed that surfacedefects like steps influence the pattern formation mainly close to the critical temperature of the order-disorder transition. It could be shown that all adsorbate-adsorbate interactions are connected by a straightforward scaling in the critical temperature, whereas the adsorbate-substrate interaction is of a more complicated nature, especially in the presence of surface defects.

O 15.41 Fr 17:00 Poster TU D

**In-situ X-ray Diffraction study of organic-organic heterostructures of Diindenoperylene and copper-hexadecafluorophthalocyanine** — ●ESTHER BARRENA<sup>1</sup>, DIMAS GARCÍA DE OTEYZA<sup>1</sup>, J. ORIOL OSSÓ<sup>2</sup>, STEFAN SELLNER<sup>1</sup>, and HELMUT DOSCH<sup>1,3</sup> — <sup>1</sup>Max-Planck-Institut für Metallforschung, Heisenbergstr.3, 70569 Stuttgart, Germany — <sup>2</sup>Institut de Ciència de Materials de Barcelona CSIC, 08190 Bellaterra, Spain — <sup>3</sup>Institut für Theoretische und Angewandte Physik, Universität Stuttgart, 70550 Stuttgart, Germany

Many organic devices like Light-Emitting Diodes (OLEDs), solar cells or ambipolar transistors are based on p-n junctions of organic semiconductors. Here we present an in-situ X-ray diffraction study of the structure of bilayers of Diindenoperylene (DIP) and copper-hexadecafluorophthalocyanine (F16PcCu), p-type and n-type semiconductors, respectively. The molecular films have been grown at different temperatures on silicon oxide by Organic Molecular Beam Deposition. We show that DIP on F16PcCu grows in the Stransky-Krastanov growth mode at 120°C. Interestingly, a change in the F16CuPc structure at the organic-organic interface is induced. At 25°C and -10°C, DIP molecules form a well ordered film and no structural rearrangement of F16PcCu is observed. For bilayers grown in the inverse order, i.e. F16CuPc on DIP, changes on the F16CuPc structure are observed as well. Complementary studies by AFM support the results.

O 15.42 Fr 17:00 Poster TU D

**Laser induced local decomposition of octadecylsiloxane monolayers: Patterning in an ultra-high vacuum environment** — ●RAFAEL BAUTISTA MESTER, THORSTEN BALGAR, NILS HARTMANN and ECKART HASSELBRINK — Universität Duisburg-Essen, Campus Essen, Fachbereich Chemie, Universitätsstr. 5, 45141 Essen

A procedure for direct patterning of octadecylsiloxane (ODS) monolayers has been developed. Silicon substrates were coated with ODS in a millimolar solution of octadecyltrichlorosilane [1]. Subsequently, patterning was carried out at ambient conditions using a highly focused laser beam of an argon ion laser operated at 514 nm [2]. In order to investigate the specific role of oxygen and water in the overall patterning process additional experiments were carried out at well-defined conditions in an ultra-high vacuum environment. Similar to the results at ambient conditions here structures with lateral dimensions well below the laser spot diameter can be prepared. A general mechanism of the patterning process is discussed.

[1] Th. Balgar, R. Bautista, N. Hartmann and E. Hasselbrink, Surf. Sci. 532-535 (2003) 963.

[2] N. Hartmann, Th. Balgar, R. Bautista, S. Franzka and E. Hasselbrink, Proc. SPIE 5223 (2003) 9.

O 15.43 Fr 17:00 Poster TU D

**Combined Normal and Torsional NC-AFM Measurements: PTCDA on KBr(001)** — ●TOBIAS KUNSTMANN, ANDREAS SCHLARB, and ROLF MÖLLER — Universität Duisburg-Essen, D-45141 Essen, Germany

Dissipative lateral forces provide the main contribution to friction. To measure these forces the tip has to move parallel to the surfaces. This can be achieved either by using the "q-plus sensor" [1], or torsional modes of a cantilever [2]. The normal and torsional modes of a commercially available cantilever have been excited simultaneously. For our measurements we have used the frequency shift ( $\Delta f$ ) of the normal mode to control the tip sample distance. Additionally the energy dissipated in the normal mode has been recorded. The frequency shift and the damping of the lateral oscillation were measured independently providing the conservative as well as the dissipative lateral forces. The experiments have been performed on PTCDA on a KBr(001) surface. While the dissipation in normal mode does not show a difference between plain KBr and PTCDA-crystallites, the dissipation for the torsional mode shows a significant increase on top of the PTCDA islands.

This work was funded by the SFB616 "Energy dissipation at surfaces" of the Deutsche Forschungsgemeinschaft.

[1] F.J.Giessibl et al., Proc. Nat. Acad. Sci. US 99 (19), 12006 (2002)

[2] O. Pfeiffer et al., Phys. Rev. B 65 (16), 161403 (2002)

O 15.44 Fr 17:00 Poster TU D

**NMR and XAFS Investigation of the Structure of Mo(allyl)<sub>4</sub> Followed by Wet Chemical Deposition of the Complex on a Thin Al<sub>2</sub>O<sub>3</sub> Film and Subsequent Characterisation Using XPS** — ●KARIFALA DUMBUYA<sup>1</sup>, SVEN SCHROEDER<sup>2</sup>, NORBERT WEIHER<sup>2</sup>, KLAUS CHRISTMANN<sup>1</sup>, and TAL PERRY<sup>1</sup> — <sup>1</sup>Free University Berlin, Institute of Chemistry, Department of Physical and Theoretical Chemistry, Takustrasse 3, 14195 Berlin — <sup>2</sup>University of Manchester, School of Chemical Engineering and School of Chemistry, PO Box 88 Sackville Street, Manchester M 60 1 QD, UK

We report the synthesis and structural elucidation of Mo(C<sub>3</sub>H<sub>5</sub>)<sub>4</sub> using solid and liquid state NMR (13C, 1H) and XAFS of the complex in solution. The NMR results agree remarkably well with previous work with the 1H showing five resonances (four doublets and a multiplet) indicating five different protons. The 13C also revealed three different carbons, suggesting that all four allyl groups are equivalent. To our knowledge, this is the first attempt at solid state NMR study on this complex. XAFS investigation of the Mo k-edge revealed a coordination number of 3.6 for molybdenum in the first coordination shell, i.e., an average of 11 C-atoms. The average Mo-C distance was 2.35 Å, a value which compares well with Mo-C distances in related molybdenum complexes and supports the case for a symmetrical pi-allyl system. Deposition of the complex from a solution of pentane on a freshly prepared Al<sub>2</sub>O<sub>3</sub> surface in ultra high Vacuum with the help of a specially designed transfer cell proved very successful, albeit significant silicon contamination. Investigation of the contaminant is in progress.

O 15.45 Fr 17:00 Poster TU D

**Surface Structures and Atomic Details of CeO<sub>2</sub>(111) revealed by Dynamic Force Microscopy** — ●S. GRITSCHNEDER<sup>1</sup>, Y. NAMAI<sup>2</sup>, Y. IWASAWA<sup>2</sup>, and M. REICHLING<sup>1</sup> — <sup>1</sup>Fachbereich Physik, Universität Osnabrück, Barbarastrasse 7, 49076 Osnabrück, Germany — <sup>2</sup>Department of Chemistry, The University of Tokyo, 7-3-1 Hongo, Bunkyo-ku, Tokyo 113-0033, Japan

Ceriumdioxide is a catalytically active material with unique properties that allow it to store and release oxygen. It is highly interesting to analyse this catalytic surface on the atomic level to gain an in-depth understanding of the involved chemical processes and help to establish structure-function relationships for catalysis. In this contribution we present highly resolved images and atomic details of surface features on CeO<sub>2</sub>(111) like terrace structures, step edges, kinks and hexagonally shaped pits that are naturally formed during surface preparation by sputtering and annealing cycles. We find that such structures can well be imaged with atomic resolution and exhibit a morphological characteristics that is in details significantly different from that of cleaved CaF<sub>2</sub>(111), a surface with exactly the same crystallographic structure and a very similar lattice constant and ionic radii. We demonstrate that the non-contact, constant-height mode is the preferable mode of operation for dynamic force microscopy imaging at room temperature as it allows maximum resolution and undesired regulation artefacts can be minimized by carefully choosing scanning parameters, like detuning, scanning speed, and the gain of

the distance regulation loop.

O 15.46 Fr 17:00 Poster TU D

**Investigation of the  $\text{La}_{0.7}\text{Sr}_{0.3}\text{MnO}_3/\text{SrTiO}_3(100)$ -interface by X-ray photoelectron spectroscopy under optical excitation** — ●ELKE BEYREUTHER<sup>1</sup>, STEFAN GRAFSTRÖM<sup>1</sup>, CHRISTIAN THIELE<sup>2</sup>, KATHRIN DÖRR<sup>2</sup>, and LUKAS ENG<sup>1</sup> — <sup>1</sup>Institut für Angewandte Photo-physik, Technische Universität Dresden, D-01062 Dresden — <sup>2</sup>IFW Dresden, Postfach 270116, D-01171 Dresden

The functional properties (conductivity, spin polarisation) of layered perovskite structures are crucially influenced by the electronic state distribution at internal interfaces.

The shift of an X-ray photoelectron spectrum under simultaneous optical excitation in the ultraviolet and visible range is equivalent to a surface photovoltage (SPV) and hence provides information about electronic surface and interface states, barrier heights and relaxation times. So far, semiconductor surfaces as well as the interface between organic films and semiconducting or metallic substrates have been characterized successfully by the technique [1].

Here, we report on SPV measurements on epitaxially grown 15 nm thick  $\text{La}_{0.7}\text{Sr}_{0.3}\text{MnO}_3$  layers on undoped and Nb-doped  $\text{SrTiO}_3(100)$  substrates. The plot of the SPV versus the excitation wavelength reflects the absorption characteristics of the substrate and reveals a continuous distribution of interface states in the sub-bandgap range. The interpretation of the results within the Schottky theory of classical metal-semiconductor contacts is discussed critically.

[1] S. Teich *et al.*, Surf. Sci. **552**, 77-84 (2004)

O 15.47 Fr 17:00 Poster TU D

**Growth and electronic structure of epitaxial  $\text{Ba}_{0.7}\text{Sr}_{0.3}\text{O}$  layers on the Si(001) surface** — ●ANDREAS GERDES, JAN ZACHARIAE, and HERBERT PFNÜR — Institut für Festkörperphysik, Universität Hannover, Appelstr. 2, 30167 Hannover

We investigated the growth conditions, crystalline quality and stoichiometry of the medium  $k$  ( $\epsilon_r \approx 30$ )  $\text{Ba}_{0.7}\text{Sr}_{0.3}\text{O}$  films using high resolution LEED, UPS, XPS and EELS. Lattice matched  $\text{Ba}_{0.7}\text{Sr}_{0.3}\text{O}$  layers were grown on an intermediate layer on the Si(001) substrate in UHV by evaporation of the metals in an ambient oxygen pressure. The quality of oxide layers depends on two conditions: the kind of the intermediate layer and the accurate oxygen dose, which was determined by mass accumulation on a quartz crystal micro balance. A correct fraction of Ba and Sr in the mixed oxide layers leads to well ordered and lattice matched oxide films from a few monolayers up to 20 nm and more. To obtain monocry-stalline  $\text{Ba}_{0.7}\text{Sr}_{0.3}\text{O}$  layers, although of different quality, it is necessary to start the growth on one of the three following types of intermediate layers: strontium silicide layers  $\Theta \leq 1$  ML grown at  $T \geq 750^\circ\text{C}$ , strontium metal layers  $\Theta > 1$  ML grown at  $T \leq 650^\circ\text{C}$  and the silicate layers (1 ML of  $\text{Sr}_2\text{SiO}_4$ ). The electronic structure, surface roughness and interface oxidation for the growth on different intermediate layers will be discussed. First results of the growth of  $\text{Ba}_{0.7}\text{Sr}_{0.3}\text{O}$  on vicinal Si(001) surfaces to generate a stepped insulator surface and the formation mechanism of surface F-centers will also be presented.

O 15.48 Fr 17:00 Poster TU D

**Charged and non-charged surface defects on NiO(001) investigated by AFM** — ●UWE KAISER, NICO PLOCK, ALEXANDER SCHWARZ, and ROLAND WIESENDANGER — Institut für Angewandte Physik, Universität Hamburg, Jungiusstr. 11, 20355 Hamburg

Surface defects of transition-metal oxides like NiO are important for their catalytic behavior as they strongly enhance the reactivity of the surface. In this study, we investigated the (001)-surface of NiO under UHV-conditions with our home-built atomic force microscope. Typical AFM-images show flat terraces of monatomic height with widths of some ten nanometers. The image quality strongly depends on the tip condition, which could be improved by repeatedly touching the surface with the tip. With such tips, it was possible to detect extended vacancy-islands and point defects down to the atomic scale. The circumferences of some of the vacancies appear elevated, while others do not show this specific feature. In some cases, very faint elevated circular contrasts on terraces can be found without the presence of a vacancy. As ionic crystals can trap charges like electrons in positively charged vacancy sites, these different contrasts can be interpreted as differently charged vacancies at or just below the surface.

O 15.49 Fr 17:00 Poster TU D

**Surface and Interface Structures of  $\text{ZrO}_2(111)$  Films on Pt(111)** — ●K. MEINEL<sup>1</sup>, A. EICHLER<sup>2</sup>, K.-M. SCHINDLER<sup>1</sup>, H. NEDDERMEYER<sup>1</sup>, and W. WIDDRÄ<sup>1</sup> — <sup>1</sup>Martin-Luther-Universität Halle-Wittenberg, FB Physik, D-06099 Halle, Germany — <sup>2</sup>Institut für Materialphysik und Center for Computational Material Science, Universität Wien, Sensengasse 8/12, A-1090 Wien, Austria

$\text{ZrO}_2$  films are prepared on Pt(111) by reactive deposition of Zr in an  $\text{O}_2$  atmosphere followed by post-annealing and characterized by STM, LEED and DFT calculations. After deposition, the films display a slightly rotated  $p(1 \times 1)$  structure. Post-annealing of submonolayer films yields  $\text{ZrO}_2$  films having a slightly compressed  $(4 \times 4)$  structure, which is commensurate to a  $(5 \times 5)$  structure of the Pt(111) interface. Post-annealing of thicker films yields a  $(2 \times 2)$  structure, which is slightly expanded and commensurate to a  $(\sqrt{7} \times \sqrt{7})$  structure of the Pt(111) interface. Continuing the annealing induces the formation of domains possessing a  $(1 \times 1)$  structure rotated by  $\pm 6.6^\circ$ . These domains are energetically favored and grow at the expense of the  $(2 \times 2)$  areas. With the film rotation, a  $(3\sqrt{3} \times 3\sqrt{3})$  film structure develops, which is slightly compressed and commensurate to a rotated  $(\sqrt{19} \times \sqrt{19})R \pm 36.6^\circ$  structure of the Pt(111) interface. High temperature annealing ( $T > 1200$  K) finally yields incommensurate structures of expected  $\text{Zr}_x\text{O}_y\text{Pt}_z$  phases.

O 15.50 Fr 17:00 Poster TU D

**Thick Titanium Oxide Films by Unfiltered Arc Deposition** — ●PETER DRECHSLER and ROGER THULL — Abteilung für Funktionswerkstoffe der Medizin und Zahnheilkunde, Universitätsklinikum Würzburg, Pleicherwall 2, 97070 Würzburg

Thick titanium oxide (Rutile) films have attractive properties like good blood compatibility and good corrosion resistance which are very suitable for medical implants. A sufficient thickness supplies the essential wear resistance.

The presented titanium oxide films are deposited by means of unfiltered arc sputtering technique on polycrystalline titanium and steel surfaces. The film thickness is 3–6 microns depending on the deposition time with a deposition rate of 4 microns/hour. The substrate temperature was varied from room temperature to 870 K. The ratio of the anatase to rutile phases depends on the substrate temperature as XRD measurements revealed. Above 670 K no anatase phase could be found. The polycrystalline rutile films grew predominately in (110)-direction.

The optical band gap of the rutile films was measured by means of UV-VIS spectroscopy. The band gap was found at  $3.00 \pm 0.02$  eV with low variation with the film thickness.

O 15.51 Fr 17:00 Poster TU D

**Applications of High Speed Scanning Capacitance Spectroscopy for the analysis of semiconductor microdevices** — ●MARTIN VON SPREKELSEN and ROLAND WIESENDANGER — University of Hamburg, Institute of Applied Physics and Microstructure Research Center, Jungiusstrasse 11, D-20355 Hamburg, Germany

High spatial resolution down to the nanometer scale becomes essential for analytical tools for semiconductor devices. On the other hand, in the semiconductor industry, scanning capacitance microscopy (SCM) is an established analytical method to obtain 2D-dopant profiles of charge carrier concentrations; these profiles are usually taken at a constant bias voltage ( $V_{\text{bias}}$ ). However the spatial resolution of SCM is limited by unavoidable side effects such as mobile surface charges or the strong influence of  $V_{\text{bias}}$  on the SCM profiles. To overcome these restrictions, we develop High-speed Scanning Capacitance Spectroscopy (HSSCS) which is performed by modulating the  $V_{\text{bias}}$  voltage at a frequency in the kHz-range. The modulated electric field virtually traps mobile surface charges. Furthermore, the highspeed method allows us to measure capacitance spectra for  $V_{\text{bias}}$ , by which we can analytically get rid of the influence of  $V_{\text{bias}}$ .

We present HSSCS dopant profiles on Si-semiconductor samples of ultra-shallow junctions with high resolution down to 10 nm. Further results of HSSCS on III-V-semiconductors samples are also discussed.

O 15.52 Fr 17:00 Poster TU D

**Influence on alkali dopants on  $\text{V}_2\text{O}_5$ . DFT cluster model studies.** — ●MALGORZATA WITKO and ROBERT GRZYBOS — Institute of Catalysis and Surface Chemistry, PAS, ul. Niezapominajek 8, 30 239 Kraków, Poland

Selectivity to partially oxidized products in oxidative dehydrogenation (ODH) depends on basicity of the surface (nucleophilicity of oxygen atoms). From the experiment it is known that alkali metal dopants change the

basicity of the surface and thus influence the selectivity. To understand the role of alkali additives on the behavior of the (010)V<sub>2</sub>O<sub>5</sub> surface cluster DFT calculations are carried out. Alkali metal is approach to the surface and its position is optimized. Changes in electronic structures for systems without and with alkali are discussed in terms of electronic structure, electrostatic potentials and total energy of the systems. It is found that alkali adsorbs on the surface in the "hole" site between four vanadyl oxygen atoms sticking out of the surface. Only slightly less favored site is the "hole" between four bridging oxygen atoms. Alkali metal transfers an electron to the empty d-band of vanadium ions leading to its reduction. Through a polarization effect the negative charge accumulates on O atoms increasing their nucleophilicity, however this influence is very short-range. As a result, the oxygen atoms affected by dopant are at the same time blocked by them. Blocking of the most active sites may be the main reason behind increased selectivity of doped catalyst.

O 15.53 Fr 17:00 Poster TU D

**Effect of support and additives on properties of molybdena-based catalysts.** — ●RENATA TOKARZ-SOBIERAJ and MALGORZATA WITKO — Institute of Catalysis and Surface Chemistry, PAS, ul. Niezapominajek 8, 30 239 Kraków, Poland

Molybdenum oxide-based catalysts are active and selective in many reactions of very different types e.g. selective oxidation, oxidative dehydrogenation. The catalytic properties of such catalysts strongly depend on acid-base properties of catalysts surfaces, which determine the strength of surface-substrate interactions and facilitate the desorption of products from the surface. Experiment shows that acid-base properties of an oxide catalyst can be controlled by the introduction of additives or usage of different supports. In the present work, the effect of additives (K, Ni, Cr, Pt) and effect of the support (SiO<sub>2</sub>, Al<sub>2</sub>O<sub>3</sub>, TiO<sub>2</sub>, MgO) on the electronic and geometric structures is discussed by means of quantum chemical calculations based on the density functional theory (DFT), using cluster model. Theoretical data shows that substitution of molybdenum atom(s) in the cluster by additive atoms or atoms from different supports changes the local electronic state and, what follows, the local reactivity of different surface oxygen sites (Mo=O and Mo-O-X) that are present at the catalyst surface. The results of calculations are compared with the experimental findings.

O 15.54 Fr 17:00 Poster TU D

**Simulations of Analogue Control Circuits for the Dynamic Scanning Force Microscope** — ●REBECCA KASTEBO and MICHAEL REICHLING — Fachbereich Physik, Osnabrück Universität, Barbarastr.7, 49069 Osnabrück

We study the behaviour of an analogue control circuit presently used in our dynamic scanning force microscope (SFM) by performing simulations of the circuit in the framework of a SPICE program. We devote our simulations to the separation regulator circuit which is responsible for controlling the distance between the cantilever and the sample. In detail, we investigate the response time and the stability conditions in order to avoid oscillations in the circuit, which may cause damage to both, the cantilever and the sample. We compare the results of our simulation to tests performed on the physical circuit of the SFM. It is the aim to optimise the circuits and control parameters depending on the experimental conditions, i.e. the sample and the imaging goal.

O 15.55 Fr 17:00 Poster TU D

**Testing SFM-Cantilevers in the Ultra-High Vacuum** — ●HEINER LINDEMANN, LUTZ TRÖGER, SEBASTIAN GRITSCHNER, and MICHAEL REICHLING — Fachbereich Physik, Universität Osnabrück, Barbarastr. 7, D-49076 Osnabrück

For taking high-resolution images with a dynamic scanning force microscope (SFM) operated in the so-called non-contact mode, cantilevers with a high Q-factor (about 100.000) are required, i.e. the response function should exhibit a very narrow peak. When detecting the oscillation with a light source operating in the infrared ( $\lambda \sim 800\text{nm}$  or higher), it is essential to use reflex-coated cantilevers as in this wavelength region the material of the cantilever (silicon) is nearly transparent. The reflex-coating, however, decreases the effective Q of the cantilever.

To determine the Q-factor before installing the cantilever into the SFM, cantilevers are tested in a separate ultra-high vacuum (UHV). We designed a setup where cantilevers of different SFM types can be fixed to measure the response function. We describe the design of the test station including a laser light source, a four-quadrants-photodiode and electronics to detect the oscillation of the cantilever that is excited by a piezo ceramic and present testing results obtained with various types of can-

tilevers.

O 15.56 Fr 17:00 Poster TU D

**Detailed analysis of the response characteristic of a dynamic scanning force microscopy feedback control system** — ●FRANK OSTENDORF, SABINE HIRTH, and MICHAEL REICHLING — Fachbereich Physik, Universität Osnabrück, Barbarastr. 7, 49076 Osnabrück

To obtain high resolution dynamic scanning force microscopy (SFM) images, the understanding and optimisation of the feedback control system is very important. Therefore, we analysed in detail the response characteristic of our electronic circuits. A typical feedback control system for dynamic SFM consist of three independent loops: amplitude control, demodulation control, and distance control. These three loops were analysed by means of a measurement simulation and under realistic imaging conditions. By optimising various components of the feedback control system, we enhance the signal-to-noise-ratio and improve SFM imaging stability.

O 15.57 Fr 17:00 Poster TU D

**Development of a high-resolution SFM for use in a UHV cryogenic temperature environment** — ●LUTZ TRÖGER und MICHAEL REICHLING — Universität Osnabrück, Barbarastr. 7, 49076 Osnabrück

We describe the development of a high-resolution SFM for use in a UHV cryogenic temperature environment. The design concept aims at highest resolution studies and is optimised for atomic precision force spectroscopy. The microscope utilises a laser interferometer for cantilever oscillation detection and an integrated eddy current damping stage to reduce mechanical noise. Additionally the commercial LHe/LN<sub>2</sub>-bath-cryostat providing the cooling is equipped with a second stage of external kinematic vibration damping. We demonstrate the capability of the detection and scanning system and show first test measurements concerning mechanical stability and functionality.

O 15.58 Fr 17:00 Poster TU D

**Lokal aufgelöste berührungslose Leitfähigkeitsmessungen (Wirbelstrommikroskopie)** — ●TINO ROLL, MARTIN GÖRLICH und MARIKA SCHLEBERGER — Universität Duisburg-Essen, Fachbereich Physik, 45117 Essen

Bei der Wirbelstrommikroskopie wird ein Rasterkraftmikroskop mit einem magnetischen AFM-Cantilever im non-contact-Modus betrieben. Dessen Oszillation führt zu Wirbelströmen in leitenden Materialien. Aufgrund dieser Wirbelströme kommt es zu einer zusätzlichen Wechselwirkung zwischen Spitze und Probe. Die Dämpfung der Cantilever-Oszillation dient als Messgröße für die mikroskopische Leitfähigkeit der Probe, das heißt Flächen konstanter Dämpfung entsprechen Flächen konstanter Leitfähigkeit. Ebenso ist es möglich, magnetische Domänen mit Hilfe leitender oszillierender AFM-Spitzen abzubilden. Experimentelle Daten zeigen, dass die Wirbelstrommikroskopie eine geeignete Methode zur Untersuchung der Leitfähigkeit ohne Kontakt zur Oberfläche ist.

O 15.59 Fr 17:00 Poster TU D

**Construction of an Atomic Force Microscope combined with a Field Ion Microscope** — ●DANIEL BRAUN, ANDRÉ SCHIRMEISEN, HENDRIK HÖLSCHER, and HARALD FUCHS — Physikalisches Institut, WWU Münster, Wilhelm-Klemm-Str. 10, 48149 Münster

While the atomic force microscope (AFM) is capable of resolving surfaces with atomic resolution, the exact configuration of the tip is entirely unknown. But it is necessary to know the exact position and identity of the tip atoms to understand the contrast mechanisms in atomic force microscopy. A method that allows to determine the position of the tip atoms with atomic precision is the field ion microscope (FIM).

We build an AFM according to a design previously published [1] for operation at low temperatures under an ultra high vacuum (UHV) conditions. The construction of the microscope body features a very high mechanical stability that makes an external damping mechanism unnecessary. The original design uses a silicon cantilever as the force sensor; its bending is detected by an optical interferometer. However, it is very difficult to use conventional silicon tips in a FIM. Therefore we intend to use a tuning fork [2], which allows us to use an appropriate material, e.g. tungsten, as the tip material of the force sensor. Our goal is to investigate how the contrast mechanism in AFM is influenced by the exact geometry of the last atoms of the tip.

[1] W. Allers et al., Rev. Sci. Instrum. 69 (1998) 221

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

O 15.60 Fr 17:00 Poster TU D

**An approach on near-field Raman spectroscopy using the tetrahedral SNOM tip** — ●STEFAN KLEIN<sup>1</sup>, ULRICH FISCHER<sup>1</sup>, DANIEL MOLEND<sup>1</sup>, HARALD FUCHS<sup>1</sup>, and MICHAEL HIETSCHOLD<sup>2</sup> — <sup>1</sup>Physikalisches Institut, Westfälische-Wilhelms-Universität Münster, Wilhelm-Klemm-Str. 10, D-48149 Münster — <sup>2</sup>Institut für Physik, TU Chemnitz, D-09107 Chemnitz

The effect of field enhancement at nanoscale metallic structures is critical to optical phenomena such as surface-enhanced Raman scattering (SERS). Assemblies of coupled metal nanoparticles attracted high interest as SERS active systems supporting so called hot-spots of the electric field. Most recently tip-enhanced Raman scattering (TERS), where a metallic tip is situated near a smooth surface covered by Raman active species has been reported. The experimental results show, that only a small amount of molecules in the near-field of the laser irradiated tip-apex contributes to an observed characteristic Raman spectrum. The tip acts in these experiments similar to a single particle supporting a single hot-spot, which enhances the incident electric field. Different experimental approaches on TERS have been realized using metal coated AFM cantilevers or STM tips. Here we present an approach on near-field Raman spectroscopy using the tetrahedral SNOM tip to investigate molecular monolayers on gold films.

O 15.61 Fr 17:00 Poster TU D

**Accuracy and Resolution Limits of Kelvin Probe Force Microscopy** — ●CHRISTIAN LOPPACHER, ULRICH ZERWECK, TOBIAS OTTO, STEFAN GRAFSTRÖM, and LUKAS ENG — Institut für Angewandte Photophysik, Technische Universität Dresden, D-01062 Dresden

Kelvin probe force microscopy is a scanning probe technique capable of mapping the local surface potential or workfunction on various surfaces with high spatial resolution. This technique can be realized on the basis of either an amplitude-sensitive method or a frequency modulation method, which are sensitive to the electrostatic force and its gradient, respectively. We present a detailed experimental and theoretical study of the accuracy and resolution provided by the two methods, including a novel setup for the frequency modulation technique. Au(111) with a submonolayer coverage of KCl serves as a test sample exhibiting extended sharply bounded areas that differ in workfunction by an amount well known from ultraviolet photoelectron spectroscopy. The experimental results are compared with the predictions of a numerical simulation based on a realistic model for the tip-sample geometry. Good agreement is found. The experimental analysis allows us to specify the lateral, vertical and potential resolution that can be achieved with the two methods for a given tip size. Our work clearly proves that the frequency modulation method is preferable in most applications because it (i) provides much higher lateral resolution, (ii) yields quantitative surface potential values on areas larger than the tip radius, and (iii) is little affected by variations of the tip-sample distance during topographic imaging.

O 15.62 Fr 17:00 Poster TU D

**Accuracy and Resolution Limits of Kelvin Probe Force Microscopy** — ●CHRISTIAN LOPPACHER, ULRICH ZERWECK, TOBIAS OTTO, STEFAN GRAFSTRÖM, and LUKAS ENG — Institut für Angewandte Photophysik, Technische Universität Dresden, D-01062 Dresden

Kelvin probe force microscopy is a scanning probe technique capable of mapping the local surface potential or workfunction on various surfaces with high spatial resolution. This technique can be realized on the basis of either an amplitude-sensitive method or a frequency modulation method, which are sensitive to the electrostatic force and its gradient, respectively. We present a detailed experimental and theoretical study of the accuracy and resolution provided by the two methods, including a novel setup for the frequency modulation technique. Au(111) with a submonolayer coverage of KCl serves as a test sample exhibiting extended sharply bounded areas that differ in workfunction by an amount well known from ultraviolet photoelectron spectroscopy. The experimental results are compared with the predictions of a numerical simulation based on a realistic model for the tip-sample geometry. Good agreement is found. The experimental analysis allows us to specify the lateral, vertical and potential resolution that can be achieved with the two methods for a given tip size. Our work clearly proves that the frequency modulation method is preferable in most applications because it (i) provides much higher lateral resolution, (ii) yields quantitative surface potential values on areas larger than the tip radius, and (iii) is little affected by variations of the tip-sample distance during topographic imaging.

O 15.63 Fr 17:00 Poster TU D

**Accuracy and Resolution Limits of Kelvin Probe Force Microscopy** — ●CHRISTIAN LOPPACHER, ULRICH ZERWECK und STEFAN GRAFSTRÖM — Institut für Angewandte Photophysik, Technische Universität Dresden, D-01062 Dresden

Kelvin probe force microscopy is a scanning probe technique capable of mapping the local surface potential or workfunction on various surfaces with high spatial resolution. This technique can be realized on the basis of either an amplitude-sensitive method or a frequency modulation method, which are sensitive to the electrostatic force and its gradient, respectively. We present a detailed experimental and theoretical study of the accuracy and resolution provided by the two methods, including a novel setup for the frequency modulation technique. Au(111) with a submonolayer coverage of KCl serves as a test sample exhibiting extended sharply bounded areas that differ in workfunction by an amount well known from ultraviolet photoelectron spectroscopy. The experimental results are compared with the predictions of a numerical simulation based on a realistic model for the tip-sample geometry. Good agreement is found. The experimental analysis allows us to specify the lateral, vertical and potential resolution that can be achieved with the two methods for a given tip size. Our work clearly proves that the frequency modulation method is preferable in most applications because it (i) provides much higher lateral resolution, (ii) yields quantitative surface potential values on areas larger than the tip radius, and (iii) is little affected by variations of the tip-sample distance during topographic imaging.

O 15.64 Fr 17:00 Poster TU D

**Formation of Ag islands on Ag(111) using atomic force microscopy in the dynamic mode** — MICHAELA ZEYER-DÜSTERER, ●RENE SCHMIDT, ALEXANDER SCHWARZ, and ROLAND WIESEN-DANGER — Institut für Angewandte Physik, Universität Hamburg, Jungiusstr. 11, 20355 Hamburg

Ag vacancy and adatom islands on Ag(111) have been frequently regarded as a test system to study the growth and dynamics of 2D-nanostructures. Conventionally, such structures are created by argon ion bombardment and subsequent heating. However, in this study we utilized atomic force microscopy in the dynamic mode to create and image vacancy and adatom islands on flat Ag(111) terraces. Their formation occurs when the tip enters the repulsive interaction regime. Non-invasive stable imaging on the resulting structures is possible in the non-contact attractive regime. The application of local force spectroscopy enables to examine the growth mechanism in more detail. Particularly, the influence of external parameters like the applied repulsive force and the oscillation amplitude on the island size are evaluated.

O 15.65 Fr 17:00 Poster TU D

**Surface investigations of single junction thermal converters in the infrared spectral range** — ●VIKTOR SCHLOSSER<sup>1</sup>, GERNOT HEINE<sup>2</sup>, M. GARCOCZ<sup>2</sup>, W. WALDMANN<sup>2</sup>, and GERHARD KLINGER<sup>3</sup> — <sup>1</sup>Institut für Materialphysik, Universität Wien — <sup>2</sup>Bundesamt für Eich- und Vermessungswesen, Wien — <sup>3</sup>Institut für Meteorologie und Geophysik, Universität Wien

The ac-dc transfer standard is one of the basic electrical standards, by which the ac voltage and ac current are deduced from their dc counterparts. A well established method is the comparison of electrical power between ac- and dc- voltage by converting the power to force or heat. Converters may be recognised as reference standard and the system is called "ac-dc transfer standard". Differences in the signal between ac- and dc- power generation depend on frequency and waveform. In the low frequency regime the thermal ripple dominates the error introduced by the thermal converter. Thermocouple measurements of the bulk temperature of a bead of a single junction thermal converter suggest that a significant thermal ripple exists only at frequencies below 20Hz. A scanning infrared radiation imaging set up was used to investigate the bead's surface. By this method frequency dependent temperature modulations were observed up to frequencies of 200Hz. The experimental method will be presented and the results will be discussed.

O 15.66 Fr 17:00 Poster TU D

**Stack-type vibration decoupling for scanning probe applications** — ●F. MÜLLER<sup>1</sup>, A.-D. MÜLLER<sup>1</sup>, D. BILLEP<sup>2</sup>, ST. KURTH<sup>3</sup>, A. SHAPORIN<sup>2</sup>, M. HIETSCHOLD<sup>1</sup>, and W. DÖTZEL<sup>2</sup> — <sup>1</sup>Chemnitz University of Technology, Institute of Physics, Solid Surfaces Analysis Group, 09107 Chemnitz — <sup>2</sup>Chemnitz University of Technology, Faculty of Electrical Engineering and Information Technology, Microsystems and Device Technology Group, 09107 Chemnitz — <sup>3</sup>Fraunhofer IZM, Micro Devices and Equipment, Reichenhainer Strasse 88, 09126 Chemnitz

In Scanning Tunneling Microscopy (STM), a stack of mechanically coupled metal plates is commonly used as vibration isolation to obtain atomically resolved images. In this work, the transmission of mechanical vibrations through this stack is studied in dependence on its geometrical dimensions and material properties [1, 2]. A phase sensitive correlation analysis between a defined mechanical excitation and the resulting movement of different plates in vertical and lateral directions allows to quantify the efficiency of the vibration damping in a frequency range till 200 Hz. From the characteristics obtained at the example of the Pocket STM, the typical frequency response function (FRF) of the stack is obtained. For optimization purposes, a finite element model of the device was used. Modal and transient analysis of the device were performed for various combinations of geometrical parameters and material properties. Modelling results show satisfactory similarities with the measurements taken at the STM stack.

[1] S.I. Park, C.F. Quate, Rev. Sci. Instrum. 58, 2004-2009 (1987). [2] D.W. Pohl, IBM J. Res. Develop. 30 (4), 417-427 (1986).

O 15.67 Fr 17:00 Poster TU D

**Tribological properties of amorphous and crystalline antimony nanoparticles studied by SFM and TEM** — ●CLAUDIA RITTER<sup>1</sup>, UDO D. SCHWARZ<sup>2</sup>, BERT STEGEMANN<sup>1,3</sup>, MARKUS HEYDE<sup>1,4</sup>, and KLAUS RADEMANN<sup>1</sup> — <sup>1</sup>Humboldt-Universität zu Berlin, Institute of Chemistry, Brook-Taylor-Str. 2, D-12489 Berlin, Germany — <sup>2</sup>Department of Mechanical Engineering, Yale University, P.O. Box 208284, New Haven, CT 06520-8284, USA — <sup>3</sup>Federal Institute of Materials Research and Testing (BAM), D-12200 Berlin, Germany — <sup>4</sup>Fritz-Haber-Institute of the Max-Planck-Society, Faradayweg 4-6, D-14195 Berlin, Germany

The fundamentals of friction, in particular, the interplay between friction, adhesion, true contact area and crystalline structure at the interface, are still insufficiently understood. In this investigation, antimony nanoparticles grown on HOPG and MoS<sub>2</sub> were used as a model system. The morphology of the nanoparticles was characterized by SFM, SEM and TEM. Thus, both the interface structure and the real contact area were accurately determined. The TEM study revealed a size dependent amorphous-polycrystalline phase transition. Controlled translation of the particles was induced by the action of the oscillating tip in dynamic mode SFM. During manipulation, the power dissipated due to tip-sample interactions was recorded. Particles with contact areas below 10000 nm<sup>2</sup> were much easier to move compared to their larger counterparts. We suggest that structural lubricity might be the reason for the low dissipation in the small amorphous particles, while elastic multistabilities might dominate energy dissipation in the larger polycrystalline particles.

O 15.68 Fr 17:00 Poster TU D

**Abbildung biologischer Proben mit dem CE-Modus in der Rasterkraftmikroskopie** — ●JENS FALTER, JAN-ERIK SCHMUTZ, DANIEL EBELING, MARCUS SCHÄFER und HENDRIK HÖLSCHER — Center for NanoTechnology (CeNTech) und Physikalisches Institut der Universität Münster, Gievenbecker Weg 11, 48149 Münster

Die dynamische Rasterkraftmikroskopie ermöglicht neue Einblicke und Erkenntnisse in die Oberflächenphysik. Die Wechselwirkungen an Oberflächen können mit der dynamischen Kraft-Spektroskopie ausgemessen werden. Bei tiefen Temperaturen im Hochvakuum ist dies sogar mit dreidimensionaler Auflösung möglich [1]. Aufgrund verschiedener experimenteller Probleme war diese Methode aber auf das Vakuum beschränkt. Um dynamische Rasterkraftspektroskopie auch an Luft und in Flüssigkeiten zu ermöglichen, haben wir den sogenannten CE-Modus implementiert. Mit dieser Technik ist die Rekonstruktion der Spitzen-Proben-Wechselwirkung ebenfalls möglich [2]. Wir haben die Möglichkeiten dieses Ansatzes insbesondere für biologische Proben untersucht. Im Vordergrund stehen dabei Messungen in Flüssigkeiten, dem natürlichen Medium für biologische Proben.

[1] H. Hölscher, S. M. Langkat, A. Schwarz, R. Wiesendanger, Appl. Phys.

Lett. 81, 4428 (2002)

[2] H. Hölscher, B. Gotsmann, A. Schirmeisen, Phys. Rev. B 68, 153401 (2003)

O 15.69 Fr 17:00 Poster TU D

**Adhesion forces studied with colloid probe atomic force microscopy** — ●BERT STEGEMANN, HENRIK BACKHAUS, HEINZ KLOSS, and ERICH SANTNER — Bundesanstalt für Materialforschung, BAM - VIII.1 Tribologie und Verschleißschutz, Unter den Eichen 44-46, D-12205 Berlin

Adhesion is of fundamental importance for the tribological behavior, e.g., in nanomechanical devices. A promising approach to determine interfacial adhesion at sub-micron scale is to measure pull-off forces with an atomic force microscope (AFM). As adhesion depends on numerous factors, such as contact area, environment and dynamics, there is still a lack of reliable quantitative data. Here, we report on a systematic analysis of AFM pull-off forces for well-defined systems under ultrahigh vacuum conditions. Interaction geometry is controlled by means of colloid AFM probes, i.e., microspheres attached at the end of bare AFM cantilevers. Clean sample surfaces of a wide range of single crystal metals and compound materials were prepared by subsequent Ar ion sputtering and annealing as affirmed by surface analytical techniques. The influence of experimental parameters, like applied load, contact time and contact area on the pull-off forces is discussed. The results obtained are compared with predictions from theoretical models and correlated with macroscopic mechanical properties of the materials.

O 15.70 Fr 17:00 Poster TU D

**Optical properties of silver cluster ensembles** — ●HADJ MOHAMED BENIA, NIKLAS NILIUS, and HANS-JOACHIM FREUND — Fritz-Haber-Institut der Max-Planck-Gesellschaft, Faradayweg 4-6, 14195 Berlin

By means of photon emission spectroscopy with an STM, we have studied the electromagnetic coupling in silver cluster ensembles. The ensembles were prepared by two techniques: (i) atom deposition on a thin alumina film in UHV and (ii) deposition of size-selected silver colloids, prepared by a reverse micelle technique, on gold and HOPG substrates. Silver on alumina grows with a very low cluster density. The corresponding cluster ensemble shows one plasmon resonance, indicative for weak cluster-cluster coupling. In contrast, measurements on dense colloidal cluster arrays reveal two plasmon peaks, shifted to higher and lower energies with respect to the one observed for alumina-supported Ag clusters. The presence of two resonance peaks is explained by considerable electromagnetic coupling in the cluster ensemble.

O 15.71 Fr 17:00 Poster TU D

**Charge Carrier Dynamics at Silicon surfaces: A Time-Resolved Photoemission Study with Combined Laser and Synchrotron Radiation.** — ●TATJANA GIESSEL<sup>1</sup>, DAVID BRÖCKER<sup>1</sup>, HELENA PRIMA GARCIA<sup>1</sup>, RAMONA WEBER<sup>1</sup>, MARTIN WEINELT<sup>1,2</sup>, and WOLF WIDDRA<sup>3</sup> — <sup>1</sup>Max-Born-Institut, Berlin, Germany — <sup>2</sup>Freie Universität, Berlin, Germany — <sup>3</sup>Martin Luther Universität, Halle, Germany

Charge carrier dynamics at the Si(100) surface and for thin oxide layers on Si(100) have been studied by probing the time-dependent surface photovoltage (SPV). Electron-hole pairs are excited in the near-surface region by femtosecond lasers pulses and the subsequent dynamics of charge carrier recombination is determined by time-resolved Si 2p core-level photoemission using synchrotron radiation. For laser fluences up to 60 μJ/cm<sup>2</sup> the observed non-exponential decay of the SPV can be described within a model based on thermionic emission. For higher laser fluences up to 60 mJ/cm<sup>2</sup> an oscillation of the SPV in time is observed. A fast drop of the SPV within 100 ps is followed by a slow increase reaching its maximum at several 100 nanoseconds. An even slower decay in the microsecond range then restores the primary SPV. The decay time of the initial fast drop of the SPV decreases with increasing sample temperature, which suggests a phonon mediated charge-carrier recombination-process. The subsequent SPV dynamics on the time scale of hundreds of nanoseconds to microseconds are assigned to diffusion-limited processes.

O 15.72 Fr 17:00 Poster TU D

**Electron-electron correlations at the LiF(100) surface probed via (e,2e) spectroscopy** — ●FRANK O. SCHUMANN, JAMAL BERAKDAR, and JÜRGEN KIRSCHNER — MPI f. Mikrostrukturphysik, Weinberg 2, 06120 Halle

Electronic correlations manifest themselves in many-body effects like

superconductivity and magnetism. Due to the Coulomb and exchange interaction two electrons tend to avoid each other leading to an exchange-correlation hole. We studied the correlation between two electrons by probing the emission of electron pairs from a LiF(100) surface upon excitation with 32 eV primary electrons. The set-up consists of a channelplate, followed by a central collector and a pulsed electron gun. The energy of the electrons follows from their flight times. We find correlation in energy and k-space of an electron pair, where one electron originates from the top of the valence band. We selected the energies of the ejected electron pair to be  $E_1=9$  eV and  $E_2=8$  eV, respectively. Mapping the correlation as a function of the in-plane momentum of the second electron results in the observation of a zone of reduced intensity. The extension of this exchange-correlation hole is  $\sim 1 \text{ \AA}^{-1}$  which is in the range of theoretical predictions on double photoemission. Another experimental fact is the sensitivity of the correlation hole to decoherence effects, an aspect which is largely unexplored theoretically. Increasing the impinging electron energy to 33.7 eV allows for inelastic scattering of the electron pair. This opens up a decoherence channel and the correlation hole vanishes. Varying the primary energy is therefore a tool for tuning on or off decoherence effects.

O 15.73 Fr 17:00 Poster TU D

**Electron coincidence spectroscopy on Xe/Cu(111)** — ●CARSTEN WINKLER and JÜRGEN KIRSCHNER — MPI f. Mikrostrukturphysik, Weinberg 2, D-06120 Halle

Correlation between electrons is a fundamental characteristics of systems containing many electrons. In the present experiments, electron coincidence spectroscopy (e,2e) has been carried out in order to study energy distributions of correlated electrons ejected from condensed Xe films. The films have been prepared by dosing 20 L of Xe onto a Cu(111) single crystal surface that was cooled down by  $\ell$ He to a temperature of  $T_p \simeq 50$  K. The incoming (primary) electrons are generated by a pulsed electron source with a kinetic energy in the range of  $20 \text{ eV} \leq E_p \leq 35$  eV. The scattered (secondary) coincident electrons, on the other hand, are detected by using two reflection time-of-flight (TOF) spectrometers. With that, the kinetic energies  $E_1$  and  $E_2$  of the corresponding coincident electrons can be calculated from its flight time from sample to the detector.

As a first step, TOF spectra were taken for Xe adsorbed on Cu(111) at energies of  $E_p = 20$  eV and  $E_p = 25$  eV. Compared to the corresponding data of metals like Cu or Co, these measurements show rather high coincidence count rates. The data generally show a distinct feature in the region  $(E_1 + E_2) = E_p - W$  with  $E_1 = E_2$ . Here,  $W$  is the work function that was determined to be  $W \simeq 8$  eV. These promising results of the very first (e,2e)-coincidence studies on solid Xe are an encouragement for further systematic investigations, namely varying the Xe film thickness. (2004)

O 15.74 Fr 17:00 Poster TU D

**Manipulation of ultrafast surface processes using fs-pulse shaping** — ●FELIX STEEB, MARLIES WESSENDORF, JÖRG LANGE, ALEXANDER MÖNNICH, STEFAN MATHIAS, MARTIN AESCHLIMANN, and MICHAEL BAUER — FB Physik, TU Kaiserslautern, Erwin-Schrödinger-Str. 46, 67663 Kaiserslautern

In recent years, coherent control of ultrafast processes in the gas phase [1] or in the liquid phase [2] by means of adaptive femtosecond pulse shaping has been demonstrated.

In this paper, we present first attempts to employ the pulse shaping technique to the manipulation of ultrafast surface processes, such as surface chemical reactions.

For the Two-Photon-Photoemission (2PPE) yield from the occupied shockley surface state of a Cu(111) surface, we find a complex dependence on the spectral phase of the exciting pulse, modulated by a programmable 640-stripe liquid crystal spatial light modulator incorporated into a conventional 4f-setup. Resonance enhanced excitation induced by an unoccupied adsorbate state, e.g. Cs/Cu(111), modifies this dependence. Model calculations within the framework of the Liouville-von-Neumann equations can qualitatively reproduce the experimental data. Future prospects, e.g. possible schemes to control a surface chemical reaction using pulse-shaping techniques and other potential applications are discussed.

[1] - A. Assion et al.: Science 282, 919 (1998)

[2] - T. Brixner et al: Nature 414, 57 (2001)

O 15.75 Fr 17:00 Poster TU D

**Limitations in the use of a 2D hemispherical energy analyser for PES in combination with a low-repetitive ultrashort photon source** — ●S. MATHIAS<sup>1</sup>, O. HEINZ<sup>2</sup>, S. PASSLACK<sup>1</sup>, D. MITTNACHT<sup>1</sup>, V. TEMNOV<sup>2</sup>, M. BAUER<sup>1</sup>, D. VON DER LINDE<sup>2</sup>, and M. AESCHLIMANN<sup>1</sup> — <sup>1</sup>FB Physik, TU Kaiserslautern, 67663 Kaiserslautern — <sup>2</sup>Institut für experimentelle Physik, Uni Duisburg Essen, 45117 Essen

One of the main advantages of hemispherical electron analysers equipped with a 2D detector is their high efficiency due to the parallel detection scheme with respect to energy and momentum. It makes these systems highly preferable for specific applications e.g. for the use with low-repetitive photon sources such as laser-based femtosecond UV-sources. In this study a 2D analyser has been used for 2 Photon Photoemission spectroscopy from an occupied surface state of Cu(111) using a 1 kHz laser amplifier system. For comparison, corresponding data have also been recorded using a ToF electron analyzer and a high repetitive (80 MHz) Ti:Sapphire laser. Particular focus has been set on the spectral broadening due to space charge effects which become apparent at sufficient high pulse intensities from the 1 kHz amplifier. The experimental data are compared with numerical simulations which support the relevance of space charge effects. Our results show that the 2D analyzer scheme is suitable for high-resolution angular-resolved electron spectroscopy in combination with low repetitive laser sources and may in the future be used complementary to conventional ToF-detectors.

O 15.76 Fr 17:00 Poster TU D

**New measurements on the Casimir-van der Waals potential** — ●LODEWIJK ARNTZEN — Physikalisches Institut, Heidelberg University, 69120 Heidelberg

We recently measured quantum reflection of cold helium atoms from a purely attractive potential. The interaction could be identified as originating from the Casimir force between a single atom and semi-conducting surface. We are now specifically investigating the temperature behavior of the Casimir-van der Waals potential. Within the incident energy range between  $\mu\text{eV}$  and  $\text{neV}$ , the surface temperature is varied from 300 K to 1200 K. These new measurements show that the quantum reflected intensities decrease sharply and reproducibly with increasing temperature. We will present different mechanisms that may account for this observation. In addition the Debye-Waller effect, the temperature dependence of the electric permittivity and magnetic effects will be addressed.

O 15.77 Fr 17:00 Poster TU D

**Force microscopy analysis of etch pits for crystal defect assignment** — ●CHRISTIAN MOTZER und MICHAEL REICHLING — Fachbereich Physik, Universität Osnabrück, Barbarastr. 7, 49069 Osnabrück

Ex-situ scanning force microscopy analysis of etched (111)  $\text{CaF}_2$  cleavage plates were carried out to study crystal defects. Etch figures are well known to be related to certain crystal defects and were studied by several microscopy methods to determine the etch pit density (EPD) which relate to the dislocation density in a crystal. Force microscopy enables us to investigate in detail the etch figures and reveal more than the occurrence of dislocation etch pits. We found several types of etch pits which relate to different kinds of defects. Point bottom etch pits and flat pits are discussed in relation to their crystal defect origins. Segregation connected with dislocations alter the kinetic during dissolution and hence change the appearance of etch pits, e.g. etch pits appear with multiple inner walls.

O 15.78 Fr 17:00 Poster TU D

**A setup for grazing incidence x-ray scattering measurements at the SAW2 beamline of DELTA** — ●CHRISTOF KRYWKA<sup>1</sup>, MICHAEL PAULUS<sup>1</sup>, CHRISTIAN STERNEMANN<sup>1</sup>, MICHAEL VOLMER<sup>1</sup>, OLIVER H. SEECK<sup>2</sup>, and METIN TOLAN<sup>1</sup> — <sup>1</sup>Experimentelle Physik I, DELTA, Universität Dortmund, Maria-Goeppert-Mayer Strasse 2, 44221 Dortmund, Germany — <sup>2</sup>HASYLAB am DESY, Notkestraße 85, 22603 Hamburg

We report on an experimental setup installed at the SAW2 (Superconducting Asymmetric Wiggler) beamline of the Dortmund Electron Accelerator DELTA that allows grazing incidence small angle scattering (GISAXS) experiments on liquid surfaces. GISAXS is a unique technique to probe surface and near-surface structures of soft materials. The setup was designed for photon energies between 8 and 15keV using a six circle diffractometer in combination with a focussing mirror. First GID experiments have already been successfully performed on water and aqueous NaJ solution as well as on polypropylenglycol (PPG) samples.

O 15.79 Fr 17:00 Poster TU D

**Time-Resolved Reflection High-Energy Electron Diffraction – Pump-Probe Experiments on Clean and Bi-covered Si Surfaces** — ●A. JANZEN, B. KRENZER, and M. HORN-VON HOEGEN — Universität Duisburg-Essen, Institut für Experimentelle Physik, 45117 Essen

Time-resolved Reflection High-Energy Electron Diffraction opens a new pathway to investigate the structural dynamics at surfaces subsequent to an intense electronic excitation by a fs-laser pulse. By variation of the time delay between a fs-laser-pump pulse and a ps-electron-probe pulse the transient state of the surface under examination can be determined. The construction of a laser-driven electron gun providing picosecond electron pulses and the setup of an electron diffraction apparatus has already been successfully accomplished.

We are now conducting studies of ultrafast heating phenomena after laser excitation of clean Si surfaces and thick Bi-films epitaxially grown on Si. The last step in the chain of processes following the excitation is the transient heating of the lattice, leading to a drop in the diffraction spot intensity (*Debye-Waller effect*). Since Bi has a much lower Debye temperature than Si,  $\Theta_{D,Bi} = 119$  K compared to  $\Theta_{D,Si} = 652$  K, the Debye-Waller effect is much more pronounced on Bi surfaces than on Si surfaces. First results of the pump-probe experiments and a discussion of the encountered problems will be presented.

O 15.80 Fr 17:00 Poster TU D

**Contrast mechanisms in imaging spectroscopy using the nanoESCA** — ●S. SCHMIDT<sup>1</sup>, F. FORSTER<sup>2</sup>, F. REINERT<sup>2</sup>, M. ESCHER<sup>3</sup>, N. WEBER<sup>3</sup>, M. MERKEL<sup>3</sup>, D. FUNNEMANN<sup>4</sup>, B. KRÖMKER<sup>4</sup>, CH. ZIETHEN<sup>5</sup>, P. BERNHARD<sup>5</sup>, H.-J. ELMERS<sup>5</sup>, G. SCHÖNHENSE<sup>5</sup>, and S. HÜFNER<sup>1</sup> — <sup>1</sup>Universität des Saarlandes, D-66041 Saarbrücken — <sup>2</sup>Universität Würzburg, D-97074 Würzburg — <sup>3</sup>Focus GmbH, D-65510 Hünstetten — <sup>4</sup>OmicronNanoTechnology GmbH, D-65232 Taunusstein — <sup>5</sup>Universität Mainz, D-55128 Mainz

We present the results obtained during synchrotron measurements using the *nanoESCA* prototype for imaging XPS to demonstrate its imaging capabilities of elemental, chemical, magnetic and orientational contrast in prototypical samples with a spatial resolution better than 120 nm, an energy resolution of  $\Delta E \leq 110$  meV and the ability to image electrons with kinetic energies up to 1.6 keV [1]. We demonstrate the extension of the standard applications of imaging ESCA systems to the use of MCD and MLDAD contrast in the Fe 2p XPS core-level spectra to map ferromagnetic domains. We also show how the *nanoESCA* setup can be used to distinguish between different grain orientations in poly-crystalline materials by measuring the electronic structure of single grains [2].

[1] M. Escher *et al.*, J. Phys.: Condens. Matter, in print.

[2] M. Escher *et al.*, J. Electron Spectrosc. Relat. Phenom., in print

O 15.81 Fr 17:00 Poster TU D

**A multichannel detection photoemission experiment** — ●MICHAEL HELLE, MARTIN MARCZYNSKI, MATTHIAS KALLÄNE, SÖNKE HARM, KAI ROSSNAGEL, and LUTZ KIPP — Institut für Experimentelle und Angewandte Physik, Universität Kiel, D-24098, Germany

It is possible to reduce the data collection times of angle-resolved photoelectron spectroscopy (ARPES) by means of parallel detection of electron energy and angle by at least a factor of ten. Parallel detection is implemented by equipping a hemispherical analyzer which is rotatable about the sample in ultrahigh vacuum with a position and time sensitive microchannel plate detector with delay-line readout (DLD: delay-line detector).

The construction and the characterization of a home-built hemispherical analyzer with DLD from the Roentdek company will be presented. First measurements of the layered transition metal dichalcogenide  $TiTe_2$  before and after adsorption of potassium will be shown.

This work was supported by the BMBF proj. no. 05 KS1 FKB.

O 15.82 Fr 17:00 Poster TU D

**Scaling laws of the angular emission distribution of laser ablated plasma pulses from monoatomic and binary targets in a mass range from 27 to 184** — ●SHAIENDRA NATH SRIVASTAVA and KLAUS ROHR — Technical University of Kaiserslautern, D 67663 Kaiserslautern, Germany

In the present experiment we have investigated emission characteristics of laser produced plasma pulses quantitatively and over a wide mass range. Targets have been monoatomic Al, Ti, Cu, Mo, W and compounds of these with different stoichiometric ratios. Thereby the (average) mass

covers a range from 27 to 184. The following major results are observed: (1) The emission cones of all species steepen continuously as a function of the (average) atomic mass. Thereby, for the first time, the widths can be well described by a general scaling law namely  $k/A + c$ . Here  $k$  and  $c$  systematically depend on the size of the ablation area. (2) The measured widths of the compound systems agree with averaged data of its single pure component if the corresponding stoichiometric ratios of the pure targets are used. This suggests that stoichiometry is essentially conserved. (3) All emission shapes can be fitted uniquely by Gauß-functions which reflects the dominating effect of the spatial shape of the laser pulse on the shape of the emission distribution. The result are essential for practical applications, they allows quite simply predictions of emission distributions of monoatomic species hardly to measure otherwise (e.g. gases) and of compound systems of arbitrary compositions.

O 15.83 Fr 17:00 Poster TU D

**UHV compatible high-pressure reaction cell for in-situ IR and kinetic studies of single model catalysts** — ●THOMAS HÄRING, THOMAS DIEMANT, ZHONG ZHAO, HUBERT RAUSCHER, and R. J. BEHM — Abt. Oberflächenchemie und Katalyse, Universität Ulm, 89069 Ulm

We have designed and constructed a high pressure reaction cell for in-situ IR (PEM-IRAS) and kinetic measurements at pressures up to 100 mbar. The cell is attached to a UHV system equipped with standard facilities for sample preparation and characterization. The small volume of the cell and the low leak rate over the differentially pumped seal allows to follow reactions under batch conditions for several hours; well-defined gas flow rates can be established by calibrated capillaries. We present details of the setup of the reaction cell and discuss the performance of the system.

O 15.84 Fr 17:00 Poster TU D

**Advances in nanofocusing with reflective photon sieves** — ●JAN BARTUSSEK, JENS BUCK, MATTHIAS KALLÄNE, SÖNKE HARM, KAI ROSSNAGEL, and LUTZ KIPP — Institut für Experimentelle und Angewandte Physik, Universität Kiel, D-24098 Kiel

Photon sieves are a new type of diffraction optics for focusing synchrotron radiation to submicrometer dimensions. They appear especially promising for future angle and spatially resolved photoemission experiments at the VUV-FEL at HASYLAB, because side lobes in the intensity pattern in the focal plane can be suppressed almost completely by applying smooth window functions. In addition, by separating zero from first order light the background can be reduced significantly. Using a knife edge scanner we measured focal spots for photon sieves optimized for a photon energy of 100 eV. Experiments were carried out at beamline BW3 at HASYLAB. The results are discussed in the context of numerical simulations. Work is supported by BMBF proj. no. 05 KS1 FK1.