

## 7 SURFACES, BOUNDARY LAYERS AND THIN FILMS

*Wednesday, 2. Sept. 2009, Room E*

Time	ID	SURFACES, BOUNDARY LAYERS AND THIN FILMS <i>Chair: E. Zojer, TU Graz</i>
<b>09:00</b>		<b>PLENARY SESSION</b>
<b>12:40</b>		<b>Postersession, Lunchbuffet</b>
<b>14:00</b>	<b>701</b>	<p style="text-align: center;"><b>Interfaces and surfaces in organic molecular crystals: their crucial role in organic field effect devices</b></p> <p style="text-align: center;"><i>Bertram Batlogg</i> <i>ETH Zürich, Laboratorium für Festkörperphysik, 8093 Zürich, Switzerland</i></p> <p>The performance of organic electronics is to a high degree determined by the interfaces between organic semiconductors, dielectrics and metal contacts. An overview will be given over the recent progress in identifying, quantifying and ultimately (almost) eliminating the detrimental electronic trap states associated with structural and chemical defects.</p>
<b>14:40</b>	<b>702</b>	<p style="text-align: center;"><b>Direct relation between energy level alignment and device performance</b></p> <p style="text-align: center;"><i>Anna M. Track<sup>1</sup>, Philipp Stadler<sup>2</sup>, Ullah MuJeeb<sup>3</sup>, Gebhard J. Matt<sup>3</sup>, Niyazi Serdar Sariciftci<sup>2</sup>, Michael G. Ramsey<sup>1</sup></i></p> <p><sup>1</sup> <i>Insitut für Physik / Surface Science Group, KFU Graz, Universitätsplatz 5, 8010 Graz, Austria</i></p> <p><sup>2</sup> <i>Linzer Institut für organische Solarzellen (LIOS) / Physikalische Chemie, Altenbergerstraße 69, 4040 Linz, Austria</i></p> <p><sup>3</sup> <i>Institut für Festkörperphysik, Altenbergerstr. 69, 4040 Linz, Austria</i></p> <p>Interface engineering in organic thin film transistors has become the key issue in designing devices with acceptable electrical transport properties. In this work we present two different OFETs with fullerene as semiconductor and electrochemically grown alumina oxide as well as alumina oxide passivated with divinyltetramethyldisiloxane-bis(benzocyclobutene) (BCB) as gate insulator. These interfaces are studied in detail by X-ray and ultraviolet photoemission spectroscopy (XPS and UPS) and compared to the transistor transport characteristics. Here we can show that the device performance can be directly related to the measured electronic level alignment at the dielectric interface. The threshold voltage of the transistor characteristics is shifted by 0.8V to more positive values when the BCB is used. We correlate the different transport performance to the reduction of the work function and concomitant shift in the photoemission features of the semiconductor of 0.8 eV due to a build-in potential at the BCB/fullerene interface.</p>

15:00	703	<p style="text-align: center;"><b>Growth of sexithiophene films on Cu(110)-(2x1)O at elevated substrate temperatures</b></p> <p style="text-align: center;"><i>Günther Weidlinger, Harald Zaglmayr, Lidong Sun, Daniel Roman Fritz, Thorsten Wagner, Peter Zeppenfeld</i>  <i>Institut für Experimentalphysik, Johannes Kepler Universität Linz, Altenberger Straße 69, 4040 Linz, Austria</i></p> <p>Sexithiophene (6T) thin films were grown on the Cu(110)-(2x1)O surface in UHV with the substrate held at 380K. Ex-situ atomic force microscopy (AFM), fluorescence microscopy (FM) and laser scanning confocal microscopy (LSCM) reveal elongated 6T islands with a height of up to a few hundreds of nanometers. These needles consist of crystallites of two distinct orientations with respect to the main axes of the substrate surface. However, polarization dependent FM shows that the 6T molecules in the needles are exclusively aligned along the [001] direction of the substrate. Comparing AFM and FM images, regions of maximum fluorescence emission correspond to defects where light can couple out of the needles due to the waveguiding effect such as the needle ends or grain boundaries within the needles. Photoluminescence spectra obtained by LSCM are in qualitative agreement with reference spectra of single crystalline 6T. No wetting layer of 6T was observed with LSCM. After a short exposure to air and a transfer back to UHV, reflectance difference spectra show, indeed, a complete quenching of the characteristic signal of the wetting layer of 6T. This suggests that the wetting layer is removed as soon as the sample is exposed to ambient conditions.</p>
15:20	704	<p style="text-align: center;"><b>Alkanethiols SAM formation on gold: Growth from solution versus physical vapor deposition</b></p> <p style="text-align: center;"><i>Johanna Stettner<sup>1</sup>, Paul Frank<sup>1</sup>, Franz Nußbacher<sup>1</sup>, Thomas Griesser<sup>2</sup>, Gregor Trimmel<sup>2</sup>, Adolf Winkler<sup>1</sup></i>  <sup>1</sup> <i>Institute of Solid State Physics, Petersgasse 16, 8010 Graz, Austria</i>  <sup>2</sup> <i>Institut für Chemische Technologie von Materialien, Stremayrgasse 16, 8010 Graz, Austria</i></p> <p>We present a survey about undecanethiol (UDT) and mercaptoundecanoic acid (11-MUA) SAM formation on gold, using wet chemical preparation methods and physical vapour deposition in UHV. Two different substrates were investigated: Polycrystalline gold foils and an Au(111) single crystal. The substrate quality is checked by AFM.</p> <p>AES shows a shift of the sulphur peak of a monolayer in comparison to sulphur of the multilayer, indicating sulphur bonded to the substrate.</p> <p>The TD spectra for in situ evaporated UDT and 11-MUA - SAMs on Au(111) are quite similar, showing two main desorption features: A peak around 400 K, stemming from desorption of disulfides, and a monolayer peak at 550 K. On the recrystallized gold foil, a third desorption feature at 580 K exists, which is attributed to cracking of the sulphur – carbon bond. For SAMs grown in solution, a considerable influence of the substrate cleanliness can be found: When the substrate is only cleaned by Piranha solution, a peak around 700K appears. The concomitant desorption of m = 197 suggests desorption of Au – containing molecules.</p>

15:40	705	<p style="text-align: center;"><b>Organic semiconductor growth on Graphene studied by LEEM and <math>\mu</math>LEED</b></p> <p style="text-align: center;"><i>Gregor Hlawacek<sup>1</sup>, F. S. Khokhar<sup>2</sup>, Raoul van Gastel<sup>2</sup>, Bene Poelsema<sup>2</sup>, Christian Teichert<sup>1</sup></i></p> <p style="text-align: center;"><sup>1</sup> <i>Institute of Physics, University of Leoben, Franz Josef Str. 18, 8700 Leoben, Austria</i></p> <p style="text-align: center;"><sup>2</sup> <i>Institute for Solid State Physics, University of Twente, Veldmaat 10, 7522 Enschede, Netherlands</i></p> <p>Organic electronics market is demanding for powerful and flexible devices based on small conjugated molecules. To achieve this, a proper substrate has to be chosen. For para-sexiphenyl (6P), graphene is an ideal substrate for two reasons, namely -- its unique properties and the similarity between the structure of the molecule and the graphene lattice.</p> <p>Here, 6P was deposited at various substrate temperatures onto graphene flakes grown on Ir(111) [1]. The dynamics of the deposition process and the crystallographic structure was observed in-situ by means of Low Energy Electron Microscopy (LEEM) and micro Low Energy Electron Diffraction (<math>\mu</math>LEED). Layer-by-layer growth of lying molecules is observed for low temperatures. At higher temperatures the growth of -- for 6P typical -- 1D needles on a wetting layer is observed.</p> <p>This work is supported by the FWF project S9707-N08 and FOM project 04PR2318. [1] Coraux, J. et al., New J. Phys., 2009, 11, 023006.</p>
16:00		<b>Coffee Break</b>
		<i>Chair: T. Greber, Uni Zürich</i>
16:30	706	<p style="text-align: center;"><b>Ambient Pressure Surface Science of Catalytically Active Nanostructures</b></p> <p style="text-align: center;"><i>Günther Rupprechter, Christian Weilach, Karin Föttinger, Yuri Suchorski</i> <i>Institute of Materials Chemistry, Vienna University of Technology, Veterinärplatz 1, 1210 Vienna, Austria</i></p> <p>Advances in the preparation of planar nanostructured surfaces (single crystals, thin films, supported nanoparticles) under ultrahigh vacuum enable us to model an increasing number of technical catalysts. Significant advances have also been made in carrying out Surface Science at ambient pressure. Polarization-modulated infrared reflection absorption spectroscopy (PM-IRAS) and sum frequency generation (SFG) vibrational laser spectroscopy, complemented by high-pressure X-ray photoelectron spectroscopy (HP-XPS), have been utilized for studies of surface reactions at near atmospheric pressure. This allows us to investigate a functioning surface in its active state. Increasing attention is directed towards comparing global reaction properties with local activity (as revealed by photoemission electron microscopy PEEM), as well as towards contrasting model systems and industrial-grade catalysts. A number of case studies are presented illustrating the dynamic behavior of catalytically active surfaces, including surface alloys and surface oxides for methanol and CO surface reactions.</p>

17:10	707	<p style="text-align: center;"><b>ZnO films on Pd(111) studied by TPD, RAIRS and STM</b></p> <p style="text-align: center;"><i>Frederik Weber<sup>1</sup>, Gunther Weirum<sup>1</sup>, Svetlozar Surnev<sup>2</sup>, Robert Schennach<sup>1</sup></i>  <sup>1</sup> <i>Solid State Physics, Graz University of Technology, Petersgasse 16/2, 8010 Graz, Austria</i>  <sup>2</sup> <i>Institute of Physics, Karl Franzens Universität, Universitätsplatz 5, 8010 Graz, Austria</i></p> <p>Zinc oxide has attracted significant scientific and technological interest, since it is widely used in catalysis, gas sensing, and in the fabrication of optoelectronic devices. If the wurtzite ZnO crystal is cleaved parallel to the basal plane (0001), two structurally and chemically different surfaces are created on each side of the crystal, which are Zn- and O-terminated. The structure stabilisation mechanism of these two polar surfaces has been extensively investigated, but consensus models have not evolved yet. Here we have investigated the surface structure of zinc oxide nanolayers grown on a Pd(111) surface by reflection absorption infra red spectroscopy (RAIRS), scanning tunneling microscopy (STM) and temperature programmed desorption. The ZnO layers have been prepared by reactive evaporation of Zn in an oxygen atmosphere (<math>5 \times 10^{-8}</math> – <math>5 \times 10^{-6}</math> mbar) onto the Pd substrate. In the submonolayer coverage range two 2D hexagonal ZnO<sub>x</sub> phases coexist on the Pd(111) surface: one with an open honeycomb (4x4) structure, and the other one with a close-packed structure with a lattice constant of 3.3 Å, which is close to the bulk value of ZnO(0001) surfaces (3.25 Å). The latter phase displays a (6x6) Moiré structure (6 Pd lattice spacing = 5 ZnO unit cells) and appears as a single layer at low oxygen pressures (<math>p &lt; 1 \times 10^{-7}</math> mbar), but converts to a bi-layer at <math>p(\text{O}_2) &gt; 1 \times 10^{-6}</math> mbar. The structure of the second layer is also strongly dependent on the oxygen pressure: at <math>p &lt; 1 \times 10^{-7}</math> mbar two surface terminations are present and display different contrast and apparent height in the STM images, whereas at <math>p(\text{O}_2) &gt; 1 \times 10^{-6}</math> mbar only a single termination is observed. These structures are further analysed with TDS and RAIRS using pyridine as a probe molecule.</p>
17:30	708	<p style="text-align: center;"><b>Co-adsorption of atomic H and CO on Ni/Cu(110) bimetallic surfaces</b></p> <p style="text-align: center;"><i>Erkan Demirci<sup>1</sup>, Christian Carbogno<sup>2</sup>, Axel Gross<sup>2</sup>, Adolf Winkler<sup>1</sup></i>  <sup>1</sup> <i>Institute of Solid State Physics, TU Graz, Petersgasse 16, 8010 Graz, Austria</i>  <sup>2</sup> <i>Institute for Theoretical Chemistry, Ulm University, 89069 Ulm, Germany</i></p> <p>The adsorption of CO, atomic hydrogen and the co-adsorption of H/CO on Cu(110), Ni/Cu(110) and epitaxially grown Ni(110) surfaces has been studied using AES, TDS and LEED. Adsorption of CO at 180 K on a Ni/Cu(110) bimetallic surface yields three new adsorption states with adsorption energies between that of CO on clean Cu(110) and clean Ni(110). The interaction of atomic and molecular hydrogen has been investigated on this special surface. While H<sub>2</sub> does not adsorb on clean Cu(110), it can adsorb on nickel. This difference is used to get further information about the Ni/Cu adsorption sites. The interaction between CO and atomic H has also been investigated on Cu(110), Ni(110) and Ni/Cu(110) surfaces. Increasing amount of atomic H reduces the CO desorption from the CO preadsorbed Cu(110) surface. In addition we have carried out DFT calculations in order to identify the Cu/Ni atomic arrangement and the adsorption sites of CO on these bimetallic surfaces using VASP.</p>

17:50	709	<p style="text-align: center;"><b>Growth of One-Dimensionally Ordered Au Clusters on Carbon-Modified W(110)</b></p> <p style="text-align: center;"><i>Magdalena Bachmann, Norbert Memmel, Erminald Bertel Institute of Physical Chemistry, Innrain 52a, 6020 Innsbruck, Austria</i></p> <p>The growth of gold nanodots on a carburized tungsten surface ((15x12)C/W(110)) is studied by scanning tunneling microscopy (STM). At 700 K we observe formation of uniformly sized clusters on a rectangular grid defined by the template unit cell (1.4 x 3.1 nm<sup>2</sup>), with the clusters nucleating in the carbon-poor regions of the (15x12) unit cell. At lower temperatures also formation of "interstitial" clusters on less favorable sites is observed. This behavior parallels the growth of Ag and Co clusters on the same substrate. However, the present results for Au contradict to some extent a recent STM study by Varykhalov et al. [Phys. Rev. B 77, 035412 (2008)] with respect to size, ordering and preferred alignment of the quasi-one dimensionally ordered cluster lines. Reasons for these discrepancies are discussed.</p>
18:10	710	<p style="text-align: center;"><b>Proof of liquid layering in nanometre confinement</b></p> <p style="text-align: center;"><i>Edith Perret <sup>1</sup>, Kim Nygard <sup>1</sup>, Dillip Satapathy <sup>1</sup>, Tobias Balmer <sup>2</sup>, Oliver Bunk <sup>1</sup>, Manfred Heuberger <sup>3</sup>, Johannes Friso van der Veen <sup>1</sup> <sup>1</sup> Paul Scherrer Institute, Villigen, 5232 Villigen, Switzerland <sup>2</sup> ETH Zürich, Wolfgang-Pauli-Str. 10, 8093 Zürich, Switzerland <sup>3</sup> EMPA, Lerchenfeldstrasse 5, 9014 St.Gallen, Switzerland</i></p> <p>The lubricating properties of a molecular liquid between two surfaces may change if the surfaces approach each other to within a few molecular diameters. The question arises whether the liquid remains 'liquid' in this case. We performed the first synchrotron X-ray reflectivity (XRR) study of a liquid under extreme confinement in order to determine the density profile of the liquid's layer structure. We show that squeezing a tetrakis-trimethylsiloxy silane (TTMSS) drop between two mica single crystals causes the liquid's molecules in the film region to order in discrete layers parallel to the surfaces. Electron density profiles determined across gaps of 8.6 and 11.2 nm reveal hydrated mica surfaces which confine 8 respectively 10 equidistant monolayers of TTMSS. The monolayer densities suggest closed-packed ordering, while the measured interlayer distance of 1.0 nm sterically enables sliding of single layers out of the film.</p>
18:30		<b>Jahreshauptversammlung des Fachausschusses OGD</b>
18:45		<b>END</b>

Time	ID	<b>SURFACES, BOUNDARY LAYERS AND THIN FILMS</b> <i>Chair: G. Rupprechter, Uni Wien</i>
09:00		<b>PLENARY SESSION</b>
12:40		<b>Postersession, Lunchbuffet</b>
14:00	711	<p><b>Nanostructures at surfaces and their scanning probe microscopy based characterization</b></p> <p><i>Christian Teichert</i> <i>Institute of Physics, Montanuniversität Leoben, Franz Josef Str. 18, 8700 Leoben, Austria</i></p> <p>Surface nanostructures play an important role in high-technology applications from nanoelectronics to nanocoatings. Atomic-force microscopy (AFM) and its derivatives like conductive AFM (C-AFM), magnetic force microscopy (MFM), and friction force microscopy yield reliable data on the structures' size, shape and arrangement and allow to characterize their physical properties. Examples - to obtain integral structure information - will be presented for the self-organized heteroepitaxial growth of inorganic and organic semiconductors as well as for ion-eroded compound semiconductors. The resulting nanostructure ensembles can serve as templates to grow, e.g., nanomagnet arrays which than can be studied by MFM. Detailed analysis of nanostructure shape and arrangement can also yield insight into basic atomic and molecular diffusion processes as it will be illustrated for the growth of organic semiconductor films. It is further demonstrated that AFM can even be applied to characterize ensembles of free standing nanowires.</p> <p>Research supported by FWF, European Community, and ÖAD. <a href="http://www.unileoben.ac.at/~spmgroup">www.unileoben.ac.at/~spmgroup</a></p>
14:40	712	<p><b>H adsorption induced fcc-nanomartensitic transition in 4-5 ML Fe films</b></p> <p><i>Albert Biedermann</i> <i>Faculty of Physics, University of Vienna, Boltzmanngasse 5, 1090 Wien, Austria</i></p> <p>Fe films on Cu(100) admit the study of phase transitions between the fcc phase and different ferromagnetic bcclike phases with atomic detail. Such transitions may prove useful for the microscopic control of magnetization by ion beams, temperature variation, or gas adsorption. In this work, the near reversible transition between the fcc and the bcclike nanomartensitic (NM) phase induced by hydrogen adsorption is imaged by variable temperature scanning tunneling microscopy. The phase transition is described by combining surface chemistry and solid state physics of the films in a simple 2-parameter statistical mechanical model yielding the free energy difference between fcc and NM in dependence of temperature. The fcc and NM film phases show a relative stability similar to bulk Fe, but only above 200 K. This difference between bulk and ultrathin films is discussed in terms of the magnetic structure, which is thought to control phase stability in Fe.</p>

15:00	713	<p><b>Shape Dependent Thermal Magnetization Reversal Mechanism</b></p> <p><i>Fabian Donat Natterer<sup>1</sup>, Safia Ouazi<sup>1</sup>, Géraud Moulas<sup>1</sup>, Anne Lehnert<sup>1</sup>, Stefano Rusponi<sup>1</sup>, Stanislas Rohart<sup>2</sup>, Wulf Wulfhekel<sup>3</sup>, Harald Brune<sup>1</sup>,  <sup>1</sup> Institut de Physique de la Matière Condensée (IPMC), EPFL, Station 3,  1015 Lausanne, Switzerland  <sup>2</sup> Laboratoire de Physique des Solides, Université Paris Sud et CNRS, Bât. 300,  91405 Orsay, France  <sup>3</sup> Physikalisches Institut, Universität Karlsruhe (TH), Wolfgang-Gaede Strasse 1,  76131 Karlsruhe, Germany</i></p> <p>The transition state for thermally induced magnetization reversal in nanostructures can be mono-domain where all magnetic moments are turned coherently. This has an energy barrier which is dependent on the sum of the anisotropy energy of all constituent atoms (Néel-Brown). Alternatively, the transition state may involve a propagating domain wall turning the magnetization with an energy barrier that is linked in a less trivial way to the anisotropy energy. We report on the magnetization reversal in monolayer high Co islands on Pt(111). By kinetically controlled growth we have realized compact islands and fractal ones (<math>D \sim 1</math>), which have only initial branching. With in-situ STM and MOKE we show that the first island type rotates coherently while the second one reverses its magnetization by domain wall nucleation and propagation, once the length of the branches have reached a critical value of 15 nm.</p>
15:20	714	<p><b>Near field emission scanning electron microscopy</b></p> <p><i>Taryl Kirk<sup>1</sup>, Urs Ramsperger<sup>1</sup>, Lorenzo De Pietro<sup>1</sup>, Olivier Scholder<sup>1</sup>, Urs Maier<sup>2</sup>, Danilo Pescia<sup>1</sup>  <sup>1</sup> ETH Zürich, Mikrostrukturen, Laboratorium für Festkörperphysik,  Wolfgang-Pauli-Strasse 16, 8093 Zürich, Switzerland  <sup>2</sup> Ferrovac GmbH, Thurgauerstrasse 72, 8050 Zürich, Switzerland</i></p> <p>We present a simple "near field emission scanning electron microscope" (NFESSEM) capable of imaging conducting surfaces with high spatial resolution. In this instrument electrons are excited from the sample surface after undergoing interactions with a low-voltage (&lt; 60V) primary beam of electrons field-emitted from a tungsten tip positioned tens of nanometers above the sample. Topographic images, determined from the intensity variations of secondary and backscattered electrons, yield a vertical resolution on an atomic scale and a lateral resolution of less than two nanometers. We report on the first topographic electron intensity images of terraces and mono-atomic steps on a single crystal substrate, not yet attained with a remote electron gun in conventional scanning electron microscopy. The topographic contrast of the extracted electrons and the field emission current are indistinguishable, in agreement with theoretical models of optimal spatial resolution.</p>

15:40	715	<p style="text-align: center;"><b>Atomic Layer Deposition: Thin film- and interface engineering for the post-silicon era</b></p> <p style="text-align: center;"><i>Stephan Abermann, Christoph Henkel, Ole Bethge, Emmerich Bertagnolli, Institute for Solid State Eletronics, Vienna University of Technology, Floragasse 7/1, 1040 Vienna, Austria</i></p> <p>Atomic Layer Deposition (ALD) experienced a tremendous increase of interest on the part of the semiconductor science community within the last years, and with its the introduction as a key technology for HfO<sub>2</sub>-based gate dielectrics [1], intel© ushered in a new era of semiconductor processing. The ability to control film deposition on an atomic scale, almost independent of the surface morphology, makes ALD to the method of choice in this field. Additionally, by optimizing precursor chemistry and cycling schemes, interface characteristic and film stoichiometry can widely be engineered.</p> <p>We will present our results on ALD of high-k/metal-gate stacks on materials considered as alternatives to silicon in future semiconductor technologies, like Ge, or InAlN/GaN. We will show that stack and interface composition can be tailored and optimized by precursor chemistry and the applied ALD cycling schemes, thus leading to improved electrical device behaviour.</p> <p>[1] <a href="http://www.intel.com/technology/silicon/high-k.htm?iid=tech_arch_45nm+body_hik">http://www.intel.com/technology/silicon/high-k.htm?iid=tech_arch_45nm+body_hik</a></p>
16:00		<p><b>Coffee Break</b></p>
		<p><i>Chair: C. Teichert, Uni Leoben</i></p>
16:30	716	<p style="text-align: center;"><b>sp<sup>2</sup> hybridized single layer templates: Hexagonal Boron Nitride and Graphene</b></p> <p style="text-align: center;"><i>Thomas Greber Physik Institut, University of Zürich, Winterthurerstrasse 190, 8057 Zürich, Switzerland</i></p> <p>sp<sup>2</sup> hybridized single layers of hexagonal boron nitride and graphene on Rh(111) and Ru(0001) form corrugated superstructures with about 3nm lattice constant. These structures were stable in air and may be used as templates for supramolecular architectures. The peculiar trapping mechanism for single molecules with a diameter of 1 to 2 nm is traced back to strong lateral electric fields within the nanostructure that can be measured with photoemission from adsorbed xenon. Graphene is metallic and reveals weaker lateral electric fields above the corrugated surface. From this a three level hierarchy of bonds that is important for the template function is proposed.</p>



17:10	717	<p style="text-align: center;"><b>Graphene on Ru(0001): A surface x-ray diffraction study of a corrugated surface structure</b></p> <p style="text-align: center;"><i>Domenico Martocchia<sup>1</sup>, Matts Björck<sup>1</sup>, Christian M. Schlepütz<sup>1</sup>, Bruce D. Patterson<sup>1</sup>, Philip R. Willmott<sup>1</sup>, Thomas Brugger<sup>2</sup>, Thomas Greber<sup>2</sup></i>  <sup>1</sup> Paul Scherrer Institut, 5232 Villigen, Switzerland  <sup>2</sup> Physik-Institut, Universität Zürich, Winterthurerstrasse 190, 8057 Zürich, Switzerland</p> <p>Nanostructured materials have attracted increasing interest in recent years due to their potential in practical electronic applications. Graphene is a single sheet of carbon atoms arranged in a honeycomb structure. Corrugation of graphene sheets is believed to strongly influence the electronic properties of the system. Recently, it has been reported that graphene grown on transition metals form single-domain moiré patterns with high structural perfection. It was suggested that graphene on Ru(0001) forms a moiré structure in which (12 x 12) unit cells of graphene sit on (11 x 11) unit cells of Ru (called an "12-on-11" superstructure). Other studies proposed an 11-on-10 structure.</p> <p>We present here a detailed structure of graphene/Ru(0001) using surface x-ray diffraction (SXRD). Surprisingly, the superstructure is shown unambiguously to be 25-on-23, whereby each supercell contains four crystallographically distinct but chemically almost identical substructures. Strong oscillations on the SXRD superstructure rods indicate significant corrugation of the Ru-substrate.</p>
17:30	718	<p style="text-align: center;"><b>A surface chemical approach to the fabrication of 2D superhoneycomb polymer networks</b></p> <p style="text-align: center;"><i>Marco Bieri<sup>1</sup>, M. Treier<sup>1</sup>, J. Cai<sup>1</sup>, K. Ait-Mansour<sup>1</sup>, Pascal Ruffieux<sup>1</sup>, Oliver Gröning<sup>1</sup>, Pierangelo Gröning<sup>1</sup>, M. Kastler<sup>2</sup>, K. Müllen<sup>2</sup>, Roman Fasel<sup>1</sup></i>  <sup>1</sup> EMPA, Swiss Federal Laboratories for Materials Testing and Research, Feuerwerkerstrasse 39, 3602 Thun, Switzerland  <sup>2</sup> Max-Planck-Institute for Polymer Research, Ackermannweg 10, 55128 Mainz, Germany</p> <p>Structuring matter down to the scale of single atoms is the ultimate goal of nanotechnology. There exist nowadays a variety of top-down and bottom-up approaches that allow for a structuring of matter on length scales ranging over several orders of magnitude. To this end, the ability to structure matter at sub-nanometer dimensions with atomic precision is required. At these length scales, geometrical dimensions and topology are inherently linked to the electronic properties, with the exciting opportunity to engineer the latter such as, e.g. in semiconductor quantum dots. Whereas lithographic techniques – often referred to as top-down approaches – are inherently limited with respect to their ultimate resolution and precision, bottom-up approaches can be used down to the smallest length scales. We demonstrate this by the fabrication of the first member of an up to this date elusive class of materials, the hydrocarbon superhoneycomb polymer networks.</p>

17:50	719	<p><b>Evolution of electronic structure on Transition Metal doped Titanium Disulfide by angle-resolved photoemission spectroscopy study</b></p> <p><i>Xiaoyu Cui, Vladimir Strocov, Luc Patthey</i>  <i>Paul Scherrer Institut, Swiss Light Source, 5232 Villigen, Switzerland</i></p> <p>We will present ARPES results on the intercalated compound <math>\text{Fe}_x\text{TiS}_2</math> (<math>0 \leq x \leq 0.33</math>) in Swiss Light Source (SLS). A semiconductor band structure was revealed for the undoped sample, which resolves a long-standing controversy in this system. We discuss the modification of the valence bands around the several high symmetric points (G, L). The Fe 3d-Ti 3d hybridized states are observed in the larger binding energy region (500 meV) and near the Fermi level. The electronic structure for high doping (<math>x=0.33</math>) was calculated in the framework of the density functional theory with the use of the full-potential augmented-plane-wave method. Knowledge of hybridization among the Fe 3d, Ti 3d, and S 3p states is very important to understand the physical properties of <math>\text{Fe}_x\text{TiS}_2</math> system.</p>
18:10	720	<p><b>Microwave plasma synthesis – a versatile technique for fabricating nanocrystalline oxides and composites</b></p> <p><i>Ulrich Brossmann<sup>1</sup>, Martin Sagmeister<sup>1</sup>, Markus Postl<sup>2</sup>, Dorothee Szabó<sup>3</sup>, Rolf Ochs<sup>3</sup>, Emil List<sup>2</sup>, Roland Würschum<sup>1</sup></i></p> <p><sup>1</sup> Institute of Materials Physics, Graz University of Technology, Petersgasse 16, 8010 Graz, Austria</p> <p><sup>2</sup> Institute of Solid State Physics, Graz University of Technology, Petersgasse 16, 8010 Graz, Austria</p> <p><sup>3</sup> Institute for Materials Research III, Forschungszentrum Karlsruhe, Hermann-von-Helmholtz-Platz 1, 76344 Eggenstein-Leopoldshafen, Germany</p> <p>Microwave plasma (MWP) synthesis was used to obtain a wide range of nanocrystalline oxides and nano-composite materials. Low processing temperatures in the range of 250° - 400°C and electric charging in the non-equilibrium plasma contribute to a small grain size and narrow size distribution of the oxide core particles which can be coated in-situ with another oxide (forming, e.g., <math>\text{ZrO}_2/\text{Al}_2\text{O}_3</math> core shell particles) or a functional organic shell, e.g. pentacene. Uncoated oxide nanoparticles of <math>\text{Al}_2\text{O}_3</math>, pure and <math>\text{Y}_2\text{O}_3</math>-alloyed <math>\text{ZrO}_2</math> as well as <math>\text{WO}_3</math> were prepared from a range of inorganic and organic precursor chemicals. XRD and TEM studies confirm initial grain sizes in the range of 3-5 nm. The in-situ coating of <math>\text{ZrO}_2</math> core particles with a luminescent organic shell, e.g. pentacene was confirmed by optical spectroscopy. Stable dispersions with a small agglomerate size, as required for subsequent solution processing steps, e.g. spin-coating, were obtained by in-situ dispersion in ethylene glycol.</p>
18:30		<b>END</b>
19:30		<b>Conference Dinner</b>

**Friday, 4. Sept. 2009, Room E**

Time	ID	<b>SURFACES, BOUNDARY LAYERS AND THIN FILMS</b> <i>Chair: P. Willmott, PSI Villigen</i>
<b>09:00</b>	<b>PLENARY SESSION</b>	
<b>12:40</b>	<b>Postersession, Lunchbuffet</b>	
<b>14:00</b>	<b>721</b>	<p style="text-align: center;"><b>Controlling the Electronic Structure of Metal/Organic Interfaces</b></p> <p style="text-align: center;"><i>Egbert Zojer, Institute of Solid State Physics, Petersgasse 18, 8010 Graz, Austria</i></p> <p>Two approaches for modifying the electrode work-functions in organic (opto)electronic devices are the use of polar self-assembled monolayers (SAMs) and the deposition of (sub)monolayers of strong organic donors or acceptors as interfacial layers between the metal and an organic semiconductor. To understand the processes that determine how work function modification and level alignment depend on the chemical and morphological structure of the adsorbate layer, we rely on quantum-mechanical modelling. Whenever possible, the obtained results are compared to experimental data. For SAMs, aspects like the impact of substituents, the role played by the conjugated backbone and the docking groups and the influence of coverage will be discussed. For flat-lying chemisorbed molecules, the situation can be complicated by a superposition of charge forward and backward donation processes involving different regions of the molecules. Moreover, molecule/metal combinations will be presented in which the electronic states at the Fermi energy extend onto the adsorbate layer.</p>
<b>14:40</b>	<b>722</b>	<p style="text-align: center;"><b>Reconstruction of Molecular Orbitals from Photoemission Data</b></p> <p style="text-align: center;"><i>Peter Puschnig<sup>1</sup>, Stephen Berkebile<sup>2</sup>, Alexander Fleming<sup>2</sup>, Georg Koller<sup>2</sup>, Claudia Ambrosch-Draxl<sup>1</sup>, Falko Netzer<sup>2</sup>, Michael Ramsey<sup>2</sup></i></p> <p style="text-align: center;"><sup>1</sup> <i>University Leoben, Franz-Josef-Strasse 18, 8700 Leoben, Austria</i> <sup>2</sup> <i>Karl-Franzens University Graz, Universitätsplatz 5, 8010 Graz, Austria</i></p> <p>Photoemission spectroscopy is a direct method to study the band structure of solids by measuring the kinetic energy versus angular distribution of the photoemitted electrons. Recording the photoemission intensity over a hemispherical region, i.e., measuring the 2D momentum distribution for a given electron kinetic energy, generates reciprocal space maps of the emitting orbital. With examples from both thick crystalline films and strongly bound organic adsorbate layers we establish this simple approach that allows the real space electron distribution of molecular orbitals, via a Fourier transform, to be obtained in good agreement with density functional calculations.</p>

15:00	723	<p style="text-align: center;"><b>A detailed analysis of the bonding of chemisorbed conjugated molecules on noble metals</b></p> <p style="text-align: center;"><i>Gerold M. Rangger, Oliver T. Hofmann, Anna M. Track, Ferdinand Rissner, Egbert Zojer</i>  <i>Institut für Festkörperphysik Technische Universität Graz, Petersgasse 16, 8010 Graz, Austria</i></p> <p>The deposition of organic monolayers on metals is of interest for modifying surface properties in molecular electronics. We present a theoretical study of acceptor and donor molecules (F4TCNQ/TTF) on Ag/Au(111). Experiments show pronounced changes in the UPS spectra of the molecules due to strong interactions with the surfaces. To understand the bonding mechanism, we use a projection of the density of states onto atomic and molecular orbitals in combination with a crystal orbital overlap type population analysis. This allows analyzing the molecular orbital occupation and the determination of bonding and anti-bonding contributions of molecular/atomic orbitals on the energy scale. Only a simultaneous examination of adsorption induced changes of the molecular geometry (including a bending of the molecule) and of the interaction between molecule and metal allows to arrive at a consistent picture for the investigated chemisorption processes.</p> <p>European Commission support through ICONTROL (EC-STREP-033197) is gratefully acknowledged.</p>
15:20	724	<p style="text-align: center;"><b>Band structure effects in electronic stopping</b></p> <p style="text-align: center;"><i>Peter Bauer, Sergey Markin, Michael Spitz, Daniel Primetzhofner</i>  <i>Johannes Kepler Universität - Inst. f. Experimentalphysik, Altenbergerstraße 69, 4040 Linz, Austria</i></p> <p>We present LEIS-experiments to determine the electronic energy loss of H and He ions in noble metals such as Cu or Au. Absolute energy loss data were obtained from backscattering measurements at energies of 8-10 keV, using nm-films of Cu and Au. High accuracy in thickness calibration was obtained by a high resolution RBS spectrograph. For very low projectile velocities relative measurements were performed to deduce the electronic energy loss in Cu by comparison to previously obtained Au data.</p> <p>For both metals investigated we found a pronounced change in the velocity dependence of the electronic stopping power, <math>dE/dx</math>, for very low velocities. This can be directly attributed to the density of states, i.e. an excitation threshold for d-electrons, situated 1-2 eV below EF.</p>

15:40	725	<p><b>Vanishing energy loss for slow ions in large band gap insulators</b></p> <p><i>Daniel Primetzhofer, Sergey Markin, Michael Spitz, Peter Bauer Johannes Kepler Universität - Inst. f. Experimentalphysik, Altenbergerstraße 69 , 4040 Linz, Austria</i></p> <p>If ions move in matter they usually get decelerated by different energy transfer mechanisms with the electrons of the target. We present LEIS-experiments to determine the electronic energy loss of H and He in matter. Recently, a pronounced change in the velocity dependence of the electronic stopping power, <math>dE/dx</math>, was reported for very slow ions in Au. This can be directly attributed to the density of states.</p> <p>We have observed vanishing electronic energy loss in different large band gap insulators such as LiF, KCl or SiO<sub>2</sub> for very low projectile energies, i.e. <math>E &lt; 500</math> eV deuterons. This is an outstanding result since it shows for the first time that ions can travel in an insulator without transferring any energy to the electronic system of the sample. However, the question remains, why the threshold is found at velocities much lower than expected.</p>
16:00		<p><b>Coffee Break</b></p>
		<p><i>Chair: A. Winkler, TU Graz</i></p>
16:30	726	<p><b>PbTiO<sub>3</sub>/SrTiO<sub>3</sub> superlattices and their interfaces</b></p> <p><i>Pavlo Zubko<sup>1</sup>, Matthew Dawber<sup>2</sup>, Nicolas Stucki<sup>1</sup>, Celine Lichtensteiger<sup>1</sup>, Stefano Gariglio<sup>1</sup>, Jean-Marc Triscone<sup>1</sup>, Eric Bousquet<sup>3</sup>, Patrick Hermet<sup>3</sup>, Philippe Ghosez<sup>3</sup></i></p> <p><sup>1</sup> University of Geneva, DPMC, 24 Quai E.-Ansermet, 1211 Geneva, Switzerland  <sup>2</sup> Stony Brook University, Department of Physics and Astronomy, Stony Brook, 11794, NY, United States  <sup>3</sup> Universite de Liege, Physique Theoretique des Materiaux, Allee du 6 Aout, 4000 Sart Tilman, Belgium</p> <p>PbTiO<sub>3</sub>/SrTiO<sub>3</sub> superlattices have proven to be an exciting system, both as a way of creating new artificial materials with desirable properties, as well as for their interesting new physics. By simply changing the relative layer thicknesses of the two parent compounds, the structural and electrical properties can be tuned over a wide range of values on demand [1]. For a constant SrTiO<sub>3</sub> layer thickness, reducing the thickness of the PbTiO<sub>3</sub> layers leads to a lowering of the tetragonality, remnant polarization and transition temperature. However, below a certain thickness, when the interface density becomes large, a deviation from the expected behaviour is observed as the properties of the interfaces themselves become significant. A recovery of ferroelectricity is observed and has been linked to an improper ferroelectric state where the polarization is coupled to oxygen octahedral rotations at the interfaces, as predicted from ab-initio calculations [2]. The above properties will be discussed together with recent electrical and structural measurements aimed at better understanding this fascinating system.</p> <p>[1] M. Dawber et al., Adv. Mater. 19, 4153 (2007).  [2] E. Bousquet et al., Nature 452, 732 (2008).</p>

17:10	727	<p style="text-align: center;"><b>The growth and electronic structure of porphyrins: From ordered monolayers to epitaxially oriented crystalline films</b></p> <p style="text-align: center;"><i>G. Koller<sup>1,2</sup>, S. Berkebile<sup>1</sup>, S. Gusenleitner<sup>1</sup>, P. Puschnig<sup>3</sup>, K. Emtsev<sup>4</sup>, T. Seyller<sup>4</sup>, T. Bauert<sup>2</sup>, K. H. Ernst<sup>2</sup>, M. G. Ramsey<sup>1</sup></i></p> <p style="text-align: center;"><sup>1</sup> <i>Institute of Physics, Karl-Franzens University Graz, Universitätsplatz 5, 8010 Graz, Austria</i></p> <p style="text-align: center;"><sup>2</sup> <i>EMPA, Swiss Federal Laboratories for Materials Testing and Research, Laboratory for Nanoscale Materials Science, Überlandstrasse 129, 8600 Dübendorf, Switzerland</i></p> <p style="text-align: center;"><sup>3</sup> <i>Chair of Atomistic Modelling and Design of Materials, University of Leoben, Franz-Josef-Straße 18, 8700 Leoben, Austria</i></p> <p style="text-align: center;"><sup>4</sup> <i>Lehrstuhl für Technische Physik, Universität Erlangen-Nürnberg, Erwin-Rommel-Str. 1, 91058 Erlangen, Germany</i></p> <p>Here an extensive study of pure and metal tetraphenyl-porphyrins (H<sub>2</sub>TPP and Pt(II)-TPP) on both the clean and (2x1)O reconstructed Cu(110) surfaces is presented. The in-situ growth has been investigated by LEED, XPS, NEXAFS, and ARUPS. On both substrates well ordered monolayers are formed, with the macrocycles flat on the surface and the phenyl rings tilted from the surface. Both molecules adopt particular but different azimuthal orientations: for H<sub>2</sub>TPP it is driven by the phenyls, while for Pt(II)-TPP the peculiar orientation observed will be argued to result from the orbital symmetry.</p> <p>This work was supported by the European Community - Research Infrastructure Action under the FP6 "Structuring the European Research Area" Programme (through the Integrated Infrastructure Initiative" Integrating Activity on Synchrotron and Free Electron Laser Science - Contract R II 3-CT-2004-506008) and the Austrian Science Funds FWF (NFN "Interface Controlled and Functionalized Organic Films" and project P21330-N20).</p>
17:30	728	<p style="text-align: center;"><b>Growth and magnetic properties of metallo-porphyrins on magnetic substrates</b></p> <p style="text-align: center;"><i>Christian Wäckerlin, Dorota Chylarecka, Kathrin Müller, Nirmalya Ballav, Timur Kim, Frithjof Nolting, Thomas Jung Paul Scherrer Institute, 5232 Villigen PSI, Switzerland</i></p> <p>X-ray Magnetic Circular Dichroism (XMCD) is a very powerful tool used for studying the coupling between organic molecules and magnetic substrates. Not only allows it for detection of magnetic moments of individual species, but it is also sensitive to small amounts (sub-monolayer) of molecules.</p> <p>In this study the properties of manganese (III) tetraphenyl porphyrin chloride (MnTPPCL) molecules evaporated on cobalt thin films are investigated. We are the first group to show, by means of XMCD, the magnetic coupling between molecules and the substrate at room temperature and without applying an external magnetic field. X-ray Absorption Spectroscopy (XAS) results suggest a chemical reaction of the molecules with underlying cobalt. Images taken by Scanning Tunneling Microscope (STM) show the adsorption geometry of molecules on magnetic surfaces.</p>

17:50	729	<p style="text-align: center;"><b>Self-assembly of a large porphyrin derivative containing pentafluoro-phenyls studied by STM on Ag(111) and Cu(111)</b></p> <p style="text-align: center;"><i>Jérôme Wiss<sup>1</sup>, Tomas Samuely<sup>1</sup>, Tobias Voigt<sup>2</sup>, Jens Hornung<sup>2</sup>, Mihaela Enache<sup>1</sup>, Nikolai Wintjes<sup>1</sup>, Jorge Lobo-Checa<sup>1</sup>, François Diederich<sup>2</sup>, Thomas Jung<sup>3</sup>, Meike Stöhr<sup>1</sup></i></p> <p style="text-align: center;"><sup>1</sup> Institute of Physics, Klingelbergstr. 82, 4056 Basel, Switzerland  <sup>2</sup> Laboratorium für Organische Chemie, ETH Zürich, Hönggerberg, 8093 Zürich, Switzerland  <sup>3</sup> Laboratory for Micro- and Nanotechnology, Paul-Scherrer-Institute, 5232 Villigen, Switzerland</p> <p>Electronic devices built up from organic building blocks are promising candidates for addressable devices at the nanoscale. To create them based on self-assembly would be a very elegant method to generate a functional material, thus exploiting the principles of supramolecular chemistry.</p> <p>Molecule 1 ((5,15-Bis(2,6-dimethoxy-4-phenylphenyl)-10,20-bis[4-(2,3,4,5,6-pentafluorophenyl)-phenyl]porphyrinato(2-)-kN21,kN22,kN23,kN24}zinc(II)) was studied on Ag(111) and Cu(111) single crystals under UHV conditions. With STM experiments three different assemblies of molecule 1 were found on Ag(111). The observed assemblies depend on the deposition rate of 1. Of special interest was a hexagonal porous network which was stable up to annealing temperatures of 300°C. A pore of the network had a diameter of about ~2nm. Because of the large pores and the stability it is suited to accommodate guest molecules.</p> <p>The same molecule forms on Cu(111) only close-packed assemblies which display similarities to the patterns obtained on Ag(111).</p> <p>Molecule 1 is the first example of a highly fluorinated porphyrin derivative which arranges on a surface in a porous network. Furthermore, it creates a surprising arrangement of the molecules with the fluorine residues quite close to each other.</p>
18:10	730	<p style="text-align: center;"><b>Charge exchange in the reionization regime in LEIS</b></p> <p style="text-align: center;"><i>Michael Spitz, Daniel Primetzhofer, Sergey Markin, Peter Bauer</i>  <i>Johannes Kepler Universität - Inst. f. Experimentalphysik, Altenbergerstraße 69, 4040 Linz, Austria</i></p> <p>In Low-energy ion scattering (LEIS) very efficient neutralization of primary ions is responsible for the high surface sensitivity obtained. We present an investigation of the neutralization of He<sup>+</sup> ions scattered from noble metal surfaces in the reionization regime. Experiments were performed for a Cu<sub>0.5</sub>Au<sub>0.5</sub>(100) single crystal and polycrystalline Au and Cu. Probabilities for collision induced neutralization and reionization processes were deduced from TOF-LEIS spectra. The probability for collision induced neutralization is increasing with primary energy. The reionization probability is found to be low in the whole range of energies investigated (&lt; 10%). A strong increase in subsurface contributions due to decreasing Auger neutralization efficiency is observed. This may lead to an increase in the ion yield, depending on scattering geometry. The impact of these findings on quantitative surface analysis by LEIS will be discussed.</p>
18:30		<b>END</b>
19:30	21	<b>Public Lecture</b>

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**Rubrene on SiO<sub>2</sub>: from the early growth stage to late crystallization**

*Shaima Abd Albaqi<sup>1</sup>, Helmut Sitter<sup>1</sup>, Barbara Stadlober<sup>2</sup>, Clemens Simbrunner<sup>1</sup>, Gregor Hlawacek<sup>3</sup>, Christian Teichert<sup>3</sup>*

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The fabrication of Rubrene thin films is of interest because of the high mobility observed for Rubrene single crystals. Here, we report on an atomic force microscopy (AFM) investigation of the growth of Rubrene thin films by Hot Wall Epitaxy on Mica and SiO<sub>2</sub>. During the initial formation of amorphous islands, a nonconstant growth rate is observed due to changes in the sticking coefficient. Saturation density has been determined and the island size has been extracted by applying the scale theory.

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**Conductive AFM investigations of arrowhead defects in GaInP/Ge structures**

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Polar semiconductor heterostructures grown on Germanium nonpolar substrates are of great interest for application in electronic devices. The limiting factor with respect to their prosperous usage is the presence of defects, such as antiphase domains (APD) and arrowhead defects [1], which diminish the quality of the resultant epitaxial layer. Here, we present conductive atomic force microscopy (C-AFM) investigations of GaInP thin films conventionally grown (by MOVPE) on Ge (100) substrate misoriented 6° towards (111) to study their electrical properties. C-AFM measurements were mainly performed under UHV conditions [2]. Two-dimensional C-AFM current maps reveal specific electrical behavior from the different facets of the arrowhead defects. Detailed discussion of the electrical behavior is based on local I-V curves recorded from specific areas.

[1] B. Galiana, et al., Superlattices Microstructures **45** (2009) 277.

[2] S. Kremmer, et al., Mat. Sci. Eng. B **102** (2003) 88.

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**Modification and nano-patterning of high-T<sub>c</sub> superconducting thin films by masked ion beam irradiation**

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Ion irradiation of the high-temperature superconductor (HTS) YBa<sub>2</sub>Cu<sub>3</sub>O<sub>7</sub> (Y-123) creates different types of defects depending on ion mass, energy and dose. Irradiation with Helium



	<p>ions of moderate energy (75 keV) primarily creates point defects. We measure in situ the modification of electrical transport properties of Y-123 thin films (thickness 200 nm) during ion irradiation. The He ions penetrate thin films and produce collision cascades with small lateral straggle that allow for patterning of nanostructures in the HTS layer. We present features smaller than 100 nm in size produced by masked ion beam irradiation of Y-123 films. Computer simulations indicate that nano-patterning of Y-123 thin films with 10 nm lateral resolution is achievable.</p>
<p><b>754</b></p>	<p><b>Assignment of electronic surface resonances: Br/Pt(110) as a case study.</b></p> <p><i>Christian Braun<sup>1</sup>, Peter Amann<sup>1</sup>, Alexander Menzel<sup>1</sup>, Erminald Bertel<sup>1</sup>, Rinaldo Zucca<sup>2</sup>, Josef Redinger<sup>2</sup></i></p> <p><sup>1</sup> <i>Institute for Physical Chemistry, Innrain 52a, 6020 Innsbruck, Austria</i>  <sup>2</sup> <i>Center for Computational Materials Science, Wiedner Hauptstr. 8, 1040 Wien, Austria</i></p> <p>Finding and investigating low-dimensional model systems is essential to improve the understanding of materials with strong electron correlation. It has been shown that electronic resonances on anisotropic transition metal surfaces represent such model systems [1]. In investigating the characteristic properties of these surfaces, it is important to disentangle bulk and surface-localized electronic states.</p> <p>To this end, we compare the experimental electronic band structure measured by angle resolved photoemission (ARPES) with theory (DFT) for the case of Br/Pt(110). Most of the dispersion features can be explained with a calculated one-dimensional density of states which indicates near surface transitions. Comparing different surfaces we show that most of the electronic states are sensitive to the symmetry of the surface. Thus these states most likely derive from surface resonances which are promising candidates to investigate electron correlation.</p>
<p><b>755</b></p>	<p><b>Tailoring the work function of noble metals using a cyano-based molecular acceptor: HAT-CN on Au(111) and Ag(111)</b></p> <p><i>Paul Frank<sup>1</sup>, Markus Koini<sup>1</sup>, Tatjana Djuric<sup>1</sup>, Norbert Koch<sup>2</sup>, Ralph Rieger<sup>3</sup>, Klaus Müllen<sup>3</sup>, Roland Resel<sup>1</sup>, Adolf Winkler<sup>1</sup></i></p> <p><sup>1</sup> <i>Institute of Solid State Physics, TU Graz, Petersgasse 16, 8010 Graz, Austria</i>  <sup>2</sup> <i>Institut für Physik, Humboldt Universität zu Berlin, Newtonstrasse 15, 12489 Berlin, Germany</i>  <sup>3</sup> <i>Max Planck Institute of Polymer Research, Ackermannweg 10, 55128 Mainz, Germany</i></p> <p>Ultra-thin films of hexaazatriphenylene-hexacarbonitrile (HAT-CN) were prepared on a Au(111) single crystal and on a Ag(111) single crystal utilizing organic molecular beam deposition (OMBD) under well defined ultra high vacuum (UHV) conditions. The thin films were investigated by thermal desorption spectroscopy (TDS), X-ray photoelectron spectroscopy (XPS), X-ray diffraction (XRD) and atomic force microscopy (AFM). XPS in combination with TDS was applied to reveal the kinetics of the layer growth. Additionally, the HAT-CN growth characteristics were studied as a function of substrate temperature. From TDS, the pre-exponential factor and the heat of evaporation for the individual layers could be determined experimentally. Ex-situ AFM and XRD were used to determine the morphology and the crystal structure of the grown films. A Kelvin probe (KP) was used to follow the change of the work function with increasing film thickness.</p> <p>The HAT-CN molecules exhibit a quite unusual layer growth behaviour which features coverage- and temperature-dependent rearrangements of the molecules. The change of the work function of the Au(111) and the Ag(111) surface due to HAT-CN adsorption is explained by the use of the presented growth model.</p>

<p><b>756</b></p>	<p style="text-align: center;"><b>Characterization of Titanium and Silicon Nanoparticle Films by STM and XPS techniques</b></p> <p style="text-align: center;"><i>Michaela Hager, Stefan Jaksch, Paul Scheier, Radula Stijepovic, Nikolaus Endstrasser, Institut für Ionen und Angewandte Physik, Technikerstraße 25, 6020 Innsbruck, Austria</i></p> <p>Nanoparticle films of titanium are produced by DC magnetron sputtering onto HOPG. The size, shape and electrical properties of the nanoparticles are investigated as a function of the plasma parameters. Without breaking the vacuum the sample is transferred to the STM- or XPS- chamber.</p> <p>By Scanning Tunneling Microscopy (STM) surface characterization, manipulation of the film and sample stability are investigated. X-ray Photoelectron Spectroscopy (XPS) measurements provide information on the chemical composition of the surface layers. In combination with Ar ion beam sputtering depth profiles of the nanoparticle films are obtained. Particular attention is given to the oxidation of the films. Even long term exposure of the samples to ambient air only leads to the oxidation of the surface of the nanoparticles, however with a constant level throughout the whole film thickness. Charging of the films by electron irradiation and STM imaging at increased bias voltages modifies the properties of the films. We observe increased oxidation at the irradiated regions and with the STM an increase of the local density of states is measured.</p> <p>Acknowledgments: work was supported by the FWF, Wien and the European commission Brussels via the project ITS-LEIF and the cost network CM0601 (ECCL)</p>
<p><b>757</b></p>	<p style="text-align: center;"><b>Integration of High-k/Metal Gate Schottky Barrier MOSFET</b></p> <p style="text-align: center;"><i>Christoph Henkel, Ole Bethge, Stephan Abermann, Emmerich Bertagnolli Institute for Solid-State Electronics, Floragasse 7, 1040 Vienna, Austria</i></p> <p>Only recently, CMOS technology put a new focus on Schottky Barrier Metal Oxide Semiconductor Field Effect Transistors (SBMOSFET) due to their excellent scalability to sub-10 nm channel lengths, and their drastically reduced source/drain parasitic resistance [1]. Moreover, since the overall thermal budget of the integration process of SBMOSFET can be reduced to temperatures below 600°C, an easy integration of high-k dielectrics in the sub nm regime is possible, as it is recommended by the ITRS roadmap [2].</p> <p>This work addresses the integration of high-k dielectrics into p-SBMOSFET on Silicon-on-Insulator substrates. The gate stack incorporates a tungsten metal gate and an Atomic Layer Deposited ZrO<sub>2</sub> gate oxide. The impact of different process parameters, e.g. annealing conditions for the deposition of the ZrO<sub>2</sub> gate dielectrics, and for the formation of the platinum silicide source/drain contacts is discussed.</p> <p>[1] J. M. Larson and J. P. Snyder, IEEE Trans. on Electron Devices, 53 (2006) [2] International Technology Roadmap for Semiconductors, 2007, <a href="http://public.itrs.net/">http://public.itrs.net/</a></p>
<p><b>758</b></p>	<p style="text-align: center;"><b>Transverse Shear Force Microscopy investigation of tiophene based Self Assembled Monolayers</b></p> <p style="text-align: center;"><i>Gregor Hlawacek<sup>1</sup>, Q. Shen<sup>1</sup>, H. Flesch<sup>2</sup>, Roland Resel<sup>2</sup>, Christian Teichert<sup>1</sup></i> <i><sup>1</sup> Institute of Physics, University of Leoben, Franz Josef Str. 18, 8700 Leoben, Austria</i> <i><sup>2</sup> Institute of Solid State Physics, Graz University of Technology, Petersgasse 16, 8010 Graz, Austria</i></p> <p>Transverse Shear Force Microscopy (TSM) allows to investigate crystallographic domains in thin organic films [1]. Here, TSM has been used to characterize a tiophene based self assembled monolayer (SAM), which has been used in the fabrication of a SAM based</p>

	<p>transistor [2]. The performance of such a device depends strongly on the domain size within the SAM. Using TSM, the domain size was evaluated in dependence of the SAM preparation method. A clear correlation between domains size, annealing and preparation time as well as electrical device performance is found. The SAM thickness as measured by Atomic Force Microscopy is compared to X-Ray reflectivity investigations.</p> <p>This work is supported by the FWF project S9707-N08 and S9702-N08.  [1] Last, J. et al., <i>Advanced Materials</i>, 1996, 8, 730.  [2] Smith, E. C. J., et al., <i>Nature</i>, 2008, 455, 956.</p>
759	<p style="text-align: center;"><b>Self-assembled nanopatterning in Si(001) homoepitaxy</b></p> <p style="text-align: center;"><i>Yanfang Hu, Reinhold Koch</i>  <i>Institut für Halbleiter- und Festkörperphysik, Johannes Kepler Universität Linz,</i>  <i>Altenbergerstr. 69, 4040 Linz, Austria</i></p> <p>The nanopatterning of the Si(001) surface with a periodic superstructure has become a challenging research topic as it can improve spatial ordering and size uniformity for nanostructure growth on the leading substrate of semiconductor technology. Combined scanning tunneling microscopy investigations and Monte Carlo simulations revealed that the surface configuration of the Si(001) depends on the Si coverage of the topmost surface layer. [1] In a narrow coverage window a (2 x n) superstructure— consisting of elongated (2x1) reconstructed stripes separated by a dimer-vacancy line every few nanometers— is formed. Here we show that the dimer-vacancy concentration in the surface layer can be tuned by Si deposition onto Si(001). As predicted by the Monte Carlo simulations at certain Si coverages long-range (2 x n) reconstructed terraces are formed, thus providing an alternative for nanopatterning of the Si(001) surface.</p> <p>[1] R. Koch, <i>Surf. Sci.</i> 600, 4694(2006)</p>
760	<p style="text-align: center;"><b>Image contrast dependence on the field emitter in near field emission scanning electron microscopy</b></p> <p style="text-align: center;"><i>Taryl Kirk, Lorenzo De Pietro, Olivier Scholder, Urs Ramsperger, Danilo Pescia</i>  <i>ETH Zürich, Mikrostrukturen, Laboratorium für Festkörperphysik, Wolfgang-Pauli-Strasse 16,</i>  <i>8093 Zürich, Switzerland</i></p> <p>In conventional scanning electron microscopy the lateral resolution is limited by the electron beam diameter impinging on the specimen surface. Near field emission scanning electron microscopy (NFSEEM) provides a simple means of overcoming this limit; however the most suitable field emitter remains to be determined. NFSEEM has been used in this work to investigate the W (110) surface with single crystal tungsten tips of (310), (111), and (100)-orientations. The topographic images generated from both the electron intensity variations and the field emission current indicate higher resolution capabilities with decreasing tip work function than with polycrystalline tungsten tips. The confinement of the electron beam transcends the resolution limitations of the geometrical models, which are determined by the minimum beam width. Moreover the electron intensity images show more detail with higher resolution than field emission current imaging, which implies additional parameters, such as the beam energy and detector sensitivity, must be considered.</p>

761	<p style="text-align: center;"><b>Sub-monolayer growth investigations of 6P on SiO<sub>2</sub></b></p> <p style="text-align: center;"><i>Stefan Lorbek, Gregor Hlawacek, Christian Teichert</i>  <i>Institute of Physics, University of Leoben, Franz Josef Strasse 18, 8700 Leoben, Austria</i></p> <p>Although, progress has been made in the recent years in the understanding of fundamental growth processes in organic molecular beam epitaxy, the underlying details are still unknown [1]. Especially, understanding of the island nucleation on the substrate during the deposition of oligomere thin films is crucial for the design of growth routes that will avoid the undesired formation of 3D structures.</p> <p>Here, the rod like model molecule para-sexiphenyl (6P) has been deposited onto the isotropic surface of silicon dioxide (SiO<sub>2</sub>) at various temperatures between 300K and 430K under ultra-high vacuum. Islands size, -distribution and fractal dimension are then obtained by in-situ and ex-situ atomic force microscopy in intermittent mode. Scaling laws and capture zone analysis using Voronoi tessellation have been used to obtain the critical nucleus size <math>r^*</math>.</p> <p><small>This work is funded by the FWF project "Organic thin films" S9707-N08.  [1] G. Hlawacek, et al., Science 321, 108 (2008)</small></p>
762	<p style="text-align: center;"><b>Low-temperature scanning tunneling microscopy and spectroscopy of single adsorbed metallo-porphyrin molecules</b></p> <p style="text-align: center;"><i>Stefan Müllegger<sup>1</sup>, Mohammad Rashidi<sup>1</sup>, Lorenz Michael Reith<sup>2</sup>, Wolfgang Schöfberger<sup>3</sup>, Reinhold Koch<sup>1</sup></i></p> <p style="text-align: center;"><sup>1</sup> <i>Institut für Halbleiter- und Festkörperphysik, Johannes-Kepler-Universität Linz, Altenbergerstraße 69, 4040 Linz, Austria</i></p> <p style="text-align: center;"><sup>2</sup> <i>Institut für Organische Chemie, Johannes-Kepler-Universität Linz, Altenbergerstraße 69, 4040 Linz, Austria</i></p> <p style="text-align: center;"><sup>3</sup> <i>Institut für Anorganische Chemie, Johannes-Kepler-Universität Linz, Altenbergerstraße 69, 4040 Linz, Austria</i></p> <p>Metallo-porphyrins are well-known to play important roles in such fundamental biological processes as photosynthesis, cell respiration or bio-catalysis. They have been used as model systems to study in vivo photoactivation of drug precursors (photodynamic therapy). The high analogy to Pt(II) compounds makes Au(III) complexes good candidates for development and testing as anticancer drugs. Especially Au(III) porphyrins exhibit interesting photocatalytic oxidative properties serving therefore as potential photonucleases.</p> <p>As a model system, Au(III) meso-tetraphenylporphyrin (Au-TPP) was synthesized to study the reduction mechanism on the central Au(III) metal ion and the reduction process on the ligand's macrocyclic ring system. Complementing recent wet-electrochemical analysis, we have performed low-temperature scanning tunneling microscopy and -spectroscopy studies on individual Au-TPP molecules adsorbed on monocrystalline Au(111) under ultra-high vacuum conditions at 8 K. In particular, the electronic properties of the central Au ion and the macrocyclic ring system have been investigated with submolecular resolution on individual Au-TPP molecules.</p>

<p><b>763</b></p>	<p><b>Conductive Atomic Force Microscopy investigations of organic thin films</b></p> <p><i>Andreas Pavitschitz<sup>1</sup>, Igor Beinik<sup>1</sup>, Markus Kratzer<sup>1</sup>, Christian Teichert<sup>1</sup>, Günther Schwabegger<sup>2</sup>, Clemens Simbrunner<sup>2</sup>, Helmut Sitter<sup>2</sup>, Thomas Griesser<sup>3</sup>, Wolfgang Kern<sup>3</sup></i></p> <p><sup>1</sup> <i>Institute of Physics, University of Leoben, Franz Josef Str. 18, 8700 Leoben, Austria</i>  <sup>2</sup> <i>Institute of Semiconductor and Solid State Physics, Johannes Kepler Universität, Altenbergstraße 69, 4040 Linz, Austria</i>  <sup>3</sup> <i>Institute of Chemistry of Polymeric Materials, University of Leoben, Franz Josef Str. 18, 8700 Leoben, Austria</i></p> <p>Organic materials are already used in electronic devices as dielectrics, semiconductors and conductive materials. The device performance depends on the electrical properties and the surface morphology of the organic thin film. Conductive Atomic Force Microscopy (C-AFM) allows simultaneous mapping of the morphology and the local film conductivity on the nanometre-scale. The details of carrier transport can be explored by measuring local current-voltage (I/V) curves.</p> <p>In this study, C-AFM was used to investigate dielectric parylene layers and the UV sensitive conductive polymer blend poly(diphenyl bicyclo[2.2.1]hept-5-ene-2,3-dicarboxylate) (PPNB)/ Poly (N-vinylcarbazole) (PVK) thin films. Parylene films were grown by polymerization of parylene-C on Si (100) and on Ag/glass, the PPNB/PVK layers were prepared by spin coating on p-doped Si(100). Both parylene films were found to be continuous and insulating. For the PPNB/PVK film C-AFM revealed a change in conductivity after UV-exposure.</p> <p>Support by the FWF projects S9702, S9706, S9707 and P19636-N20 is acknowledged.</p>
<p><b>764</b></p>	<p><b>Nucleation studies of para-hexaphenyl growth on mica(0001)</b></p> <p><i>Thomas Potocar<sup>1</sup>, Paul Frank<sup>1</sup>, Stefan Lorbek<sup>2</sup>, Christian Teichert<sup>2</sup>, Adolf Winkler<sup>1</sup></i></p> <p><sup>1</sup> <i>Institute of Solide State Physics, TU Graz, Petersgasse 16, 8010 Graz, Austria</i>  <sup>2</sup> <i>Institute of Physics, University of Leoben, Franz-Josef-Straße 18, 8700 Leoben, Austria</i></p> <p>The initial states of para-hexaphenyl (p-6P) growth on mica(0001) has been studied by thermal desorption spectroscopy (TDS) and atomic force microscopy (AFM). Submonolayers of p-6P were grown under ultra-high vacuum conditions by physical vapour deposition (PVD). The coverage was determined quantitatively by a quartz microbalance. It was recently shown that modifications of the mica surface, either by contamination with carbon or by surface roughening via Ar<sup>+</sup> sputtering, can considerably influence the layer formation. In particular the orientation of the molecules changes from flat lying on the freshly prepared surface to standing molecules on the modified surface. TDS is a powerful method to discriminate between these two growth modes. From the temperature and flux dependence of the island density, as determined by AFM, the critical cluster size for nucleation has been determined. In addition, from TDS the pre-exponential factor of the desorption rate can be calculated, which gives valuable information on the mobility of the molecules and clusters prior to desorption.</p>

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### Low-energy muSR as a new local probe technique to study photo-induced phenomena in thin films and heterostructures

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In a large variety of physical systems small changes in charge carrier densities may induce dramatic changes of the physical properties. Prominent examples are the high-T<sub>c</sub> cuprates representing strongly correlated electron systems close to a metal-insulator transition, or Mn-doped dilute magnetic (III,Mn)V semiconductors where the Mn impurities are coupled ferromagnetically by delocalized charge carriers. Photogenerated charge carriers open the fascinating possibility to change charge carrier concentrations in situ in a controlled way, which provides a convenient way to tune the physical properties of the system. A local probe such as the muon will provide complementary information to macroscopic measurements, and potentially new insights due to its high sensitivity to local magnetic fields. The results of a prototype experiment on Si clearly demonstrate the capability of the low-energy muSR technique to study photo-induced phenomena on thin films and heterostructures in a 100 nm region close to the surface. This will allow to open new fields of LE-muSR applications.

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### Self-Assembled Monolayers on Surfaces: Effect of the Molecular Conformation on the Interface Energetics.

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In the field of organic electronics, the use of self-assembled monolayers (SAMs) is common practice to enhance device performance. In particular, it has been shown that the deposition of SAMs on metals can cause significant modifications of the metal work-functions,  $\Delta\Phi$ . We use slab-type band-structure calculations to show that the effect of a SAM depends significantly on the interfacial geometry. For example, at low coverage the calculated  $\Delta\Phi$  can vary by about 100% depending on the tilt angle of the SAM forming molecules. The crux hereby is that often different conformations turn out to be energetically (almost) equivalent, which makes the determination of the equilibrium structures particularly difficult. Thus, we study various systems adopting two different geometry optimization schemes; (i) a damped molecular dynamics procedure in Cartesian coordinates and (ii) an internal-coordinate based strategy using GDIIIS (geometrical direct inversion in the iterative subspace). We find that, since the latter is capable of describing molecular degrees of freedom more efficiently, it typically provides more reliable results.

<p><b>767</b></p>	<p><b>Along the complexity axis in catalytic CO oxidation on Pt: single crystal, polycrystalline foil, model of a catalytic particle</b></p> <p><i>Yuri Suchorski <sup>1</sup>, Wolfgang Drachsel <sup>1</sup>, Christian Spiel <sup>1</sup>, Diana Vogel <sup>1</sup>, Robert Schlögl <sup>2</sup>, Günther Rupprechter <sup>1</sup></i></p> <p><i><sup>1</sup> Institute of Materials Chemistry, Vienna University of Technology; Veterinärplatz 1, 1210 Vienna, Austria</i></p> <p><i><sup>2</sup> Department of Inorganic Chemistry, Fritz-Haber-Institut der MPG; Faradayweg 4-6, 14195 Berlin, Germany</i></p> <p>To bridge the structural complexity gap between single crystals and industrial oxide supported metal catalysts, various metal/oxide model systems were developed, enabling us to study structure-reactivity relationships by surface science techniques. In the present contribution we compare the CO oxidation activity of various model systems with increasing complexity: (i) Pt(111) single crystal, (ii) polycrystalline Pt foil consisting of [100]-, [110]- and [100]-oriented grains, and (iii) the apex of a [110] and [100]-oriented Pt nanotip. Such an apex exhibits a heterogeneous surface formed by differently oriented nanofacets, and can thus serve as model for a metal nanoparticle. CO oxidation on planar surfaces was studied by photoemission electron microscopy (PEEM) and mass-spectroscopy (MS), whereas field emission (FEM) and field ion (FIM) microscopies were used for nanotips. The influence of the heterogeneity of the sample surface on kinetic phase transitions is discussed in terms of grain- and facet-boundary effects, and is compared to metal-oxide interfaces.</p>
<p><b>768</b></p>	<p><b>Molecular Dynamics Simulations of Self Assembled Conjugated Thiols on an Au(111) Surface</b></p> <p><i>Lukas Wittwer, Ferdinand Rissner, Egbert Zojer</i></p> <p><i>Institut für Festkörperphysik, Technische Universität Graz, Petersgasse 16, 8010 Graz, Austria</i></p> <p>The opportunity to modify surface properties by covering a substrate with self-assembled monolayers has lead to increased interest in interfaces between metals and organic monolayers.</p> <p>While the electronic properties of such systems can be investigated in detail using density-functional theory (DFT) calculations, the investigation of structural and dynamic properties of is a prohibitive task within DFT. Molecular dynamics simulations (MD) allow for computer experiments at finite temperatures and reasonable system sizes, without intrinsically assuming crystallinity of the monolayer. Therefore, MD was employed to examine conformational properties of conjugated thiols on gold. In particular, we focus on the impact of defects, like missing molecules or imperfect substrate surfaces and also discuss their consequences for the electronic properties of the SAM-covered surfaces.</p>
<p><b>769</b></p>	<p><b>Spatially resolved photoluminescence studies on rubrene micro-crystals</b></p> <p><i>Harald Zaglmayr <sup>1</sup>, Lidong Sun <sup>1</sup>, Helmut Sitter <sup>2</sup>, Shaima'a Abd Al-Baqi <sup>2</sup>, Peter Zeppenfeld <sup>1</sup></i></p> <p><i><sup>1</sup> Institut für Atom- und Oberflächenphysik, Altenbergerstr. 69, 4040 Linz, Austria</i></p> <p><i><sup>2</sup> Institut für Halbleiter- und Festkörperphysik, Altenbergerstr. 69, 4040 Linz, Austria</i></p> <p>Rubrene single crystals with size of several tens of micrometers on mica substrates have been prepared by hot wall epitaxy. Epi-fluorescence microscopy and laser scanning confocal microscopy are applied to investigate the morphology and the optical properties of these crystals. The spatially resolved photoluminescence spectrum shows a strong dependence on the orientation which can be attributed to (1) the optical anisotropy of the crystal and (2) different states of oxidation on the different crystal planes.</p>

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### Competing Orders in a Quasi-1D System: A Microscopic View

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We report on a low-temperature order-order transition in a quasi-one-dimensional (1D) surface system, which allows to study the microscopic details of the phase transition with atomic resolution by scanning tunneling microscopy. The competing ordered states are a quasi-hexagonal  $c(2 \times 2)$  structure favoured by inter-adsorbate repulsion and a rectangular  $(2 \times 1)$  phase stabilized by a charge density wave in the substrate [1]. Cooling the room-temperature long-range ordered  $c(2 \times 2)$  phase gives rise to rapid fluctuations which slow down as the critical temperature of about 50 K is approached. At 50 K the STM images reveal a striped phase exhibiting all hallmarks of quasi-1D critical fluctuations. This is at variance with the Landau theory of phase transitions, which would predict order-order transitions to be discontinuous. The results signal a break-down of the mean-field approximation in this system.

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

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### Electro-optical properties of dendritic materials and their use in high efficiency OLEDs

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Organic light-emitting devices (OLEDs) have attracted much attention in the past decades, being an alternative to silicon-based LEDs. They exhibit superior properties with respect to high contrast, low fabrication cost, adaptive device design and flexible structure. Recent developments have drawn a focus on conjugated dendritic materials constituting a one-molecule-host-guest system. By virtue of a well controllable synthesis process the adaptive design of dendrimers by tailored combinations of cores, dendrons and surface groups becomes feasible.

We have studied the optical properties of one specific dendritic material using spectroscopic methods as well as its behaviour when integrated into an OLED structure. By adding charge transport and charge injection layers to the structure the device luminance and efficiency could be significantly enhanced. The results suggest a strong Förster energy transfer coupling between the non-emissive dendron shell and the core giving rise to a single, stable emission peak.



**Ag induced structures on oxygen precovered Cu(110)**

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The Cu(110) surface can be readily structured by adsorbing oxygen: If the coverage of oxygen is less than required to form a complete (2x1) overlayer, CuO stripes are formed which are separated by bare copper areas. These stripes are uniformly distributed and parallel to the [001] direction.

On such an oxygen pre-covered surface silver was adsorbed at 660K. As revealed by scanning tunneling microscopy, submonolayer silver coverages lead to a phase separation between CuO and Ag/Cu alloy areas. The original Cu-CuO stripe phase is destroyed and larger CuO areas ('ponds') are formed. They are separated by Ag like stripes which are again parallel to the [001] direction.

The use of this structure as a template for additional adsorption of Ag at 300K leads to the formation of 3D nanorods along the perpendicular [1-10] direction as known for Ag grown on clean Cu(110). Since on our template the nanorods only grow on the Ag like stripes, their length is limited by the width of these stripes. With this technique one can even change the aspect ratio of the rods such that their longer axis is now parallel to the [001] direction.