

**O 42: Poster Session II (Nanostructures at surfaces: arrays; Nanostructures at surfaces: Dots, particles, clusters; Nanostructures at surfaces: Other; Nanostructures at surfaces: Wires, tubes; Metal substrates: Adsorption of O and/or H; Metal substrates: Clean surfaces; Metal substrates: Adsorption of organic/bio molecules; Metal substrates: Solid-liquid interfaces; Metal substrates: Adsorption of inorganic molecules; Metal substrates: Epitaxy and growth; Heterogeneous catalysis; Surface chemical reactions; Ab-initio approaches to excitations in condensed matter; Organic, polymeric, biomolecular films— also with adsorbates; Particles and clusters)**

Time: Wednesday 17:45–20:30

Location: P2

O 42.1 Wed 17:45 P2

**Realization of Large-Scale Nano-Patterned Surfaces by the UTAM-Technique** — ●STEFAN OSTENDORP, YONG LEI, and GERHARD WILDE — Institut für Materialphysik, Westfälische Wilhelms-Universität Münster, Wilhelm-Klemm-Str. 10, 48149 Münster, Germany

Using an UTAM (ultra-thin alumina membrane) surface nano-patterning technique, large-scale arrays of highly regular metallic and semiconductor nano-particles were fabricated on silicon and sapphire substrates. The structural parameters of the synthesized nano-particles are controllable, including the diameter, spacing, and shape. Different metallic nano-particles have been oxidized using a well-controlled oxidation process in a modified CVD-system. The aim of the experiment is to obtain a core-shell nanostructure with a metallic core and an oxide shell. During the oxidation of some metallic nano-particles (chromium and nickel) on a silicon substrate, an interesting nano-porous silicon oxide surface structure with embedded metallic oxide nano-particles evolved. These surface nano-porous structures are under investigation now by AFM, EFM, SEM and TEM to determine the details of their growth mechanism.

O 42.2 Wed 17:45 P2

**Terephthalic acid (TPA) on Si(111)- $\alpha$  and  $\beta$ -( $\sqrt{3} \times \sqrt{3}$ )-Bi surfaces** — ●TAKAYUKI SUZUKI<sup>1</sup>, THERESA LUTZ<sup>1</sup>, GIOVANNI COSTANTINI<sup>1,2</sup>, and KLAUS KERN<sup>1,3</sup> — <sup>1</sup>Max Planck Institute for Solid State Research, Heisenbergstrasse 1, 70569 Stuttgart, Germany — <sup>2</sup>Department of Chemistry, University of Warwick, Coventry, CV4 7AL, United Kingdom — <sup>3</sup>Institute de Physiques des Nanostructures, Ecole Polytechnique Fédérale de Lausanne, CH-1015 Lausanne, Switzerland

We have carried out scanning tunneling microscopy (STM) experiments of terephthalic acid (TPA) adsorption on Si(111)- $\alpha$  and  $\beta$ -( $\sqrt{3} \times \sqrt{3}$ )-Bi surfaces in order to study supramolecular self-assembly on passivated semiconductor surfaces. Both Si(111)- $\alpha$  and  $\beta$ -( $\sqrt{3} \times \sqrt{3}$ )-Bi are passivated semiconductor surfaces without highly reactive Si dangling bonds, and have Bi coverages of 1/3 and 1 monolayer, respectively. The TPA molecules adsorb randomly on  $\alpha$ -( $\sqrt{3} \times \sqrt{3}$ )-Bi and do not form any ordered supramolecular layer. On the other hand, they form ordered supramolecular layers on  $\beta$ -( $\sqrt{3} \times \sqrt{3}$ )-Bi with at least four different types of coexisting structures. This completely different supramolecular self-assembly behavior on the  $\alpha$  and  $\beta$ -( $\sqrt{3} \times \sqrt{3}$ )-Bi surfaces is quite striking since the two substrates are composed by the same atomic species and are characterized by the same unit cell. The different behavior is related to the differences in the electronic structure of these surfaces. Similar to the Si dangling bond states on Si(111)-7 $\times$ 7, localized surface states exist on Bi adatoms on  $\alpha$ -( $\sqrt{3} \times \sqrt{3}$ )-Bi, but not on Bi trimers on  $\beta$ -( $\sqrt{3} \times \sqrt{3}$ )-Bi.

O 42.3 Wed 17:45 P2

**Faceted Lead Clusters on Nano Structured HOPG** — ●NIKLAS GRÖNHAGEN, FARHAD GHALEH, and HEINZ HÖVEL — Technische Universität Dortmund, Experimentelle Physik I, 44221 Dortmund

Lead as a cluster material shows an interesting behavior which distinguishes it from other metals. Lead starts diffusing at quite low temperatures and tends to form facets very easily. This is because Pb atoms can reorganize within or between clusters, consequently lowering their surface energy and thus transform into clusters with improved stability.

In the present study we produced faceted lead clusters by deposition of lead atoms on graphite (HOPG) samples, prestructured with nanometer sized pits [1]. The nano-pits were either distributed randomly on the sample or produced in an array using focussed ion beam lithography (ionLiNE system, Raith GmbH) [2].

Subsequently the clusters were investigated by scanning tunneling microscopy. We observed a fine structure in the height distribution given by Pb monolayer steps and an odd-even-oscillation. By measurements with scanning tunneling spectroscopy we were able to show that "Quantum Well States" are responsible for this growth behavior.

[1] H. Hövel, Appl. Phys. A 72, 295 (2001) [2] F. Ghaleh, R. Köster, H. Hövel, L. Bruchhaus, S. Bauerdick, J. Thiel, R. Jede: J. Appl. Phys. 101, 044301 (2007)

O 42.4 Wed 17:45 P2

**Selective and Hierarchical Bonding Interactions in 2D Multi-Component Supramolecular Networks at Surfaces** — ●ALEXANDER LANGNER<sup>1</sup>, STEVEN L. TAIT<sup>1</sup>, CHANDRASEKAR RAJADURAI<sup>2</sup>, NIAN LIN<sup>1</sup>, MARIO RUBEN<sup>2</sup>, and KLAUS KERN<sup>1,3</sup> — <sup>1</sup>Max-Planck-Institut für Festkörperforschung, Stuttgart — <sup>2</sup>Institut für Nanotechnologie, Forschungszentrum Karlsruhe — <sup>3</sup>Ecole Polytechnique Fédérale de Lausanne, Switzerland

Self-assembly of organic molecules is an efficient bottom-up approach to pattern surfaces with unique two-dimensional (2D) architectures at the nanometer scale. In order to achieve extended and highly ordered supramolecular networks, the spontaneous self-organization process has to be steered by selective, directional and strong, but non-covalent bonding interactions, such as hydrogen bonding or metal-organic complex formation. Here we concentrate on the surface supported self-assembly of aromatic ligand mixtures studied by scanning tunneling microscopy (STM) under ultra high vacuum (UHV) conditions. The various molecular building blocks are provided with either carboxylic acid or pyridyl moieties. In these ligand mixtures, selectivity of the functional groups towards different co-evaporated metal coordination centers is observed, which can lead to ligand separation or the formation of complex multi-component networks, stabilized by hierarchical bonding (i.e. hydrogen bonding as well as metal-ligand coordination). We will demonstrate that the selective and hierarchical character of the bonding interactions allow the controlled manipulation of structural network parameters.

O 42.5 Wed 17:45 P2

**In-situ scanning tunneling microscope growth studies of InAs and InN quantum dots during MOVPE growth** — ●MATTHIAS SCHMIES, RAIMUND KREMZOW, MARKUS PRISTOVSEK and MICHAEL KNEISSL — TU Berlin, Institut für Festkörperphysik, EW 6-1, Hardenbergstr. 36, D-10623 Berlin, Germany

Novel optoelectronic devices, like single-photon emitters and semiconductor lasers demand a better understanding of the growth process and control of quantum dots (QD). Most optoelectronic devices are grown by metal organic vapour phase epitaxy (MOVPE) systems which allows mass fabrication for industrial applications. While QD growth has been studied intensively for InGaAs, the understanding of the mechanisms responsible for the formation of the QDs and especially of the ripening process during annealing and cooling down after growth is still relatively poor. The InGaN material system is even less understood. In order to investigate the growth dynamics and to clarify the theory of QD ripening we employed a in-situ scanning tunnelling microscope (STM) which allows measurements during MOVPE growth. In this paper we will discuss the ripening process of InAs QDs on GaAs(001):Si at 475°C. For the InAs/GaAs system the development of the structure density agrees to the mean field theory of Lifshitz, Slyozov and Wagner (LSW-theory) of the Ostwald ripening process for three dimensional island on a two dimensional substrate. Additionally, we will present first experiments of InN QDs grown on GaN/templates sapphire using tertiarybutylhydrazine (tBHy) as nitrogen precursor.

O 42.6 Wed 17:45 P2

**Monodisperse micro-island formation on Ni/Ru(0001) mono-**

**layers** — ●PETER JAKOB<sup>1</sup>, KAI ANHUT<sup>1</sup>, SEBASTIAN SCHNUR<sup>2</sup>, and AXEL GROSS<sup>2</sup> — <sup>1</sup>Fachbereich Physik, Philipps-Universität Marburg, D-35032 Marburg, Germany — <sup>2</sup>Institut für Theoretische Chemie, Universität Ulm, D-89069 Ulm, Germany

The formation of virtually identical and thermally stable Ni micro-islands (trimers) is presented. In our combined experimental and theoretical investigation we define the conditions for their unusual creation (expulsion of Ni atoms or trimers from the underlying substrate by means of adsorbate induced compressive stress) and give a detailed characterization of the micro-islands' structural properties, chemical composition and electronic/magnetic properties [1]. Specifically, we show that their exceptional structural and thermal stability can be ascribed to oxygen attached to the islands, thereby forming (metallic) Ni-oxygen composites. Our observation of a high density of identical clusters represents a major contribution to overcome a common challenge in materials science related to establishing a correlation between structural and catalytic/electronic properties of nanoscale objects. Usually, the various approaches lead to a dazzling array of sizes and shapes rather than monodisperse particles in a well-defined environment.

[1] P. Jakob, K. Anhut, S. Schnur, and A. Groß, Phys. Rev. Lett. 101, 206101 (2008).

O 42.7 Wed 17:45 P2

**Theoretical study of nucleation processes on patterned surfaces** — ●STEFAN FRIEDER HOPP and ANDREAS HEUER — Institut für Physikalische Chemie, Universität Münster, 48149 Münster, Germany

The properties of template-directed nucleation are studied in the transition region where full nucleation control is lost and additional nucleation beyond the pre-patterned structure is observed. To get deeper insight into the microscopic mechanisms, Monte Carlo simulations are performed. In this context, the previously used continuous algorithm [1] is replaced by a discrete one to reduce simulation time and to allow more detailed calculations. The applied method is based on the assumption that the molecules on the surface occupy the sites of a simple fcc lattice. It is shown that the simulation results presented in [1],[2] can be reproduced quite well by the discrete algorithm. Furthermore, the new method facilitates the calculation of the distribution of nuclei on the surface by using the radial distribution function  $g(r)$  which provides another possibility of comparison with experimental data.

[1] F. Kalischewski, J. Zhu, A. Heuer. Loss of control in pattern-directed nucleation: a theoretical study. Phys. Rev. B 77, 155401, (2008).

[2] F. Kalischewski, A. Heuer. Dynamic effects on the loss of control in template-directed nucleation, preprint (2008)

O 42.8 Wed 17:45 P2

**Nanopartikel - eine Perspektive für die tribologische Anwendung in der Industrie?** — ●SVEN MARTIN PROPPERT, KATJA TÖNSING und DARIO ANSELMETTI — Universität Bielefeld, Experimentelle Biophysik und angewandte Nanowissenschaften, Deutschland

Angestoßen durch wiederholte Medienberichte über nanopartikuläre Festschmierstoffe für Verbrennungsmotoren[1] wird in dieser Arbeit in einem kombinierten mikroskopischen (AFM) und makroskopischen (Pin on Disk Tribometer) Ansatz untersucht, inwieweit sich Schmier- und Verschleißschutzwirkung bei der Verwendung unterschiedlicher Nanopartikel nachweisen lassen.

Wir untersuchten mittels AFM in Modellversuchen das Adsorptionsverhalten auf glatten Oberflächen wie Glas oder Glimmer und quantifizierten sowohl mikro- als auch makroskopisch die Reibwerte der gebildeten Oberfläche. Darüber hinaus wurden die Oberflächen auch auf mechanische- sowie Temperaturstabilitätseigenschaften geprüft.

[1] Wirtschaftswoche Nr.047, Seite 106, 2008-11-17

O 42.9 Wed 17:45 P2

**Local spectroscopy of metallic thin layers and clusters on semiconducting surfaces** — ●JEDRZEJ SCHMEIDEL, MATHIAS MENDE, CHRISTOPH TEGENKAMP, and HERBERT PFNÜR — Institut für Festkörperphysik, Leibniz Universität Hannover, Abteilung Oberflächen, Appelstrasse 2, 30167 Hannover, Germany

Many physical and chemical properties of metallic nanostructures depend strongly on their size and the coupling to their supports. Although transport concepts, like Schottky barriers and Coulomb blockade effects, are understood on a mesoscopic scale, the knowledge of influence of atomic sized defect structures (islands, steps, grains) is still

lacking. Using Ag wetting layers on Si(111), we have investigated the adsorption sites and I(V) characteristics of silver clusters adsorbed at different lattice sites by means of STM and STS. Using Ag  $\sqrt{3} \times \sqrt{3}$  reconstruction on Si(111), strong band bending leads to charge depletion in Si close to the hybrid interface, i.e. the 2d template is electrically isolated. It was noticed in the I(V) curves, that the Debye length is around 100nm (10G $\Omega$ ) for properly n-doped samples.

Additional evaporation of Ag followed by annealing to 300K results in the formation of nm-sized Ag clusters on top. Using the STM tip as a second tunneling junction, Coulomb blockade effects at 100K have been found in form of dI/dV resonance structures within the Si band gap range. The separation of these peaks in inversely proportional to the dot size as classically expected.

O 42.10 Wed 17:45 P2

**One-dimensional Structure of Boron Nitride on Chromium (110): A Study of the Growth of Boron Nitride by Chemical Vapour Deposition of Borazine** — ●FRANK MÜLLER<sup>1</sup>, HERMANN SACHDEV<sup>2</sup>, and STEFAN HÜFNER<sup>1</sup> — <sup>1</sup>Institut für Experimentalphysik, Universität des Saarlandes, 66041 Saarbrücken — <sup>2</sup>Institut für Anorganische Chemie, Universität des Saarlandes, 66041 Saarbrücken

In a recent study [1], the nucleation and growth of boron nitride films on a Chromium (110) surface by thermal decomposition of borazine, (HBNH)<sub>3</sub>, was investigated by low energy electron diffraction (LEED), X-ray photoelectron spectroscopy (XPS) and X-ray photoelectron diffraction (XPD). The boron nitride film forms a chemically non-uniform one-dimensional superstructure with short range order along the [1-10] direction and long range order along [001]. Also the thermal stability of the resulting BN film was investigated and a chemical reaction with the substrate was observed leading to the formation of Cr-B- and Cr-N- bonds at the interface, indicating the onset of the formation of hard boride and nitride phases in the system Cr-B-N.

[1] F. Müller, S. Hüfner, H. Sachdev, Surf. Sci. 602 (2008) 3467

O 42.11 Wed 17:45 P2

**Epitaxial Growth of Boron Nitride on a Rh-YSZ-Si(111) Multilayer System: Formation and Fine Tuning of a BN NanoMesh by Substrate Effects** — ●FRANK MÜLLER<sup>1</sup>, HERMANN SACHDEV<sup>2</sup>, and STEFAN HÜFNER<sup>1</sup> — <sup>1</sup>Institut für Experimentalphysik, Universität des Saarlandes, 66041 Saarbrücken — <sup>2</sup>Institut für Anorganische Chemie, Universität des Saarlandes, 66041 Saarbrücken

The epitaxial growth of boron nitride on the surface of a Rh-YSZ-Si(111) multilayer system by CVD of borazine (HBNH)<sub>3</sub> was investigated by low energy electron diffraction (LEED). The formation of a (14x14) h-BN on (13x13) Rh superstructure was observed, which is different in size from an already reported (13x13) h-BN on (12x12) Rh(111) superstructure grown on a Rh(111) single crystal substrate ("h-BN nanomesh"). We found hints that differences between the thermal expansion behaviour of the multilayer substrates and the single crystal substrate can be the reason for the formation of different sized superstructures [1].

[1] F. Müller, S. Hüfner, H. Sachdev, Surf. Sci. in press (doi:10.1016/j.susc.2008.10.033)

O 42.12 Wed 17:45 P2

**A liquid phase injection method for the deposition of molecules and clusters on atomically defined Si/Ag surfaces** — ●MATHIAS MENDE, JEDRZEJ SCHMEIDEL, HERBERT PFNÜR, and CHRISTOPH TEGENKAMP — Institut für Festkörperphysik, Universität Hannover, Abteilung Oberflächen, Appelstrasse 2, 30167 Hannover, Germany

Techniques for the deposition of nano-sized objects with limited thermal stability like organic molecules, metallic clusters and functionalized CNT's are highly needed and therefore in the focus of current research. Besides electrospray ion beam deposition [1] also pulse valve injection is used [2].

We developed a technique for the soft deposition of neutral molecules and clusters out of a solvent in a controlled Argon atmosphere. Using a microdispenser system, droplets of different solvents with a diameter of 55  $\mu\text{m}$  were reliably injected onto any surface, which can be prepared under UHV conditions. In order to correlate the concentration of Au clusters (3-5nm) on the surface with the concentration in the solvent, the droplets have been investigated by SEM and XPS. The distribution of height and size of the clusters was determined by STM on clean Si(111) 7x7 and Si(111) Ag  $\sqrt{3} \times \sqrt{3}$  surfaces. To test the functionality of the Au clusters and to demonstrate the preservation of the atomic structure in the vicinity of the nano-sized objects, STS

measurements have been performed.

[1] S. Rauschenbach et al., *Small* 2, 540 (2006)

[2] Y. Terada et al., *e-J. Surf. Sci. Nanotech.* 2, 28 (2004)

O 42.13 Wed 17:45 P2

**Winkel- und Impulsverteilungen von Photoelektronen aus Metallclustern** — ●BERNHARD FABER, PHILIPP WOPPERER und PAUL-GERHARD REINHARD — Institut für Theoretische Physik II, Uni Erlangen, Staudtstr. 7, 91058 Erlangen, Deutschland

Die Winkel- und Impulsverteilung der Photoelektronen aus kleinen  $\text{Na}_N$ -Clustern werden untersucht. Die Anregung durch einen linear polarisierten fs-Laser und die nachfolgende Clusterdynamik werden mit zeitabhängiger Dichtefunktionaltheorie simuliert. Für freie Cluster wird über ein Ensemble von Orientierungen gemittelt. Es bleibt eine reine Polarwinkelabhängigkeit, die im Detail vom emittierenden Einzelchenzustand bestimmt ist.

Es werden auch Cluster betrachtet, die auf einer Ar(001) oder MgO(001) Oberfläche deponiert sind. (Dabei kann, als weitere Variante, unter der Isolatorschicht noch eine Metallunterlage folgen.) Hier ist die Orientierung wohldefiniert und die Winkelverteilungen zeigen wesentlich reichere Strukturen in Polar- und Azimutwinkel. Die Emission wird von Oberflächenabstoßung und anziehender Bildladungskraft stark beeinflusst.

O 42.14 Wed 17:45 P2

**STM/STS Investigations of early stage of the growth of silicides** — ●MACIEJ CEGIEL, MACIEJ BAZARNIK, JAN RÖNSPIES, and HERBERT PFNÜR — Leibniz Universität Hannover, Institut für Festkörperphysik, Appelstr. 2, 30167 Hannover, Germany

Investigations of transition metals and their silicides are extremely interesting as for certain transition metals stable, lattice matched and metallic structures can be grown. In general this process is compatible with silicon technology, i.e. these silicides can be used as contacts and interconnects in electric circuits. Furthermore, using lattice anisotropies can be used skilfully to grow either quantum dots or atomic wires with extraordinary high aspect ratios and one-dimensional band structures simply by self-organization. This fact facilitates silicides even for applications in nanoelectronics devices. In particular, the shape and the electronic properties of these objects depend not only on the annealing temperature but also on the initial amount of the deposited material. In this contribution we report on Co, Ti and Dy silicide formation on Si(111) and vicinal Si(111) surfaces. For the former the diffusion dependent formation of silicide islands have been investigated for both  $(7 \times 7)$  and Ni  $(\sqrt{19} \times \sqrt{19})$  substrates. For submonolayer coverage of Ti the early state of growth on Si(111)  $7 \times 7$  has been studied by STM. Using STS resonant states with maxima at  $-1,19\text{eV}$  (HOMO),  $+0,49\text{eV}$  and  $+1,51\text{eV}$  (LUMO) were found in between Ti clusters and discussed as quantum well states. On the contrary, this states were not found in between Ti clusters grown Si(111)- $(\sqrt{19} \times \sqrt{19})$

O 42.15 Wed 17:45 P2

**Topography dependent distribution of Ag on Si surfaces during surfactant sputtering** — ●TAHA YASSERI<sup>1</sup>, KUN ZHANG<sup>2</sup>, HANS HOFSSÄSS<sup>2</sup>, and REINER KREE<sup>1</sup> — <sup>1</sup>Institute for Theoretical Physics, University of Göttingen, Friedrich-Hund Platz 1, D-37077 Göttingen, Germany. — <sup>2</sup>2nd Institute of Physics, University of Göttingen, Friedrich-Hund-Platz 1, D-37077 Göttingen, Germany.

Surface pattern formation by ion beam sputtering (IBS) can be modified by a mono layer steady-state coverage of surfactant atoms during the erosion (Surfactant Sputtering). An experimental set-up which allows a systematic study of this effect for various substrates and surfactants has been recently realized by us. Meanwhile we also extended a continuum theory and a Monte Carlo model to include surfactant effects, which makes it possible to compare experimental and theoretical findings.

Here, we present the case study of a Si substrate irradiated by 5keV Xe ions and Ag surfactants. We discuss the distribution of Ag atoms on the structured (rippled) Si surface using SEM and AFM imaging, MC data and numerical solutions of the continuum theory. We find that Ag is clustering preferentially on the crests of ripples, in accordance with a simple physical picture.

O 42.16 Wed 17:45 P2

**Optical spectroscopy of single laser-trapped gold nanoparticles** — ●NINET BABAJANI, STEPHAN EIFEL, MAXIMILIAN REISMANN, and GERO VON PLESSEN — Inst. of Physics (IA), RWTH Aachen Uni-

versity, 52056 Aachen, Germany

The plasmon lines of chemically synthesized noble-metal nanoparticles of nearly spherical shape and approximately equal size exhibit surprisingly large particle-to-particle variations of their resonance peak positions and line widths [1].

The reasons for these spectral variations are still unknown. Possible explanations include faceting of the nominally spherical particles, charges and chemical effects within the suspension, and interactions with the substrate.

In this work, a method is presented in which a single gold nanoparticle suspended in an aqueous environment is trapped by an optical tweezer and its light-scattering spectrum, which is free of substrate effects, is measured. Subsequently the trapped nanoparticle is deposited onto a substrate using the optical tweezer and its spectrum is measured again. A comparison of the single-particle spectra allows us to draw conclusions about the origin of the spectral differences between the particles.

[1] C. Sönnichsen et al., *New J. Phys.* (2002) vol. 4 pp. 93

O 42.17 Wed 17:45 P2

**Localized plasmons in defined silver microdisks investigated by PEEM** — ●FLORIAN SCHERTZ<sup>1</sup>, JOCHEN MAUL<sup>1</sup>, NOELIA BOCCIO<sup>2</sup>, ANDREAS UNGER<sup>2</sup>, GERD SCHÖNHENSE<sup>1</sup>, and MAX KREITER<sup>2</sup> — <sup>1</sup>Institut für Physik, Johannes Gutenberg-Universität, D-55099 Mainz — <sup>2</sup>Max-Planck-Institut für Polymerforschung, D-55128 Mainz

Well-defined silver-disks with a diameter of 1micrometer and a height of 40nm deposited on a Si substrate are illuminated by Ti-sapphire femtosecond-laser pulses with a wavelength of 400nm corresponding to a photon energy of 3.1 eV. The emitted electrons are detected by means of a photoelectron emission microscope (PEEM).

As the electric field vector of the photons changes from p- to s-polarization, a bimodal electron emission pattern emerges, indicating the excitation of nanoplasmonic fields in the Ag particles. In addition, we observe a correlation between elliptical deformation of the area of the Ag disks with distinct photoelectron emission and the fraction of the s-polarization of the impinging photons.

Furthermore, the photoemission yield was investigated as a function of laser power revealing different power exponent dependencies for s- and p-polarized light.

O 42.18 Wed 17:45 P2

**Klusterexperimente an dünnen Co-PLD-Schichten und Schichtsystemen** — MARKUS TRAUTMANN, ROBER HÄHLE, JANINE FISCHER, INGO SILL, ANDRE BIKOWSKI, THOMAS SCHMIDT, VEIT GROSSE, ●FRANK SCHMIDL und PAUL SEIDEL — FSU Jena, Institut für Festkörperphysik, Helmholtzweg 5, 07743 Jena, Germany

Für das gezielte Wachstum von Kohlenstoffnanoröhren (CNT's) spielen ferromagnetische Kluster (Co,Fe,Cr) eine entscheidende Rolle. Wir stellen Untersuchungen zur strukturierten Abscheidung von dünnen Co-Schichten mittels lasergestützter Abscheidung (PLD) vor. Es wurden Klusterexperimente auf Si-Substraten mit und ohne  $\text{SiO}_2$ -Einzelschichten bzw. Schichtsystemen durchgeführt. Wir diskutieren die Messungen zur Klustergröße in Abhängigkeit von Ausgangsschichtdicke, Klustertemperatur und Substratmaterial im Hinblick auf eine mögliche in-situ Abscheidung von CNT's mittels PLD.

O 42.19 Wed 17:45 P2

**Electron beam induced deposition: How to use an electron beam as a pen and precursor molecules as ink to write nanopatterns** — MICHAEL SCHIRMER<sup>1,2</sup>, MARIE-MADELEINE WALZ<sup>1,2</sup>, THOMAS LUKASCZYK<sup>1,2</sup>, FLORIAN VOLLNHALS<sup>1,2</sup>, HANS-PETER STEINRÜCK<sup>1,2</sup>, and ●HUBERTUS MARBACH<sup>1,2</sup> — <sup>1</sup>Lehrstuhl für Physikalische Chemie II — <sup>2</sup>Interdisciplinary Center for Molecular Materials (ICMM), Universität Erlangen-Nürnberg, Egerlandstr. 3, D-91058 Erlangen

The fabrication of chemically and structurally well-defined nanostructures is still a challenge and important for a large number of envisioned technological applications. We explore the technique of electron-beam induced deposition (EBID) to realize the engineering of such nanostructures: By exploiting a highly focused electron-beam of a scanning electron microscope (SEM) we directly write nanostructures by locally dissociating adsorbed precursor molecules. In contrast to previous studies our novel approach is to work in an ultra high vacuum (UHV) environment. This allows us to overcome the hitherto existing limitation concerning the rather poor cleanliness of the deposits

[1]. In this work, we present the successful generation of clean metallic (Fe) and oxidic nanostructures (TiOx, FeOx) with lithographically controlled shapes and lateral dimensions partially smaller than 10 nm on different substrates. The concept of EBID, basic physical principles and the promising perspectives and applications of this nanostructuring tool will be presented. This work was supported by the DFG under grant MA 4246/1-1.[1] T. Lukaszczuk, et al., *Small* 4(6) (2008) 841.

O 42.20 Wed 17:45 P2

**Surface energy gradient produced by collision cascades: effects on pattern formation by ion beam sputtering** — REINER KREE<sup>1</sup>, •TAHA YASSERI<sup>1</sup>, and ALEXANDER K. HARTMANN<sup>2</sup> — <sup>1</sup>Institute for Theoretical Physics, University of Göttingen, Friedrich-Hund Platz 1, D-37075 Göttingen, Germany. — <sup>2</sup>Institute for Physics, University Oldenburg, Carl-von-Ossietzky Strasse 9-11, D-26111 Oldenburg, Germany

In the existing theories of pattern formation due to ion beam sputtering, the energy of collision cascades leads to sputtering of atoms. But the lateral displacements at the surface due to the excess energy are not taken into account. We provide a continuum and a Monte Carlo model, which include this effect. Both models are based on standard transport theory.

We discuss the importance of the additional lateral transport on ripple formation using results of MC simulations and numerical (finite element) solutions of the continuum model.

O 42.21 Wed 17:45 P2

**Nanostructuring of thin V2O3 films on Au(111) by sputtering** — •LIZ MICHAELA RÖSKEN, FLORIAN LOVIS, ARMIN FELDHOFF, and RONALD IMBIHL — Institut für Physikalische Chemie und Elektrochemie, Leibniz-Universität Hannover, Callinstr. 3-3a, D-30167 Hannover, Germany

Thin V2O3 films of approximately 1 - 100 ML thickness on Au(111) were prepared by evaporation of vanadium in an O2 atmosphere (p(O2) = 10<sup>-7</sup> mbar). The films were characterized by LEED, Auger electron spectroscopy and photoelectron emission microscopy (PEEM). With annealing at T = 350° C epitaxial V2O3 films were found exhibiting (sqrt(3) x sqrt(3))R30° and (2x2) structures. Only after longer exposure to hydrogen (1-3 h) some reduction of the V2O3 film could be seen as evidenced by an increase of the PEEM brightness corresponding to a work function decrease. Upon sputtering the film displayed some unexpected optical effects: depending on the angle of observation the films appeared red or green. Secondary electron microscopy (SEM) revealed that the sputtering has led to island formation on the surface. The islands exhibit an average diameter of 20 nm and an average separation from each other of 20 nm. As possible mechanisms causing the island formation selective sputtering and the transformation of the 2D layer V-oxide into a 3D layer are discussed.

O 42.22 Wed 17:45 P2

**Laser induced backside wet etching of transparent materials with ultrashort laser pulses** — •MARTIN EHRHARDT and KLAUS ZIMMER — Leibniz-Institut für Oberflächenmodifizierung, Leipzig

The surface micro structuring of transparent dielectric materials with lasers can be achieved by direct laser ablation using VUV - wavelength or ultrashort pulses. Another approach to structuring these materials are indirect laser processing methods. Such methods use an enhanced absorption at interface of the material which can be achieved by an additional liquid, temporary plasma or absorption layer. At LIBWE (Laser induced backside wet etching) the backside of the transparent material is immersed to an absorbing liquid. That results in an intense energy deposition near the interface. For LIBWE with ns laser pulse the influence of several process parameters on e.g. etch rate, surface morphology were investigated in detail by Zimmer et al for a number of materials. However, for an improved understanding of the involved time processes an investigation of the influence of the pulse length for e.g. etch rate and surface morphology is important. In this presentation we will show recent results of the investigation of fused silica etched by LIBWE with ultrashort pulses. In particular the influence of the laser fluence and pulse number of the etch characteristic were investigated in detail and discussed. Furthermore morphological investigations were performed on the etched surface by different analytic techniques to characterize the surface quality. The results will be discussed with respect to the etch model for LIBWE with ns pulse to figure out the influence of the ultrashort pulse effects of the etching process.

O 42.23 Wed 17:45 P2

**Laser-induced mechanical excitation of nanostructures (and their measurement by means of SXM)** — •MARKUS SCHMOTZ<sup>1</sup>, TOBIAS GELDHAUSER<sup>1</sup>, PATRICK BOOKJANS<sup>2</sup>, and PAUL LEIDERER<sup>1</sup> — <sup>1</sup>Universität Konstanz, Deutschland — <sup>2</sup>James Madison University, USA

Information about deformations of nanostructures in the Gigahertz regime is rather sparse until now. Especially irradiation with short laser pulses is hardly studied. Our work aims at creating Surface Acoustic Waves (SAW) in the Gigahertz range based on short laser pulse techniques and using them to excite nanostructures. Generation and optically based detection of SAWs by single shot experiments showed first results. A new approach to the GHz regime is to utilize raster-probe techniques. Therefore we are developing a new detection method based on a homebuilt, variable temperature Scanning Tunneling Microscope (STM). Exploiting the highly non-linear I(z)-characteristic of the tunnelling-gap allows us to determine elongation in the sub-Å regime with high lateral resolution. Since the STM lacks a suitable temporal resolution for GHz-waves, we started to investigate vibrational modes in thin, free standing silicon membranes (thickness some hundred nm) in the kHz to MHz regime. In this range our STM electronics are fast enough to resolve the vibrations almost one-to-one. Comparison between optically gained information and corresponding STM data show excellent agreement. Measurements with the STM and according optical techniques at frequencies up to the GHz regime are currently under investigation.

O 42.24 Wed 17:45 P2

**Investigations on Focused Electron and Focused Ion Beam Induced Deposition of WC, PdC and PtC** — •HOLGER MOTZKAU<sup>1,2</sup> and DETLEF SPÖDDIG<sup>2</sup> — <sup>1</sup>Experimental Condensed Matter Physics, Department of Physics, Stockholm University, Roslagstullsbacken 21, SE-104 06 Stockholm, Sweden — <sup>2</sup>Abteilung für Supraleitung und Magnetismus, Institut für Experimentelle Physik II, Universität Leipzig, Linnéstr. 5, D-04103 Leipzig, Germany

Metallic nanostructures were grown by means of Focused Electron and Focused Ion Beam Induced Deposition (FEBID/FIBID) in a Dual Beam Microscope (DBM). The used precursors were tungsten hexacarbonyl, palladium(II) bis-(hexafluoroacetylacetonate) and methylcyclopentadienyl(trimethyl)platinum(IV). This investigation will present an optimization of the growth rates and homogeneities on an insulating SiN-surface. The chemical composition of the nanostructures were discussed by means of Energy Dispersive X-Ray Spectroscopy (EDX). Detailed AFM-scans reveal strong inhomogeneities for the W and Pd deposits as well as a small nonlinear growth at small thicknesses below 50 nm for all used precursors.

O 42.25 Wed 17:45 P2

**Coverage-Dependent Faceting of Au Chains on Si(557)** — •I. BARKE<sup>1</sup>, F. ZHENG<sup>2</sup>, S. BOCKENHAUER<sup>2</sup>, K. SELL<sup>1</sup>, V. v. OEYNHAUSEN<sup>1</sup>, K. H. MEIWES-BROER<sup>1</sup>, and F. J. HIMPSEL<sup>2</sup> — <sup>1</sup>Universität Rostock, Institut für Physik, 18051 Rostock — <sup>2</sup>Dept. of Physics, University of Wisconsin Madison, 1150 University Ave, Madison, WI 53706

The structural and electronic phase diagram of Au on Si(557) is established using scanning tunneling microscopy (STM) and angle-resolved photoemission (ARPES). Five phases consisting of altogether seven facets are observed in the sub-monolayer regime. Four of them consist of two coexisting structures. In order of increasing Au coverage the five phases are: Si(111)7x7 + Si(112), Si(557)1x2-Au, Si(111)5x2-Au + Si(335)-Au, Si(111)sqrt(3)xsqrt(3)-Au + Si(335)-Au, and Si(111)sqrt(3)xsqrt(3)-Au + Si(5 5 11)-Au. The relative surface areas of the five phases and seven facets are determined accurately by depositing a Au wedge ranging from 0 to 0.8 monolayer and performing automatic pattern recognition on large-scale STM images. Angle-resolved photoemission spectra are decomposed into contributions from the five phases. The Fermi wave vectors of various facets are identified. Using Si(557)1x2-Au as reference we find a coverage of 3 Au chains per unit cell for the frequently-studied Si(111)5x2-Au surface (instead of the widely-used value of 2 Au chains). The impact of this finding on structural models is discussed.

O 42.26 Wed 17:45 P2

**Temperature- and adatom-induced conductance modification of In/Si(111)-(4x1) nanowires** — •NADJA KOCH, SIMONE SANNA, STEFAN WIPPERMANN, and WOLF GERO SCHMIDT — Lehrstuhl für theoretische Physik, Universität Paderborn, Warburger Str. 100, 33098 Paderborn

Quasi one-dimensional structures, such as artificial atomic-scale wires, attract considerable attention due to their fascinating physical properties and large technological potential [1]. Highly anisotropic surface superstructures such as the In/Si(111)-(4x1) nanowire array are suitable model systems to explore atomic-scale wires both experimentally and computationally [2,3]. As a contribution to the understanding of the controversially discussed low-temperature phase transition of the In nanowires, we present ab-initio calculations of their temperature-dependent Landauer conductance. Additionally, we calculate the influence of adatoms (In, Pb, H, O) on the nanowire cond. [4]. Our results for In deposition, where exp. data are available, agree very well with the measurements [5]. The cond. drop due to adatoms is explained in terms of potential-well scatt. and/or structural deform. of the nanowires.

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[5] T Tanikawa et al., Phys Rev Lett 93, 016801 (2004).

O 42.27 Wed 17:45 P2

**Electron beam stimulated thermal desorption of oxygen: a lithographic method** — ●JAN RÖNSPIES, TAMMO BLOCK, and HERBERT PFNÜR — Leibniz Universität Hannover, Institut für Festkörperphysik, Appelstr. 2, 30167 Hannover, Germany

We explored the structural limits of unconventional electron beam lithography by directly writing with an electron beam into ultra-thin  $SiO_2$  films. These bare silicon window structures are suitable for growing contiguous metallic nanowires with thickness of a few monolayers. These uncovered structures with lateral dimensions down to 10nm were analyzed further by tunneling microscopy. The Auger excitation process (Knotek-Feibelman mechanism) necessary for electron-beam stimulated thermal desorption of oxygen (EBSTD) allows generation of ultra-small structures. The subsequent processing step combines thermal desorption of the remaining monoxide and simultaneous etching promoted by thermally activated silicon atoms, which turns out to be a strongly anisotropic process close to step edges [1]. Applying this combination of processes to a regularly stepped  $Si(557)$  sample which consists of a periodic array of small (111) and (112) oriented mini-facets with an average periodicity of 5.7nm normal to the steps, line widths close to the resolution of the electron microscope of 5nm were obtained. Thus exploitation of the quantized nature of ultrasmall structures far above liquid He temperatures becomes feasible as well as contacting of single molecules.

[1] *J.Appl.Phys.* 103, 064303(2008)

O 42.28 Wed 17:45 P2

**The formation of Au nanowires on Ge(001): an ab-initio study** — ●SIMEON SAUER<sup>1</sup>, FRANK FUCHS<sup>1</sup>, JÜRGEN FURTHMÜLLER<sup>1</sup>, FRIEDHELM BECHSTEDT<sup>1</sup>, CHRISTIAN BLUMENSTEIN<sup>2</sup>, SEBASTIAN MEYER<sup>2</sup>, JÖRG SCHÄFER<sup>2</sup>, and RALPH CLAESSEN<sup>2</sup> — <sup>1</sup>Institut für Festkörpertheorie und -optik, Universität Jena, D-07743 Jena — <sup>2</sup>Physikalisches Institut, Universität Würzburg, D-97074 Würzburg

Deposition of approximately 0.5 ML of Au on the Ge(001) surface leads to self-organized formation of chains along the [110] direction [1]. These chains are characterized by some unprecedented features: low-defect growth, high aspect ratio and rather high spacing between adjacent chains. This system seems to be a possible candidate for the formation of a Luttinger liquid.

Assuming a  $c(8x2)$  translational symmetry we propose several models of Au chain structures. They are investigated in the framework of a density functional theory approach. For each model, different features including surface energy, STM images, band structure, etc. are calculated. The computed properties are compared to experimental data and used to evaluate the different models.

[1] J. Schäfer, C. Blumenstein, S. Meyer, M. Wisniewski, and R. Claessen, Phys. Rev. Lett. 101, in press (Dec. 2008).

O 42.29 Wed 17:45 P2

**Large Area Growth of Pt-induced Atomic Nanowires on Ge(001)** — ●SEBASTIAN MEYER<sup>1</sup>, KATHRIN ROENSCH<sup>1</sup>, MARC WISNIEWSKI<sup>1</sup>, CHRISTIAN BLUMENSTEIN<sup>1</sup>, JÖRG SCHÄFER<sup>1</sup>, ANDREJ STEKOLNIKOV<sup>2</sup>, FIEDHELM BECHSTEDT<sup>2</sup>, and RALPH CLAESSEN<sup>1</sup> — <sup>1</sup>Physikal. Institut, Universität Würzburg, 97074 Würzburg — <sup>2</sup>Inst. f. Festkörpertheorie u. -optik, Universität Jena, 07743 Jena

The structural properties of atomic nanowires are closely affecting both self-organized growth and resulting conduction behavior. A fascinating case are Pt nanowires on the Ge(001) surface. A dimerization along the chains observed in scanning tunneling microscopy (STM) is reminiscent of a charge density wave. However, sideways dimer elements also exist, which indicate dimerized back-bonds. Near the Fermi level, dimerization is not observed, and a spatially rather uniform charge density exists. It is consistent with metallic character at room temperature, as is confirmed by tunneling spectroscopy. Concerning the bonds involved, rather high substrate temperatures ( $\sim 700^\circ\text{C}$ ) are needed to initiate large-area growth. The experimental findings can be understood within a structural model obtained from ab-initio simulation [1]. It turns out that Pt-Ge bonds are favored. Moreover, the prominent dimerization along the chain is explained by Ge dimers rather than Pt ones. Instead, the metal atoms are incorporated as chain of alternating Pt and Ge atoms adjacent to the top ridge. Such complex bond rearrangement makes it plausible that high activation energies are needed for a structural reorganization.

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O 42.30 Wed 17:45 P2

**Suppression of phase transition by doping: atomic Pb chains on Si(557)** — MARCIN CZUBANOWSKI, ●MELANI GAUCH, CHRISTOPH TEGENKAMP, and HERBERT PFNÜR — Leibniz Universität Hannover, Festkörperphysik, Abteilung Oberflächen

The adsorption of Pb on Si(557) substrate leads to the formation of anisotropic metallic structures as reveal by conductivity measurements, SPA-LEED and ARPES. The annealing of at least 1.3ML Pb at 640K forms atomic chain structure within a (223) facet, which shows below  $T_c = 78\text{K}$  a metallic conductance along the wires, whereas the perpendicular direction is insulating. As revealed by ARPES and LEED, the interplay between the filling of the surface bands, determined by the Pb coverage, and the reciprocal lattice vector, defined by the inter-chain spacing, results below  $T_c$  in a perfect nesting condition. Due to a temperature driven refaceting transition, the system switches into a 2d regime, where conductivity is seen in both direction. In our recent experiments, the influence of additional Pb atoms on the phase transition at  $T_c$  has been investigated by means of SPA-LEED. The electronically stabilized system at 1.3ML has been doped by a small amount of addition Pb (in steps of 0.01ML). The structural phase transition is gradually suppressed as the coverage reaches 1.5ML. As judged from SPA-LEED the excess coverage starts to decorate the steps, obviously changing the filling factors of the surface states.

O 42.31 Wed 17:45 P2

**Surface Photo Voltage and Local Work Function Variations of Nanostructures on Si(111) measured by STM** — ●KRISTIAN SELL, INGO BARKE, STEFAN POLEI, VIOLA VON OEYNSHAUSEN, and KARL-HEINZ MEIWES-BROER — Universität Rostock, Institut für Physik, 18051 Rostock, Germany

We present surface photo voltage (SPV) and local work function (LWF) measurements of Si(111)5x2-Au atomic chains and deposited clusters on a Si(111)7x7 surface. Quantitative results are obtained from spatially resolved I(V) spectra. On a Si(111) surface partially covered by the quasi one-dimensional Si(111)5x2-Au structure we determine the SPV as a function of laser power at different locations. Based on these results we establish and discuss a simple model for the band bending which leads to LWF variations on a sub-nanometer scale. This model is confirmed by spatially resolved LWF measurements using I(Z) spectroscopy. In addition we present preliminary SPV measurements on clusters produced in an arc cluster ion source (ACIS) and deposited on Si(111)7x7.

O 42.32 Wed 17:45 P2

**Field Emission Resonances on Junctions between Si(111)7x7 and Si(111)5x2-Au** — ●STEFAN POLEI, INGO BARKE, KRISTIAN SELL, VIOLA V. OEYNSHAUSEN, and KARL-HEINZ MEIWES-BROER — Institut für Physik, Universität Rostock, Universitätsplatz 3, D-18051 Rostock

The image state derived field emission resonances (FER) are investigated on a Si(111)7x7 substrat which is partially covered by the quasi one-dimensional Si(111)5x2-Au structure. These states can be observed by  $dI/dV$  measurements of the unoccupied energy range if the STM is operated in a field emission mode. A shift of the FER peak positions on Si(111)7x7 patches vs. Si(111)5x2-Au patches is found which happens on a scale of one nanometer. The origin of that shift is attributed to work function differences [1] caused by the different Fermi level pinning. The results are discussed in view of local work

function changes determined by I(Z) spectroscopy across a (7x7)-(5x2-Au) junction.

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O 42.33 Wed 17:45 P2

**Investigation of self-sustained molecular wires by STM** — ●KERRIN DÖSSEL<sup>1</sup>, MAYA LUKAS<sup>1</sup>, ALEXANDRINA STUPARU<sup>1</sup>, CHRISTOPHE STROH<sup>1</sup>, MARCEL MAYOR<sup>1,2</sup>, and HILBERT V. LÖHNESEN<sup>3,4</sup> — <sup>1</sup>Forschungszentrum Karlsruhe, Institut für Nanotechnologie, D-76021 Karlsruhe — <sup>2</sup>Universität Basel, Department of Chemistry, CH-4056 Basel — <sup>3</sup>Universität Karlsruhe, Physikalisches Institut, D-76128 Karlsruhe — <sup>4</sup>Forschungszentrum Karlsruhe, Institut für Festkörperphysik, D-76021 Karlsruhe

In recent years the electronic structure and in particular the conductance of organic molecules have been investigated in a growing number of experiments. A method frequently used to measure molecular conductance is the mechanically controlled break junction (MCBJ) technique. However, in MCBJs the nature of the contact of the molecule to the electrodes is not known. Theory is thus lacking important information to exactly model and thus understand molecular conductance. It is therefore desirable to fully characterize molecular wires which are binding stably to the electrodes. We investigate self-sustained molecules, that are designed to stand upright on a conducting substrate, which serves as one electrode, while the head-group is sticking out freely from the surface, accessible by the tip of our UHV STM. We used STM and STS to investigate the molecules' position and surrounding on the surface, the bond to the surface and the electronic properties of our tripod molecules on several metallic surfaces at low temperature (30K).

O 42.34 Wed 17:45 P2

**Growth of horizontally aligned carbon nanotubes on single crystalline surfaces** — ●FLORIAN SZILLAT, HANS KLEEMANN, PHILIPP ZEIGERMANN, MICHAEL BLECH, MATHIAS STEGLICH, and BERND SCHROETER — Universitaet Jena, Institut fuer Festkoerperphysik, Max-Wien-Platz 1, 07743 Jena, Deutschland

A controlled growth of aligned carbon nanotubes with particular structural and electronic properties at predefined positions is a prerequisite to utilize them in electronic or nanooptical devices. Alignment could be reached by applying electric fields during growth via chemical vapor deposition or by using single crystalline substrates. In the latter case the anisotropic arrangement of the surface atoms create an intrinsic electric field. An easy and fast way to analyze the crystallographic orientation of the substrate is the use of electron channeling pattern. The metal catalyst is deposited and prestructured at the substrate surface to support the aligned growth of CNTs. The carbon nanotubes are produced by catalytic chemical vapor deposition using ethanol or methane as precursor gas. The quality of these nanotubes is tested by raman and x-ray spectroscopy. Morphology and orientation of the nanotubes are characterized by scanning electron and atomic force microscopy.

O 42.35 Wed 17:45 P2

**Oxide formation on reconstructed Au(110) surfaces** — ●MARC LANDMANN, EVA RAULS, and WOLF GERO SCHMIDT — Lehrstuhl für Theoretische Physik, Universität Paderborn

The stability of oxygen adstructures on the unreconstructed (1x1) and the "missing row" type reconstructed (1x2) and (1x3) Au(110) surfaces [1,2] has been investigated by density-functional theory calculations, considering experimentally typical ultra high vacuum conditions. Three Au-O chain like structures have been identified to be especially stable under specific (T,p) conditions. These chain structures, oriented along the atomic ridges of the reconstructed surfaces, are clearly favored over oxygen conglomerates on (1xr) surfaces and represent the most stable form of chemisorbed atomic oxygen on Au(110) surfaces.

Our investigation of surface oxidation directly connects the adsorption of atomic oxygen on Au(110) single-crystal surfaces to experimental [3] and theoretical [4] results that have recently shown that oxygen incorporation in freely suspended atomic gold chains results in a stabilization of these structures.

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O 42.36 Wed 17:45 P2

**Entropy changes stability of Au(110) surface reconstructions** — EVA RAULS, ●MARC LANDMANN, and WOLF GERO SCHMIDT — Lehrstuhl für Theoretische Physik, Universität Paderborn

In contrast to the unreconstructed single-crystal surfaces of Cu and Ag, the Au(110) surface is subject to short range reconstructions of a missing row type. Even the lowest energy surface in (111) direction shows a long range surface reconstruction. Experimentally, Au(110) reconstructions with (1x2) and (1x3) periodicity are observed [1,2], while in theoretical works, the stability order is discussed controversially [3].

We have carried out density-functional theory calculations to resolve this controversy. If we consider the contributions of vibrational entropy, we find different stabilizations for the different reconstructions. This leads to a temperature dependent stability order, with the (1x3) reconstruction being the most stable structure at zero temperature, while, at room temperature, the most often observed (1x2) reconstruction is most stable, demonstrating the crucial role of entropy.

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O 42.37 Wed 17:45 P2

**STM/CITS Characterization of 1D and 2D Superstructures Evolving on Pure Highly Ordered Pyrolytic Graphite** — ●AARON GRYZIA, MARC D. SACHER, ARMIN BRECHLING, and ULRICH HEINZMANN — Molecular and Surface Physics, Bielefeld University

The last decades have shown highly ordered pyrolytic graphite (HOPG) as one of the most important substrates for studying adsorbates such as metal atoms, organic molecules, polymers and many others by Scanning Tunneling Microscopy (STM) and Scanning Tunneling Spectroscopy (STS) techniques. Although HOPG is in use for many years, known effects such as 1D[1] and 2D[2] superstructures have been studied very sparsely. These native HOPG superstructures are often very similar to the investigated adsorbates. Therefore the understanding of the properties of the substrate and its special features is of vital importance. In reverse the effects themselves may lead to new applications e.g. in using these 2D-superstructures as templates for adsorbing molecules in array like structures[3]. We focus our research on chain like structures and arrays on HOPG measured by STM and Current Image Tunneling Spectroscopy (CITS) under UHV conditions in order to understand the origin of these effects. First results of these measurements will be presented.

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O 42.38 Wed 17:45 P2

**STM study of the adsorption of phthalocyanine molecules on anisotropic surfaces** — ●TOBIAS PERTRAM<sup>1</sup>, QIHUI WU<sup>2</sup>, CONRAD BECKER<sup>1</sup>, and KLAUS WANDELT<sup>1</sup> — <sup>1</sup>Institute of Physical and Theoretical Chemistry, University of Bonn, Wegelerstr. 12, 53115 Bonn, Germany — <sup>2</sup>Department of Physics, La Trobe University, Victoria 3086, Australia

The {110} surfaces of fcc metals show an intrinsic anisotropy due to the rectangular surface unit cell. This anisotropy can be even more pronounced in the case of the (1x2) missing row reconstruction, which has been found for metals such as Pt and Au. In contrast, on Pd(110) this reconstruction is only stable after the adsorption of hydrogen [1]. The clean Pd(110) does not show the tendency to reconstruct. After deposition of small amounts of Au (< 1 ML) on the unreconstructed Pd(110) surface pseudomorphic Au islands are observed, whereas in the case of higher Au amounts (> 2 ML) the resulting Au layer shows the characteristic (1x2) reconstruction, which however is still remains pseudomorphic to Pd(110) [2]. We used both reconstructed surfaces, the hydrogen induced Pd(110)-(1x2) surface and the Au modified one as a substrate for the deposition of phthalocyanine molecules. STM investigations under UHV conditions reveal a specific adsorption behaviour of the phthalocyanine molecules, which are oriented along rows of the reconstructed surfaces ("template effect").

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O 42.39 Wed 17:45 P2

**Puzzling effects of side chains on self-assembled molecular nanostructures** — ●STEPHAN BLANKENBURG, EVA RAULS, and WOLF GERO SCHMIDT — Theoretische Physik, Universität Paderborn, Germany

Molecular self-assembly and self-organization is presently seen as a promising alternative to the top-down design for future electronic devices. The experimental and theoretical study of well-defined model systems is an essential step for understanding the basic mechanisms responsible for the formation of complex supramolecular structures [1-4]. In this context, the influence of alkyl side chains on hydrogen bonded molecular surface networks were analyzed with scanning tunneling microscopy [5]: the adsorption of cyanuric (CYA), diethylbarbituric (DEB) and butylcyanuric acid (BuCYA) at Au(111) show large differences in their ordering at the surface. Here we use density-functional theory calculations within the generalized-gradient approximation to rationalize these differences in terms of hydrogen bonds as well as intermolecular H-H interactions.

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O 42.40 Wed 17:45 P2

**Charge transfer in the TCNQ-sexithiophene complex** — ●KAI-FELIX BRAUN and SAW-WAI HLA — Nanoscale & Quantum Phenomena Institute and the Department of Physics & Astronomy, Ohio University, Athens, Ohio 45701, USA.

Molecular crystals from thiophene molecules can be doped with TCNQ-F4 molecules for use in all-organic opto-electronic and semiconductor devices. The charge transfer and the molecular orbital energy level formation in between these two organic molecules is investigated here by density functional theory calculations (DFT). The isolated molecules are calculated non-bonded and bonded together forming a charge transfer complex (CTC). The relaxed structure of the complex shows essentially coplanar and centered molecules with the  $\alpha$ -sexithiophene rings tilted alternately by  $4.8^\circ$ . The bond formation of these molecules results in a charge transfers of  $\sim 0.4 e^-$  from the  $\alpha$ -sexithiophene to the TCNQ-F4 molecule. The HOMO-LUMO gap width is reduced as compared to the isolated molecules due to the newly formed orbitals in the CTC complex. Upon adsorption on a Au(111) surface electrons are transferred onto the molecule complex thereby causing the molecular levels to align asymmetric with respect to the charge neutrality level. The theoretical results for the single molecule and CTC layer are compared to experimental photoemission and scanning tunneling spectroscopy results. Journal of Chemical Physics 129 (2008), 064707.

O 42.41 Wed 17:45 P2

**Two dimensional structure formation controlled by metal-ligand interactions** — ●ACHIM BREITRUCK, HARRY E. HOSTER, and R. JÜRGEN BEHM — Institute of Surface Chemistry and Catalysis, Ulm University, D-89069 Ulm

Using highly oriented pyrolytic graphite (HOPG) as substrate, two dimensional structure formation of bisterpyridine (BTP) molecules in the presence of metal atoms was studied by scanning tunnelling microscopy (STM) under ultrahigh vacuum (UHV) conditions. BTP molecules form highly ordered networks stabilized by C-H...N type hydrogen bonds. [1,2] Upon metal deposition (Ag, Cu), these hydrogen bonds are partially lifted in favour of metal...N-pyridine interactions. This results in new network structures that strongly depend on the metal-to-molecule ratio. Surprisingly, we find the same sequence of metal coverage dependent structures for Ag and Cu addition, while theory predicts the Cu...N-pyridine interaction to be about 3 times stronger than the Ag...N-pyridine interaction.[3] Possible reasons for this will be discussed.

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O 42.42 Wed 17:45 P2

**Spatial modulation of molecular adsorption energies due indirect interactions** — ●STEPHAN BLANKENBURG and WOLF GERO SCHMIDT — Theoretische Physik, Universität Paderborn, Germany

The autonomous ordering and assembly of atoms and molecules on

atomically well-defined surfaces appears as a very promising alternative route to even smaller functional systems with nanometre dimensions. However, the mechanisms controlling the self-ordering phenomena need to be thoroughly understood in order to use them for nanofabrication processes. In this context we investigate computationally the origin of long-range order observed experimentally for the adsorption of (i) (s)-glutamic acid on Ag(110) [1] and (ii) phenylglycine and adenine on Cu(110) [2,3]. In both cases we find long-wave oscillations of the substrate charge density to be decisive for the adsorption configuration. In case of glutamic acid adsorbed on Ag(110), long-range strain field are very important as well, while they are nearly negligible for phenylglycine and adenine adsorbed on Cu(110).

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O 42.43 Wed 17:45 P2

**2D chemistry on Au(111) surfaces** — ●EVA RAULS, STEPHAN BLANKENBURG, and WOLF GERO SCHMIDT — Theoretische Physik, Universität Paderborn, Germany

The design of functional two-dimensional molecular networks has become an area of intense research [1,2]. The constraint to 2 in contrast to the availability of 3 dimensions has a large impact on many chemical reactions. Chemical reactions between surface adsorbed molecules may lead to products very different from those obtained in solutions or the gas phase. The imide formation between a diaminoterphenyl (DATP) and a PTCDA molecule [3] is one very interesting example in this respect. In scanning tunneling microscopy (STM) experiments, it has been observed that the Au surface changes both the reaction path and the reaction product compared to 3D. In order to understand these experimental observations, we have studied the chemical reactions both in solution and on the Au(111) surface by density-functional theory calculations in the generalized-gradient approximation.

- [1] S. Blankenburg and W. G. Schmidt, PRL 99, 196107 (2007).
- [2] E. Rauls and W.G. Schmidt, J. Phys. Chem C 112, 11490 (2008).
- [3] M. Treier, N.V. Richardson, and R. Fasel, JACS 130, 14054 (2008).

O 42.44 Wed 17:45 P2

**Adsorption geometry and self assembly of corrole molecules on different copper facets** — ●LEONID LICHTENSTEIN, STEFAN KUCK, GERMAR HOFFMANN, and ROLAND WIESENDANGER — Institute of Applied Physics, University of Hamburg

A new member of the metalloporphyrinoid class is the one-carbon short corrole which is a very accessible, easily tunable compound with many potential applications in material science and catalysis. These molecules differ from the parent porphyrin molecules [1] mainly by their lower inherent symmetry and the smaller cavity. In this study using STM we address the conformation (orientation and chirality) and self assembly of iron-triphenylcorrole (FeTPC) molecules on Cu(100) and Cu(111). At low coverage FeTPC molecules show restricted symmetry and can be controllably switched among different conformations [2]. At higher coverage formation of regular aggregates can be observed. We will present the results of the growth study in dependence of surface geometry and coverage and discuss results of scanning tunneling spectroscopy investigations of these systems.

- [1] W. Auwärter et al., Int J. Nanotechnology Vol. 5, 1171 (2008).
- [2] S. Kuck et al., J. Am. Chem. Soc., 130, 14072 (2008).

O 42.45 Wed 17:45 P2

**Adsorption of metal phthalocyanines on Cu(111) and Cu(100): A STM study** — ●SHIH-HSIN CHANG, JENS BREDE, JÖRG SCHWÖBEL, STEFAN KUCK, GERMAR HOFFMANN, and ROLAND WIESENDANGER — Institute of Applied Physics, University of Hamburg, Jungiusstrasse 11 D-20355 Hamburg, Germany

The temperature dependent adsorption behavior of 4-fold symmetric metal phthalocyanines (MPcs) on metals with commensurate and incommensurate symmetries was investigated by means of scanning tunneling microscopy. On the 4-fold symmetric Cu(100) surface, planar and 4-fold molecular structures in two equivalent orientations were found for MPcs when prepared at room temperature. In addition, two metastable orientations were identified when prepared at low temperature which can be depopulated upon annealing. MPcs adsorbed on the 6-fold symmetric Cu(111) surface showed a disturbed molecular appearance. The symmetry of molecular structures changed from 4-fold



to 2-fold which is discussed in terms of molecule-substrate interaction.

O 42.46 Wed 17:45 P2

**Coverage-dependence adsorbed structure of tetracene on Ag(110)** — •HAN HUANG<sup>1,2</sup>, FEI SONG<sup>1,3</sup>, QIAO CHEN<sup>4</sup>, WUZONG ZHOU<sup>5</sup>, and SHING BAO<sup>1</sup> — <sup>1</sup>Department of Physics, Zhejiang University, Hangzhou 310027, P. R. China — <sup>2</sup>Department of Physics, National University of Singapore, 117542, Singapore — <sup>3</sup>ISA and iNANO, University of Aarhus, 8000C, Denmark — <sup>4</sup>Department of chemistry, University of Sussex, Sch Life Sci, Brighton BN1 9QJ, E Sussex England — <sup>5</sup>School of Chemistry, University of St Andrews, St Andrews KY16 9ST, Fife Scotland

The ordered adsorption structures of tetracene on Ag(110) have been studied by low energy electron diffraction (LEED), scanning tunneling microscopy (STM) and density functional theory (DFT) calculations. At a low coverage, as calibrated with LEED, both p(4 x 4) and c(8 x 4) ordered structures are simultaneously formed on an Ag(110) surface at room temperature. STM images suggest the molecular plane is parallel to the Ag surface with its long molecular axis aligned along the [001] azimuth. DFT optimization reveals a separation of 0.3 nm between the molecular plane and substrate surface while the center of the tetracene molecule is on the long bridge site. Increasing coverage slightly, a (6,2;2,5) structure is formed while the adsorbed molecules maintain the flat-lying geometry with adjacent molecules alternating their height relative to the surface.

O 42.47 Wed 17:45 P2

**Photoemission studies of ex-situ prepared butanethiol and azobenzene derivative SAMs on Au(111): heat- and light-induced modifications of electron spectra** — •TILL LEISSNER, NILS HEINEMANN, TIMM ROHWER, OLEKSIY ANDREYEV, and MICHAEL BAUER — Institut für Experimentelle und Angewandte Physik, Uni Kiel

Molecular switches and their intriguing properties attract much interest in the field of molecular electronics. Wet chemical deposition is a generally used method for coating of metallic surfaces with azobenzene-based switching molecules. In fact, the obtained SAMs are often imperfect and very inhomogeneous.

In this contribution we will present an improved technology of the ex-situ SAMs preparation. For our studies we choose butanethiol molecules as a model system for the molecular switch 3-(4-(4-Hexylphenylazo)phenoxy)propan-1-thiol adsorbed on a Au(111) surface. The quality of the obtained butanethiol and molecular switch SAMs was checked by means of two photon photoemission (2PPE) and LEED.

Furthermore, we will present data showing the impact of annealing and laser illumination (80 MHz fs-laser system) on butanethiol/Au(111) samples. In contrast to butanethiol, the molecular switch revealed strong irreversible modifications of the electronic structure under laser irradiation. This result will be discussed particularly in the context of a potential switching mechanism.

O 42.48 Wed 17:45 P2

**Scanning tunneling microscopy of polyoxometalates on Au(111)** — •LEONID KLIUIENKO<sup>1</sup>, PAUL KÖGERLER<sup>2</sup>, and BERT VOIGTLÄNDER<sup>1</sup> — <sup>1</sup>Institute of Bio- und Nanosystems (IBN) and JARA-Fundamentals of Future Information Technology, Forschungszentrum Jülich, D-52425 Jülich, Germany — <sup>2</sup>Institute of Solid State Research (IFF) and JARA-Fundamentals of Future Information Technology, Forschungszentrum Jülich, D-52425 Jülich, Germany

Single and aggregated {Mo<sub>72</sub>Fe<sub>30</sub>} · H<sub>2</sub>O polyoxometalate (POM) clusters have been studied by low-temperature ultra high vacuum (UHV) scanning tunneling microscope (STM). Several methods were tried to deposit polyoxometalates on the Au(111) surface. "Drop casting" from a water solution in N<sub>2</sub> atmosphere and pulse injection techniques were used for POM cluster deposition onto a previously cleaned Au(111) surface. After subsequent annealing in UHV samples were studied in the STM. STM images show that POM clusters were adsorbed on clean Au(111) surface and reveal a strong affinity towards cluster agglomeration. Nevertheless it was possible to image single POM clusters.

O 42.49 Wed 17:45 P2

**STM study of growth, structure, and stability of DMDS on Au(111)** — •PATRICK MEHRING, AXEL BEIMBORN, DANIEL WEIER, FRANK SCHÖNBOHM, TOBIAS LÜHR, and CARSTEN WESTPHAL —

Fakultät Physik - Technische Universität Dortmund, Otto-Hahn-Str. 4, D 44221 Dortmund, Germany

Systems of self-assembled monolayers (SAM) are in the focus of present research activities due to their potential applications in fields like molecular electronics, bio-sensing, and the manipulation of metallic surface characteristics. Therefore, monolayers of linear alkanethiols are considered as ideal model systems. In this study the growth, structure, and stability of Dimethyldisulfide (DMDS) layers on Au(111) were investigated by scanning tunneling microscopy. SAMs were formed by solution deposition methods at room temperature. We varied the deposition time from 6h to 24h. Subsequently, several thermal annealing steps with increasing temperatures were performed in vacuum. After each step, the monolayer was investigated by STM. A stripe phase with increasing coverage as a function of the deposition time was observed. After annealing at 80°C molecular islands were observed at the surface. After island formation the stripe phase is removed completely due to the rearrangement of molecules at the surface. Between the islands an amorphous phase was found. Increasing the temperature to 150°C leads to a disappearance of the islands. The herringbone reconstruction of the gold surface reappeared.

O 42.50 Wed 17:45 P2

**Comparison of Different Porphyrin Derivatives in Scanning Tunneling Microscopy** — •FLORIAN VOLLNHALS, FLORIAN BUCHNER, INA KELLNER, YUN BAI, MARTIN SCHMID, J. MICHAEL GOTTFRIED, HANS-PETER STEINRÜCK, and HUBERTUS MARBACH — Lehrstuhl für Physikalische Chemie II, Interdisciplinary Center of Molecular Materials (ICMM), Universität Erlangen-Nürnberg, Egerlandstr. 3, D-91058 Erlangen

Porphyrin derivatives are considered as ideal building blocks for the self-assembly of molecular devices due to their rigid structure triggering long range order and versatile functionalities. Here we explore the appearance of different porphyrin derivatives, namely octaethylporphyrins (OEP) and tetraphenylporphyrins (TTP), on Ag(111) in scanning tunneling microscopy (STM). Additional information concerning the electronic structure, in particular the density of states close to the Fermi level, was acquired by means of ultraviolet photoelectron spectroscopy (UPS) and scanning tunneling spectroscopy (STS). It will be shown that the contrast in a layer of intermixed CoTPP and 2HTPP [1] and the appearance of individual CoTPP molecules in STM depends on the applied bias voltage. The comparison in particular of CoTPP and CoOEP reveals similar signatures in UPS but different bias dependent appearance in STM. These findings will be discussed in terms of intramolecular conformation, molecule substrate interaction and the corresponding electronic structure. Supported by the DFG through SFB 583. [1] K. Comanici et al., Langmuir, 24(2008), 1897.

O 42.51 Wed 17:45 P2

**Organic-Metal Interface: Cysteine on Au(110)** — •BENJAMIN HÖFFLING, FRANK ORTMANN, KARSTEN HANNEWALD, and FRIEDHELM BECHSTEDT — Institut für Festkörpertheorie und -optik, Friedrich-Schiller-Universität, Jena, Germany

The interaction of thiol groups with gold surfaces is of particular importance in the research of transport properties of organic materials (organic electronics) since the sulfur-gold interaction is strong and establishes a link between electrode and organic semiconductor. Additional functional groups, however, might have an influence on this bond and deserve attention in adsorption studies. By means of density functional calculations, we study such an interplay of different functional groups upon adsorption for the model system of the amino acid cysteine on the Au(110) surface. The interaction of the functional groups with the surface is investigated in detail. We present results on the electrostatic potential, the charge redistribution upon adsorption, and induced changes in the density of states. Finally, we predict four qualitatively different adsorption configurations for cysteine on Au(110) and compare their characteristics.

O 42.52 Wed 17:45 P2

**Room temperature STM investigation of organic molecules deposited by pulse injection** — •CARMEN PÉREZ LEÓN<sup>1</sup>, CHRISTOPH SÜRGER<sup>1</sup>, MARCEL MAYOR<sup>2,3</sup>, and HILBERT V. LÖHNESEN<sup>1,4</sup> — <sup>1</sup>Physikalisches Institut and DFG-Center for Functional Nanostructures (CFN), Universität Karlsruhe, D-76128 Karlsruhe, Germany — <sup>2</sup>Forschungszentrum Karlsruhe, Institut für Nanotechnologie, D-76021 Karlsruhe, Germany — <sup>3</sup>Department of Chemistry, University of Basel, CH-4056 Basel, Switzerland — <sup>4</sup>Forschungszentrum Karlsruhe, Institut für Festkörperphysik, D-



76021 Karlsruhe, Germany

$\pi$ -conjugated oligomers  $C_{114}H_{158}O_8S_2Si_2$  (CHOSSi) have been deposited on clean Cu(111) at room temperature using the pulse-injection method with tetrahydrofuran (THF) as solvent. Scanning tunneling microscopy measurements in ultra-high vacuum at room temperature demonstrate that the CHOSSi and THF molecules coadsorb on the copper surface. The solvent molecules form ordered structures with distinct orientations and domain boundaries suggesting a strong interaction of THF with the substrate. Individual and small clusters of CHOSSi molecules appear randomly distributed on the surface with no apparent correlation with the solvent. A detailed study of the self-organized adsorption of the THF molecules on Cu(111) will be presented.

O 42.53 Wed 17:45 P2

**Self-assembly of amino acids on noble metal surfaces: universality of the amino acid bonding scheme** — ●JOACHIM REICHERT<sup>1</sup>, AGUSTIN SCHIFFRIN<sup>1,2</sup>, YAN PENNEC<sup>2</sup>, WILLI AUWÄRTER<sup>1</sup>, ALEXANDER WEBER-BARGIONI<sup>2</sup>, MATTHIAS MARSCHALL<sup>1</sup>, DEAN CVETKO<sup>3</sup>, ALBANO COSSARO<sup>3</sup>, ALBERTO MORGANTE<sup>3</sup>, and JOHANNES V. BARTH<sup>1</sup> — <sup>1</sup>Physik Department, TU München, Germany — <sup>2</sup>Chemistry Department, University of British Columbia, Vancouver, Canada — <sup>3</sup>INFN/TASC, Trieste, Italy

We investigated the molecular self-assemblies of L-methionine on Cu(111) and L-tyrosine on Ag(111) by means of STM, HAS, XPS and NEXAFS in UHV. The self-assembly of L-methionine on Cu(111) is strongly influenced by the substrate reactivity and reveals a temperature dependent structural transformation involving a chiral orientational switch and the emergence of an ordered 1D high temperature phase. XPS data show that this transformation is triggered by a thermally activated deprotonation of the  $NH_3^+$  group. The ordered phase shows noncovalent molecular dimerization and alignment into chains which are commensurate with the underlying substrate. L-tyrosine on Ag(111) self-assembles into linear nanoribbons primarily following the substrate crystalline symmetry. A zwitterionic noncovalent molecular dimerization is observed, and NEXAFS data provide evidence of a non-flat adsorption of the phenol ring. This dimerization scheme is reminiscent of methionine on Cu(111) and Ag(111), and supports a universal self-assembling trend for amino acids on close-packed noble metal surfaces.

O 42.54 Wed 17:45 P2

**Substrate Effect in the structure of ordered Bis-terpyridine monolayer networks** — ●THOMAS WALDMANN<sup>1</sup>, DANIELA KÜNZEL<sup>2</sup>, HARRY E. HOSTER<sup>1</sup>, AXEL GROSS<sup>2</sup>, and R. JÜRGEN BEHM<sup>1</sup> — <sup>1</sup>Institute of Surface Chemistry and Catalysis, Ulm University, D-89069 Ulm, Germany — <sup>2</sup>Institute of Theoretical Chemistry, Ulm University, D-89069 Ulm, Germany

We present different supramolecular networks formed by monolayers of a Bis-terpyridine derivative (2,4'-BTP)[1,2] on the (100) and (111) surfaces of Ag and Au. On all four substrates, ordered and disordered structures are observed by STM and LEED under UHV conditions at  $T = 300$  K and at 90 K. On Ag(111) and Au(111) surfaces, single 2,4'-BTP molecules are observed in 12 different orientations with 30° difference. This is explained by a best fit of the molecules to the substrate, maximizing the number of N atoms being adsorbed a-top of substrate atoms [3,4]. This simple model fully explains the resulting molecular networks on Ag(111) and Au(111). Its suitability for rationalizing monolayer networks on the (100) surfaces of Ag and Au is tested.

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

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

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

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

O 42.55 Wed 17:45 P2

**Substrate-induced molecular orientation of ClGa-phthalocyanine studied by MAES and UPS** — ●T. HOSOKAI<sup>1</sup>, A. GERLACH<sup>1</sup>, H. MACHIDA<sup>2</sup>, Y. SUZUKI<sup>2</sup>, S. DUHM<sup>2</sup>, N. KOCH<sup>3</sup>, S. KERA<sup>2</sup>, U. NOBUO<sup>2</sup>, and F. SCHREIBER<sup>1</sup> — <sup>1</sup>Institut für Angewandte Physik, Universität Tübingen, Germany — <sup>2</sup>Graduate School of Advanced Integration Science, Chiba university, Japan — <sup>3</sup>Institut für Physik, Humboldt-Universität zu Berlin, Germany

Understanding the substrate-molecule interactions is a prerequisite for the control of organic film growth. Here we report the substrate-induced molecular orientation of the non-planar chlorogallium phthalocyanine (ClGaPc) molecules on Cu(111) and graphite by means of UPS and metastable atom electron spectroscopy (MAES). In the monolayer MAES shows distinctively different features on Cu(111) and graphite: On the Cu(111) surface bands corresponding to non-bonding orbitals of the Cl-atom, i.e. those largely distributed parallel and perpendicular to the molecular plane, are not observed, whereas on the graphite both bands can be found. Because of the high surface sensitivity of the MAES technique these results indicate a different orientation of ClGaPc on Cu(111) and graphite. On Cu(111) ClGaPc molecules orient with the Cl-atom directed towards the Cu surface, whereas on the graphite ClGaPc molecules orient with the Cl-atom directed towards the vacuum. Although it is often found that Pc molecules orient to maximize the overlap with the substrate electrons, we show that the central atoms also play a role for the orientation of polar Pc molecules on different substrates.

O 42.56 Wed 17:45 P2

**Organic and Metal-Organic Networks Based on NC - Ph - CN** — ●MATTHIAS MARSCHALL<sup>1</sup>, JOACHIM REICHERT<sup>1</sup>, WILLI AUWÄRTER<sup>1</sup>, KNUD SEUFERT<sup>1</sup>, FLORIAN KLAPPENBERGER<sup>1</sup>, SVETLANA KLYATSAKYA<sup>2</sup>, MARIO RUBEN<sup>2</sup>, ALEXANDER WEBER-BARGIONI<sup>3</sup>, and JOHANNES V. BARTH<sup>1</sup> — <sup>1</sup>Physik Department, TU München, Germany — <sup>2</sup>Institut für Nanotechnologie, Karlsruhe, Germany — <sup>3</sup>Department of Physics and Astronomy, University of British Columbia, Vancouver, Canada

The assembly of metal-organic networks is a promising method to fabricate well defined, highly stable supramolecular nanostructures. We investigated the molecular structures by means of Scanning Tunneling Microscopy (STM) and Near Edge X-ray Adsorption Fine Structure (NEXAFS). A systematic investigation of such a metal organic network on Ag(111) and Cu(111) revealed several highly ordered and complex networks. The complexity and the variety of the observed molecular networks is presumably caused by the numerous degrees of freedom of the investigated molecules. Upon absorption the molecules obtain a surface induced chirality and their supramolecular assemblies were studied in dependence of the coverage and preparation parameters. At certain conditions even highly stable macromolecules were formed.

O 42.57 Wed 17:45 P2

**Conformation-controlled networking of H-bonded assemblies on surfaces** — MANFRED MATENA<sup>1</sup>, MIHAELA ENACHE<sup>1</sup>, ANNA LLANES-PALLAS<sup>2</sup>, DAVIDE BONIFAZI<sup>2</sup>, THOMAS A. JUNG<sup>3</sup>, and ●MEIKE STÖHR<sup>1</sup> — <sup>1</sup>University of Basel, Switzerland — <sup>2</sup>University of Trieste, Italy — <sup>3</sup>Paul-Scherrer-Institute, Switzerland

In order to prepare networks that could undergo phase transitions through a thermally-induced inversion of the molecular conformation leading to a variation of the intermolecular interactions, directional intermolecular forces can be regarded as promising candidates. In particular, H-bonding interactions will be exploited since their intermolecular interaction strength and geometry can be controlled by the number and arrangement of available H-bonding donor or acceptor moieties. We studied the 2D self-organization of a conjugated molecule bearing terminal 2,6-di(acylamino)pyridine moieties [1], which are well-known to form H-bonds, on a Ag(111) surface by STM. The hexagonal porous network, which is formed for room temperature deposition, is transformed into a close-packed rhombic pattern by a thermally induced trans-cis inversion of the terminal groups. This transformation can be explained by the fact that the system wants to minimize its energy: at the same time the free surface energy is minimized while the number of H-bonds per terminal group is doubled from two to four. [1] A. Llanes-Pallas et al., Angew. Chem. Int. Ed. 2008, 47, 7726

O 42.58 Wed 17:45 P2

**Porphine on Copper (110) - Adatoms make the difference** — ●ABEL ROBIN, MATTHEW STEPHEN DYER, SAM HAQ, MATS PERSSON, and RASMITA RAVAL — University of Liverpool, Liverpool, U.K.

We have studied the adsorption of free-base ( $H_2$ -P) and copper porphine (Cu-P) molecules on a Cu(110) surface.

Using scanning tunnelling microscopy (STM), reflection absorption infrared spectroscopy (RAIRS) and density functional theory (DFT) calculations we gain insight into the details driving the adsorption and organization of porphine molecules on metal surfaces. Interestingly, we find Cu-P molecules organizing upon adsorption in regular 2D assemblies whereas  $H_2$ -P only exhibits local ordering - even after annealing.

Experiments and calculations reveal another major difference between the two investigated systems, that is Cu-adatoms are attracted by  $H_2$ -P molecules; a process not observed for Cu-P adsorption. The

adatom-attachment to H<sub>2</sub>-P has - next to a number of interesting features - an influence on the ability of the porphine molecule to self-assemble into a regular structure. Metallization experiments of H<sub>2</sub>-P do not lead to a significant improvement in molecular ordering, suggesting that the molecules do remember the original adsorption environment, therefore, the adatom attachment to H<sub>2</sub>-P induces irreversible adsorption features.

Finally, we will present experimental and theoretical details of the highly organized Cu-P assembly. This structure is promising for technological applications since it does not require complicated functional groups attached to the porphyrin molecule for self-assembly.

O 42.59 Wed 17:45 P2

**Self-assembly of highly ordered ferrocenyl nanostructures monitored by second harmonic generation** — ●ROBERT OSSIG<sup>1</sup>, FLORIAN VOGEL<sup>1</sup>, JENS HOSSBACH<sup>2</sup>, ULRICH SIEMELING<sup>2</sup>, and FRANK TRÄGER<sup>1</sup> — <sup>1</sup>Institut für Physik and Center for Interdisciplinary Nanostructure Science and Technology – CINSaT, Universität Kassel — <sup>2</sup>Institut für Chemie and Center for Interdisciplinary Nanostructure Science and Technology – CINSaT, Universität Kassel

Custom-made molecules are ideal candidates to prepare stable self-assembled monolayers (SAM), which yield a wide range of applications, for example, as electronic or sensoric devices. In this contribution we present two recently synthesized ferrocene-functionalized tripod ligands with ferrocene as a reactive head group. The anchor groups of the ligands consist of three thioether-chains, each with 8 or 12 carbon atoms, respectively. Due to their structure, these molecules show a very high rigidity, which is an important pre-condition to form stable SAMs. To monitor the SAM formation, second harmonic generation (SHG) has been applied. The in situ SHG measurements show an initial fast decrease of the signal followed by a slower decrease as a function of immersion time. For a deeper insight of the involved processes, concentration dependent measurements have been performed. From these measurements we conclude that the SAM formation of both molecules occurs in a two-step process, a fast adsorption and a subsequent slow ordering. Further ex situ measurements (ellipsometry and scanning-tunneling-microscopy) confirm the formation of highly ordered monolayers.

O 42.60 Wed 17:45 P2

**Diffusion of 1,4-butanedithiol on unreconstructed Au(111)** — ANDREAS FRANKE and ●ECKHARD PEHLKE — Institut für Theoretische Physik und Astrophysik, Christian-Albrechts-Universität zu Kiel

Extending our previous density-functional studies on the diffusion of alkanethiols on gold surfaces, we now focus on more complex sulfur anchored molecules diffusing on the unreconstructed Au(111) surface. As a benchmark system we choose 1,4-butanedithiol radicals (BDT: S-(CH<sub>2</sub>)<sub>4</sub>-S) which bind to the gold surface via two sulfur atoms. Molecules that bind to the surface via more than one site are expected to show diffusion properties beyond isotropic diffusion of single adsorbate atoms (e.g. [1]). Unreconstructed Au(111) exists under certain electrochemical conditions [2]. Density functional calculations are carried out using the VASP code by Hafner, Kresse *et al.* [3]. We compare various adsorption geometries of one BDT per (4x3) unit cell. For the most favourable geometry both S-atoms bind close to fcc-hollow sites with  $d_{S-S}=4.9\text{\AA}$ . Taking the free, spinpolarized radical as reference, the adsorption energy was calculated to be -3.3 eV. Due to lateral interactions, the adsorption energy changes to -3.8 eV in a (6x6) surface unit cell. We found a diffusion path with a small maximum energy barrier of 0.3 eV which results in a translation perpendicular to the S-S-axis of the molecule. Notably, the energy barrier increases to approx. 0.5 eV in case of the larger (4x6) surface unit cell.

[1] K.-Y. Kwon, *et al.*, *Phys. Rev. Lett.* **95**, 166101 (2005).

[2] M. A. Schneeweiss, *et al.*, *Appl. Phys. A* **69**, 537 (1999).

[3] <http://cms.mpi.univie.ac.at/vasp/>

O 42.61 Wed 17:45 P2

**Surface mobility and its impact on the stability of oligopyridine mono- and multilayer phases on HOPG - a thermal desorption study** — ●MICHAEL ROOS, HARRY E. HOSTER, and R. JÜRGEN BEHM — Institute of Surface Chemistry and Catalysis, Ulm University, D-89069 Ulm, Germany

We report on the temperature and coverage dependent desorption rates from layers of two types of Bis(terpyridine)derivatives (BTP) on HOPG [1-4]. These rates are much higher for thicker films than for monolayers. These variations do not predominantly arise from changes in the energetic desorption barriers but are dominated by the frequency

factors. Due to the large mass (618 amu) and the correspondingly large moments of inertia of the BTP molecules, the frequency factor approaches 10<sup>26</sup> Hz for desorption from an immobile initial state (multilayer), whereas it is changed by a factor of 10<sup>-9</sup> for desorption out of a mobile state (monolayer). This fits to STM observations at 300 K, which revealed that the most stable phase for both molecules is not a close packed hydrogen bonded one, but a dilute 2D gas, where translation and planar rotation are active. We compare the frequency factors and activation energies for desorption of the two types of BTP, which differ in the position of the peripheral N atoms, and discuss possible reasons for the differences.

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

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

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

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

O 42.62 Wed 17:45 P2

**Co-porphyrin molecules on metal surfaces: from single molecules to molecular arrays and bilayer islands** — ●WILLI AUWÄRTER, KNUD SEUFERT, FLORIAN KLAPPENBERGER, JOACHIM REICHERT, and JOHANNES V. BARTH — Physik Department, TU München, Germany

We report on scanning tunneling microscopy (STM) and spectroscopy (STS) experiments on Co-tetraphenylporphyrin (CoTPP) molecules adsorbed on Ag(111) and Cu(111) surfaces. Starting by a characterization of the electronic and geometric structure of individual CoTPP's, we proceed to CoTPP arranged in highly organized arrays, where we discuss subtle modifications of the electronic structure induced by the packing of CoTPP. The inequivalent adsorption sites of CoTPP assembled in islands on Ag(111) results in a moire-type modulation of the lowest unoccupied molecular orbital. In a next step we address the imaging of CoTPP molecules immobilized on a CoTPP monolayer. The modification of the electronic structure clearly indicates that these 2nd layer molecules are electronically decoupled from the metal substrate. In addition, we compare the morphology of CoTPP on Cu(111) and Ag(111) with free-base porphyrins, which allows us to discuss the influence of specific molecule-substrate interactions on the molecular conformation and the mobility.

O 42.63 Wed 17:45 P2

**Formation of metal-organic networks of azobenzene molecular switches on a Au(111) surface** — ●CHRISTOPH LIMBACH, NILS HENNINGSEN, KATHARINA J. FRANKE, and JOSE IGNACIO PASCUAL — Freie Universität Berlin, Berlin, Germany

Azobenzene is a model molecular system for conformational switches, whose adsorption on metal surfaces has lately attracted a lot of interest due to its possible application to switchable molecular electronic devices. Using low temperature scanning tunnelling microscopy and spectroscopy (STM/STS) we investigate the coadsorption of di-metacyano azobenzene (DMC) molecules and cobalt atoms on a Au(111) surface. Room temperature co-deposition of both species results in the formation of metal-organic chains as well as small clusters. dI/dV spectroscopy and conductance maps plotting the distribution of unoccupied resonances are used to localize the coordination bonds between Co atoms and DMC. We find that coordination bonds can be formed indistinguishably at two intramolecular sites: the cyano termination and the di-azo bridge (N=N). This leads us to conclude that the metal organic bond is probably mediated by the lone-pair electrons of nitrogen atoms, as found recently [1]. We envision a controlled modification of the transition metal properties by switching the molecular ligands.

[1] U. Schlickum *et al.* *Nano Lett.* **7**, 3813, 12007

O 42.64 Wed 17:45 P2

**Structure-function relation in the photoswitch tetra-tert-butyl-azobenzene (TBA) on Au(111)** — ●ROLAND SCHMIDT<sup>1,2</sup>, DANIEL BRETE<sup>1,2</sup>, SEBASTIAN HAGEN<sup>2</sup>, ROBERT CARLEY<sup>1</sup>, CORNELIUS GAHL<sup>1</sup>, PETRA TEGEDER<sup>2</sup>, and MARTIN WEINELT<sup>1,2</sup> — <sup>1</sup>Max-Born-Institut, Berlin — <sup>2</sup>Freie Universität-Berlin, Berlin

We have investigated tetra-tert-butyl-azobenzene (TBA) adsorbed on Au(111) by X-ray absorption (XAS) and autoionization spectroscopy at the Berlin synchrotron facility BESSY. In TBA the azobenzene photoswitch is decoupled from the substrate by four tert-butyl legs. XAS reveals a slight bending of the azo group of the trans isomer towards the Au(111) surface. The interaction of the N=N bond with the gold substrate is also reflected by an interchange of HOMO and HOMO-1, as identified from participator decay in Resonant-Raman-Auger. Autoionization of the C1s<sup>-1</sup>π<sup>+1</sup> excited state mainly occurs

via spectator and participator decay, while the  $N1s^{-1}\pi^{+1}$  state shows an additional non-resonant Auger contribution of comparable strength. This demonstrates that charge transfer from the LUMO to the substrate is faster when exciting at the nitrogen edge and can explain the quite exceptional dependence of the TBA photoisomerization yield on photon energy [1].

[1] S. Hagen, P. Kate, F. Leyssner, D. Nandi, M. Wolf, and P. Tegeder *J. Chem. Phys.* (2008), **129**, 164102

O 42.65 Wed 17:45 P2

**In situ STM study of Cu modified Au(100) electrodes in alkaline solution** — ●CHRISTIAN SCHLAUP and KLAUS WANDEL — Institute for Physical and Theoretical Chemistry, University of Bonn, Wegelerstr. 12, D-53115 Bonn

Ultrathin Cu layers were prepared on Au(100) electrodes using the well-known Cu underpotential deposition. After a two step electrolyte exchange process these Cu modified Au(100) electrodes were exposed to a 0.01 M NaOH electrolyte. In dependence on the electrochemical potential different surface structures were found and characterized. Starting at low potentials where the adsorbate free pseudomorphic Cu adlayer remains stable, two barely ordered structures were formed during potential increase. In a first step  $OH^-$  ions are adsorbed, forming an largely disordered overlayer with a next neighbor distance of about 0.6 nm. During further potential increase the Cu layer is oxidized yielding a CuO film, which shows a characteristic stripe structure. In contrast to bulk Cu(100) electrodes, where a two step oxidation process via an intermediate  $Cu_2O$  species was found, the CuO film is formed directly under these conditions. However, an additional structure was found in the transition regime between the uncovered and  $OH^-$  covered Cu layer. After keeping the potential constant for at least 20 minutes, islands with a hexagonal lattice and a next neighbor distance of about 0.3 nm appear. Both, the small lattice constant and the slow kinetic may point to the formation of a Au/Cu surface alloy.

O 42.66 Wed 17:45 P2

**Structural transitions of Heptyl Viologen adlayers on a Cu(100) electrode: In situ STM study** — ●MIN JIANG, KNUD GENTZ, and KLAUS WANDEL — Institute for Physical and Theoretical Chemistry, University of Bonn, Wegelerstr.12, D-53115 Bonn

Surface redox processes and structural transitions of heptyl viologen ( $1,1'$ -Diheptyl-4,4'-bipyridinium dichloride,  $DHV^{2+}$ ) was studied on a Cu(100) electrode by cyclic voltammetry (CV) and in situ scanning tunneling microscopy (STM). Typical for a redox-active molecule,  $DHV$  in KCl electrolyte solution exhibited two pairs of spike-like current waves and two-step one-electron redox processes. The  $DHV^{2+}$  species spontaneously formed four kinds of highly ordered phases on the preadsorbed chloride  $c(2 \times 2)$  adlayer under non-reactive condition, which were composed of two mirror domains and two rotational domains. One-electron reduction of the dication  $DHV^{2+}$  caused a phase transition to a stripe pattern which arises from a  $\pi - \pi$  stacking of the corresponding monocation radical  $DHV^+$  species. This phase transition involved not only reduction of the pre-adsorbed  $DHV^{2+}$  species but also a further adsorption and reduction of  $DHV^{2+}$  species from the solution phase. During the cathodic sweep, the stripe pattern of the cation radicals changed from a loose array to a more compact structure. At more negative potential, the ordered stripe pattern disappeared gradually and a reversible order-disorder transition happened. This is caused by chloride desorption-adsorption through the viologen film.

O 42.67 Wed 17:45 P2

**Water clusters and thin films on clean and oxygen-adsorbed Ni(111) surfaces** — ●STEFAN WIPPERMANN und WOLF GERO SCHMIDT — Lehrstuhl für theoretische Physik, Universität Paderborn, Warburger Str. 100, 33098 Paderborn

Despite the importance of water-surface interaction for many technological applications and surface science, it is only poorly understood in many instances. Inspired by recent experimental [1] and theoretical work [2], we explore the adsorption of water on clean and oxygen-adsorbed Ni(111) surfaces using density functional theory. Calculations on the water adsorption geometries and vibrational frequencies were performed for a wide range of monomer, dimer, trimer and hexamer structures adsorbed on the  $p(2 \times 2)$ -Ni(111)-O and clean Ni(111) surfaces [3]. While our results agree well with the experimental findings of Nakamura and Ito [1], they suggest a different interpretation in terms of mainly two candidate structures: (i) Formation of an ice Ih-like bilayer structure with the free OH-bonds pointing upwards along the

surface normal, and (ii) Formation of cyclic buckled hexamers similar to the ones discussed in Ref. [4]. In the latter case, each water molecule forms an  $OH-O_{ad}(2 \times 2)$  hydrogen bond with two different hydrogen bond types depending on the water molecule's normal position in the buckled hexamer.

[1] M Nakamura and M Ito, *Phys Rev Lett* 94, 035501, 2005.

[2] D Sebastiani et al., *J Chem Theory Comput* 1, 78, 2005.

[3] S Wippermann and W G Schmidt, *Phys Rev B* (submitted)

[4] A Michaelides and K Morgenstern, *Nature Materials* 6, 597, 2007.

O 42.68 Wed 17:45 P2

**SXPS Studies of Porphyrin Adsorption on Copper/Electrolyte Interfaces** — ●STEPHAN BREUER<sup>1</sup>, DUC THANH PHAM<sup>1</sup>, GENNADY CHERKASHININ<sup>2</sup>, THOMAS MAYER<sup>2</sup>, and KLAUS WANDEL<sup>1</sup> — <sup>1</sup>Universität Bonn, Institut für Physikalische und Theoretische Chemie, Wegelerstraße 12, 53115 Bonn — <sup>2</sup>Technische Universität Darmstadt, FB Materialwissenschaft, Petersenstraße 23, 64284 Darmstadt

We have studied electrochemically prepared Tetra-(methylpyridinium)-porphyrin (TMPyP) adsorbates on anion precovered copper surfaces by Synchrotron X-ray Photoelectron Spectroscopy (SXPS) at the synchrotron light source BESSY II. In order to correlate existing structural data with the chemical composition of the adsorbate layer we have systematically changed the underlying anion coverage (sulphate, chloride), the substrate symmetry (Cu(100), Cu(111)) and the applied potential. In contrast to vapour deposition, electrochemistry offers a pathway to deposit also thermolabile organic molecules. Our studies have revealed that the N1s signal, that indicates the presence of TMPyP on the surface, can be deconvoluted in several signals which are very sensitive to changes of the chemical environment and the redox state. As TMPyP counterion we have used tosylate which stabilizes the adsorbate layer.

O 42.69 Wed 17:45 P2

**A new in-situ X-ray diffraction setup: Electrodeposition of Zn from ionic liquids** — APARNA PAREEK, DIMITAR BORISOV, MICHAEL ROHWERDER, DIRK VOGEL, and ●FRANK RENNER — Max-Planck Institut für Eisenforschung, Max-Planck Strasse 1, 40237 Düsseldorf

To facilitate the investigation of the UHV prepared electrochemical interfaces by in situ x-ray diffraction using synchrotron radiation, an electrochemical cell setup combined with a portable UHV chamber was reported earlier. In the current work, we re-engineered the above electrochemical setup to investigate the Zn electrodeposition on the Au (111) surface from ionic liquids. Ionic liquids have very low vapor pressure, which means they can be handled in UHV environments. A smart addition of heating stage was used to overcome the problems like high viscosity and less conductivity, which are usually associated with ionic electrolytes. Furthermore, with this setup, the electrolyte contact with the sample surface can be attained in the controlled gas atmosphere. Here we report the first results of Zn electrodeposition and re-dissolution obtained using this new setup. In-situ x-ray diffraction enabled to track the initial steps of Zn deposition on the Au (111) surface, where the growth of an epitaxially ordered Zn film was observed.

O 42.70 Wed 17:45 P2

**Surface-enhanced resonators for microfluidic and nanofluidic applications** — ●BEYNOR ANTONIO PAEZ-SIERRA<sup>1</sup> and VIKTORIIA KOLOTOVSKA<sup>2</sup> — <sup>1</sup>QUBITON Laboratories KG, 4040 Linz, Austria — <sup>2</sup>Zentrum für Biomedizinische Nanotechnologie, Upper Austrian Research, Austria, 4020 Linz, Austria

Revealing and understanding phenomena at interfaces is an important issue concerning biology, chemistry, engineering, physics, and many other disciplines. Science and technology at the nano- and micro-scale have myriads of proven examples where surface-to-volume ratio becomes dominant for process performance. Thereby, it is of great interest to pursue surface chemistry, tuning of energetic surface levels, control of trap states, or engineering of interface barriers among others, in order to overcome into stable and high efficient optoelectronic processes. We report simulations on surface-enhanced Raman resonators (SERRs) for microfluidic and nanofluidic applications. The process has its origins on the surface-enhanced Raman spectroscopy (SERS) phenomenon, where one main feature consists on the coupling between external electric fields with surface plasmons at structured metallic surfaces or colloids, resulting in strong local electric fields. The implementation of surface-enhanced reservoirs or enhanced walls

at the fluidic chip, allow to acquire more intense signals of various spectroscopic probes, and hence to reduce the acquisition time.

O 42.71 Wed 17:45 P2

**Homoepitaxial electrodeposition on Cu(001) in different electrolytes** — ●ARNE DRÜNKLER, FREDERIK GOLKS, YVONNE GRÜNDER, DANIEL KAMINSKI, KLAUS KRUG, JOCHIM STETTNER, and OLAF M. MAGNUSSEN — Christian-Albrechts Universität Kiel, Germany

Cu electrodeposition is used for the defect-free filling of trenches with dimensions <100nm on ultra large scale integrated (ULSI) microchips [1]. Multicomponent electrolytes containing organic additives are used cause a faster growth at the bottom of the trench than at the upper walls resulting in void free filling of the trench. Even though the influence of the additives combination on the shape evolution of the Cu deposit was subject of numerous studies [2,3], their precise role during the elementary steps of the deposition is largely not understood. Surface X-Ray diffraction (SXRD) is ideal for the investigation of electrochemical metal deposition on atomic scale, as buried interfaces and structural information of the interface are accessible. In a first step the potential dependent interface structure of Cu(001) was investigated in copper free electrolyte. Furthermore, kinetic growth investigations in HCl and H<sub>2</sub>SO<sub>4</sub> solution are presented. Electrodeposition studies of Cu(001) in CuSO<sub>4</sub> containing HCl indicated step flow growth over a wide potential regime. In a Cu containing electrolyte mixture of H<sub>2</sub>SO<sub>4</sub> and HCl evidence for a transition from 2D- to 3D-growth is found.

References: [1] P.C. Andricacos, et al., *Electroch. Microf.* 42, 567 (1998), [2] T.P. Moffat, D. Wheeler, M.D. Edelstein, D. Josell, *IBM J. Res. Develop.* 49, 19 (2005), [3] D. Josell, D. Wheeler, W.H. Huber, T.P. Moffat, *Phys. Rev. Lett.* 87, 016102-1 (2001)

O 42.72 Wed 17:45 P2

**(111)-Textured Platinum Thin-Layer Electrodes on  $\alpha$ -Al<sub>2</sub>O<sub>3</sub>(0001) for Spectro-Electrochemistry** — ●BJÖRN BRAUN-SCHWEIG, ALEXEJ MITIN, and WINFRIED DAUM — Institut für Physik und Physikalische Technologien, TU Clausthal, Leibnizstrasse 4, D-38678 Clausthal-Zellerfeld

The use of infrared vibrational spectroscopy to study electrochemical reactions on surfaces of bulk metal electrodes in aqueous electrolytes is often impaired by diffusion limitations as thin-layer electrolytes are required to minimize IR absorption in the liquid. Alternatively, thin-layer electrodes on IR-transparent substrates may be used to access the metal-electrolyte interface by IR transmission through the solids. While the latter strategy does not suffer from diffusion limitations of the electrolyte, it usually lacks the advantages of well-defined, single-crystalline electrode surfaces desired for model studies. We report the preparation of well-characterized Pt thin-film electrodes suitable for spectro-electrochemistry. Thin Pt layers with a thickness of 3 to 15 nm were grown by vapor deposition on atomically smooth  $\alpha$ -Al<sub>2</sub>O<sub>3</sub>(0001) single crystal surfaces and characterized by AES, cyclic voltammetry, AFM and STM. We used iodine adsorption to characterize the crystallographic surface orientation of our Pt films. Atomically resolved STM images of the iodine adlayer on the thin films reveal the same superstructures as found on Pt(111) bulk single crystals and demonstrate high structural order and (111) texture of our films. The effects of growth temperature and film thickness on the surface morphology of the thin-film electrodes are discussed.

O 42.73 Wed 17:45 P2

**The adsorption of CO<sub>2</sub> and CO on Ca and CaO films studied with MIES, UPS and XPS** — ●SEBASTIAN DAHLE<sup>1</sup>, FLORIAN VOIGTS<sup>1</sup>, KAI VOLGMANN<sup>1</sup>, FABIAN BEBENSEE<sup>2</sup>, and WOLFGANG MAUS-FRIEDRICHS<sup>1</sup> — <sup>1</sup>Institut für Physik und Physikalische Technologien, TU Clausthal, Leibnizstrasse 4, 38678 Clausthal-Zellerfeld, Germany — <sup>2</sup>Lehrstuhl für Physikalische Chemie II, Universität Erlangen-Nürnberg, Egerlandstrasse 3, 91058 Erlangen, Germany

The adsorption of different atmospheric molecules on metals is both of fundamental and of technological interest that arises from several applications. Ca especially is used to enhance the performance of high temperature oxygen sensors based on SrTiO<sub>3</sub>, as a promoter in many catalytic reactions and as a metal electrode in different organic or polymeric semiconductor components. A lot of studies of the effect of Ca on different catalysts neglect the interaction of Ca itself with different gases, although this might contribute considerably to the role of Ca as a promoter in catalysis.

Our results for the interaction of Ca and CaO films with CO<sub>2</sub>

and CO are presented in this poster. For our studies, we employed Metastable Induced Electron Spectroscopy (MIES), Ultraviolet Photoelectron Spectroscopy (UPS), and X-ray Photoelectron Spectroscopy (XPS). Both CO<sub>2</sub> and CO lead to the formation of CO<sub>3</sub><sup>2-</sup> complexes on top of the surface while being exposed to Ca or CaO.

O 42.74 Wed 17:45 P2

**Interaction of Fe and Fe<sub>2</sub>O<sub>3</sub> with reactive gases** — ●KAI TRISTAN VOLGMANN, FLORIAN VOIGTS, and WOLFGANG MAUS-FRIEDRICHS — Institut für Physik und Physikalische Technologien, TU Clausthal, Leibnizstr. 4, 38678 Clausthal-Zellerfeld

Mars' atmosphere contains a rather high portion of methane and formaldehyde with 10 ppb respectively 100 ppb. Different sources including extraterrestrial life have been proposed, but the origin of these gases is still unknown. It has been found earlier that methane and formaldehyde can be produced through a photocatalytic process on a hematite surface with adsorbed water in a CO<sub>2</sub> atmosphere.

The scope of this work is to examine the underlying processes which happen on granular powders of hematite. As a first step thin films of iron and Fe<sub>2</sub>O<sub>3</sub> are examined.

These thin films are investigated by means of their interaction with reactive gases like O<sub>2</sub>, CO<sub>2</sub> and H<sub>2</sub>O. These reactions have been studied with photoelectron spectroscopy. X-ray photoelectron spectroscopy is used to determine stoichiometry of the samples, while Ultraviolet photoelectron spectroscopy and Metastable Induced Electron Spectroscopy are used to analyse the valence band region and to gain information about changes in workfunction due to reactions on the surfaces.

O 42.75 Wed 17:45 P2

**Characterization and catalytic properties of bimetallic Au-Pd(111) surfaces** — ●MARCO MOORS<sup>1</sup>, TOMASZ KOBIELA<sup>2</sup>, CONRAD BECKER<sup>1</sup>, and KLAUS WANDEL<sup>1</sup> — <sup>1</sup>Institute of Physical and Theoretical Chemistry, University of Bonn, Wegelerstr. 12, D-53115 Bonn, Germany — <sup>2</sup>Faculty of Chemistry, Warsaw University of Technology, Noakowskiego 3, 00 664, Warsaw, Poland

Investigations of bimetallic systems with regard to their surface composition and morphology are of great importance for the development of new catalysts. In this work the compositional, electronic and structural properties of thin Au films deposited on a Pd(111) single crystal have been studied by ultraviolet photoelectron spectroscopy (UPS), photoemission of adsorbed xenon (PAX) and CO titration as a function of film thickness (ranging from submonolayer amounts up to multilayers) and temperature. The surface morphology of the system Au on Pd(111) exhibits a strong temperature dependence. Depositing Au at 150 K results in closed films, which undergo a smoothening of the topmost atomic layer by annealing the sample up to 250 K. At a surface temperature of 450 K the Au-Pd intermixing begins at the interface between substrate and overlayer eventually reaching the outermost surface at annealing temperatures of 650 K. Annealing to 850 K and above results in a fast Au depletion in the surface region, which is completed at 1050 K. Additionally performed reaction studies of the partial hydrogenation of butadiene to 1-butene using temperature programmed desorption (TPD) have shown a significant improvement of the catalytic properties of the alloyed Au-Pd surface compared to pure Pd(111).

O 42.76 Wed 17:45 P2

**Growth of ultrathin well-ordered Ni-Al alloyed layers on Ni(111) : a Grazing Incidence X-ray Diffraction study** — ●SÉVERINE LE MOAL<sup>1</sup>, GEOFFROY PRÉVOT<sup>2</sup>, DIDIER SCHMAUS<sup>2</sup>, RÉMI LAZZARI<sup>2</sup>, and BERNARD CROSET<sup>2</sup> — <sup>1</sup>Institute of Physical and Theoretical Chemistry, University of Bonn, Wegelerstr. 12, D-53115 Bonn, Germany — <sup>2</sup>Institut des NanoSciences de Paris, Universités Paris 6 et Paris 7, CNRS, 140 rue de Lourmel, F-75015 Paris, France

Ni-Al alloys are of great technological interest because of their remarkable mechanical and thermal properties. They are also resistant to corrosion due to the formation at their surface of a passive ultrathin film of aluminum oxide that acts as a diffusion barrier. Previously, we reported the epitaxial growth of NiAl and Ni<sub>3</sub>Al films on a Ni(111) single crystal [Le Pévédic et al, *Surf. Sci.* 600 (2006) 565 and *Surf. Sci.* 601 (2007) 395]. We recently studied their structure and the kinetics of formation by Grazing Incidence X-ray Diffraction (ESRF, ID03). Starting from an initial Al deposit, the growth and the structural and chemical ordering of the Ni<sub>3</sub>Al and NiAl layers are followed upon annealing. Disordered NiAl already forms at room temperature. In the 573-673 K temperature range the thickness of the NiAl layer increases and chemical ordering takes place. Once NiAl has grown up to the

surface, ordered Ni<sub>3</sub>Al starts to form. Simultaneously, the diffraction signal of NiAl decreases and characteristic diffraction spots of Ni<sub>3</sub>Al appear and get sharper. The Ni<sub>3</sub>Al layer is stable up to 773 K. The lattice constants of the films were measured throughout growth and annealing time.

O 42.77 Wed 17:45 P2

**Vibrational spectroscopy of the rough Cu(111) surface** — ●DIANA VOGEL, OLAF SKIBBE, and ANNEMARIE PUCCI — Kirchhoff-Institut für Physik, Universität Heidelberg, Im Neuenheimer Feld 227, D-69120 Heidelberg

It is known that defect sites on a surface have a strong influence on adsorbates due to the changed electronic structure compared to the clean surface. In this work we characterize the rough Cu(111) surface by using High-Resolution Electron Energy Loss Spectroscopy (HREELS). The roughness has been produced by evaporating small amounts of copper onto the cooled surface so small islands are assumed to be grown. In our spectroscopic study, a vibrational state has been found at a quite high loss energy compared to the bulk phonon band. After annealing of the surface another vibrational state at an even higher energy has been detected. In analogy to known investigations on stepped copper surfaces the observed vibrational modes can be attributed to low coordinated step atoms of the islands [1]. The observed change of the vibrational spectra with increasing annealing temperature can be related to a morphology change of the islands. Measurements of the work function change of the surface after evaporating and annealing confirmed this result.

[1] A. Kara, P. Staikov and T. S. Rahman, Phys. Rev. B 61, 5714 (2000).

O 42.78 Wed 17:45 P2

**Surface phases and structure determination of thin silver films grown on the Re(10 $\bar{1}$ 0) surface** — ●VIKTOR SCHERF, LYRIA MESSAHEL, CHRISTIAN PAULS, and KLAUS CHRISTMANN — Institut für Chemie und Biochemie der FU Berlin, Takustr.3, D-14195 Berlin

We have examined the growth of silver films on the Re(10 $\bar{1}$ 0) surface under UHV conditions by means of electron diffraction techniques (MEED and LEED), and carried out a quantitative structure determination of the (1 $\times$ 1)-Ag phase by LEED. In the submonolayer range, the following LEED phases were observed with increasing silver coverage: c(2 $\times$ 2), p(1 $\times$ 4), p(1 $\times$ 5) and p(1 $\times$ 1), their I,V curves will be presented here. The in situ measured MEED curves of the (0,0) beam at 700 K show with increasing Ag coverage permanently two local maxima and minima; both maxima correlate with the formation of c(2 $\times$ 2) structure at different surface coverages. Once the p(1 $\times$ 1) phase is formed, the MEED intensity decreases almost linearly with the deposited amount of Ag indicating the formation of rough silver multilayers which grow according to a Stranski-Krastanov mechanism. We will also present the first dynamic LEED calculation for the Ag p(1 $\times$ 1) structure which clearly suggests the formation of a silver bilayer. The results will be discussed and compared with previous work on the same system as well as on the Au/Re(10 $\bar{1}$ 0) system [1].

[1] C. Pauls and K. Christmann, J. Physics Condensed matter, submitted

O 42.79 Wed 17:45 P2

**Kinetic Monte Carlo study of growth of Co on Cu(110) at room temperature** — OLEG V. STEPANYUK<sup>1</sup>, ●NIKOLAY N. NEGULYAEV<sup>2</sup>, ALEXANDER M. SALETSKY<sup>1</sup>, and WOLFRAM HERGERT<sup>2</sup> — <sup>1</sup>Faculty of Physics, Moscow State University, 119899 Moscow, Russia — <sup>2</sup>Fachbereich Physik, Martin-Luther-Universität, D06099 Halle, Germany

During the last decade many experimental and theoretical studies have been performed on Co/Cu heterostructures which are of great interest for spintronic applications. While the formation of thin Co films during thermal deposition on Cu(100) and Cu(111) has been investigated and understood at the atomic scale [1,2], our knowledge about growth process of Co on Cu(110) is still missing.

Here, performing atomic-scale simulations we study the growth of Co on Cu(110) in the early stages of heteroepitaxy. The energetics of various diffusion processes relevant for this system is investigated by means of molecular dynamics simulations and density functional theory. We show that the interface intermixing occurs at room temperature [3]. Our results reveal that embedded Co atoms serve as nucleation centers for substituted Cu atoms. Surface diffusion of expelled Cu adatoms rules an elongated along the [1-10] direction shape of nanoislands consisting mainly of Cu atoms [3].

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[2] N.N. Negulyaev et al., Phys. Rev. B 77, 125437 (2008).

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O 42.80 Wed 17:45 P2

**Preparation and electrical characterization of BaO, SrO and Ba<sub>0.7</sub>Sr<sub>0.3</sub>O thin films on Si(001)** — ●DIRK MÜLLER-SAJAK<sup>1</sup>, ALEXANDR COSCEEV<sup>2</sup>, HERBERT PFNÜR<sup>1</sup>, and KARL R. HOFMANN<sup>2</sup> — <sup>1</sup>Leibniz-Universität Hannover, Inst. f. Festkörperphysik — <sup>2</sup>Leibniz-Universität Hannover, Bauelemente der Mikro- und Nanoelektronik

In context with the search for alternative gate oxides in CMOS technology, we have grown high-k BaO, SrO and Ba<sub>0.7</sub>Sr<sub>0.3</sub>O films of thickness between 5 and 20 nm on clean Si(001) using molecular beam epitaxy of pure metals in ambient oxygen pressure. Especially the BaSr mixture oxide is of high interest, because it grows epitaxially and crystalline on Si(001).

Using Si(001) samples with thick SiO<sub>2</sub> films in combination with lithography, windows of clean Si(001) have been fabricated. Our thin films were only generated on these small squares using a tungsten mask. After preparation, the oxides were capped with 350nm Au and electrically characterized ex-situ.

From capacity-voltage (CV) measurements dielectric constants near the values for volume material were obtained. Furthermore we found very low hysteresis (<5mV) and flatband voltages close to that of the work function difference between Si and Au (+0.65eV). Due to the stoichiometry of these films and well defined interfaces, low leakage current densities (<10<sup>-5</sup>A/cm<sup>2</sup>) have been found by current-voltage (IV) measurements. The density of residual defect states at the interface have been derived from CV measurements and will be discussed.

O 42.81 Wed 17:45 P2

**Nucleation of Cu on Cu(001) by pulsed laser deposition** — ●ANDREAS DOBLER and THOMAS FAUSTER — Lehrstuhl für Festkörperphysik, Universität Erlangen-Nürnberg, Staudtstr. 7, 91058 Erlangen

For submonolayer homoepitaxial growth, nucleation theory allows to extract the critical island size by scaling island densities with the deposition rate. Pulsed laser deposition provides instantaneous deposition rates up to 10<sup>4</sup> ML/s and particle energies up to hundreds of eV.

We measured island densities after pulsed laser deposition of Cu on Cu(001) at 300 K. For best focus conditions ( $I \approx 10$  J/cm<sup>2</sup>), we varied the average deposition rate  $F$  from 10<sup>-5</sup> to 10<sup>-2</sup> ML/s at 1 Hz repetition rate. The saturation island density scales as  $n_x \propto F^p$  with an exponent near the value for thermal deposition of  $p = 0.4$ . However, the experimental island density is two orders of magnitude lower than expected by considering the instantaneous flux. This result is in good agreement with a theoretical study of nucleation for pulsed fluxes considering dimer mobility [1].

[1] N. Combe and P. Jensen, Phys. Rev. B 57 (1998) 15553

O 42.82 Wed 17:45 P2

**Adsorption Geometry and Molecular Orbital Structure of Fluorinated Cobalt Phthalocyanine (F16CoPc) Layers on HOPG Substrate.** — ●MAHMOUD ABDEL-HAFIEZ<sup>1</sup>, MARIUS TOADER<sup>1</sup>, THIRUVANCHERIL G.GOPAKUMAR<sup>2</sup>, AFSHIN ABBASI<sup>1</sup>, and MICHAEL HIETSCHOLD<sup>1</sup> — <sup>1</sup>Solid Surfaces Analysis Group and Theoretical Physics Group, Institute of Physics, Chemnitz University of Technology, D-09107,-Chemnitz, Germany — <sup>2</sup>Christian-Albrechts-Universität zu Kiel, Institute of Experimental and Applied Physics, D-24118 Kiel, Germany

The adsorption geometry and electronic structure of isolated fluorinated Cobalt Phthalocyanine (F16CoPc) molecules adsorbed on the basal plane of HOPG (highly oriented pyrolytic graphite) substrate was studied. Monolayers were prepared using organic molecular beam epitaxy (OMBE) under UHV conditions at room temperature and investigated at 40 K using an Omicron VT-STM. At a thickness of around one monolayer, F16CoPc forms perfect quadratic phase superstructures on HOPG films. Adsorption geometry of molecules within the adlayer shows the influence of fluorine atoms on the packing. Single molecule calculations are employed to understand the type of interactions between F16CoPc and the substrate, as well as the effects of fluorine atoms on the geometric configurations of the adsorbed F16CoPc molecules.

O 42.83 Wed 17:45 P2

**Structure and energetics of bimetallic surface confined alloys** — ●ANDREAS BERGBREITER<sup>1</sup>, RALF T. RÖTTER<sup>1</sup>, ALBERT K. ENGSTFELD<sup>1</sup>, HARRY E. HOSTER<sup>1</sup>, AXEL GROSS<sup>2</sup>, and R. JÜRGEN

BEHM<sup>1</sup> — <sup>1</sup>Institute of Surface Chemistry and Catalysis, Ulm University, D-89069 Ulm — <sup>2</sup>Institute for Theoretical Chemistry, Ulm University, D-89069 Ulm

The atomic distribution in a number of  $A_xB_{1-x}/B$  type surface alloys was determined by STM imaging with chemical contrast and statistically evaluated. Whereas in the systems  $Au_xPt_{1-x}/Pt(111)$ ,  $Ag_xPt_{1-x}/Pt(111)$ , and  $Pd_xRu_{1-x}/Ru(0001)$  we find preferences for larger homoatomic aggregates, the atom distribution in  $Pt_xRu_{1-x}/Ru(0001)$  and  $Ag_xPd_{1-x}/Pd(111)$  is very close to a random one [1]. In  $Ag_xPd_{1-x}/Pd(111)$ , our data show a small tendency towards clustering for  $x_{Ag} < 0.5$ , whereas at  $x_{Ag} > 0.5$  this is reversed to a slight preference for heteroatomic neighborhoods. Based on these experimental results, we have derived effective cluster interaction energies for all surface alloys [2]. These allow us to calculate phase diagrams for the surface alloys that we compare to predictions from theoretical work and to the behaviour of the corresponding bulk systems. We also discuss in how far the different atom distributions affect chemical and catalytic properties of the surface alloys.

- [1] H.E. Hoster et al., *Phys.Chem.Chem.Phys* 10 (2008) 3812.  
 [2] A. Bergbreiter et al., *Phys.Chem.Chem.Phys* 9 (2007) 5127.

O 42.84 Wed 17:45 P2

**Heterogeneously Catalysed Process for HCl Oxidation over Stabilised RuO<sub>2</sub>(110)** — ●STEFAN ZWEIDINGER<sup>1</sup>, JAN PHILIPP HOFMANN<sup>1</sup>, MARCUS KNAPP<sup>1</sup>, DANIELA CRIHAN<sup>1</sup>, ARI PAAVO SEITSONEN<sup>2</sup>, KEES-JAN WESTSTRATE<sup>3</sup>, EDWIN LUNDGREN<sup>3</sup>, JESPER ANDERSEN<sup>3</sup>, MICHAEL SCHMID<sup>4</sup>, PETER VARGA<sup>4</sup>, and HERBERT OVER<sup>1</sup> — <sup>1</sup>Physikalisch-Chemisches Institut, Justus-Liebig Universität Gießen, Heinrich-Buff-Ring 58, D-35392 Gießen — <sup>2</sup>IMPMC, CNRS & Université Pierre et Marie Curie, 4 place Jussieu, case 115, F-75252 Paris — <sup>3</sup>Dept. of Synchrotron Radiation Research, Lund University, Sölvegatan 14, S-22362 Lund — <sup>4</sup>Institut für Allgemeine Physik, TU Wien, Wiedner Hauptstraße 8-10, A-1040 Wien

High-resolution core-level shift spectroscopy and temperature-programmed reaction experiments together with density functional theory calculations reveal that the oxidation of HCl with oxygen producing Cl<sub>2</sub> and water proceeds on the chlorine-stabilised RuO<sub>2</sub> (110) surface via a one-dimensional Langmuir-Hinshelwood mechanism [1]. The recombination of two adjacent chlorine atoms on the catalyst's surface constitutes the rate-determining step in this novel Deacon-like process. The stability of RuO<sub>2</sub>(110) is related to the selective replacement of bridging O atoms at the catalyst surface by chlorine atoms [2], as evidenced by high-resolution core-level shift spectroscopy, scanning tunnelling microscopy and density functional theory simulations.

- [1] Crihan, D. et al.; *Angew. Chemie Int. Ed.* 2008, 47, 2131-2134.  
 [2] Zweidinger, S. et al.; *J. Phys. Chem. C* 2008, 112, 9966-9969.

O 42.85 Wed 17:45 P2

**Nanoporous Gold: XPS and In-situ XPS Investigation** — ●KARIFALA DUMBUYA<sup>1</sup>, ARNE WITTSTOCK<sup>2,3</sup>, VOLKMAR ZIELASEK<sup>2</sup>, JÜRGEN BIENER<sup>3</sup>, ALEX HAMZA<sup>3</sup>, MARCUS BÄUMER<sup>2</sup>, MICHAEL GOTTFRIED<sup>1</sup>, and HANS-PETER STEINRÜCK<sup>1</sup> — <sup>1</sup>Universität Erlangen-Nürnberg, Lehrstuhl für Physikalische Chemie II, Egerlandstr. 3, 91058 Erlangen, Germany — <sup>2</sup>Institute for Applied and Physical Chemistry, University of Bremen, Leobener Strasse NW2, 28359 Bremen, Germany — <sup>3</sup>Nanoscale Synthesis and Characterization Laboratory, Lawrence Livermore National Laboratory, P.O. Box 808, Livermore, California 94550, United States of America

Recent reports [1] have revealed that monolithic nanoporous gold (npAu) exhibits remarkably high catalytic activity for CO oxidation. This observation is surprising because the traditional catalyst is of the oxide-supported type. The specific particle-support interactions, which apparently play important roles in the standard Au catalyst, are absent for the nanoporous Au. If this is the case, then why does it display such high activity? The answer is most likely related to traces of residual Ag in the npAu. To highlight the role played by each metal in the catalytic process, we have investigated npAu with respect to changes in the chemical and electronic states of both metals with and without CO and O<sub>2</sub> using in-situ XPS (1 mbar) and XPS, respectively. Our results confirm previous XPS results in that segregation of Ag occurs in the surface region. HP-XPS data suggests that this residual Ag plays a significant role in activating molecular oxygen. [1] V. Zielasek et al., *Angew. Chem. Int. Ed.* 2006, 45, 8241-8244.

O 42.86 Wed 17:45 P2

**Nanoporous Gold: XPS and In-situ XPS Investigation** —

●KARIFALA DUMBUYA<sup>1</sup>, ARNE WITTSTOCK<sup>2,3</sup>, VOLKMAR ZIELASEK<sup>2</sup>, JÜRGEN BIENER<sup>3</sup>, ALEX HAMZA<sup>3</sup>, MARCUS BÄUMER<sup>2</sup>, MICHAEL GOTTFRIED<sup>1</sup>, and HANS-PETER STEINRÜCK<sup>1</sup> — <sup>1</sup>Universität Erlangen-Nürnberg, Lehrstuhl für Physikalische Chemie II, Egerlandstr. 3, 91058 Erlangen, Germany — <sup>2</sup>Institute for Applied and Physical Chemistry, University of Bremen, Leobener Strasse NW2, 28359 Bremen, Germany — <sup>3</sup>Nanoscale Synthesis and Characterization Laboratory, Lawrence Livermore National Laboratory, P.O. Box 808, Livermore, California 94550, United States of America

Recent reports [1] have revealed that monolithic nanoporous gold (npAu) exhibits remarkably high catalytic activity for CO oxidation. This observation is surprising because the traditional catalyst is of the oxide-supported type. The specific particle-support interactions, which have been shown to play important roles in the standard Au catalyst, are absent for the nanoporous Au. This being the case, then why does it display such high activity? The answer is most likely related to traces of residual Ag in the npAu. To highlight the role played by each metal in the catalytic process, we have investigated npAu with respect to changes in the chemical and electronic states of both metals with and without CO and O<sub>2</sub> using in-situ XPS (1 mbar) and XPS, respectively. Our results confirm previous XPS results in that segregation of Ag occurs in the surface region. HP-XPS data suggests that this residual Ag plays a significant role in activating molecular oxygen. [1] V. Zielasek et al., *Angew. Chem. Int. Ed.* 2006, 45, 8241-8244.

O 42.87 Wed 17:45 P2

**Nanostructuring of Cu Planar Surfaces With Pt For The Investigation of Hydrogen Related Reactions** — ●ODYSSEAS PASCHOS<sup>1</sup>, HOLGER WOLFSCHMIDT<sup>1</sup>, RAINER BUSSAR<sup>1,2</sup>, and ULRICH STIMMING<sup>1,2</sup> — <sup>1</sup>Department of Physics E19, Technische Universität München, James-Franck-Str. 1, 85748, Garching, Germany — <sup>2</sup>Bavarian Center for Applied Energy Research (ZAE Bayern), Walther-Meißner Str. 6, 85748, Garching, Germany

Recent advances in electrochemistry show that nanostructuring surfaces with metallic catalysts can enhance their electrocatalytic activity. This is advantageous for various applications such as fuel cells and electrolyzers, since it can improve their performance with simultaneous decrease in the amount of precious metal catalysts that is used. Previous work on Pd decorated Au(111) surfaces showed that by decreasing the Pd amount on Au(111), an increase of the activity for hydrogen evolution reaction (HER) occurred for very small coverages. A similar trend was observed for the case of Pt nanostructured Au(111) surfaces. However more research needs to be done in order to obtain a better understanding of this effect. The choice of the substrate material is an important factor for the design of the catalyst structure. In this work we will present results on hydrogen related reactions for Pt nanostructured Cu surfaces. Pt deposited on Cu results in a compressed lattice of Pt and hence the electrochemical behavior of the catalyst system is altered compared to bulk Pt and Pt deposited on Au(111). The results will be compared to the Pt/Au(111) system and hence useful conclusions can be drawn for the choice of substrate material.

O 42.88 Wed 17:45 P2

**Vibrational Spectroscopy of Adsorbates on Roughened Cu(111)** — ●OLAF SKIBBE, DIANA VOGEL, and ANNEMARIE PUCCI — Kirchhoff-Institut für Physik, Universität Heidelberg, Im Neuenheimer Feld 227, 69120 Heidelberg

Rough surfaces are known to provide properties different from those found on low-index pristine single crystal surfaces. These defect determined properties are often responsible for the chemical activity of the surface in heterogeneous catalysis. In this work we present vibrational spectra taken with high-resolution electron energy loss spectroscopy (HREELS) of different adsorbates (e.g. CO, C<sub>2</sub>H<sub>4</sub>) on roughened Cu(111). The roughening was performed by evaporating small amounts of copper on the cooled Cu(111) surface. In addition, we performed measurements of the work function change by using the highly monochromated electron beam of the HREELS in the retarding potential method. The structure of the  $I(U)$  curve can be assigned to different morphologies of the substrate.

O 42.89 Wed 17:45 P2

**Pressure gap in electrochemically induced oxygen spillover at Pt/YSZ electrodes** — ●ARAFAT TOGHAN, LIZ RÖSKEN, and RONALD IMBHL — Institut für Physikalische Chemie und Elektrochemie, Leibniz-Universität Hannover, Callinstr.3-3a, D-30167 Hannover, Germany

Upon application of a pumping voltage to Pt electrodes on the oxygen-conducting solid electrolyte YSZ (yttria-stabilized zirconia) we observe the spillover of discharged oxygen atom onto the Pt surface. The spillover which represents the basis of the electrochemical promotion of heterogeneously catalyzed reactions has been investigated in the past at low pressure, at  $p < 10^{-4}$  mbar. We extend here these studies up to 1 mbar using in situ XPS at BESSY. We use (111) oriented YSZ single crystals, oriented Pt (111) electrodes were prepared by sputtering of Pt target on the surface of a single crystal YSZ (111) using magnetron sputtering technique in inert argon atmosphere at room temperature. The electrodes were characterized by scanning electron microscope (SEM) and by photoelectron emission microscopy (PEEM).

O 42.90 Wed 17:45 P2

**Study of atomic adsorption on graphite monolayer by computer simulation** — ●VITALIY GORBENKO — Classical Private University, Zaporozhye, Ukraine

Understanding of chemical interaction of various atoms with graphite and carbon-based structures is both scientifically and technologically important [1]. The calculations by semiempirical (PM3, PM6), ab-initio (Hartree-Fock) and density functional theory (DFT) methods have been used for study of main properties of the interaction and changes in electronic density of nanographite layers. The MOPAC2007 and GAMESS program packages have been used.

In graphite layers every carbon atom is bounded with three other carbon atoms via  $sp^2$  hybridization. Breaking the  $\pi$ -bonds and producing additional  $\sigma$ -bond is the main mechanism of chemisorption of atoms on graphite monolayers. The three typical adsorption sites have been found. Namely, first is single carbon atom, next is bridge between nearest carbon atoms and last is center of hexagonal carbon cell. Cluster geometry, total energy, atom bonds orders, value of the electron density, atom orbital populations and molecular localized orbitals were obtained. The obtained results of calculations will be detailed and discussed.

[1] J.C. Meyer, A. K. Geim, M. I. Katsnelson, K. S. Novoselov, T. J. Booth, S. Roth, Nature Lett. 2007; 446:60.

O 42.91 Wed 17:45 P2

**Reaction of Methanol on functionalized Ruthenium** — ●PAWEŁ GAZDZICKI and PETER JAKOB — Fachbereich Physik, Philipps-Universität Marburg, D-35032 Marburg, Germany

Infrared Absorption Spectroscopy and Temperature-Programmed Desorption were used to study the adsorption and reaction of methanol on various functionalized Ru(0001) surfaces. The used substrates were the clean Ru(0001) surface, Ru(0001) precovered with 0.5 and 1 ML D, Ru(0001)-(2 × 2)-O, Ru(0001)-(2 × 1)-O and a pseudomorphic Cu monolayer on the Ru(0001) surface.

From the vibrational modes of the isotopes  $CH_3OH$  and  $CH_3OD$  clear evidence for intact adsorption at  $T = 80$  K has been found for all investigated substrates. This finding contradicts previous studies which suggested an OH (OD) bond scission upon adsorption of methanol on Ru(0001) and Ru(0001)-(2 × 2)-O, even at low temperatures, as well as recombinative desorption at elevated  $T$ .

The thermal evolution varies considerably for the individual surfaces with the prominent methoxy ( $CH_3O$ ) species being produced on clean Ru(0001) and Cu/Ru(0001) only. On the oxygen (pre)covered surfaces methanol predominantly desorbs without reaction; a small fraction decomposes directly to form CO and H without forming any detectable intermediates. Finally, 1 ML D/Ru(0001) largely passivates the surface and methanol adsorption is fully reversible.

O 42.92 Wed 17:45 P2

**Chemical trends in the metal-substrate interaction for adsorbed Pt atoms** — ●CHONG GAO and AXEL GRÖSS — Institut für Theoretische Chemie, Universität Ulm, \*D-89069 Ulm, Germany

Catalysts typically consist of small metal particles deposited on an oxide substrate. In this context, the so-called strong metal support interaction (SMSI) has been discussed intensively [1] which significantly influences the catalytic properties of group VIII metals. Using density functional theory, we have performed a systematic study of chemical trends in the metal-support interaction. As a first step, we considered a single Pt atom adsorbed on  $TiO_2$ , Si and Au substrates, thus making also contact to systems that are of interest in electrocatalysis. As a probe of the chemical reactivity, we determined the electronic structure of the adsorbed Pt atoms and evaluated CO adsorption energies on these metal-support systems. The results are compared to recent results of the local reactivity of surface alloy systems [1,2].

[1] S. Sakong, C. Mosch, and A. Groß, Phys. Chem. Chem. Phys. **9**, 2216 (2007).

[2] Y. Gohda and A. Gross Surf. Sci. **601**, 3702 (2007).

O 42.93 Wed 17:45 P2

**Pushing and Pulling a Sn Ion through an Adsorbed Phthalocyanine Molecule** — ●YONGFENG WANG<sup>1</sup>, JÖRG KRÖGER<sup>1</sup>, RICHARD BERNDT<sup>1</sup>, and WERNER A. HOFER<sup>2</sup> — <sup>1</sup>Institut für Experimentelle und Angewandte Physik, Christian-Albrechts-Universität zu Kiel, D-24098 Kiel, Germany — <sup>2</sup>Surface Science Research Center, University of Liverpool, Liverpool L69 3BX, United Kingdom

Molecule-based functional devices on surfaces may take advantage of bistable molecular switches. The conformational dynamics and efficiency of switches are radically different on surfaces compared to liquid phase. We present a design of molecular layers, which enables bistable switching on a surface, and, for the first time, demonstrate control of a single switch in a dense and ordered array at the spatial limit. Up and down motion of a central Sn ion through the frame of a phthalocyanine molecule is achieved via resonant electron or hole injection into molecular orbitals.

O 42.94 Wed 17:45 P2

**Micrometer-scale parallel studies on microstructured model catalysts** — ●MATTHIAS ROOS, STEFAN KIELBASSA, MENHILD EYRICH, JOACHIM BANSMANN, and R. JÜRGEN BEHM — Institute of Surface Chemistry and Catalysis, Ulm University, D-89069 Ulm

To study mesoscopic effects in catalytic reactions, a spatially resolving scanning mass spectrometer was developed, which allows to quantitatively determine reaction rates above model catalysts. Using microstructured model systems with catalytically active fields separated by inert areas, transport effects will be evaluated from the variation in local reaction rates with size and separation of the active fields [1,2]. Experimental data on microstructured Pt films on  $SiO_2$  are presented, and compared with results of simulations. Moreover, first measurements on Au/ $TiO_2$  model catalyst are shown.

[1] M. Roos et al., Rev. Sci. Instrum. **78** (2007) 084104

[2] S. Kielbassa et al., Langmuir **20** (2004) 6644

O 42.95 Wed 17:45 P2

**DFT Studies of  $TiO_2$  (110) and Cu Surfaces** — ●PIOTR KOWALSKI<sup>1</sup>, BERND MEYER<sup>2</sup>, and DOMINIK MARX<sup>1</sup> — <sup>1</sup>Lehrstuhl für Theoretische Chemie, Ruhr-Universität Bochum, D-44780 Bochum — <sup>2</sup>Interdisziplinäres Zentrum für Molekulare Materialien und Computer-Chemie-Centrum, Department Chemie und Pharmazie, Friedrich-Alexander-Universität Erlangen-Nürnberg

Using DFT-based ab-initio calculations in combination with a thermodynamic formalism we investigate the properties of  $TiO_2$  (110) and Cu surfaces. We have calculated the relative stability of various structural models of the nonpolar, mixed-terminated  $TiO_2$  (110) surface in contact with a surrounding gas phase at finite temperature and pressure. Adsorption and desorption of H,  $H_2O$ , CO, simple alcohols as well as the formation of O vacancies were considered. Assuming thermodynamic equilibrium between the surface and an oxygen, hydrogen and water containing atmosphere, we constructed a phase diagram of the lowest free energy surface structures. Cu surfaces are interesting from technological point of view as methanol, a key material for the synthesis of organic materials, is made catalytically from gas containing CO,  $CO_2$  and  $H_2$  in presence of a Cu/ZnO/ $Al_2O_3$  catalyst. It is believed that the morphological changes of the Cu particles on the ZnO support due to a strong metal-support interaction (wetting/dewetting) is the source of higher catalytic activity. We use DFT-based ab-initio calculations to identify the reactive sites on the Cu particles. In particular we investigate the adsorption of hydrogen and dissociated formic acid on clean as well as defective (steps/terraces) Cu surfaces.

O 42.96 Wed 17:45 P2

**The interaction of HCOOH with oxygen-terminated ZnO(000-1)** — ●HENGSHAN QIU, YUEMIN WANG, and CHRISTOF WÖLL — Physical Chemistry I, Ruhr-University Bochum, 44780 Bochum, Germany

Zinc oxide is one of the most important metal oxides due to its electrical, optical and catalytic properties as well as potential applications [1]. The clean, adsorbate-free polar O-terminated ZnO(000-1) surface is electrostatically unstable due to uncompensated surface charges and adopts a (1×3) structure with an abundance of oxygen vacancies [1]. It has been proposed that these vacancy sites exhibit high catalytic activ-



ity toward methanol synthesis and formate species could be one of the important intermediates in this process. In this work, the interaction of HCOOH with O-ZnO(000-1) has been studied by high resolution electron energy loss spectroscopy (HREELS) and thermal desorption spectroscopy (TDS). Exposing ZnO(000-1) surface to HCOOH at 100 K leads to the formation of physisorbed multilayers, chemisorbed monolayer and bidentate formate species. The latter can only be formed at oxygen vacancies through a dissociative adsorption of HCOOH with the ionized H diffusing into the bulk. Heating the sample to higher temperatures induces a thermally activated conversion from the bidentate to a monodentate formate species. At 550 K further decomposition occurs releasing CO, CO<sub>2</sub> and H<sub>2</sub>. In addition, an adsorbate-induced Zn desorption was also observed along with the formate dissociation. [1] Ch. Wöll, Prog. Surf. Sci. 82 (2007) 55.

O 42.97 Wed 17:45 P2

**In-situ investigations of adsorbed benzene on silver modified Pt(322) surfaces** — ●SANDRA KÜNZEL<sup>1</sup>, MATTHIAS SCHÖPPKE<sup>1</sup>, REGINE STREBER<sup>2</sup>, MICHAEL PETER ANDREAS LORENZ<sup>2</sup>, HANS-PETER STEINRÜCK<sup>2</sup>, and REINHARD DENECKE<sup>1</sup> — <sup>1</sup>Wilhelm-Ostwald-Institut für Physikalische und Theoretische Chemie, Universität Leipzig, Linnestraße 2, 04103 Leipzig — <sup>2</sup>Lehrstuhl für Physikalische Chemie II, Universität Erlangen-Nürnberg, Egerlandstraße 3, 91058 Erlangen

In a previous study the site-specific adsorption of benzene on Ni(111) has been investigated by in-situ x-ray photoelectron spectroscopy (XPS) [1]. In an attempt to study lateral confinement on the adsorption properties of larger molecules, we applied such detailed analysis of C 1s core levels (excited by synchrotron radiation at BESSY II) to benzene adsorption on stepped Pt(322). The effective terrace width was modified from five atomic rows to zero by different amounts of Ag (from 0.2 to 1 ML) deposited at 300 K, which form monatomic rows along the step edges [2]. Adsorption of benzene on clean Pt(322) at 190 to 300 K yields only a single C 1s peak with no indication of specific step related adsorption. Increasing amounts of Ag result in a monotonous decrease of benzene adsorption at 300 K (no adsorption on Ag). Since complete site blocking was already observed for Ag coverages exceeding 0.6 ML (i.e. three monorows), a horizontal adsorption geometry and, thus, a minimum free Pt area required can be proposed.

This work was supported by BMBF (05 ES3XBA/5).

[1] C. Papp et al., Phys. Rev. B 73 (2006) 235426.

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

O 42.98 Wed 17:45 P2

**Pulsed laser modification of the steel-polymer interface** — ●CHRISTIAN HOLZHEU, MATTHIAS LASKE, and OTHMAR MARTI — University of Ulm, Institute of Experimental Physics

Laser treatment of stainless steel and the resulting material changes are studied. The irradiation of steel surfaces with short laser pulses improves the adhesion of polymers and especially of fluorinated polymers. Several experiments helped to elucidate the main parameters responsible for polymer adhesion. A setup for laser conditioning under well defined atmospheres was developed. Chemical changes and changes in surface topography caused by laser treatment are analyzed and compared with relevant adhesion data. Measuring the reflectance by the surface allowed to get a relative measure of chemical changes at the surface of the material. For quantitative material characterization GDOES (Glow Discharge Optical Emission Spectroscopy) is used. The durability of the steel before and after laser treatment is evaluated in long time tests applying mechanical pulses.

O 42.99 Wed 17:45 P2

**excited states of the chromophores within many-body perturbation theory** — ●YUCHEN MA and MICHAEL ROHLFING — Fachbereich Physik, Universität Osnabrück, Germany

Although the chromophores of photoactive yellow proteins and rhodopsin proteins have been the subject of numerous spectroscopic investigations because of their unique biochemistry and photophysical properties, the position in energy of their excited states are still not well-defined in theory. We use the *ab-initio* many-body perturbation theory (GW approximation and Bethe-Salpeter equation) to study the excited states of these chromophores, which taking into account electronic exchange, correlation, and electron-hole interaction effects.

Calculations show that the resonant-antiresonant coupling beyond the commonly employed Tamm-Dancoff approximation is needed for an accurate description of the lowest  $\pi \rightarrow \pi^*$  excitations, which affects the excitation energy by up to 0.4 eV. The huge exchange interaction

between the electron and hole leads to the unnegligible coupling between the resonant transition and the antiresonant counterpart. The lowest  $n \rightarrow \pi^*$  excitation for the chromophores of photoactive yellow proteins is composed from free electron-hole transitions with very different quasiparticle transition energies. An accurate description of the lowest  $n \rightarrow \pi^*$  excitation requires inclusion of the dynamics effect in the electron-hole screening, which affects the excitation energy by up to 0.3 eV.

O 42.100 Wed 17:45 P2

**Perturbative approach for electronic excitations in adsorption on metal surfaces** — ●PETER KRATZER and MATTHIAS TIMMER — Fachbereich Physik - Theoretische Physik and Centre for Nanointegration (CeNIDE), Universität Duisburg-Essen, Lotharstr. 1, 47048 Duisburg, Germany

When molecules or atoms adsorb on a metal surface electronic excitations will appear. We have developed and implemented a new method, which is able to calculate the spectra of these excitations. Here, we present the method, which is based on first-order time-dependent perturbation theory, and ground-state density-functional theory (DFT) calculations. It is simple enough to be applied to a wide class of adsorbates and surfaces, while at the same time allowing us to extract system-specific information. We show results for the adsorption of atomic hydrogen isotopes on-top the Al(111) surface. The experimentally observed isotope effect can be explained. At the same time, the method avoids many of the problems of earlier approaches.

It can be implemented with reasonable effort within existing DFT codes, as a post-processing tool [1].

[1] <http://arXiv.org/abs/0810.5248>

O 42.101 Wed 17:45 P2

**Quasiparticle band-structures and lifetimes in noble metals using GW approximation** — ●ZHILUN YI<sup>1</sup>, YUCHEN MA<sup>1</sup>, MICHAEL ROHLFING<sup>1</sup>, VIATCHESLAV SILKIN<sup>2</sup>, and EVGENI CHULKOV<sup>2</sup> — <sup>1</sup>Universität Osnabrück, Osnabrück, Germany — <sup>2</sup>Donostia International Physics Centre, San Sebastian, Spain

We present the calculations of quasiparticle bandstructures and lifetimes for noble metals Cu and Ag within the GW approximation. For Cu, Both the calculated positions of the *d* bands and the width of the *d* bands is within 0.1 eV compared to the experimental results. For Ag, partial core correction should be included in the pseudopotential to get reliable positions of the *d* bands. The calculated lifetime agree with the experiment in the energy region away from the Fermi level, but deviates from the experimental results near the Fermi level where short range interactions which GW approach fails to describe play an important role. For a better description of the lifetime near the Fermi level, higher terms beyond the GW approximation in the many body perturbation theory need to be considered.

O 42.102 Wed 17:45 P2

**Structural Dependence of Optical Properties of Tellurium** — ●STEPHAN BLANKENBURG<sup>1,2</sup>, WOJCIECH WELNIC<sup>1</sup>, and LUCIA REINING<sup>1</sup> — <sup>1</sup>Laboratoire des Solides Irradiés, École Polytechnique, Paris, France — <sup>2</sup>Theoretische Physik, Universität Paderborn, Paderborn, Germany

The further miniaturization of electronic and optoelectronic devices needs the understanding of fundamental material properties to open up new avenues for the nano-fabrication process. Essential steps for understanding the basic mechanisms are the experimental and theoretical study of well-defined model systems [1,2]. In this context, tellurium with its several chemical and physical properties is one of the elemental materials of interest. Due to the discrepancies between the theoretical and experimental determined optical parameters in the literature of Te [3,4], we used time-dependent density-functional theory to reveal the origin of this effect. The puzzling interplay between structural parameters and optical properties as well as the transition to one-dimensional Te nanowires are analyzed in detail.

[1] W. Welnic, et. al., Nature Materials 5, 56 (2006).

[2] W. Welnic, S. Botti, L. Reining, M. Wuttig, PRL 98, 236403 (2007).

[3] S. Tutuhashi, et. al., Phys. Rev. 3, 177 (1969).

[4] P. Ghosh, M. Upadhyay, U. V. Waghmare, PRB 75, 245437 (2007).

O 42.103 Wed 17:45 P2

**Solving the Bethe-Salpeter equation for Wannier-Mott like excitons in InN, ZnO, and MgO.** — ●FRANK FUCHS, CLAUDIA RÖDL, ANDRÉ SCHLEIFE, JÜRGEN FURTHMÜLLER, and FRIEDHELM

BECHSTEDT — Institut für Festkörpertheorie und -optik, Friedrich-Schiller-Universität Jena, Max-Wien-Platz 1, 07743 Jena, Germany

The accurate calculation and parameter-free prediction of optical spectra including excitonic effects is highly desirable for both fundamental and applied research. Excitonic effects can be treated in the framework of many-body perturbation theory and the Bethe-Salpeter equation (BSE), by solving an eigenvalue problem for the electron-hole Hamiltonian  $\hat{H}$ .

In this study we investigate the formation of Wannier-Mott like excitonic states below the optical absorption edge for InN, ZnO, and MgO. Using a recently developed numerically efficient method [1] it is possible to obtain converged results for the binding energies of the first shells of Wannier-Mott excitons.

The results are critically compared to the predictions based on the Wannier-Mott two-band model and available experimental data. In comparison to the latter the computed binding energies, if converged, appear to be significantly overestimated. We discuss this with respect to a deficiency in the underlying approximation of a static screening and investigate the possibility to go beyond.

[1] F. Fuchs, C. Rödl, A. Schleife, and F. Bechstedt Phys. Rev. B 78, 085103 (2008)

O 42.104 Wed 17:45 P2

**2nd-order Møller-Plesset perturbation theory applied to extended systems** — ●ANDREAS GRÜNEIS, MARTIJN MARSMAN, and GEORG KRESSE — Faculty of Physics, University Vienna, and Center for Computational Materials Science, Sensengasse 8/12, A-1090, Vienna, Austria

The use of wave function based methods, such as Møller-Plesset perturbation theory, to add electronic correlation to the Hartree-Fock (HF) approximation is common practice in the computational quantum chemistry of molecular systems. Due to the computational cost involved, however, these methods have hardly been applied to extended systems.

Recently, we have implemented 2nd-order Møller-Plesset (MP2) perturbation theory within the framework of the full-potential Projector-Augmented-Wave (PAW) method, using periodic boundary conditions and a plane wave basis set.

The present implementation allows for the calculation of total energies as well as quasiparticle energies. In order to determine the accuracy of this method we calculated lattice constants, bulk moduli, band gaps, and atomization energies of several semiconducting and insulating systems, including hexagonal Ice. Compared to HF, HF+MP2 yields an improved description of the aforementioned structural properties.

Regarding band gaps, HF+MP2 band gaps present an improvement over the corresponding HF results. Nevertheless, the underestimated static dielectric screening properties of the employed HF wave functions are reflected in underestimated band gaps.

O 42.105 Wed 17:45 P2

**Optical Spectra and Band Structure of Anatase and Rutile TiO<sub>2</sub>** — ●ANDREAS GREULING<sup>1</sup>, PATRICK RINKE<sup>2</sup>, and MICHAEL ROHLFING<sup>1</sup> — <sup>1</sup>Universität Osnabrück, Barbarastr.7,D-49069,Osnabrück — <sup>2</sup>University of California, Santa Barbara

TiO<sub>2</sub> is a semiconductor which is used in many applications (e.g. in biotechnology, cosmetic industry, paint industry, in catalysis or photocatalysis). Therefore, the (optical) properties of TiO<sub>2</sub> are of great interest. As these are still not fully understood in theory we address its excited electronic states and optical spectra with ab initio methods beyond DFT.

We present results of first principles calculations for anatase und rutile TiO<sub>2</sub>. Starting from the electronic ground state, which is calculated within DFT(LDA), we describe the single particle excitations with an GWA approach. We use Gaussian basis-sets because this results in reasonable computational cost. Then we calculate the electron-hole interaction and solve the Bethe-Salpeter Equation (BSE) in order to obtain coupled electron-hole excitations. Based on the resulting data we evaluate the optical spectra and compare them with experimental data.

O 42.106 Wed 17:45 P2

**IRRAS studies on a new emitter material for OLEDs** — ●TOBIAS GLASER<sup>1</sup>, MARTIN BINDER<sup>1</sup>, ANNEMARIE PUCCI<sup>1</sup>, CHRISTIAN LENNARTZ<sup>2</sup>, and CHRISTIAN SCHILDKNECHT<sup>2</sup> — <sup>1</sup>Kirchhoff-Institut für Physik, Universität Heidelberg — <sup>2</sup>BASF SE, 67056 Ludwigshafen

A new emitter material for organic light emitting devices (OLEDs) called CN-PMBIC is investigated by infrared (IR) spectroscopy. Experiments were performed under UHV conditions with a commercial FT IR spectrometer flanged to the chamber. Thin films of the organic material were deposited by vapor sublimation on different substrates. Especially infrared reflection absorption spectroscopy (IRRAS) is a well-suited method to investigate the growth of the organic films. Furthermore, the influence of Ca on CN-PMBIC was studied at room temperature and at 100 K. Ca plays an important role as cathode material in OLED fabrication. The evaporation of Ca onto a film of CN-PMBIC gives rise to new IR features that strongly depend on the sequence in which the various materials are deposited and on the sample temperature. The new features are supposed to be related to dynamic charge transfer effects.

O 42.107 Wed 17:45 P2

**Design of composite materials via textured polymer brushes** — ●MANUELA PLUNTKE<sup>1</sup>, SABINE LETSCHE<sup>2</sup>, DIRK VOLKMER<sup>2</sup>, and OTHMAR MARTI<sup>1</sup> — <sup>1</sup>Institute of Experimental Physics, Ulm University, Albert-Einstein-Allee 11, 89069 Ulm — <sup>2</sup>Institute of Inorganic Chemistry II, Ulm University, Albert-Einstein-Allee 11, 89069 Ulm

Acidic matrix macromolecules are involved in the production of biomaterials such as bone and nacre. Therefore polyelectrolyte brushes exposing a multitude of acidic groups are attractive tools to control the growth of biogenic minerals.

To obtain crystalline thin mineral films we deposit inorganic material in a lithographically structured organic matrix of polymer brushes grown by surface-initiated atom-transfer radical polymerisation. The initial metastable amorphous thin film is converted into a polycrystalline phase by thermal treatment.

To find optimal conditions for the specific deposition of different minerals we varied the matrix properties by altering the functional groups of the brushes and the experimental parameters.

Our current studies focus on the analysis of the brush swelling behaviour in the mineralization media by AFM as well as on the mechanical properties of the materials.

After all our investigations contribute to the understanding of the interactions between the inorganic minerals and the organic matrix molecules and offer attractive perspectives for potential applications like optical information processing and regenerative medicine.

O 42.108 Wed 17:45 P2

**Experimentelle Untersuchungen der Adsorption und des Kristallwachstums von Komponenten epikutikularer Wachse.** — ●ALEXANDER HOMMES<sup>1,2</sup>, WILHELM BARTHLOTT<sup>3</sup> und KLAUS WANDEL<sup>2</sup> — <sup>1</sup>FGAN, Wachtberg, Germany. — <sup>2</sup>Institut für Theoretische und Physikalische Chemie, Surfaces and Interfaces, University of Bonn, Germany. — <sup>3</sup>Nees-Institut für Biodiversität der Pflanzen, University of Bonn, Germany.

Im Rahmen dieser Arbeit wurde das konzentrationsabhängige Phasenverhalten von adsorbiertem Octacosan-1-ol und Octacosan-1-ol Derivaten an der fest/flüssig und fest/gas Grenzfläche eines künstlichen Substrats mittels AFM/STM/REM untersucht. Octacosan-1-ol ist Hauptbestandteil der epikutikularen Wachse auf Weizenblättern, und bildet somit die äußerste Barriere zur Umwelt und bestimmt die Hydrophobizität der Blattoberfläche. Die Nukleations- und Wachstumsbedingungen auf der nativen Oberfläche führen zur Ausbildung von kristallinen "Platelets", die aufgrund einer komplexen mikro- und nanoskopische Architektur einen Superhydrophoben Effekt auslösen. Um diesen Effekt grundlegend zu verstehen und in einem technischen Prozeß nutzbar zu machen, muß ein Verständnis zum Wachstum von organischen Kristallen auf Oberflächen entwickelt werden. Hierzu werden verschiedene, in epikutikularen Wachsen enthaltene Moleküle auf künstlichen Oberflächen adsorbiert und das Kristallwachstum beobachtet. Die erhaltenen Erkenntnisse sind nach dem "bottom up Prinzip", von der Einzelmoleküluntersuchung über Nukleation, Aggregatbildung bis hin zum makroskopischen Kristallwachstum gegliedert.

O 42.109 Wed 17:45 P2

**On the fate of hydrogen by formation of thiol-based self-assembled monolayers: A critical in situ photoelectron spectroscopy result** — ●LAXMAN KANKATE, ANDREY TURCHANIN, and ARMIN GÖLZHÄUSER — Fakultät für Physik, Universität Bielefeld, 33615 Bielefeld

Self-assembled monolayers (SAMs) of thiols on gold are vastly utilized for the functionalization of surfaces and interfaces in interdisciplinary research for many years. However, a seminal question on the fate of

the hydrogen of the S-H groups upon SAM formation has not been answered unambiguously<sup>1</sup>. It is generally believed that the S-H bond scission takes place and the released hydrogen either sticks to the surface or desorbs in the molecular form. Some studies, however, suggest that the S-H bond scission does not occur at all. Here, we present the experimental results which clearly show that the atomic hydrogen forms upon thiol SAM formation and interacts with the monolayer terminus. Vapour phase deposition was utilized to grow 4'-nitro-1,1'-biphenyl-4-thiol, 4-nitrophenylthiol and bis-(4,4'-nitrobiphenyl)-disulphide SAMs on Au surfaces. Using in situ x-ray photoelectron spectroscopy (XPS) we found that the terminal nitro group of the thiol SAMs are partially reduced upon the self-assembly into the amino group. On the contrary, the disulphide SAMs form without any reduction.

[1] J.C. Love, L.A. Estroff, J.K. Kriebel, R.G. Nuzzo, G.M. Whitesides, *Chem. Rev.* 105 (2005) 1103

O 42.110 Wed 17:45 P2

**Study of azobenzene-containing self-assembled monolayers with surface plasmon resonance spectroscopy** — ●OLENA FILINOVA, ULRICH JUNG und OLAF MAGNUSSEN — Institut für Experimentelle und Angewandte Physik, Leibnizstraße 19, 24098 Kiel

Azobenzene-containing molecules can be switched between the trans and cis isomers by UV and visible light. Adsorbate layers of such molecular switches on surfaces are of great interest for the formation of functional nanosystems. Using surface plasmon resonance spectroscopy we have studied the kinetics of the photoisomerization processes for self-assembled monolayers containing azobenzene bound by thiol- and triazatriangulenium groups to Au surface. Using an Hg-lamp with bandpass filter the trans-cis photoswitching was monitored as a function of wavelength and radiation power. These measurements allowed to optimize the conditions for photoswitching and to determine the time constants for the first order kinetics of these processes, which allowed to estimate quantum yields of the photoisomerization reactions in the range  $10^{-5}$  to  $10^{-3}$ .

O 42.111 Wed 17:45 P2

**Reactive Sites for the Deposition of Calcium on Semiconducting Polymers** — ●FABIAN BEBENSEE<sup>1</sup>, JACK HESS BARICUATRO<sup>2</sup>, JUNFA ZHU<sup>3</sup>, JAMES SHARP<sup>2</sup>, WANDA LEW<sup>2</sup>, HANS-PETER STEINRÜCK<sup>1</sup>, J. MICHAEL GOTTFRIED<sup>1</sup>, and CHARLES T. CAMPBELL<sup>2</sup> — <sup>1</sup>Lehrstuhl für Physikalische Chemie II, Universität Erlangen-Nürnberg, Egerlandstraße 3, D-91058 Erlangen, Germany — <sup>2</sup>Department of Chemistry, University of Washington, Seattle, WA 98195, USA — <sup>3</sup>National Synchrotron Radiation Laboratory, University of Science and Technology of China, Hefei, Anhui 230029, China

Systems composed of semiconducting polymers and low work function metals - used as the cathode - are of great interest in the field of organic electronics, e.g., organic solar cells and organic light emitting diodes. The key parameter in the performance of such devices is the interface between the active polymer and the electrode. We investigated the deposition of calcium on several semiconducting polymers, including CN-MEH-PPV and P3HT, using a set of complementary experimental techniques (ISS, HR-XPS, adsorption microcalorimetry). The focus of this study is on the different adsorption or reaction sites for Ca on the polymer surface and the energetics of the interface formation. The considerable differences in the behavior of the polymers are linked to the presence of different heteroatoms. Support by the DAAD, the NSF, and the Excellence Cluster "Engineering of Advanced Materials" at the University of Erlangen-Nürnberg is gratefully acknowledged.

O 42.112 Wed 17:45 P2

**High energy photoelectron spectroscopy of HBC-C14** — ●VAJIHEH ALIJANI<sup>1</sup>, S. SHAHABEDIN NAGHAVI<sup>1</sup>, ANDREI GLOSKOVSKI<sup>1</sup>, GERHARD H. FECHER<sup>1</sup>, CLAUDIA FELSER<sup>1</sup>, KATERINA MEDYANYK<sup>2</sup>, and GERD SCHÖNHENSE<sup>2</sup> — <sup>1</sup>Institute of Inorganic and Analytical Chemistry, Johannes Gutenberg - University, 55099 Mainz — <sup>2</sup>Institute of Physics, Johannes Gutenberg - University, 55099 Mainz

A charge transfer (CT) complex is defined as an electron donor /— electron acceptor complex, characterized by electronic transitions to an excited state. In this excited state, there is a partial transfer of a charge from the donor to the acceptor. CT complexes are good candidates as photovoltaic cells, transistors and superconductors. Thin films of HBC-C14 were prepared on Si/SiO<sub>x</sub> substrate by spin coating and characterised by profilometry and atomic force microscopy. The films were investigated by X-Ray photoelectron spectroscopy with laboratory XPS source and synchrotron excitation. The excitation energy was varied in the range from 1.4 keV to 8 keV. We show that high

energy photoelectron spectroscopy at intermediate energies is better suited than at very high energies for studies of organic thin films. The reason is the enhanced contribution of the Si/SiO<sub>x</sub> substrate to the photoemission signal at higher photon energies. This is caused by very large inelastic electron mean free path that becomes comparable with the film thickness of few tens of nm at high kinetic energies of photoelectrons.

Funded by DFG through Transregio SFB TRR 49 (Project B8).

O 42.113 Wed 17:45 P2

**Valence band spectroscopy on plasma treated wood surfaces** — ●LOTHAR KLARHÖFER<sup>1</sup>, EVGENIJ PACHOMOW<sup>1</sup>, SEBASTIAN MATHES<sup>1</sup>, WOLFGANG MAUS-FRIEDRICH<sup>1</sup>, and WOLFGANG VIÖL<sup>2</sup> — <sup>1</sup>Institut für Physik und Physikalische Technologien, Leibnizstraße 4, D-38678 Clausthal-Zellerfeld, Germany — <sup>2</sup>HAWK FH Hildesheim/Holzminde/Göttingen, Fakultät Naturwissenschaften und Technik, Von-Ossietzky-Straße 99, 37085 Göttingen

Wood has been plasma treated using a dielectric barrier discharge at atmospheric pressure in ambient air, in order to improve the wettability of the surface. Chemical changes due to plasma treatment were studied by several surface sensitive techniques like XPS, UPS and MIES.

The functional groups of cellulose were identified in the valence band by fingerprints from glucose and cellobiose. The fingerprints for lignin were obtained by coniferyl alcohol, cinnamyl alcohol, phenol and benzene.

The plasma treatment in ambient air has different effects to the surface of cellulose and lignin respectively. An oxygen containing plasma reduces the cellulose surface, causes the loss of hydroxyl groups and the formation of C=O double bonds.

The lignin surface oxidizes in an oxygen containing plasma which leads to the removal of the hydrophobic phenyl groups, which react preferred with the plasma species. The destruction of the phenyl groups and therefore the molecule backbone causes the removal of the lignin from the surface, leaving a polar and rich on oxygen surface with good wetting behaviour.

O 42.114 Wed 17:45 P2

**A study of the Cobalt Phthalocyanine-Ag-Si(111) interface** — ●FEI SONG<sup>1,2</sup>, JUSTIN WELLS<sup>1,3</sup>, ZHESHEN LI<sup>1</sup>, KARSTEN HANDRUP<sup>1</sup>, SHINING BAO<sup>2</sup>, KARINA SCHULTE<sup>4</sup>, LOUISE MAYOR<sup>4</sup>, EDWARD PERKINS<sup>4</sup>, JANINE SWARBRICK<sup>4</sup>, LAUGE GAMMELGAARD<sup>5</sup>, MARJA AHOLA-TUOMI<sup>6</sup>, and PHILIP HOFMANN<sup>1</sup> — <sup>1</sup>University Aarhus, DK — <sup>2</sup>Zhejiang University, Hangzhou, CN — <sup>3</sup>Norwegian University of Science and Technology, Trondheim, N — <sup>4</sup>University of Nottingham, UK — <sup>5</sup>CARPES A/S, Kgs. Lyngby, DK — <sup>6</sup>University of Turku, FI

We describe the electronic and structural properties of the interface between Cobalt phthalocyanine(CoPc) molecules and a Si(111) surface, which is passivated by a monolayer of silver. Different photoemission-based techniques such as valence band UPS, XPS and NEXAFS are used, and the system is also investigated using nano-scale four point probes. Valence band UPS indicates a stronger bonding for the first monolayer of molecules than for subsequent monolayers. This is accompanied by a structural change from flat-lying to standing. For thicker layers, we infer the charge transfer and band alignment. Finally, the thickness-dependent surface conductance is related to these observations.

O 42.115 Wed 17:45 P2

**Infrared and Raman spectroscopy of ultrathin organic films in a liquid cell** — ●NADJA BECKER<sup>1</sup>, DENNIS AULICH<sup>1</sup>, NORBERT ESSER<sup>1</sup>, JÖRG RAPPICH<sup>2</sup>, and KARSTEN HINRICHS<sup>1</sup> — <sup>1</sup>ISAS - Institute for Analytical Sciences, Department Berlin, Albert-Einstein-Str. 9, 12489 Berlin, Germany — <sup>2</sup>Helmholtz Zentrum Berlin für Materialien und Energie GmbH, Abt. SE1, Kekuléstr. 5, 12489 Berlin, Germany

Thickness and structure of organic films is investigated by non-destructive, optical in-situ-methods. Besides molecular identification, Raman spectroscopy and infrared ellipsometry are shown to reveal complementary vibrational informations of thin films. The same in-situ cell [1] was used for characterisation of protein adsorption and the study of polymer films in contact with aqueous solutions.

Reference: [1] Y. Mikhaylova, L. Ionov, J. Rappich, M. Gensch, N. Esser, S. Minko, K.-J. Eichhorn, M. Stamm, K. Hinrichs, *Anal. Chem.* 79, 7676 (2007)

O 42.116 Wed 17:45 P2

**Nano-Mechanical Detection of (Bio-)Molecular Recognition** — ●K. GRUBER<sup>1</sup>, C. ROHR<sup>1</sup>, J. KOESER<sup>2</sup>, U. HUBLER<sup>2</sup>, T. SOBEY<sup>3</sup>, F. C. SIMMEL<sup>3</sup>, and B. A. HERMANN<sup>1</sup> — <sup>1</sup>Dept. of Physics / CeNS, LMU Munich and WMI, 85748 Garching, Germany — <sup>2</sup>Concentris GmbH, 4012 Basel, Switzerland — <sup>3</sup>Dept. of Physics, TU Munich, 85748 Garching, Germany

Based on the development of the atomic force microscope, the cantilever array technique monitors physical, chemical and biochemical processes taking place on the surface of wafer-thin and extremely sensitive silicon springs. These reactions can be measured directly without fluorescent or radioactive labels, and can be followed in real-time allowing analysis of reaction dynamics and determination of e.g. kinetic constants. The goal is to understand the chemical transduction process of a (bio-)molecular key-lock-recognition in a deflection signal by performing well defined experiments.

The hybridization signals of two 70% to 80% homologous single-stranded DNA sequences could be clearly distinguished. Each half of one cantilever array was functionalized with one of the two DNA strands. Hence, only those cantilever that bear the exact complementary to a matching single strand, offered in the sample solution, show deflection. The experiment could be successfully reproduced for several independently functionalized cantilever arrays. As one possible application, we demonstrated that a thrombin catching DNA-aptamer[1] could be successfully bound onto a cantilever surface.

[1] F. C. Simmel et al., *Angew. Chem. Int. Ed.* 2004 43, 3549 (2004)

O 42.117 Wed 17:45 P2

**Influence of supporting substrate on the shape of deposited size-selected nanoparticles** — ●CHRISTIAN KLEINHANS, WOLFGANG ROSELLEN, FURKAN BULUT, KERSTIN GEBHARDT, and MATHIAS GETZLAFF — Institute of Applied Physics, University Düsseldorf

The structure of supported clusters, significantly affecting their electronic and magnetic properties, is of large interest in today's physics, especially from a technological point of view for future applications. With a continuously working, UHV-compatible arc cluster ion source (ACIS), Fe-, Co- and FeCo-alloy-clusters have been produced and subsequently mass filtered using an electrostatic quadrupole-deflector-unit. The sizes range from 5 to 15nm. The deposition of these preformed free clusters onto a ferromagnetic Ni-thin-film prepared on a W(110)-substrate was performed under soft-landing conditions. For comparison, the clusters were additionally deposited on the bare W(110) surface. Due to the different surface energies, changes in the shape of the clusters are to be expected. The determination of size and shape of the nanoparticles was carried out by means of STM and TEM. We will also discuss the temperature dependence concerning the different nanoparticle-substrate systems.

O 42.118 Wed 17:45 P2

**Crystal structure of iron oxide nano particles synthesized from ferritin** — ●MICHAEL KRISPIN, ALADIN ULLRICH, and SIEGFRIED HORN — Lehrstuhl für Experimentalphysik II, Universität Augsburg, D-86135 Augsburg

We have investigated the local crystal structure of nanosized iron oxides by extended x-ray absorption fine structure (EXAFS). Iron oxide nanoparticles of different diameters were produced by thermal treatment of horse spleen ferritin molecules and remineralized apo-ferritin molecules, respectively. The size was determined by atomic force microscopy (AFM) as well as transmission electron microscopy (TEM). The structure of these particles was compared to various iron oxide and ferrihydrite references. The Fourier transformed (FT) EXAFS spectra of the iron oxide nanoparticles differ significantly from  $\alpha$ -Fe<sub>2</sub>O<sub>3</sub> and  $\gamma$ -Fe<sub>2</sub>O<sub>3</sub> reference spectra and change systematically as a function of particle diameter, signalling a corresponding evolution of the structure. A possible explanation could be the occurrence of a mixture of  $\alpha$ -Fe<sub>2</sub>O<sub>3</sub> and  $\gamma$ -Fe<sub>2</sub>O<sub>3</sub> phases in a core-shell model, i.e. the particle consists of a  $\alpha$ -Fe<sub>2</sub>O<sub>3</sub> core and  $\gamma$ -Fe<sub>2</sub>O<sub>3</sub> like shell. A decrease of core to shell ratio with decreasing particle size may then explain the changes in the measured FT-EXAFS. Indeed, EXAFS oscillations of samples can be fitted by a linear combination of the EXAFS oscillations of the measured  $\alpha$ -Fe<sub>2</sub>O<sub>3</sub> and  $\gamma$ -Fe<sub>2</sub>O<sub>3</sub> reference powders. This picture is supported by the fact, that x-ray diffraction (XRD) measurements on annealed native ferritin show that the  $\alpha$  and  $\gamma$  phases coexist.

O 42.119 Wed 17:45 P2

**Electronic properties of size selected Ag clusters on C<sub>60</sub> and HOPG surfaces** — ●BEN WORTMANN<sup>1</sup>, STEFANIE DUFFE<sup>1</sup>,

LUKAS PATRYARCHA<sup>1</sup>, BERND VON ISSENDORFF<sup>2</sup>, and HEINZ HÖVEL<sup>1</sup> — <sup>1</sup>Technische Universität Dortmund, Experimentelle Physik I, 44221 Dortmund, Germany — <sup>2</sup>Universität Freiburg, Fakultät für Physik, Hermann-Herder Straße 3, 79104 Freiburg, Germany

We deposited mass selected Ag clusters, which are expected to form geometrically magic icosahedra, on 1.5 ML C<sub>60</sub>/HOPG at low temperatures. On 1 and 2 ML C<sub>60</sub> we observed very narrow cluster height distributions for Ag<sub>309±3</sub> and Ag<sub>923±9</sub>. The clusters on 1 and 2 ML C<sub>60</sub> kept their original height for more than 12 hours at room temperature [1, 2]. To get information on the electronic structure of the clusters, scanning tunnelling spectroscopy measurements were performed at 5 K for Ag<sub>309±3</sub> and Ag<sub>923±9</sub>/C<sub>60</sub>/HOPG. We observed spectra with identical features for individual clusters with the same selected size. Additionally we investigated the electronic properties of size selected clusters with ultraviolet photoemission spectroscopy (UPS). Using C<sub>60</sub> as buffer layer for the cluster deposition, the dominant UPS signal of C<sub>60</sub> masks the signal of the clusters. For this reason the Ag clusters were deposited and investigated on bare HOPG at 100 K. The low temperature decreases the mobility of the clusters on HOPG and reduces coalescence. One aim of these studies is the comparison to UPS spectra of size selected clusters in free beam [3].

[1] S. Duffe et al., *EPJD* 45, 3 (2007) [2] S. Duffe et al., submitted for publication [3] O. Kostko et al., *PRL* 98, 043401 (2007)

O 42.120 Wed 17:45 P2

**Growth of magnetic clusters on a moiré pattern of graphene on Ru(0001)** — ●SIMON ALTENBURG, MARTIN ZIEGLER, JÖRG KRÖGER, and RICHARD BERNDT — Christian-Albrechts-Universität zu Kiel, D-24098 Kiel, Germany

Large areas of highly ordered single layer graphene were grown on a Ru(0001) surface by controlled segregation of Carbon from the bulk. The resulting moiré superstructure was atomically resolved by scanning tunnelling microscopy. We find that the moiré pattern acts as a template for the growth of Co clusters: Depositing Co onto the graphene layer gives rise to Co islands whose lateral dimensions are determined by the moiré pattern. The dependence of the Co island dimensions on deposition temperature and coverage was investigated. Funding by the Deutsche Forschungsgemeinschaft through SFB 668 is acknowledged.

O 42.121 Wed 17:45 P2

**Growth and Characterization of Pt Nanoparticles on CeO<sub>2</sub> (111) Films on Cu(111) by STM** — ●THORSTEN STAUDT<sup>1</sup>, YAROSLAVA LYKHACH<sup>1</sup>, LUTZ HAMMER<sup>2</sup>, M. ALEXANDER SCHNEIDER<sup>2</sup>, and JÖRG LIBUDA<sup>1</sup> — <sup>1</sup>Lehrstuhl für Physikalische Chemie II, Friedrich-Alexander-Universität Erlangen-Nürnberg — <sup>2</sup>Lehrstuhl für Festkörperphysik, Friedrich-Alexander-Universität Erlangen-Nürnberg

Precious metal nanoparticles supported on ceria films are widely used in many important applications, including three-way automotive catalysts and the catalytic oxidation of hydrocarbons. The use of ceria is motivated by its unique ability to store and release oxygen, while it is well known that metal particles supported on oxides can exhibit different chemical reactivity depending upon their size and structure.

Here we present a scanning tunnelling microscopy study on the growth of Pt nanoparticles on CeO<sub>2</sub>(111) films. These films are grown by physical vapour deposition (PVD) of cerium on a Cu(111) substrate in O<sub>2</sub> at 520 K. The recipe has been adopted from the one suggested by Matolin and coworkers [1] and modified by the use of a higher oxidation temperature to form atomically flat terraces. LEED measurements reveal a well-ordered film with a (1.5x1.5) superstructure in orientation to the underlying substrate. A Volmer-Weber growth mode of ceria is identified by STM measurements. In a next step we investigate the nucleation behaviour and growth of Pt nanoparticles, prepared by PVD. Finally, the thermal stability of these particles is studied and it is found that they are transformed into flat islands upon annealing. [1] V. Matolin et al., *Thin Solid Films* 516 (2008) 6120-6124

O 42.122 Wed 17:45 P2

**Towards an understanding of the vibrational spectrum of the neutral Au<sub>7</sub> cluster** — ●LUIS MANCERA and DAVID M. BENOIT — Nachwuchsgruppe Theorie - SFB 569, University of Ulm, Albert-Einstein-Allee 11, D-89081 Ulm, Germany

Most experimental vibrational studies on neutral gold nanoclusters have focused on charged particles. For neutral clusters, such studies have been limited in the past to Au<sub>2</sub> and Au<sub>3</sub>. Only very recently, vibrational spectra of a few small neutral gold clusters in gas-phase have

been reported, using far-infrared multiple-photon dissociation (FIR-MPD) spectroscopy [1]. Among them, Au<sub>7</sub> receives a particular attention since it is in a size regime in which anions and cations are known to adopt planar structures. In this contribution, we address the prediction of the vibrational spectrum of the Au<sub>7</sub> cluster from first principles. Since discrepancies between experimental and theoretical spectra are often attributed to anharmonic effects, we also investigate the vibrational spectrum of this cluster, using the vibrational self-consistent field method (VSCF), which includes anharmonic coupling between vibrational modes. Besides anharmonicity, we discuss other issues affecting the prediction of the spectrum, such as polymorphism and the theoretical description of the underlying potential energy surface.

[1] P. Gruene, D. M. Rayner, B. Redlich, A. F. G. van der Meer, J. T. Lyon, G. Meijer, and A. Fielicke, *Science* 321, 674 (2008)

O 42.123 Wed 17:45 P2

**HICS – Highly charged ion collisions with surfaces** — ●CHRISTIAN HAAKE, THORSTEN PETERS, JOHANNES HOPSTER, ANDREAS WUCHER, and MARIKA SCHLEBERGER — Universität Duisburg-Essen, Fachbereich Physik, 47057 Duisburg, Germany

A new ion beam installation with the name HICS (highly charged ions collisions with surfaces) has been constructed to investigate the mechanisms of energy dissipation in a substrate after the impact of highly charged ions. The set-up offers high charge states (up to Ar<sup>16+</sup> or Xe<sup>44+</sup>) and adjustable kinetic energies which can be less than 100 eV/q. These low energies are achieved by a deceleration system which uses a device we call an ion escalator. An evaporation chamber for sample preparation is mounted and a load lock system offers *in situ* transport to other vacuum systems. To analyse the irradiation effects a time-of-flight system for secondary and neutral mass spectrometry (SIMS/SNMS) is installed. Inner Electronic excitations can be detected with metal-insulator-metal junctions. These detectors offer the possibility to study excitations below the work function which limits the external emission of electrons. First data measured with Ag-AIO<sub>x</sub>-Al detectors will be presented.

O 42.124 Wed 17:45 P2

**Photochromic silver nanoparticles fabricated by nanosphere lithography** — ●MELANIE MEIXNER, ALEXANDER SPRAFKE, FLORIAN HALLERMANN, MAXIMILIAN REISMANN, MATTHIAS WÜTTIG, and GERO VON PLESSEN — Institute of Physics (IA), RWTH Aachen University, 52056 Aachen, Germany

Photochromic materials change their color under irradiation with light. In previous work [1], we have studied the photochromic transformation of silver nanoparticles embedded in transition-metal oxides prepared by dc-sputter deposition, such as TiO<sub>x</sub>, ZrO<sub>x</sub> and HfO<sub>x</sub>. The silver nanoparticles are highly inhomogeneous in shape, size and spatial distribution. The photochromic effect is based on spectral hole burning in the inhomogeneously broadened particle-plasmon band. This hole burning is probably caused by photoemission of electrons from the resonantly excited particles.

In the present work, we show that TiO<sub>x</sub>-embedded silver nanoparticles with improved photochromic properties can be fabricated through a combination of electron-beam evaporation and nanosphere lithogra-

phy. Nanosphere lithography is a method to produce hexagonal arranged and equally shaped particles [2]. The good reproducibility of this approach allows us to analyze the photochromic transformation in a more quantitative way than was possible with samples prepared by sputter deposition.

[1] C. Dahmen et al., *Appl. Phys. Lett.* 88 ,011923 (2006)

[2] J. C. Hulteen et al., *J Vac Sci Technol A* 13 pp. 1553-1558 (1995)

O 42.125 Wed 17:45 P2

**Exposure of Single-Molecule-Magnets Mn<sub>6</sub>Cr and Mn<sub>7</sub> to Soft X-Rays** — FABIAN MERSCHJOHANN<sup>1</sup>, ●ANDREAS HELMSTEDT<sup>1</sup>, AARON GRYZIA<sup>1</sup>, ANDREAS WINTER<sup>1</sup>, SEBASTIAN STEPELER<sup>1</sup>, NORBERT MÜLLER<sup>1</sup>, ARMIN BRECHLING<sup>1</sup>, MARC D. SACHER<sup>1</sup>, ULRICH HEINZMANN<sup>1</sup>, CARL-GEORG FREIHERR V. RICHTHOFEN<sup>2</sup>, THORSTEN GLASER<sup>2</sup>, SÖNKE VOSS<sup>3</sup>, MIKHAIL FONIN<sup>3</sup>, and ULRICH RÜDIGER<sup>3</sup> — <sup>1</sup>Fak. f. Physik, Uni Bielefeld — <sup>2</sup>Fak. f. Chemie, Uni Bielefeld — <sup>3</sup>Fak. f. Physik, Uni Konstanz

Mn<sub>6</sub>Cr and Mn<sub>7</sub> are two representatives of the new 7-core Single-Molecule-Magnets (SMM) with a large spin moment. Adsorbed on surfaces their electronic configuration may change depending on the substrate material. Possible modifications of the electronic configuration can be studied element-specifically by X-ray absorption spectroscopy and by measuring the spin-polarization of photoelectrons ejected by circularly polarized synchrotron radiation. Drawback of the above mentioned methods is the bad stability of the SMM during X-ray exposure. The SMM degrade due to photoreduction with increasing time of exposure. The trivalent metallic components (here Mn and Cr) become divalent ones. This degradation process was observed by using very small photon fluxes at Maxlab III. Within about one hour of X-Ray exposure the degradation saturates. The rate of degradation depends on the substrate material as well as on the SMM-concentration on the substrate. Beneath these results we will present first spin-resolved photo-emission measurements of SMM-crystals.

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**Investigation of hot electrons below the surface** — ●JOHANNES HOPSTER<sup>1</sup>, THORSTEN PETERS<sup>1</sup>, CHRISTIAN HAAKE<sup>1</sup>, DETLEF DIESING<sup>2</sup>, ANDREAS WUCHER<sup>1</sup>, and MARIKA SCHLEBERGER<sup>1</sup> — <sup>1</sup>Fachbereich Physik, Universität Duisburg-Essen, Lotharstrasse 1, 47057 Duisburg, Germany — <sup>2</sup>Physikalische Chemie, Universität Duisburg-Essen, 45117 Essen, Germany

In many physical processes energetic (hot) charge carriers play a significant role. Hot electrons may be produced in different ways, e.g. by energetic ions, laser beams or directly by a monoenergetic electron beam. Our aim is to investigate the spatial and temporal development of the electron energy distribution below the surface. To detect the hot charge carriers thin film metal insulator metal junctions (MIMs) are used. The measured yield of electron transmission through the insulator barrier depends on the initial excitation energy, the top electrode thickness, the material of the top electrode and the barrier height. By applying a bias voltage between the two metal electrodes energy dispersive measurements are possible. Corresponding data that has been obtained on various MIMs will be presented.