O 41: Poster Session I (Semiconductor Substrates: Epitaxy and growth; Semiconductor Substrates: Adsorbtion; Semiconductor Substrates: Solid-liquid interfaces; Semiconductor Substrates: Clean surfaces; Oxides and insulators: Epitaxy and growth; Oxides and insulators: Adsorption; Oxides and insulators: Clean surfaces; Organic, polymeric and biomolecular films - also with adsorbates; Organic electronics and photovoltaics, Surface chemical reactions; Heterogeneous catalysis; Phase transitions; Particles and clusters; Surface dynamics; Surface or interface magnetism; Electron and spin dynamics; Spin-Orbit Interaction at Surfaces; Electronic structure; Nanotribology; Solid/liquid interfaces; Graphene; Others)

Time: Tuesday 18:30–21:00 Location: Poster B1

O 41.1 Tue 18:30 Poster B1

SPM characterization of GaN formed by ion-beam assisted epitaxy — •Lena Neumann, Jürgen W. Gerlach, Moharram Abd El Khair, and Bernd Rauschenbach — Leibniz-Institut für Oberflächenmodifizierung e. V., Permoserstrasse 15, 04318 Leipzig

Gallium nitride (GaN) films were formed using the ion-beam assisted epitaxy technique. The influence of the nitrogen ion-to-gallium atom flux ratio (I/A ratio) on the early stages of GaN thin films nucleation and growth on super-polished 6H-SiC(0001) substrates is studied, here. The deposition process was performed by evaporation of gallium using a conventional effusion cell and irradiation with hyperthermal nitrogen ions from a constricted glow-discharge ion source at a constant substrate temperature of 630°C. The nitrogen ions flow was kept constant and their kinetic energy did not exceed 25 eV. The selection of different I/A flux ratios was done by varying the gallium effusion cell temperature in the range between 950°C and 1020°C. For comparison, a constant amount of deposited GaN was achieved by adapting the deposition time. The surface structure during the GaN growth was monitored in situ by reflection high-energy electron diffraction (RHEED). The nucleation and subsequent film formation were observed using a scanning probe microscope (SPM) attached to the deposition system. The results show that the initial stages of the ion-beam assisted GaN formation are strongly influenced by the I/A ratio.

O 41.2 Tue 18:30 Poster B1

Growth of epitaxial micrometer-sized Cu- and Cu-Ni pyramides on Silicon — •Sarah Hoffmann, Benedikt Ernst, Regina Nowak, Susanne Seyffarth, and Hans-Ulrich Krebs — Institut für Materialphysik, Universität Göttingen, Friedrich-Hund-Platz 1, D-37077 Göttingen

Thin Cu and Cu-Ni films were prepared on Si(111) substrates using pulsed laser deposition (PLD) in ultra high vacuum. At elevated substrate temperatures above 200°C, either during deposition or afterwards, epitaxial growth of three dimensional pyramides with edge lengths of about five micrometers and heights up to 500 nm is observed using scanning electron microscopy (SEM) and atomic force microscopy (AFM). In the case of pure Cu, the base area of these islands is a triangle. With increasing Ni-content, shape changes occur, which can be explained by a reduction of surface diffusion. The influence of the SiO_2 layer thickness and the formation of a Cu-Si interlayer was studied by ellipsometry. The transformation of the Cu and Cu-Ni films into the pyramids during heating were studied by resistance and x-ray measurements.

O 41.3 Tue 18:30 Poster B1

Surface analysis for the characterization of thin heteroepitaxial GaP films on Si(100) — •Henning Döscher[1], Peter Kleinschmidt[1], Anja Dobrich[1], Sebastian Brückner[1], Oliver Supplie[1], Christian Höhn[1], Ulrike Bloeck[1], Benjamin Borkenhagen[2], Gerhard Lilienkamp[2], Winfried Daum[2], and Thomas Hannappel[1] — [1]Helmholtz-Zentrum Berlin für Materialien und Energie, Hahn-Meitner-Platz 1, 14109 Berlin — [2]IEPT, TU Clausthal, Leibnizstr. 4, 38678 Clausthal-Zellerfeld

The combination of superior III-V semiconductors with Si(100) substrates via metal-organic vapour phase epitaxy (MOVPE) is a technological and scientific challenge. The growth of nearly lattice-matched GaP on Si(100) represents an important model system for the specific defect mechanisms induced by polar on non-polar epitaxy such as anti-phase disorder. Applying a contamination free transfer system between the MOVPE and ultra high vacuum (UHV), we are able to correlate UHV based surface characterization with in situ optical measurements and post-growth ex situ analysis.

The applied instruments include X-ray photoelectron spectroscopy (XPS) for chemical analysis, X-ray diffraction (XRD) and transmission electron microscopy (TEM) for film characterization, scanning tunnelling (STM) and atomic force (AFM) microscopy for surface investigations, low energy electron diffraction (LEED) and reflectance anisotropy spectroscopy (RAS) for averaged information about the anti-phase domain distribution as well as low energy electron microscopy (LEEM) and dark field TEM for its lateral resolution.

O 41.4 Tue 18:30 Poster B1

MOVPE growth processes monitored simultaneously by in-situ scanning tunneling microscope and spectroscopic ellipsometry — •Matthias Schmies, Raimund Kremzow, Markus Pristovsek, and Michael Kneissl — TU Berlin, Institut für Feskörperphysik, EW 6-1, Hardenbergstr. 36, D-10623 Berlin, Germany

Optoelectronic devices, such as single-photon emitters and semiconductor lasers, demand an excellent understanding of the growth processes during metal organic vapor phase epitaxy (MOVPE). Typical MOVPE growth conditions, e.g. 100 mbar reactor pressure and 700°C temperatures, require optical techniques for in-situ control. However, these techniques do not provide sufficient information about surface topology. Especially monitoring the changes in the InGaAs quantum dot (QD) morphology during MOVPE is very challenging. In order to obtain information about the structural changes during MOVPE, we have built a special in-situ scanning tunneling microscope (STM). In order to also measure layer thickness and composition we combined this STM with an in-situ ellipsometer and present measurements on QD formation during MOVPE containing simultaneous information of topography and layer properties. This allows us to investigate the QD shape depending on layer thickness and composition.

O 41.5 Tue 18:30 Poster B1

Adsorption Characteristics of Gallium on Si(112) — •Inga Heidmann, Moritz Speckmann, Thomas Schmidt, and Jens Falta — Institute for Solid State Physics, University of Bremen, 28359 Bremen

We studied the morphology of the clean and gallium-terminated Si(112) surface by means of scanning tunneling microscopy (STM) and low-energy electron diffraction (LEED). The Si(112) surface is of great interest for technological applications due to the fact that the clean surface is faceted [1], and the deposition of Ga atoms at the step edges of vicinal surfaces is favoured energetically. This leads to a self-organized formation of quasi one-dimensional atomic wires along the direction of the wires [2].

Our investigations on the bare surface showed two different typs of regions, one exhibiting stepped Si(112) surface areas and the other consisting of (111)-(7×7)- and (337)-(2×1)-facets orientated along the $[\bar{1}10]$ direction. Due to the adsorption of gallium the surface is smoothened and large-area (112)-orientated domains are established with a $(N \times 1)$-reconstruction, where $N = 4 - 7$ with an averaged value of roughly 5.5. The Ga atoms are arranged in rows parallel to the $[\bar{1}10]$ direction, but are interrupted by perpendicular quasiperiodic vacancy lines.

[1]: Baski et al., Phys. Rev. Lett. **74(6)**, 1995.

[2]: Snijders et al., Phys. Rev. B **72**, 2005.

O 41.6 Tue 18:30 Poster B1

Aluminium induced facetting of Si(113) studied by SPA-LEED and AFM — Inga Heidmann[1], •Moritz Speckmann[1], Tobias Nabbefeld[2], Claudius Klein[2], Michael Horn-von Hoegen[2], and Jens Falta[1] — [1]Institute of Solid State Physics, University of Bremen, 28359 Bremen — [2]Experimental Physics, University of Duisburg-Essen, 47057 Duisburg

Due to its anisotropy and lack of rotational symmetry the Si(113) surface is a candidate for the growth of low dimensional structures like nanowires. Though it is one of a very few stable high-index silicon surfaces, Si(113) appears to be unstable against facetting after adsorption of metals, e.g., Ga [1,2] or Ag [3].

By means of spot profile analysing low-energy electron diffraction (SPA-LEED) and atomic force microscopy (AFM) we analysed the Al adsorption on Si(113) in a temperature range of 600 to 800°C in dependence on both, the deposition temperature and deposition time. We find that Al, very similar to the adsorption of Ga, decomposes the Si(113) surface into a regular facet pattern along the $[1\bar{1}0]$ direction. This pattern consists of alternating (112) and (115) facets, which are (6×1) and (4×1) reconstructed, respectively. The width of the facets increases strongly with increasing deposition temperature. For temperatures above 750°C, however, only the (112) facets are found to be stable.

[1]: H. Suzuki et al., Surf. Sci. **492**, 166 (2001).
[2]: T. Clausen et al., e-J. Surf. Sci. Nanotech. **3**, 379 (2005).
[3]: M. Speckmann et al., Phys. Status Solidi RRL **3**, 305 (2009).

O 41.7 Tue 18:30 Poster B1

Influence of the pre-adsorption of group III metals on the growth of Ge nanostructures on vicinal Si surfaces — •Moritz Speckmann, Thomas Schmidt, Jan Ingo Flege, Inga Heidmann, Jan Höcker, Torsten Wilkens, and Jens Falta — Institute of Solid State Physics, University of Bremen

The employment of metals as surfactants (surface active agents) is a promising approach to influence the growth of Ge nanostructures on Si surfaces. Especially for group III and group V elements an enhanced or suppressed Stranski-Krastanov growth behaviour is found, respectively.

For all group III metal on silicon systems presented in this study we observe a drastic change of the surface morphology after adsorption of a few monolayers. For the investigations we used a variety of surface sensitive techniques, e.g., scanning tunneling microscopy (STM), spot profile analysing low-energy electron diffraction (SPA-LEED), low-energy electron microscopy (LEEM), and x-ray standing waves (XSW). On the one hand, the adsorption of Ga and In leads to a smoothening of the intrinsically unstable Si(112) surface and the development of 1D metal chains. But on the other hand, the stable Si(113) is decomposed into a regular array of nanofacets after adsorption of Ga. For all cases shown here the possibility of growing highly anisotropic Ge islands is demonstrated (Ga/Si(113) [1], Ga/Si(112) [2], In/Si(112)).

[1]: Th. Schmidt et al., New J. Phys. **9**, 392 (2007).
[2]: M. Speckmann et al., J. Phys.: Condens. Matter **21**, 314020 (2009).

O 41.8 Tue 18:30 Poster B1

STM study of Cu interaction with Pb/Si(111) surface at room and low temperatures. — •Pavel Shukrynau[1,2], Marius Toader[1], Michael Hietschold[1], and Vladimir Chab[2] — [1]Chemnitz University of Technology, Institute of Physics, Solid Surfaces Analysis Group. D-09107 Chemnitz, Germany. — [2]Institute of Physics, Academy of Sciences of the Czech Republic. CZ 162 53, Prague, Czech Republic.

Upon evaporation of a small amount of Cu on the (rt3xrt3)R30-Pb/Si(111) and (1x1)-Pb/Si(111) surfaces at room temperature followed by annealing, new clusters of hexagonal shape are formed. These clusters have a protruded border and are found randomly distributed in the (rt3xrt3)R30-Pb phase or attached to (1x1)-Pb/Si(111) islands with one side. Some of them are agglomerated in bigger clusters of a complex shape. Annealing at higher temperatures induces Pb and Cu segregation in characteristic structures observed at Si surface with a single metal adsorption. Cu atoms agglomerate in quasi-5x5 phase and Pb atoms are found in the "mosaic" structure corresponding to 1/6 ML. The formation of the clusters may be the result of Pb-Cu interaction mediated with Si substrate. Cooling the surface down to 200 K leads to significant changes in the 1x1-Pb islands. The original structure dissipates into small domains of 3x3 nm in size partially keeping the Si(111)-c(5xrt3)-Pb reconstruction. The detailed inspection of this surface reveals a local ordering in a mosaic-like pattern.

O 41.9 Tue 18:30 Poster B1

HR-EELS-study of the adsorption of propionic acid on clean and H_2O saturated Si(001) surfaces — •Bochra Boughaled Ellakhmissi[1], Miriam Lange[1], Stefan Kubsky[2], Francois Rochet[3], and Ulrich Köhler[1] — [1]Experimentalphysik IV, Ruhr-Universität Bochum, Germany — [2]Synchrotron Soleil, St. Aubin (Paris), France — [3]Laboratoire de Chimie Physique Matière et Rayonnement, Univ. P. et M. Curie, Paris, France

High resolution electron energy loss (HR-EELS) spectroscopy is used to study the reaction of propanoic acid (CH_3-CH_2-COOH) with the clean and the hydroxylated Si(001) surface. The results are compared to photoemission data. For the adsorption on the clean Si(001)-2x1 surface the results point to the simultaneous presence of different adsorption geometries, monodentate and bidentate. To circumvent the inhomogeneity caused by multiple adsorption geometries, in a second set of experiments the silicon surface was first modified by the adsorption of water leading to a grafting layer of Si-H and Si-O-H. During the reaction of the hydroxylated surface with propionic acid the strongly diminished O-H stretching mode together with the appearance of the C-H mode clearly shows a reaction of the acid with the water layer. Further information is gained by replacing the H_2O grafting layer by a D_2O layer to distinguish hydrogen (deuterium) related vibrational excitations of the grafting layers from the ones coming from the carboxylic acid. The vibrational data are consistent with the selective adsorption of the propionic acid with the Si-O-H groups via an esterification reaction in a monodentate geometry.

O 41.10 Tue 18:30 Poster B1

Investigations of PTCDA-growth on passivated silicon surfaces with SPA-LEED — •André Kubelka, Christian Schulz, and Jens Falta — Institute for Solid State Physics, University of Bremen, 28359 Bremen

Research and utilization of organic semiconductor materials have raised increasing interest in the last years. The organic molecule 3,4,9,10-perylene-tetracarboxylic-dianhydride (PTCDA) is often used as an model system for the investigation of physical and chemical properties of organic thin films. PTCDA is a promising candidate for epitaxial layer growth due to its flat molecular structure. We investigated the growth of PTCDA on passivated silicon surfaces with spot profile analysis low energy electron diffraction (SPA-LEED).

After deposition by molecular beam epitaxy on the H-passivated Si(111) the SPA-LEED images showed ring-like patterns with one visible diffuse ring, which indicates the growth of small or weakly-ordered islands with no preferential orientation with respect to the substrate. Further investigations using other experimental methods are in progress.

O 41.11 Tue 18:30 Poster B1

XPS studies of organosilanes attached to 6H-SiC(0001) — •Nabi Aghdassi[1], Deb Kumar Bhowmick[1], Steffen Linden[1], Michael Hirtz[1], André Devaux[1,2], Lifeng Chi[1,2], Luisa De Cola[1,2], and Helmut Zacharias[1,2] — [1]Physikalisches Institut, Westfälische Wilhelms-Universität Münster, Wilhelm-Klemm-Straße 10, 48149 Münster — [2]CeNTech, Center for Nanotechnology, Heisenbergstraße 11, 48149 Münster

Octadecyltrichlorosilane (OTS) represents an organic molecule which has gained much interest in respect of the formation of self-assembled monolayers on silicon dioxide substrates. Silicon carbide (SiC) is a semiconducting substrate well-suited to attach organic complexes due to its outstanding properties like a large bandgap, a high electron drift velocity and its non-toxicity. We have attached OTS molecules to the hydroxyl-terminated 6H-SiC(0001) surface via a wet chemical treatment. This system is studied by XPS. Before the functionalization of the surface the C1s region shows two peaks separated by about 2 eV. The peak with lower binding energy can be attributed to the carbidic component while the second one can be related to a silicon oxycarbide layer. After surface functionalization the peak with higher binding energy shows a large increase in intensity which can be explained by the attached alkyl chains. A covalent bonding of organosilanes with functional end groups may provide a linker for a further functionalization of the surface.

O 41.12 Tue 18:30 Poster B1

Photocatalytic CO_2 reduction investigatet with in situ ATR IR spectroscopy — •Leo Pöttinger — PCI Universität Heidelberg, Deutschland, Heidelberg

The recycling of CO_2 e.g. from exhaust gases to hydrocarbons or even fuels like methanol or methane is of high interest. The chemical storage of energy in fuels with renewable energies is considered. Cheap and good availabe semiconductors like TiO_2 are known to reduce CO_2 when illuminated with UV light to hydrocarbons. ATR IR spectroscopy is used to investigate the interface of porous TiO_2 layer and in water dissolved CO_2 . With an in situ flow through cell and light irradiation the reduction process can be tracked. With FTIR ATR spectroscopy vibrational bands are used to identify arising intermediates on the surface. The high bandgap of TiO_2 does not allow the process to run with visible light. To drive the process with visible light dye sensitsed TiO_2 porous layers are needed. Also the use of cocatalysts is under investigation.

O 41.13 Tue 18:30 Poster B1

Characterisation of a Titania(TiO_2)-Water-Interface under UV illumination in the Visible Region — •Thomas Kriesche — PCI Universität Heidelberg

Photoassisted reactions on TiO_2 have attracted much interest for e.g. decomposition of organic pollutants in wastewater. As a result of this it is necessary to understand the dynamic surface charge of titania and its interaction with water to better comprehend reactions involved. In situ ATR IR Spectroscopy is a powerful tool used to investigate the interface between TiO_2 and water. Because of the porosity of the titania powder, measurements yield information about dissolved and adsorbed species and their dynamics. LEDs with a wavelength of 350nm for photocatalytic excitation and a ZnSe-ATR-crystal were integrated in a flow cell and used in a Bruker IFS66vS spectrometer. We observed a change in absorption between 9000 and 9500cm^{-1} during UV-illumination. Additionally, we compare the results with the dynamics of the infrared region using a germanium ATR-crystal. Thin titania layer were deposited on the crystal by dropping a titania-ethanol-mixture on the ATR-surface and annealing it overnight. These layers were observed via SEM. The increase of fundamental knowledge about titania will allow a better understanding of photocatalytic reactions.

O 41.14 Tue 18:30 Poster B1

Coexistence of forward and backward buckled π-bonded chains on the Si(111)-2×1 surface — •Thomas K. A. Spaeth, Martin Wenderoth, Karolin Löser, and Rainer G. Ulbrich — IV. Physikalisches Institut, Georg-August Univ. Göttingen, Germany

The (2×1) reconstructed Si(111) surface, prepared by cleaving in ultrahigh vacuum, has been studied for more then forty years. Different models for the description of this basic reconstruction have been proposed. The model of π-bonded chains is widely accepted, but it is still an open question whether forward or backward buckled chains are formed. This ambiguity is due to the small energetic difference between the two variants. Even though the STM cannot directly distinguish between forward and backward buckled π-bonded chains, we find indications of the coexistence of both chain types by analyzing anti-phase-boundaries between domains of given buckling type on the Si(111)-2×1 surface. The anti-phase-boundaries show a lateral shift of the π-bonded chains which is not compatible with a model of only one type of buckling. But it can be readily explained by "colliding" domains of differently buckled chains. This finding is supported by STS data taken across the anti-phase-boundaries. They show different electronic structures on both sides. We acknowledge financial support by the DFG via project WE 1889/3.

O 41.15 Tue 18:30 Poster B1

Formation of the Si(111)-2×1 reconstruction — Thomas K. A. Spaeth, Martin Wenderoth, •Karolin Löser, and Rainer G. Ulbrich — IV. Physikalisches Institut, Georg-August Universität Göttingen, Germany

The Si(111)-2×1 reconstructed surface is obtained by cleavage at RT in the UHV. It consists of π-bonded chains which can run in the three equivalent lattice directions $[0\bar{1}1]$, $[\bar{1}10]$ and $[10\bar{1}]$. Different kinds of anti-phase-boundaries (APB) are theoretically possible between domains of reconstructed π-bonded chains: (i) APB separating domains of different chain orientations or (ii) APB resulting from a ‘stacking fault’ of the 2×1 reconstruction along or across the chains, i.e. the displacement can be either between two chains or within each chain. We have studied cleaved Si(111)-2×1 samples with high-resolution STM in UHV and observed APBs separating domains with different chain orientations as well as APBs with the displacement within each chain of the same direction. A displacement between two parallel chains was not found. In sample areas containing surface steps, APBs typically run parallel to the steps, within a few nm distance. We also find a clear preference for the $[\bar{1}10]$ and the $[10\bar{1}]$ direction while chains running parallel to the nominal propagation of the cleavage in $[0\bar{1}1]$ direction occur only in very few and small domains, and often linked with steps nearby. Our results provide strong indication that cleavage related surface steps control the formation of the 2×1 reconstruction domains on the Si(111) surface. We acknowledge financial support by the DFG via project WE 1889/3.

O 41.16 Tue 18:30 Poster B1

Si(100) surface preparation under VPE conditions — •Anja Dobrich, Henning Döscher, Sebastian Brückner, Christian Höhn, Peter Kleinschmidt, and Thomas Hannappel — Helmholtz-Zentrum Berlin für Materialien und Energie, Hahn-Meitner-Platz 1, 14109 Berlin

The preparation of Si(100) surfaces in vapor phase environments (VPE) suitable for subsequent III-V epitaxy was characterized by surface sensitive instruments available through a dedicated sample transfer to ultra high vacuum (UHV). Using X-ray photoelectron spectroscopy (XPS) for inspection of the chemical surface composition, we verified the ability to obtain clean Si(100) free of oxygen or other contaminations. We checked the process extensively regarding reliability, influences of the process parameters (time, surface temperature, pressure and type of process gas, presence of precursors) and dependencies on type of substrate. Because the results obtained in alternative atmospheres (N_2 and Ar) differed from those in H_2, we considered an active role of the process gas in the removal of SiO_2-layers. Fourier-transform infrared spectroscopy (FTIR) proved the presence of Si-monohydrides while low energy electron diffraction confirmed a two-domain (2x1)/(1x2) reconstruction for all Si(100) surfaces. Since these results implied a predominance of single-layer steps undesirable for subsequent III-V layers, we investigated the atomic surface structure of the samples with scanning tunnelling microscopy (STM). Depending on the off-orientation, the images revealed complex step structures and opposing trends of partial double-layer step formation.

O 41.17 Tue 18:30 Poster B1

Charge Switching of Donor Ensembles in a Semiconductor — •Karen Teichmann[1], Martin Wenderoth[1], Sebastian Loth[1], Rainer G. Ulbrich[1], Jens K. Garleff[2], A. P. Wijnheijmer[2], and Paul M. Koenraad[2] — [1]IV. Physikalisches Institut, Georg-August Universität Göttingen, Germany — [2]PSN, Eindhoven University of Technology, the Netherlands

We investigated the charge state switching behaviour of interacting donors near the GaAs (110) surface, by Scanning Tunnelling Microscopy (STM). Silicon doped ($n \approx 6 \cdot 10^{18}$ cm^{-3}) GaAs is cleaved in UHV to obtain a clean and atomically flat surface, directly afterwards the sample is transferred into a home build STM, working at 5 Kelvin. Using the STM tip as a movable gate the charge state of each donor can be switched from the neutral to the ionized state [1]. The charge configuration of a single isolated donor is unambiguously determined by the position of the tip and the applied voltage. In contrast, even a two donor system with inter donor distances smaller than 5 nm shows a more complex behavior. The electrostatic interaction of two donors close together can result in ionization gaps. In certain geometrical configurations the modified electronic properties of donors close to the surface [2] can result in bistable and time dependent charge switching behavior. We acknowledge financial support by the DFG SPP 1285.

[1] PRL 101, 076103 (2008)

[2] PRL 102, 166101 (2009)

O 41.18 Tue 18:30 Poster B1

Characterization of Oxide-based Modelcatalysts- Growth, Morphology and Structure of ultrathin Titaniumoxide- and Ceriumoxide-Films prepared by Oxidation of the Pt-based binary alloys. — •Jan Markus Essen[1], Severine Le Moal[2], Marco Moors[1], Christian Breinlich[1], Conrad Becker[2], and Klaus Wandelt[1] — [1]Institute of Physical and Theoretical Chemistry, Wegelerstr. 12, D-53115 Bonn — [2]CINaM-CNRS-UPR 3118, Case 913, Marseille Cedex 9, F-13288

Oxidation of bimetallic alloys is a versatile tool for the preparation of ultrathin oxide films. In this study we compare the growth of cerium- and titanium oxide-films obtained by oxidation of Pt_xCe/Pt(111)- or Pt_3Ti(111)-alloys. For both oxides depending on the oxidation temperature, oxygen pressure, or for the Pt_xCe-alloyphases, the amount of cerium, different structures occur. For cerium oxides only 3 different hexagonal phases are observed, while for the titanium oxides 5, hexagonal and rectangular, phases can be distinguished. This can be interpreted as a result of the interplay between the hexagonal substrate symmetry and the oxide favored symmetry, namely hexagonal for the cerium oxides and rectangular for the titanium oxides. For the cerium oxide a stoichiometric oxidation is possible, while for the titanium oxides, caused by strong realloying, this is not the case. For titanium oxides contrarily to the cerium oxides predominantly a 2D-Growth is observed. This is caused by the good matching of the lattice parameters with the underlying substrate. For cerium oxides a lattice the mismatch leads to cluster-formation and thus to a 3D growth mode.

O 41.19 Tue 18:30 Poster B1

In-situ preparation and characterisation of thick films of Calcium hydroxide — •Sebastian Dahle[1] und Wolfgang Maus-Friedrichs[1,2] — [1]Institut für Physik und Physikalische Technologien, TU Clausthal, Leibnizstr. 4, 38678 Clausthal-Zellerfeld, Germany — [2]Clausthaler Zentrum für Materialtechnik, TU Clausthal, Leibnizstr. 4, 38678 Clausthal-Zellerfeld, Germany

The interaction of Calcium hydroxide with different gases is of technological interest for various applications. For example Calcium hydroxide is used as absorbent and reacting agent for neutralisation and desulphurisation, as well as a plaster. Understanding the behaviour of Calcium hydroxide in different environments is expected to lead to increased environmental protection und energy efficiency. The investigation of the interaction processes starts in a clean environment under controlled conditions. Therefore clean films of Calcium hydroxide have to be prepared.

The preparation of thick films of Calcium hydroxide in an Ultra High Vacuum environment using a metal evaporator in combination with a gas inlet system is presented on this poster. In contrast to Calcium oxide that can easily be prepared, Calcium hydroxide shows effects of reduction via impinging Calcium atoms during the preparation. These effects have been studied with Metastable Induced Electron Spectroscopy (MIES), Photoelectron Spectroscopy (UPS(HeI) and XPS), as well as Atomic Force Microscopy (AFM).

O 41.20 Tue 18:30 Poster B1

STM and STS measurements on thin cerium oxide films grown on Pt(111) — •Christian Breinlich, Enrico Barletta, Jan Markus Essen, and Klaus Wandelt — Institute for Physical and Theoretical Chemistry, Wegelerstr. 12, 53115 Bonn, Germany

Thin oxide films, grown on a metal support, are showing interesting electronic properties. Therefore they are of great interest for the use as insulating layers in electronic devices and as a support for model catalysts. Cerium oxide has a high dielectric constant, which makes it useful in the fabrication of small capacitor devices. In this study we employed STM and STS to investigate the structural and electronic properties of thin cerium oxide films grown on Pt(111). The preparation process was studied by AES, LEED and HREELS. In a first step a Pt-Ce/Pt(111) surface alloy was prepared by evaporating a thin cerium film at 300 K with subsequent annealing to 1000 K. Then this alloy was oxidised under different conditions. Large amounts of oxygen at 900 K are leading to completely oxidised CeO_2 films, whereas smaller amounts of oxygen at 700 K are yielding mixed oxide phases. The former shows a (1.34×1.34) superstructure in LEED and rough, two to three layers high islands in STM. The mixed oxide phase shows a (4×4) superstructure and consists of flat islands with sharp edges. By employing STS it was possible to measure the band gap of the oxide films, which strongly depends on film thickness and stoichiometry.

O 41.21 Tue 18:30 Poster B1

Structural and electronic characterization of ultra thin MgO films on Mo(100) by scanning tunneling spectroscopy — •Christian Pauly, Martin Grob, Mike Pezzotta, Marco Pratzer, and Markus Morgenstern — II. Physikalisches Institut B and JARA-FIT, Otto-Blumenthal-Straße, RWTH Aachen, 52074 Aachen

We investigated MgO films on Mo(100) with a thickness of up to 11 monolayers (ML) by scanning tunneling microscopy (STM) and spectroscopy at room temperature. The MgO films were prepared by evaporation of magnesium in oxygen atmosphere.

The appearance of the MgO islands (e.g. island heights) imaged by STM strongly depends on the applied bias voltage at the onset of the conduction band. In particular, the edges appear brighter than the interior of the islands, which we attribute to a spectroscopic effect probably related to defects. The characteristic moiré pattern caused by the lattice mismatch of Mo and MgO has been found on up to 11 ML thick MgO islands. The width of the band gap was measured with respect to the film thickness by dI/dU-spectroscopy. The MgO films partly show a characteristic peak in the band gap, which could be assigned to charged defect states.

O 41.22 Tue 18:30 Poster B1

Mosaic and facet structures of epitaxial MnO films on Au(110) — •Klaus Meinel, Michael Huth, Hannes Beyer, Henning Neddermeyer, and Wolf Widdra — Institute of Physics, Martin-Luther-Universität Halle-Wittenberg, Germany

Theoretical studies of rocksalt-like MnO predict for MnO(110) surfaces a (2x1) missing row reconstruction where (100) microfacets run along the [100] direction [1]. For proving this prediction, epitaxial MnO films (thickness 5 - 10 monolayers) have been prepared on an Au(110) substrate and analyzed by means of STM and SPA-LEED. Immediately after film deposition at room temperature, a diffuse background was visible in SPALEED indicating that there is initially poor structural order. Annealing at about 750 K induces long range ordering and relaxation of film structure. Simultaneously, a partly dewetting of the Au(110) substrate occurs. The MnO(110) film displays no (110) terraces. Instead, a furrowed surface is observed with the trenches running parallel to [100]. Along this direction, the film is locally tilted by about +/- 2° due to the misfit which induces a mosaic structure. The surface of the furrows is formed by alternating stripes of (010) and (100) facets having a mean width of about 3 nm. Annealing the films at temperatures around 850 K induces a vanishing of the mosaic structure and an increasing of the width of the (001) facets. Hence, the predicted tendency of (100) faceting is confirmed by experiment. However, the facets are much broader than expected and no (2x1) missing row reconstruction is found within the investigated film thicknesses.

[1] V. Bayer et al., Phys. Rev. B 75, 035404 (2007).

O 41.23 Tue 18:30 Poster B1

Change of adsorption kinetics of CH_4 in the presence of O^- centers on MgO: a TPD study — •Philipp Giese[1], Harald Kirsch[1], Christian Frischkorn[1,2], and Martin Wolf[1,2] — [1]Institut für Experimentalphysik, FU Berlin, Arnimallee 14, 14195 Berlin — [2]Fritz-Haber-Institut, Abt. Physikalische Chemie, Faradayweg 4-6, 14195 Berlin

In order to obtain a deeper understanding of the interaction between localized holes and adsorbed CH_4, its adsorption kinetics are studied on in-situ prepared MgO/Ag(001). Different methods to increase the amount of localized holes or more specifically O^- sites on MgO-surfaces were examined. The detection method is temperature programmed desorption (TPD). After running several cycles of photoinduced N_2O reduction on MgO, the monolayer of CH_4 is slightly more strongly bound (increase of desorption temperature by ~ 5 K) compared to CH_4 adsorbed on untreated MgO. Furthermore, the whole TPD spectrum is broadened and its intensity is smaller. We conclude that the CH_4 adsorbate rearranges itself after subsequent reduction of N_2O on MgO. This behaviour cannot be induced by direct UV irradiation, so the interaction between a localized hole and CH_4 is much less favourable than the recombination of excited electron-hole pairs, in contrast to the activation of the N_2O bond in photoinduced N_2O reduction. As these localized holes reduce the activation barrier of the C-H abstraction to 0.7 eV, the aforementioned adsorbed state can be interpreted as a precursor in the process of the oxidative coupling of CH_4 on oxide surfaces.

O 41.24 Tue 18:30 Poster B1

Bond formation between single molecules on ultrathin insulating films — •Niko Pavliček, Tobias Sonnleitner, Ingmar Swart, and Jascha Repp — Institute of Experimental and Applied Physics, University of Regensburg, 93040 Regensburg, Germany

Scanning tunneling microscopy (STM) and spectroscopy (STS) studies on very thin insulating films have shown to be powerful tools in atomic-scale science [1]. These techniques have opened up exciting possibilities by enabling the investigation of the unperturbed electronic properties of single molecules [2] and artificial engineered structures.

Aromatic hydrocarbons with large delocalized π-systems are promising as functional building blocks for future molecular electronics. Consequently, bond formation between individual organic molecules is essential. First achievements in this field were the imaging of bond formation between pentacene molecules and gold atoms [3], and the formation of coordination-bonded complexes [4].

Here, we present STM and STS studies of molecules comprising nitrile groups, which facilitate the formation of direct molecule-molecule bonds, adsorbed on ultrathin insulating films. We demonstrate such synthesis, characterization, and subsequent manipulation of anthracenedicarbonitrile dimers using the STM tip.

[1] J. Repp and G. Meyer, Applied Physics A **85**, 399 (2006).
[2] J. Repp et al., Physical Review Letters **95**, 225503 (2005).
[3] J. Repp et al., Science **312**, 1196 (2006).
[4] P. Liljeroth et al., submitted (2009).

O 41.25 Tue 18:30 Poster B1

A Scanning tunneling microscope study of single Phthalocyanine molecules on ultra thin insulating layers on different metal substrates — Jens Brede, •Jörg Schwöbel, Stefan Kuck, Germar Hoffmann, and Roland Wiesendanger — Institute of Applied Physics, University of Hamburg, Jungiusstrasse 11, D-20355 Hamburg, Germany

Recent scanning tunnelling microscopy (STM) investigations of pristine molecular features probed with sub-molecular resolution have opened a gateway for future single-molecule-devices. Among these experiments are the study of electron transport via electronic and vibronic excitations [1], the current induced switching of Hydrogen atoms[2] or the spin state of a central magnetic ion[3]. It shows that a sufficient electronic decoupling of the molecule from a metallic substrate is mandatory to grant access to the immaculate molecular properties.

Here, we study single Metal-Phthalocyanine (M-Pc) molecules on insulating layers on different noble metal surfaces with a low temperature STM operated at 6K.

We use atomic resolution to determine the adsorption site of the M-Pc with respect to the underlying layer and probe locally the electronic properties, in particular the highest occupied and the lowest unoccupied molecular orbital (HOMO & LUMO), by scanning tunnelling spectroscopy (STS).

[1] Proc. Natl. Acad. Sci. U. S. A., 2005, 102, 8832-8837 [2] Science, 2007, 317, 1203-1206 [3] Phys. Rev. Lett., 2009, 102, 167203

O 41.26 Tue 18:30 Poster B1

Reduction and Reoxidation of Thin NiO Films by CO and O_2 — •Oliver Höfert, Michael Peter Andreas Lorenz, Regine Streber, Wei Zhao, Karin Gotterbarm, Andreas Bayer, Christian Papp, and Hans-Peter Steinrück — Lehrstuhl für Physikalische Chemie II, Universität Erlangen-Nürnberg, Egerlandstr. 3, 91058 Erlangen

NiO is one important material in heterogeneous catalysis. Surface defects and dislocations are considered to be the active sites; furthermore the size of particles influences the catalysts activity. We studied the reactivity of different thin NiO films on Pd(100) by in situ XPS applying synchrotron radiation at BESSY II. Due to the large lattice mismatch of 7.8% between NiO and Pd, NiO films on Pd(100) are expected to exhibit many defects such as dislocations leading to a large number of potentially active sites. To determine the reactivity of different NiO films we studied their sensitivity towards CO oxidation. Our XPS data revealed that NiO films in the submonolayer regime are indeed reduced to metallic Ni by exposure to CO at 400 K. In contrast, closed layers of NiO show a significantly lower tendency towards CO oxidation. We attribute the observed reactivity to specific sites in close vicinity of the border of uncovered Pd regions and the NiO islands. The reduction of NiO by CO is fully reversible as could be shown by subsequent reoxidation of the metallic Ni by O_2.

This work was supported by BMBF (05 ES3XBA/5) and the DFG through the Cluster of Excellence ”Engineering of Advanced Materials”.

O 41.27 Tue 18:30 Poster B1

Tunneling Spectroscopy of Cl Divacancies in Ultrathin NaCl Films — •Jascha Repp[1], Gerhard Meyer[2], Sami Paavilainen[3], Fredrik Olsson[4], and Mats Persson[5] — [1]Institute of Experimental and Applied Physics, University of Regensburg, 93040 Regensburg, Germany — [2]IBM Research - Zurich, 8803 Rüschlikon, Switzerland — [3]Institute of Physics, Tampere University of Technology, 33720 Tampere, Finland — [4]Department of Applied Physics, Chalmers University, 41296 Göteborg, Sweden — [5]Surface Science Research Centre and Department of Chemistry, The University of Liverpool, Liverpool, L69 3BX, United Kingdom

In recent years, ultrathin insulating films on metal substrates have gained appreciable attention as templates for the study of individual adsorbates. Cl-vacancies in NaCl films on copper substrates exhibit an unoccupied state localized directly at the vacancy. In this work we study pairs of Cl vacancies in NaCl layers on copper substrates with mutual distances ranging from $\sim$4 Å to $\sim$12 Å by means of scanning tunneling spectroscopy and density functional theory. The close vicinity of these vacancies results in an coupling of the electronic states associated with the individual vacancies. The unoccupied states located directly at the vacancies couple and form a symmetric and an antisymmetric state in analogy to the bonding and antibonding states in a hydrogen molecule. Theoretical analysis shows that the energy splitting of these states is appreciably increased by the zero-point fluctuations of the phonons in the polar insulator.

O 41.28 Tue 18:30 Poster B1

First-principles study of the interaction of CO, CO_2 and water with NiO surfaces — •Tobias Schaub, Volker Strauss, and Bernd Meyer — Interdisziplinäres Zentrum für Molekulare Materialien ICMM, Universität Erlangen-Nürnberg

Nickel oxide is an important catalyst for the cracking and partial oxidation of hydrocarbons. Under reaction conditions CO, CO_2 and water are frequently present in the gas phase. The formation of carbonates and the partial hydroxylation of the NiO surfaces, however, often leads to a reduction of the catalytic activity of NiO due to a blocking of available surface sites for the hydrocarbon reactions. To elucidate the nature and stability of the surface carbonates and hydroxyl groups we have used DFT+U calculations to study the adsorption of CO, CO_2 and water on different structural models of ideal and defective NiO surfaces. We find that undercoordinated Ni sites activate CO_2 and stable surface carbonates are formed which are bound in a tridentate configuration, similar as previously observed for ZnO [1]. Water adsorbs molecularly or dissociatively, depending on the surface sites with a similar binding energy as CO_2. Therefore, a strong competition between CO_2 and water for the low coordinated Ni surface sites can be expected. Finally, the influence of O vacancies on the adsorption of CO, CO_2 and water will be discussed.

[1] Y. Wang et al. *Angew. Chem. Int. Ed.* 46 (2007) 5624

O 41.29 Tue 18:30 Poster B1

High-Dimensional Neural Network Potentials for Multicomponent Systems: First Applications to Zinc Oxide — •Nongnuch Artrith, Tobias Morawietz, Marcus Maschke, and Jörg Behler — Lehrstuhl für Theoretische Chemie, Ruhr-Universität Bochum, D-44780 Bochum, Germany

Recently, artificial Neural Networks (NN) trained to first-principles data have shown to provide accurate potential energy surfaces for systems containing a single atomic species. In this work we present an extension of the NN approach to multicomponent systems by introducing physically motivated terms to deal with long-range interactions. This is a necessary condition for studying binary systems and general multicomponent systems with significant charge transfer. The capabilities of the method are demonstrated for crystal structures, amorphous structures, clusters, and surfaces of zinc oxide as a benchmark system. We show that the predicted energies and forces are in excellent agreement with reference density-functional theory calculations.

O 41.30 Tue 18:30 Poster B1

A comparative Atomic Force Microscopy study on the preparation of the polished (111) and cleaved (100) surfaces of Magnesium Fluoride (MgF2). — •Patrick Meisner, Enrico Barletta, and Klaus Wandelt — Inst. for phys. and theor. Chem., University of Bonn, Wegelerstr. 12 D-53115, Bonn, Germany

Alkaline earth fluorides are used for several applications in microelectronics, for example as protective coating and buffer layers for semiconductors. Because of its special optical attributes magnesium fluoride is also an important tool for the production of anti reflex coatings or for sealing Aluminium coated mirrors.Magnesium Fluoride is also used as catalyst in the chemical industry. Its birefringent effect makes it useful for non linear optics, and because of its wide transmitting window it is widely used for construction of high quality optical components. Consequently the finishing of the surface plays an important role on the performances of the final devices. The preparation of two different crystal faces, (111) and (100), was studied. Because of the low cleavage along the (111) surface, this surface orientation had to be prepared by cutting and polishing the crystal by abrasive submicrometer powders. On both surfaces, during cleaning of the fresh surface by thermal processes, morphological and structural effects were observed. Even during the molecular beam epitaxial growth, surfaces of different grade were achieved following different deposition conditions and post-deposition treatments. The achieved results point out to a big influence of the thermal treatments and to a better grade of the final surface after a reconstruction by MBE deposition of some mono-layers of fresh MgF2.

O 41.31 Tue 18:30 Poster B1

Temperature dependent angle resolved photo-emission spectroscopy of quasi one-dimensional organic conductor tetrathiofulvalene tetracyanoquinodimethane (TTF-TCNQ) thin films — •Martin Laux[1], Indranil Sarkar[1], Julia Demokritova[1], Jia Wei[1], Andreas Ruffing[1], Vita Solovyeva[2], Milan Rudloff[2], Michael Huth[2], and Martin Aeschlimann[1] — [1]Department of Physics and Research Center OPTIMAS, University of Kaiserslautern, Germany — [2]Physikalisches Institut, J. W. Goethe-Universität, Frankfurt am Main, Germany

The organic conductor TTF-TCNQ is known to form a classic quasi-one-dimensional metal that possibly can be used to test non-Fermi-liquid behavior in 1D Hubbard model systems [1]. Here we report on temperature dependent angle resolved photo-emission spectroscopy (ARPES) on TTF-TCNQ films deposited on KCl(100) substrate. The ARPES spectrum exhibits transfer of spectral weight near Fermi energy over a wide energy range of ~ 0.2 eV, comparable to bandwidth, for temperatures $80 \text{ K} < T < 300 \text{ K}$. Such a large spectral weight transfer compared to the thermal energy $k_B T$, indicates non-Fermi liquid behavior that cannot be explained by electron-phonon coupling and suggests the formation of 1D Hubbard model [2].

[1] N. Bulut et. al., Phys. Rev. B **74**, 113106 (2006)

[2] R. Claessen et. al., Phys. Rev. Lett. **88**, 096402 (2002)

O 41.32 Tue 18:30 Poster B1

Effects of Electron Irradiation on the Composition, Energetics and Structure of the Calcium/Poly(3-Hexylthiophene) (P3HT) Interface — •F. Bebensee[1], J. F. Zhu[2], J. H. Baricuatro[3], J. A. Farmer[3], H.-P. Steinrück[1], C. T. Campbell[3], and J. M. Gottfried[1] — [1]Universität Erlangen-Nürnberg, Lehrstuhl für Physikalische Chemie II — [2]University of Science and Technology of China — [3]University of Washington, Department of Chemistry

Energetics, composition and structure of Ca deposited on the π-conjugated polymer P3HT was studied with adsorption microcalorimetry, atomic beam/surface scattering, ion scattering spectroscopy and high-resolution XPS. Ca/P3HT is prototypical for interfaces between low work-function metals and semiconducting polymers, which are typically found in organic photovoltaic devices. The interface properties often play a crucial role with respect to the device performance, e.g. charge injection rates depend on the overlap of wave functions at the interface. Despite its outstanding importance, only little is known about the interface formation in these systems beyond their morphologies. Here, we extend our previous studies of Ca on pristine P3HT surfaces and present new results on the influence of electron irradiation (E_{kin}=100 eV) on the interface formation. While the adsorption energy of Ca remains unaltered, the sticking probability increases dramatically. This effect is related to changes in the C 1s XP spectra and, by comparison with results for pristine P3HT, provides a detailed mechanistic understanding of the impact of electron irradiation.

O 41.33 Tue 18:30 Poster B1

Metal complexation and monolayer self-assembly of the bio-organic semiconductor Alizarin — Neeti Uppal[1,5], Norbert Gast[1,3], Martin Bueno[4], Wolfgang M. Heckl[2,3], and •Frank Trixler[1,2,3] — [1]Dept. Earth and Environmental Sciences, Ludwig-Maximilians-Universität München (LMU) & Center for NanoSciences (CeNS), München, Germany — [2]Dept. of Physics, Technische Universität München (TUM), Garching, Germany — [3]Zentrum Neue Technologien, Deutsches Museum, München, Germany — [4]Fakultät Feinwerk- und Mikrotechnik, Physikalische Technik, Hochschule München, Germany — [5]Institut für Physik, Universität Augsburg, Germany

Organic Solid/Solid Wetting Deposition (OSWD) (Trixler et al.: Chem.Eur.J. 13 (2007), 7785) enables to deposit insoluble molecules such as organic pigments and semiconductors on substrate surfaces under ambient conditions. We explore the potential of OSWD to grow and manipulate monolayers of biomolecules and their chelates on graphite and use Alizarin as a model system - a natural organic compound which occurs mainly as an anthraquinone glycoside in plants.

Our investigations via Scanning Tunneling Microscopy (STM), Tunneling Spectroscopy (TS) and Molecular Modelling reveal that OSWD works also with bio-organic molecules and chelate complexes and show that the advantages of OSWD (self-assembly under ambient conditions in a non-solvent environment, nanomanipulation via molecular extraction) can all be tapped.

O 41.34 Tue 18:30 Poster B1

Self-assembled monolayers on gold containing azobenzene ligands — •Robert Ossig[1], Florian Vogel[1], Frauke Bretthauer[2], Ulrich Siemeling[2], and Frank Träger[1] — [1]Institut für Physik and Center for Interdisciplinary Nanostructure Science and Technology (CINSaT), Universität Kassel, Kassel, Germany — [2]Institut für Chemie and Center for Interdisciplinary Nanostructure Science and Technology (CINSaT), Universität Kassel, Kassel, Germany

Self-assembled monolayers (SAMs) of photoresponsive molecules yield a wide range of applications, for example, for optical devices. At present the SAMs usually consist of small anchor groups based on symmetric disulfids or thiols and large functional groups. However, the densely packed arrangement of these molecules on substrates causes a steric hindering for photoisomerisation. Hence, larger anchor groups or molecules with more than one anchor group are necessary to provide more space between the functional groups. For this purpose we have recently synthesised molecules consisting of a photoresponsive functional and two anchor groups. The functional group is based on azobenzene-derivatized 1,2-dithiolanes which can be switched between their *cis* and *trans* isomers. In this contribution we present fundamental adsorption studies of these molecules and the SAM formation, investigated by means of optical second harmonic generation. We demonstrate that for a concentration of 50 μmol/l the second order Langmuir kinetics describes the adsorption best. For a deeper insight of the involved processes concentration dependent measurements as well as ellipsometry and scanning-tunnelling microscopy have been conducted.

O 41.35 Tue 18:30 Poster B1

Dominant spin-relaxation processes in the organic semiconductor CuPc determined by means of spin-resolved two-photon photoemission — •Kathrin Koffler, Sabine Neuschwander, Jan-Peter Wüstenberg, Mirko Cinchetti, and Martin Aeschlimann — Department of Physics, University of Kaiserslautern, 67663 Kaiserslautern, Germany

Organic semiconductors (OSC) are considered as ideal materials for spintronic devices due to their chemical flexibility, their low production costs and the intrinsically low spin-orbit coupling [1]. A fundamental prerequisite for organic spintronic devices is an efficient spin injection from a ferromagnetic electrode into the OSC. With spin-resolved two-photon photoemission, a model system consisting of a thin cobalt film and the OSC copper phthalocyanine (CuPc) has been studied with focus on interfacial effects on spin injection and on the spin transport properties of CuPc [2]. In this contribution we extend the approach presented in [2] to determine the temperature dependence of the spin diffusion length in CuPc. This allows to draw conclucions about the spin relaxation mechanisms responsible for the polarization decay in the OSC CuPc.

[1] V.A. Dediu et al., Nature Mater. 8, 707-716 (2009)

[2] M. Cinchetti et al., Nature Mater. 8, 115-119 (2009)

O 41.36 Tue 18:30 Poster B1

Characterization of the Interface Interaction of Cobalt on Top of Copper- and Iron-Phthalocyanine — •Felix Schmitt, Jens Sauther, Yaou Smets, Stefan Lach, and Christiane Ziegler — Department of Physics, University of Kaiserslautern, D-67663 Kaiserslautern, Germany

A promising field of applications of organic semiconductors arises from the combination of organic materials and spintronics. In this field a deeper understanding of injection and transport as well as manipulation of spinpolarized charge carriers is necessary. The charge injection of organic semiconductor devices in general is co-determined by the geometric and the electronic structure of the specific interface and analogous behaviour is expected for the spin injection.

This motivates investigations of the interface between ferromagnetic metallic substrates and organic semiconductors. Here, a photoemission- (UPS, IPES and XPS) and IR-study of ferromagnetic cobalt on top of copper- and iron-phthalocyanine is presented. These measurements suggest chemical reactions in the interfacial region: For example, an oxidation of the Co atoms as well as a reduction of the Cu at the interface between Co and CuPc could be detected. Furthermore a diffusion of the Co into the layers of the organic substrate and the formation of Co clusters on the metal phthalocyanine surface occur.

O 41.37 Tue 18:30 Poster B1

A Fast Model for Estimating Work-Function Modifications Induced by Organic Charge-Transfer (Sub)monolayers — •Oliver T. Hofmann[1], Benjamin Bröker[2], Ralph-Peter

Blum[2], Ferdinand Rissner[1], Gerold M. Rangger[1], Ralph Rieger[3], Klaus Müllen[3], Norbert Koch[2], and Egbert Zojer[1] — [1]Institute of Solid State Physics, Graz University of Technology, Petersgasse 16, 8010 Graz, Austria — [2]Institut für Physik, Humboldt-Universität zu Berlin, Newtonstrasse 15, 12389 Berlin, Germany — [3]Max Planck Institute for Polymer Research, 55128 Mainz, Germany

Calculating work-function modifications for flat-lying conjugated molecules on extended metal surfaces using density functional theory (DFT) is an extremely resource intensive task. This prevents fast screening of new molecules for their potential to optimize metal work functions for good electron or hole injection in organic electronic devices. We present a semi-classical model, which avoids that problem. This is achieved by identifying the dominant processes occurring at the interface between metal and adsorbate in the pinning-regime, which are then parameterizing their description using band-structure DFT calculations for a small training set With the resulting interdependent equations at hand, only simple gas-phase calculations are needed to predict the work-function changes induced by new molecules. The model is tested for ten molecules on three different metal surfaces, where it shows excellent agreement with photoelectron spectroscopy data on these systems.

O 41.38 Tue 18:30 Poster B1

Tuning surface properties via distributing dipoles in self-assembled monolayers on Au(111) — •David A. Egger[1], Ferdinand Rissner[1], Gerold M. Rangger[1], Oliver T. Hofmann[1], Lukas Wittwer[1], Georg Heimel[2], and Egbert Zojer[1] — [1]Institute of Solid State Physics, Graz University of Technology, Austria — [2]Institut für Physik, Humboldt-Universität zu Berlin, Germany

Quantum-mechanical calculations are performed to study the interface between the Au(111) surface and self-assembled monolayers (SAMs) of π-conjugated molecules. Dipolar pyrimidine rings act as building units to tune the dipole moments of the SAMs in a systematic way via the number of rings in the molecular backbone. The resulting work-function modifications and the energetic alignment of the electronic states in the SAM with respect to the Fermi level are analyzed. Compared to SAMs, where strong dipole moments are introduced by end-group substitutions on otherwise non-polar molecules, an entirely different evolution of those two quantities with the backbone length is found for the present systems, where dipoles are built directly into the backbone. The distributed-dipole approach provides an additional handle for tuning surface properties and the achievable work-function modifcations can be huge. In fact, they are limited only by pinning of the metal Fermi-level at the frontier molecular states.

O 41.39 Tue 18:30 Poster B1

Study of the electronic properties of cobalt phthalocyanine thin films on poly- and single crystalline gold substrate by photoemission spectroscopies — •Fotini Petraki, Heiko Peisert, and Thomas Chassé — Institut für Physikalische und Theoretische Chemie, Universität Tübingen, Auf der Morgenstelle 8, D-72076 Tübingen, Germany

Organic electronics is a new and fast developing sector of microelectronics which aims either to cover applications that are not accessible to conventional silicon semiconductor technology or to decrease the cost of the devices with the use of organic materials. In organic devices, the interfaces between the electrodes and the organic films play an important role, as they determine the injection efficiency by establishing barriers for carrier injection in the organic active layer. Therefore, interface studies contribute to the understanding and improvement of the device performance. In the present study, model experiments concerning the interface formation between Cobalt Phthalocyanine (CoPc) ultra thin films and gold substrate were carried out by X-ray and Ultra-Violet photoelectron spectroscopies (XPS, UPS) as well as Auger spectroscopy (XAES). The experimental data indicate a quite strong interaction between the organic molecules and the metallic substrate, which is confirmed by the presence of additional features at the characteristic Co2p and CoLVV peaks of the CoPc film at the very first steps of deposition. The valence band structure of CoPc is well resolved while new features are also present for monolayer coverage. Screening mechanisms in XPS and XAES are also discussed.

O 41.40 Tue 18:30 Poster B1

Determination of Energy Levels in Organic Bulk-Heterojunction Systems — •Holger Wetzstein[1], Stefan Krause[1], Moritz Liedtke[2], Julia Kern[2], Achim Schöll[1], Carsten Deibel[2], and Friedrich Reinert[1] — [1]Experimental Physics VII, Julius-Maximilians-University of Würzburg, D-97074 Würzburg — [2]Experimental Physics VI, Julius-Maximilians-University of Würzburg, D-97074 Würzburg

In order to improve the efficiency of electronic devices based on organic semiconducting materials the detailed knowledge about the exact position of the energy levels responsible for charge transport is crucial. The experimental determination is particularly complicated for bulk heterojunctions of p- and n-conducting materials in terms of sample preparation, film morphology and distinction of the different spectroscopic signatures. We investigated four promising materials for organic photovoltaic devices: the electron donor poly(3-hexylthiophene-2,5-diyl) (P3HT) and the three electron acceptors [6,6]-phenyl-C_{61} butyric acid methyl ester ($PC_{60}BM$), its bisadduct analogue (bis-$PC_{60}BM$) and [6,6]-phenyl-C_{71} butyric acid methyl ester ($PC_{70}BM$). Thin films of pristine materials as well as bulk heterojuction samples of P3HT:$PC_{60}BM$, P3HT:bis-$PC_{60}BM$ and P3HT:$PC_{70}BM$ were examined with respect to their valence levels using ultraviolet photoelectron spectroscopy (UPS).

O 41.41 Tue 18:30 Poster B1

Preparation of $CuInS_2$ by sulfurization of CuIn samples — •Alexandra Dombrowa, Carsten Lehmann, and Christian Pettenkofer — Helmholtz-Zentrum Berlin, Berlin, Deutschland

In search for a substitute for the heavy metal Cd in thin film solar cells based on p doped $CuInS_2$ and n doped ZnO it is proposed to use ZnS instead of CdS as buffer layer material [1,2]. By applying a MOMBE process based on diethylzinc and water a ZnS buffer layer formed on an $CuInS_2$(112) topped with CuS-segregations before epitaxial ZnO growth took place. This ZnO-ZnS-CIS interface yielded a very promising band aligment for photovoltaic applications [2]. For further band aligment investigations, which are presented in a separate talk entitled 'Band alignment studies of ZnO-ZnS-CIS interfaces', we studied polycristalline CIS films prepared in-situ by sulfurization of CuIn films. We present the results of our in-situ preparation and anaylsis of on various substrates. CuIn substrate films with a thickness of 10-100nm were prepared in-situ by MBE on Mo foil and epitaxial GaAs (111) and (100) substrates. Additionally, we used production-line quality CuIn films of 1-2 μm thickness prepared ex-situ by sputtering. The substrates and the sulfurized samples were investigated in-situ by XPS and UPS. Comparing the electrical and electronic properties of ZnS/ZnO interfaces prepared by MOMBE to epitaxially interfaces we discuss the implications with respect to an in-line process for the fabrication of the thin film solar cell devices. [1] M. Bär, et. al., Journal of Applied Physics 99 (2006) [2] S. Andres, et. al., Thin Solid Films 518 (2009)

O 41.42 Tue 18:30 Poster B1

Tuning and Guiding Electron Current through Ag-SnPc-Ag Junctions — •Yongfeng Wang[1], Jörg Kröger[1], Richard Berndt[1], Héctor Vázquez[2], Mads Brandbyge[2] und Magnus Paulsson[3] — [1]Institut für Experimentelle und Angewandte Physik,Christian-Albrechts-Universität zu Kiel,D-24098 Kiel,Germany — [2]Department of Micro and Nanotechnology, NanoDTU, Technical University of Denmark, DK-2800 Kongens Lyngby , Denmark — [3]Department of Physics, Kalmar University, Sweden

The transport of electrons through molecules is relevant for processes in many branches of science and has found applications in electrical engineering. Nevertheless, the understanding and, in particular, control of electron flow through metal-molecule-metal junctions on a (sub-)nanometre scale are still incomplete. Here, we report on guided electron transport through tin phthalocyanine (SnPc) contacted by silver electrodes, the tip of a cryogenic scanning tunneling microscope and a Ag(111) single crystal. By systematically modifying molecular orientations, molecule-substrate interactions, and the electrode atomic structure, the electron conductance of Ag-SnPc-Ag junctions is tuned from 1 to 25 microsiemens. Moreover, current flow through these junctions is directionally guided as visualized by supporting nonequilibrium Green's function calculations. Funding by the Deutsche Forschungsgemeinschaft through SFB 677 is acknowledged.

O 41.43 Tue 18:30 Poster B1

Photoemission Study under Artificial Solar Irradiation: Interface Studies of the Systems Ag/C_{60}/CuPc and Ag/CuPc/C_{60} — •Mathias Fingerle[1], Felix Schmitt[1], Ingmar Bruder[2], Stefan Lach[1], and Christiane Ziegler[1] — [1]Department of Physics, University of Kaiserslautern, 67663 Kaiserslautern, Germany — [2]BASF, 67056 Ludwigshafen, Germany

During the last 3 decades research on organic solar cells has been performed and has gained increasing attention. This is due to the fact that devices can be produced at large scale and low cost. Most of today's prototype devices are of hybrid nature, i.e. the electrodes are made from inorganic materials whereas the active layers are composed by two or more organic thin films.

Here, fullerene (C_{60}) as n-type and copper phthalocyanine (CuPc) as p-type semiconductor were used as active organic materials. The electronic properties of the organic interfaces in layer structures composed of $Si/SiO_2/Ag/C_{60}/CuPc$ and $Si/SiO_2/Ag/CuPc/C_{60}$ were investigated by means of UPS and IPES. For the first time, UPS measurements were carried out under additional artificial solar irradiation. In particular for the interface $CuPc/C_{60}$, interesting changes in electron affinity and work function could be determined.

O 41.44 Tue 18:30 Poster B1

Chemical trends in the metal-substrate interaction for the reactivity of adsorbed Pt atoms — •Chong Gao and Axel Gross — Institut für Theoretische Chemie, Universität Ulm, D-89069 Ulm, Germany

Catalysts typically consist of small metal particles deposited on a 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 up to four Pt atoms adsorbed on TiO_2, Si, Ru 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 41.45 Tue 18:30 Poster B1

Non-equilibrium structures in Ultrathin V-Oxide films on Rh(111) under Reaction Conditions: The O2 + H2 reaction with and without alkali promotion — •Martin Hesse, Florian Lovis, and Ronald Imbihl — Institut für Physikalische Chemie und Elektrochemie, Leibniz-Universität Hannover, Callinstr. 3-3a, D-30167 Hannover, Germany

As a model system for vanadium-oxide based catalysts we prepared ultrathin vanadium oxide films on a Rh(111) surface1. At 400°C 0.1, 0.25 and 2.4 ML of vanadium were evaporated in oxygen with p(O2)=2*10-7 mbar. After characterization with LEED and Auger electron spectroscopy the films were subjected to the O2 + H2 reaction using photoemission electron microscopy (PEEM) as spatially resolving method. After evaporation a large variety of differently ordered Rh(111)/V/O phases were identified in LEED. The O2 + H2 reaction was studied in the 10-8 - 10-5 mbar range at temperatures between 400 and 500°C. With PEEM we observe that under reaction conditions the film is no longer homogeneous but reaction fronts and stationary Turing-like patterns develop. In the evaporated V-film we find partially ordered patterns which are very stable and change only very slowly after turning off the gases. The patterns induced by the reaction are discussed in the context of the concept of reactive phase separation. When we promote the Rh(111)/V/O-system with alkali metals turbulent spatialtemporal patterns are found.

[1] Surnev, S., M.G. Ramsey, and F.P. Netzer, Progress in Surface Science, 2003. 73, 117.

O 41.46 Tue 18:30 Poster B1

Ab initio molecular dynamics simulation of electronic energy dissipation: HCl/Al(111) — •Michael Grotemeyer and Eckhard Pehlke — Institut für Theoretische Physik und Astrophysik, Universität Kiel, Germany

The scattering of vibrationally excited HCl molecules from Au(111) has been studied experimentally and interpreted in view of electronically nonadiabatic processes [1]. We present *ab initio* molecular dynamics simulations of the scattering of highly vibrationally excited HCl molecules at Al(111). The time-dependent Kohn-Sham equations are integrated numerically for the electrons, and the positions of the ions follow Ehrenfest dynamics. The electronic excitation along the trajectory is obtained from comparison of the time-dependent electronic structure with the electronic ground state at the respective frozen-in ionic positions. Reducing numerical expenses, the simulations are carried through for mass-scaled systems. Under the assumption of linear friction, the dissipation is extrapolated to the physical masses of the ions [2]. For not vibrating HCl molecules we obtain only a faint energy transfer into electron-hole pairs. Electronic energy dissipation is significant for a strongly vibrating HCl molecule in front of Al(111). Different geometries with either the H-or Cl-atom pointing towards the surface are compared. We note that electronic friction has turned out not to be enhanced for a situation where the H-atom points towards the surface and oscillates in the charge density tail of the metal.

[1] I. Rahinov *et al.*, J. Chem. Phys. **129**. 214708 (2008).

[2] M. Lindenblatt and E. Pehlke, Surf. Sci. **23**, 5068 (2006).

O 41.47 Tue 18:30 Poster B1

Cluster-induced desorption of alkali halides from metals and insulators - influence of substrate and adsorbate configuration — B.-J. Lee[1], C.R. Gebhardt[2], H. Schröder[3], K.L. Kompa[3], and •M. Dürr[1] — [1]Fakultät Angewandte Naturwissenschaften, Hochschule Esslingen, Esslingen — [2]Bruker Daltonik GmbH, Bremen — [3]Max-Planck-Institut für Quantenoptik, Garching

Cluster-induced desorption is a versatile tool for the investigation of surface adsorbates. During cluster surface collision, the system is heated to high temperatures on a very short time scale, thus activating reactions not accessible by means of conventional heating. As an example, fragmentation-free desorption of biomolecules as large as 6000 u from various surfaces has been demonstrated [1].

For surface adsorbates prepared wet-chemically from alkali halide solutions, we show that the surface configuration, especially the influence of water molecules, can be monitored by cluster-induced desorption. As long as the anions are effectively screened by a hydration shell, they are efficiently desorbed by means of cluster impact. To higher surface temperatures, the hydration shell is lost and a strong adsorbate-surface bond prevents desorption of the anions. Cations are seen to desorb from metals via a neutral desorption channel with subsequent charge separation in the cluster whereas only a positive signal is observed for desorption from insulators.
[1] Gebhardt *et al.*, Angew. Chem. Int. Ed. **48**, 4162 (2009).

O 41.48 Tue 18:30 Poster B1

Adsorption and reactions of unsaturated hydrocarbon molecules on stepped Pt surfaces — Erik Darlatt[1], Sandra Wickert[1], Michael P. A. Lorenz[2], Regine Streber[2], Christian Papp[2], Hans-Peter Steinrück[2], and •Reinhard Denecke[1] — [1]Wilhelm-Ostwald-Institut für Physikalische und Theoretische Chemie, Universität Leipzig, Linnestr. 2, 04103 Leipzig, Germany — [2]Lehrstuhl für Physikalische Chemie II, Universität Erlangen-Nürnberg, Egerlandstr. 3, 91058 Erlangen, Germany

Using in-situ high-resolution XPS at the synchrotron radiation source BESSY II, bonding configurations of ethylene and propylene have been investigated on stepped Pt surfaces. Ethylene adsorbs on Pt(355) with significant spectral changes in C 1s compared to Pt(111), resulting from a specific step related feature. The saturation coverage related to this more strongly bound species amounts to about 1/3 of the terrace population. For propylene, two different C 1s binding energies can be related to the three carbon atoms. On Pt(355), a structureless peak results from additional step contributions. For both adsorbates, the respective alkylidin species appears as the major dissociation intermediate. Differences in thermal reactivity between flat and stepped Pt are observed for both molecules in temperature-programmed (TP-) XPS experiments.
This work was supported by BMBF (05 ES3XBA/5).

O 41.49 Tue 18:30 Poster B1

Locally resolved kinetics of catalytic CO oxidation on polycrystalline platinum — •Diana Vogel[1,2], Christian Spiel[1], Yuri Suchorski[1], Wolfgang Drachsel[1], Robert Schlögl[2], and Günther Rupprechter[1] — [1]Institute of Materials Chemistry, Vienna University of Technology, Austria — [2]Fritz Haber Institute (Max-Planck-Gesellschaft), Berlin, Germany

In this contribution we present a microscopic study of the kinetics of the catalytic CO oxidation reaction on a polycrystalline Pt foil consisting of (100)-, (110)- and (111)-type domains (∼100 μm) under reaction conditions (reactants pressure $\sim 10^{-5}$ mbar). The study was performed by combination of photoemission electron microscopy (PEEM) with mass-spectroscopy (MS). PEEM allows an *in situ* observation of the local kinetic phase transitions in the reaction, MS, in turn, provides the global kinetics. By combining the laterally resolved (PEEM) and global (MS) data we elucidate the role of the individual domains in the reaction and elaborate the contributions of the particular domains to the global kinetics. We show that the global kinetic phase diagram can be composed as a superposition of the local kinetic phase diagrams of the individual domains.

Furthermore, we compare the catalytic behaviour of the polycrystalline Pt foil with that of a Pt(111) single crystal and a sputtered Pt foil to show the influence of the surface morphology on the reaction kinetics. Increasing surface roughness shifts the kinetic phase diagram to lower temperature and higher partial CO pressure.

O 41.50 Tue 18:30 Poster B1

In-situ XPS and reactivity studies on different Au/TiO2 catalyst systems — •Martina Hank, Karif Dumbuya, Ole Lytken, Piotr Bobrowski, Bernhard Arnold, J. Michael Gottfried, and Hans-Peter Steinrück — Universität Erlangen-Nürnberg, Lehrstuhl für Physikalische Chemie II, Egerlandstr. 3, 91058 Erlangen, Germany

Nano-sized gold on oxidic substrates shows a high activity in heterogeneous catalysis which sharply contrasts the inertness of bulk gold. The origin of the catalytic activity and the nature of the active sites are still discussed controversially: Quantum size effects, low coordinated gold atoms, the substrate/gold perimeter interface or anionic as well as cationic gold species have been considered as possible candidates. We have studied surfaces of different gold-based catalysts using X-ray photoelectron spectroscopy (XPS) under ultra high vacuum conditions as well as with in-situ XPS in the presence of reactive gases (CO, O$_2$, propene and mixtures thereof) at pressures of up to 1mbar. These model systems include a Au/TiO$_2$ reference powder catalyst, a Au/TiO$_2$(110) planar model catalyst and a TiO$_2$/Au(111) inverse model catalyst. Comparison of the latter systems enables us to discriminate between cluster-size and interface related effects. Furthermore, we will discuss a novel reaction cell, which is used to study the activity of different model catalysts under ambient pressure conditions.

This work is supported by the DFG through grant GO 1812/1-1 and by the Cluster of Excellence "Engineering of Advanced Materials"

O 41.51 Tue 18:30 Poster B1

Cluster Model Studies on Catalytic Sulfidation of MoO$_3$ — Xue-Rong Shi[1,2], Mathis Gruber[2], •Klaus Hermann[2], and Jianguo Wang[1] — [1]State Key Laboratory of Coal Conversion, Institute of Coal Chemistry, Chinese Academy of Sciences, Taiyuan, Shanxi 030001, P.R. China; — [2]Fritz-Haber-Institut der MPG, Faradayweg 4-6, D-14195 Berlin and Sfb 546 "Transition Metal Oxide Aggregates", Berlin (Germany).

MoS$_2$-based catalysts, initially prepared from MoO$_3$, are known to yield high activity and selectivity for the production of mixed alcohols. This makes research on the sulfidation of MoO$_3$ quite important. Here we apply density-functional theory (DFT) together with large surface clusters (cluster code StoBe) to study the sulfidation of the MoO$_3$(010) surface as well as hydrogen adsorption at an atomic level. Surface oxygen is always found to bind more strongly with its substrate than its sulfur substitute with binding distances that are shorter for oxygen than for sulfur. Sulfur-oxygen exchange reactions are energetically preferred over sulfur adsorption at MoO$_3$(010). Further, sulfur binding is found to be facilitated by the existence of surface oxygen vacancies where sulfur substitution takes place preferentially at the singly coordinated O(1) site. Hydrogen adsorption at the perfect and sulfidic surface leads to stable OH, H$_2$O and SH, H$_2$S groups which are quite weakly bound and may easily adsorb. Thus, the presence of pre-adsorbed hydrogen facilitates oxygen and sulfur removal from the MoO$_3$(010) surface which is in qualitative agreement with earlier findings.

O 41.52 Tue 18:30 Poster B1

Homogeneity and catalytic activity of thin mesoporous Au/TiO$_2$ layers — •Matthias Roos, Menhild Eyrich, Gabriela Kucerova, Joachim Bansmann, and R. Jürgen Behm — Institute of Surface Chemistry and Catalysis, Ulm University, D-89069 Ulm, Germany

Structurally defined thin layers of homogeneous mesoporous Au/TiO$_2$ are investigated as model systems to bridge the gap between planar Au/TiO$_2$ model and powder catalysts. The dispersed mesoporous Au/TiO$_2$ catalysts were found to be significantly more active in the CO oxidation reaction [1] than catalysts based on non-porous TiO$_2$ powder (P25). Catalytically active thin Au/TiO$_2$ films are prepared by deposition of the Au/TiO$_2$ catalyst, e.g. via dip coating on planar oxide substrates. The structural integrity and the chemical properties of the obtained layers are characterized by electron microscopy methods and XPS, respectively. The local catalytic activity and homogeneity of the mesoporous Au/TiO$_2$ films for CO oxidation is studied by mass spectrometry, using a scanning mass spectrometer setup. Furthermore, IR measurements are planned in order to derive combined catalytic and in-situ spectroscopic information.

[1] Y. Denkwitz et al., *Appl.Catal.B* 91, **2009**, 470.
[2] M. Roos et al., *Rev.Sci.Instrum.* 78, **2007**, 084104.

O 41.53 Tue 18:30 Poster B1

Methanol oxidation over ZnO and Au/ZnO nanoparticles studied by vibrational spectroscopy — •Heshmat Noei[1], Martin Muhler[1], and Yuemin Wang[1,2] — [1]Lehrstuhl für Technische Chemie, Ruhr-Universität Bochum, D-44780 Bochum, Germany — [2]Lehrstuhl für Physikalische Chemie I, Ruhr-Universität Bochum, 44801 Bochum, Germany

Zinc oxide is one of the most studied materials due to its electrical, optical and catalytical properties and potential applications. The interaction of methanol with zinc oxide is a topic of fundamental and applied interest. In this work we report on the adsorption and oxidation of methanol over ZnO nanoparticles at a wide range of temperatures by employing a newly designed ultra-high vacuum infrared spectroscopy (UHV-FTIRS). Exposing the clean ZnO nanopowders to methanol at 110 K leads to the molecular adsorption, whereas at 300 K methanol is adsorbed dissociatively giving methoxy species. The FTIRS data further indicate the formation of two different methoxy species which are bound to the polar ZnO(000-1) and nonpolar ZnO(10-10) surfaces, respectively. During heating to higher temperatures, methoxy reacts partially with surface oxygen yielding formate species as confirmed by the appearance of formate-related IR bands. In addition, we could identify two different formate species, which are formed on ZnO(000-1) and ZnO(10-10) surfaces, respectively. Upon heating to 600 K, both formate species are decomposed completely. We have further studied methanol oxidation over Au/ZnO nanopartcles. The corresponding reaction mechanisms will be discussed in details.

O 41.54 Tue 18:30 Poster B1

Interaction of propene with an oxygen-precovered Au(110)*(1x2) surface — •Inga Spreine and Klaus Christmann — Institut für Chemie und Biochemie, Freie Universität Berlin, Takustr. 3, 14195 Berlin, Germany

We have studied the interaction of propene with the (1x2)-reconstructed $Au(110)$ surface covered with well-defined amounts of reactive atomic oxygen species by means of thermal reaction mass spectrometry. The chemisorbed O atoms were obtained by electron-bombarding an equilibrium coverage of physisorbed oxygen molecules at $T = 35$ K and $p(O_2) = 2 \cdot 10^{-8}$ mbar. The presence and amount of reactive O was monitored and controlled by the well-known TD states appearing between 450 and 550 K [1]. After dosing defined amounts of propene at $T = 90$ K we looked for possible partial and total oxidation products and their fragments. Desorption of the total oxidation products CO_2 (m/z 44) and H_2O (m/z 18) occurs between 170 and 520 K and represent the majority of the reaction products. Nevertheless, we were able to also detect minor amounts of partial oxidation products like propene oxide (m/z 58 and 31) and acrolein (m/z 55 and 56). The formation of acrylic acid (m/z 72) and acetone (m/z 43), however, could not be observed. Our results are discussed and compared with similar previous investigations on the $Au(111)$ [2] and the $Au(100)$ and $Au(111)$ surfaces [3].

[1] M. Gottfried et al., Surf. Sci. 511 (2002) 65 [2] X. Deng et al., J. Phys. Chem. B 110 (2006) 15982 [3] K.A. Davis and D.W. Goodman, J. Phys. Chem. B 104 (2000) 8557

O 41.55 Tue 18:30 Poster B1

Femtosecond EUV photoelectron spectroscopy of phase transitions — •Hatem Dachraoui[1], Christian Oberer[1], Günter Obermeier[2], Martin Michelswirth[1], Siegfried R. Horn[2], and Ulrich Heinzmann[1] — [1]Molecular and Surface Physics, Bielefeld University — [2]Experimental Physics II, Universität Augsburg

The thermo-induced insulator-metal phase transition in Vanadium dioxide (VO2) was investigated by use of a combination of a femtosecond EUV light source with time-of-flight (TOF) analysis of the emitted photoelectrons. The observed spectra give evidence of the changes in the electronic structure depending on temperature. Based on an analysis of the V3p- core level shift we get access to structural deviation of the VO2 and the changes of the density of states near the Fermi level responsible for the phase transition. The shift we obtained manifests this transition with its characteristic hysteresis.

O 41.56 Tue 18:30 Poster B1

In-situ XRD studies on post deposition annealed iron oxide thin films — •Florian Bertram[1], Carsten Deiter[1], Kathrin Pflaum[1], Oliver H. Seeck[1], Martin Suendorf[2], and Joachim Wollschläger[2] — [1]HASYLAB at DESY, Notkestr. 85, D-22607 Hamburg, Germany — [2]Fachbereich Physik, Universität Osnabrück, Barbarastr. 7, D-49069 Osnabrück, Germany

Because of their magnetic properties, iron oxide thin films are of interest for spintronic devices. Also, they can be used for model catalyst studies. Due to the small lattice mismatch to all iron oxide phases, MgO is a good choice as a substrate.

Here, we present studies on highly oxidized iron oxide films epitaxially grown on MgO(001), which have been annealed under vacuum conditions at beamlines BW2, W1 and P08 at DESY. For this purpose a UHV sample cell with heating and cooling capacity was developed.

Before annealing the sample it was analyzed by XRR and XRD. During the annealing process we performed CTR scans at the $(002)_{BULK}$ MgO peak, where all iron phases also have peaks. After cooling down the sample it was again analyzed by XRR and XRD.

Our analysis of the XRD measurements using kinematic diffraction theory shows a decrease in the iron oxide lattice constant pointing to a reduction of the iron oxide film.

O 41.57 Tue 18:30 Poster B1

Deposition of Fe nanoparticles on thin Co(0001) films — •Volker Hückelkamp[1], Wolfgang Rosellen[1], Christian Kleinhans[1], Furkan Bulut[1,2], Joachim Bansmann[2], Armin Kleibert[3], and Mathias Getzlaff[1] — [1]Institute of Applied Physics, University of Düsseldorf, Germany — [2]Department of Surface Chemistry, Ulm University, Germany — [3]Swiss Light Source at the Paul Scherrer Institute, Villigen, Switzerland

In recent years, 3d-metal nanoparticles are characterised by increasing importance, especially because of their magnetic properties which significantly differ from bulk behaviour. In this contribution we focus on Fe nanoparticles being deposited on thin Co films which are prepared on a W(110) crystal and exhibit a thickness between 1 and 15 ML. These films are acting as supporting material for the nanoparticles and are characterised by Auger electron spectroscopy (AES), low energy electron diffraction (LEED) and scanning tunneling microscopy (STM). Mass filtered Fe nanoparticles with a diameter ranging from 3 nm to 15 nm are produced by a continuously working arc cluster ion source (ACIS) and deposited on thin Co(0001) films under UHV condition in order to avoid any influence due to oxidation and contamination. We will discuss their structural properties and correlate them with their magnetic behaviour investigated by X-ray magnetic circular dichroism (XMCD)[J.Bansmann, A.Kleibert, Appl. Phys. A **80**, 957 (2005)].

O 41.58 Tue 18:30 Poster B1

Influence of temperature on the shape of deposited nanoparticles — •Wolfgang Rosellen[1], Georg Oeltzschner[1], Christian Kleinhans[1], Volker Hückelkamp[1], Furkan Bulut[1,2], Joachim Bansmann[2], Armin Kleibert[3], and Mathias Getzlaff[1] — [1]Institute of Applied Physics, University Düsseldorf — [2]Dep. of Surface Chemistry, Ulm University — [3]Paul Scherrer Institute, Switzerland

In this contribution we focus on the temperature behaviour of mass filtered Fe, Co and FeCo nanoparticles with diameters between 3 nm and 15 nm deposited on W(110). In RHEED experiments the orientation of mass filtered deposited Fe nanoparticles could be determined [1]. It was shown that small deposited Fe particles with diameter being less than 4 nm exhibit a spontaneously alignment, whereas larger particles with diameter of about 13 nm are randomly oriented on the W(110) surface. The temperature depending melting and orientation of deposited *3d*-metal nanoparticles produced by a continuously working arc cluster ion source (ACIS) will be discussed. The shape of the deposited nanoparticles is investigated in-situ by scanning tunneling microscopy (STM).

[1] A. Kleibert, A. Voitkans, and K. H. Meiwes-Broer, (submitted).

O 41.59 Tue 18:30 Poster B1

STM-Study of Cu growth on ZnO and TiO_2 Surfaces — •Martin Kroll[1], Abelhadi Chakir[1], Thomas Kuschel[1], Thomas Löber[1], Renate Wansing[1], Vadim Schott[2], Christof Wöll[2], and Ulrich Köhler[1] — [1]Experimental Physics IV, Ruhr-Universität Bochum, Germany — [2]Physical Chemistry I, Ruhr-Universität Bochum, Germany

The growth of Cu on $ZnO(10\bar{1}0)$ and $TiO_2(110)$ single crystal surfaces was studied as a first step to understand complex catalytically active systems often consisting of small metal clusters on metal oxide surfaces. For local STM studies flat and clean surfaces are needed. On $ZnO(10\bar{1}0)$ the influence of the UHV preparation conditions and the substrate orientation (sample miscut) on the large scale morphology was studied [1].

Cu was deposited on $ZnO(10\bar{1}0)$ by MOCVD. Thermal treatment resulted in a decreasing Cu coverage with increasing temperature up to 670K as already shown for Cu MBE depositon on ZnO(0001) [2]. Chemical analysis of the reaction of the Cu clusters with the ZnO substrate was done by XPS measurements.

Additionally, MBE Cu-growth with comparable coverage and similar thermal treatment on rutile $TiO_2(110)$ was studied. In this case no decrease in Cu coverage up to annealing temperature of 670K was detected.

[1] M.Kroll et al., Surf. Sci. **603**, L49 (2009)
[2] M.Kroll, U. Köhler, Surf. Sci. **601**, 2182 (2007)

O 41.60 Tue 18:30 Poster B1

Thermal Boundary Conductance of Bi/Si-Heterolayers: An Ultra-Fast Time-Resolved Electron Diffraction Study — •Simone Möllenbeck, Anja Hanisch-Blicharski, Annika Kalus, Boris Krenzer, Martin Kammler, and Michael Horn-von Hoegen — Department of Physics and Center for Nanointegration Duisburg-Essen (CeNIDE) Universität Duisburg-Essen, D-47057 Duisburg, Germany

The transient heating and cooling of hetero epitaxial thin film systems after fs-laser excitation with ps time resolution was studied by means of ultra fast time resolved electron diffraction in a grazing reflection geometry (RHEED). Diffraction patterns taken at different delays between pumping laser pulse and probing electron pulse are converted to the film temperature using the Debye-Waller effect. We present results on ultra thin epitaxial Bi(111) films on Si(001) and Si(111) substrates. For a 6 nm thin Bi-film a rapid increase of the surface temperature from 80 K up to 190 K upon laser excitation is followed by a slow exponential decay with a decay constant of 640 ps which is dominated by total internal reflection of the phonons at the hetero interface between film and substrate. A linear dependence, as predicted by the theoretical models, between film thickness and decay constant can be observed for the Bi-films on Si(111) down to 2.5 nm thickness. In contrast to this we observe a constant cooling rate for the Bi/Si(100) system for films thinner than 6 nm. The extreme low cooling rate for these thin films is determined not longer by the travel time through the film but by the mean free path of the phonons.

O 41.61 Tue 18:30 Poster B1

DFT calculations on influence of co-adsorbed Cl on the self-diffusion on Au(100) — •Mostafa Mesgar, Josef Anton, John A Keith, and Timo Jacob — Uni Ulm, Albert-Einstein-Allee 47

Adatom and vacancy diffusions play crucial roles in adsorption, desorption, crystal growth, and coarsening on metal surfaces. While several experimental and theoretical studies focused on the formation and diffusion of point defects on terraces, leading to a detailed understanding, much less is known about diffusion at steps and kink sites, even though this plays an important role in processes such as metal deposition and dissolution, Ostwald ripening, island and step fluctuations. Using *ab initio* density-functional theory, we investigated the self-diffusion behavior of adatoms on Au(100) surfaces with and without surface defects (e.g. steps, kinks, or vacancies) [1]. On terraced Au(100) surfaces, we find that exchange diffusion is the lowest energy mechanism while bridge diffusion is the next lowest. With surfaces in the presence of a perfect step edge, we find an even lower barrier for diffusion along the step-edge identifying that rearrangement of clusters will be faster than aggregation processes. This signifies that cluster edges might behave as catalysts. Afterwards we studied the influence of co-adsorbed Cl on the self-diffusion behavior, which turned out to have a drastic impact even on rather simple diffusion processes. Based on our present results the next aim is to perform large scale simulations, which then will provide macroscopic quantities readily comparable to experiments. [1] K. Pötting, T. Jacob, *et al.*, *High Performance Computing in Science and Engineering*, Springer-Verlag GmbH, Heidelberg, Germany (2006).

O 41.62 Tue 18:30 Poster B1

Characterisation and setup of a noncollinear optical parametric amplifier and investigation of ultrafast dynamics of Na/Cu(111) — •Daniel Wegkamp[1,3], Marcel Krenz[1,3], Uwe Bovensiepen[2,3], and Martin Wolf[1,3] — [1]Fritz Haber Institute of the MPG, Dept. of Physical Chemistry, Berlin, Germany — [2]Universität Duisburg-Essen, Dept. of Physics, Duisburg, Germany — [3]Freie Universität Berlin, Dept. of Physics, Berlin, Germany

To study ultrafast dynamics on a femtosecond timescale, laser pulses of comparable and shorter scale are used in this work in combination with 2-photon photoemission. Here, we report the principle, setup, and characterisation of a femtosecond light-source based on a noncollinear optical parametric amplifier (NOPA) and its application in studying the dynamics of Na/Cu(111) following [1]. Laser pulses with duration < 20 fs have been generated in the visible spectral range using a 300 kHz regenerative amplifier. In a single color scheme ($h\nu = 2.3$ eV) the NOPA pulses are used to excite and photoemit hot electrons, which are detected with a time of flight (TOF) spectrometer. With time independent measurements the binding energy of the adsorbate-induced resonance at 2 eV is observed in agreement with [2]. As a function of pump-probe delay a time-dependent binding energy shift of the Na resonance with -2 meV/fs is observed. This shift is explained as a pump-induced movement of the sodium adsorbate away from the surface. All experiments were conducted at the Freie Universität Berlin.

[1] H. Petek et al., Science 288 (2000) 1402
[2] N. Fischer et al., Surf. Sci. 314 (1994) 89

O 41.63 Tue 18:30 Poster B1

Ultra-Fast Time Resolved Electron Diffraction of Vibrational Dynamics in an Adsorbate Layer: $(\sqrt{3} \times \sqrt{3})$ Pb on Si(111) — •Annika Kalus, Simone Möllenbeck, Paul Schneider, Anja Hanisch-Blicharski, Boris Krenzer, Martin Kammler, and Michael Horn-von Hoegen — Department of Physics and Center for Nanointegration Duisburg-Essen (CeNIDE), Universität Duisburg-Essen, 47057 Duisburg, Germany

We use ultra-fast time resolved electron diffraction to analyze structural dynamics of adsorbates on surfaces on a ps-timescale upon excitation by fs-laser pulses. Surface sensitivity is obtained by a RHEED (reflection high energy electron diffraction)-geometry. Utilizing the Debye-Waller effect the damping of the vibrational amplitude of the adsorbate atoms could be followed as function of time in a pump probe set up. As an example we used the $(\sqrt{3} \times \sqrt{3})$ Pb/Si(111) system which was prepared by deposition of Pb on Si(111) - (7×7) at 300 K followed by an annealing step to 500 K. As a result we obtained a Pb $(\sqrt{3} \times \sqrt{3})$ reconstruction with a coverage of one monolayer and a small number of large Pb islands. After excitation we measure a relaxation time constant of the hot adsorbate system of 150 ps. This low cooling rate is explained by the huge difference in mass of Si and Pb atoms which prevents effective coupling of the Pb vibrational modes to the phonon bath in Si substrate.

O 41.64 Tue 18:30 Poster B1

Surface excitations of oxygen passivated Fe(001) — •Pavel Ignatiev, Yu Zhang, Khalil Zakeri, Valery Stepanyuk, and Jürgen Kirschner — Max-Planck-Institut für Mikrostrukturphysik, Weinberg 2, D-06120 Halle, Germany

Recent advances of spin polarized electron energy loss spectroscopy (SPEELS) [1] open up possibilities of simultaneous mapping of phonons and magnons on complex surfaces. This issues a challenge to reveal the properties of lattice dynamics, magnetic excitations and their couplings. We present a combined experimental and theoretical study of elementary excitations on the oxidized Fe(001) surface. Experimental measurements performed by means of SPEELS reveal 4 surface-related phonon branches and one magnon branch. Calculations of the force matrix from the ab initio input corroborate experimentally observed phonon dispersions. Special attention is paid to the phonons localized at oxygen atoms. Vertical vibrations of oxygen are accompanied by significant changes of the magnetic moment on the O atoms, which possibly can result in a magnon-phonon coupling.

[1] J. Prokop et al., Phys. Rev. Lett. 102, 177206 (2009).

O 41.65 Tue 18:30 Poster B1

Mechanics at the molecular scale: Insight into the physical mechanisms — •Olga A. Neucheva, Ruslan Temirov, and Stefan Tautz — Institut für Bio- und Nanosysteme (IBN-3) and JARA - Fundamental of Future Information Technology, Forschungszentrum Jülich, 52425 Jülich, Germany

The manipulation of atoms and molecules is one of the problems under investigation in a surface science. The first successful attempt to transfer an atom from a surface with use of a scanning tunneling microscope has been realized by Eigler et al [1]. An interest to understand the underlying physical mechanism from both experimental and theoretical points of view has led to investigations of many systems which can be used as atomic and molecular switches [2,3]. In our work the behaviour of a single PTCDA molecule on Ag(111) has been investigated with a LT-STM. Two level fluctuations of the conductance of the junction have been observed within a narrow range of the tip heights and bias voltages. The bistability is related to reversible switching of one of the carboxylic oxygen atoms between the surface and the STM-tip. The current passing through the junction induces vibrations of the molecule leading to weakening and breaking of a chemical bond with the surface and establishing a new one with the tip and vice versa. The switching frequency strongly depends on the bias voltages and tip heights, following a non-linear dependence on the current.

[1] D.M.Eigler, C.P. Lutz, and W.E. Rudge, Nature 352, 600 (1991)
[2] J.A. Stroscio, and R.J. Celotta, Science 306, 242 (2004)
[3] S. Gao, M. Persson, and B.I. Lundqvist, PRB 55, 7 (1997)

O 41.66 Tue 18:30 Poster B1

Rate oscillations in the O2 + H2 reaction on a Rh(111) surface alloyed with nickel — •Tim Smolinsky, Florian Lovis, and Ronald Imbihl — Institut für Physikalische Chemie und Elektrochemie, Leibniz-Universität Hannover, Callinstr. 3-3a, D-30167 Hannover, Germany

A Rh(111)/Ni surface with Ni in the submonolayer range was prepared by decomposing Ni(CO)4 at the Rh(111) surface. After characterization with low energy electron diffraction (LEED) and Auger electron spectroscopy the surface was subjected to the O2 + H2 reaction using photoemission electron microscopy (PEEM) as spatially resolving method. On a clean Rh(111) surface the O2 + H2 reaction is a bistable system. The alloying with nickel changes the system into an excitable medium. The reaction was studied in the 10-7 - 10-4 mbar range at temperatures between 300 and 700 °C. With PEEM chemical wave patterns involving simple reaction fronts have been observed. Under particular reaction conditions spiral waves and target patterns can be triggered. These spatiotemporal patterns were accompanied by rate oscillations observed with mass-spectrometry.

O 41.67 Tue 18:30 Poster B1

Time-, energy-, and angle- resolved two-photon photoemission spectroscopy on Cu(1 1 11) with the Themis 1000 — •Jens Kopprasch[1,2], Martin Teichmann[1], Kristof Zielke[1,2], Oliver Schaff[3], Sven Mähl[3], and Martin Weinelt[1,2] — [1]Max-Born-Institut, Max-Born-Straße 2a, 12489 Berlin, Germany — [2]Freie Universität Berlin, Fachbereich Physik, Arnimallee 14, 14195 Berlin, Germany — [3]SPECS GmbH, Voltastraße 5, 13355 Berlin, Germany

We present two-photon photoemission measurements with the angle-resolved time-of-flight spectrometer THEMIS 1000. The electrostatic lens system of the electron analyzer PHOIBOS (SPECS) in combination with a delay-line detector allows us to measure the kinetic energy (E_{kin}) and the wave vector parallel to the surface ($k_{\|}$) of the photoemitted electrons. Due to the axial symmetry of the spectrometer, k_x and k_y are detected without rotating the sample.
We present measurements on Cu(111), where we observe the first and second image-potential states. Furthermore, we measured the surface states at Cu(11 11), a vicinal surface with (001)-terraces. Depending on the $k_{\|}$-direction, we observe different dispersion of the surface states and lifetimes.

O 41.68 Tue 18:30 Poster B1

Design and operation of a microscopy setup for optical second harmonic generation — •Gerson Mette[1], Kristina Klass[1], Michael Dürr[1,2], Jens Güdde[1], and Ulrich Höfer[2] — [1]Fachbereich Physik und Zentrum für Materialwissenschaften, Philipps-Universität Marburg, D-35032 Marburg — [2]Fakultät Angewandte Naturwissenschaften, Hochschule Esslingen, D-73728 Esslingen

Laser-induced processes like desorption or diffusion often show a strong non-linear dependence on laser fluence. As a consequence, the desorption- or diffusion-rates differ strongly for different areas of the excited surface because of the laser's beam profile.

We present a setup for spatially resolved optical second-harmonic generation (SHG), i.e. SHG-microscopy, and illustrate its operation on the basis of our time-domain study of laser-induced diffusion of oxygen on a vicinal Pt(111) surface at low substrate temperature. Femtosecond laser pulses excite not only the diffusion of oxygen on the surface itself but also generate the second-harmonic light which is detected spatially resolved by an intensified CCD camera. Magnification of the area of interest on the sample to the CCD chip is achieved by a commercial camera lens. The fluence dependence of the diffusion process can be measured in real space across the laser's beam profile. In combination with a two-pulse correlation experiment, the fluence dependence of the energy transfer time between electronic and adsorbate system can be investigated in the same way.

O 41.69 Tue 18:30 Poster B1

Femtosecond VUV and Soft X-Ray Pulses for Surface Spectroscopy — Robert Carley[1], Kristian Döbrich[1], Cornelius Gahl[1], •Matin Teichmann[1], Kai Godehusen[2], Olaf Schwarzkopf[2], Frank Noack[1], Philippe Wernet[2], and Martin Weinelt[1,3] — [1]Max-Born-Institut, Max-Born-Straße. 2A, 12489 Berlin, Germany — [2]Helmholtz-Zentrum für Materialien und Energie, Elektronenspeicherring BESSY II, Albert-Einstein-Straße 15, 12489 Berlin, Germany — [3]Fachbereich Physik der Freien Universität Berlin, Arnimallee 14, 14195 Berlin, Germany

We present initial characterization results of a newly developed high-order harmonics (HHG) VUV beamline. It will be used to perform time-resolved studies of metal- and semiconductor surfaces, and of gas-phase molecular systems, and we show our first photoemission spectra from the W (110) surface. The HHG source is driven by the output of a commercial Ti-sapphire multipass laser amplifier generating 40 fs pulses at a repetition rate of 10 kHz, focused into an Ar-filled gas cell to create high-order harmonics. Following separation from the IR with an Al foil filter, a toroidal mirror images the HHG source onto the entrance slit of a toroidal grating monochromator, which selects a particular harmonic and the bandwidth of the transmitted radiation. A second toroidal mirror images the output slit of the monochromator onto the experimental sample housed in a custom-built UHV chamber equipped with a image-type hemispherical electron kinetic energy analyser. The VUV can be combined with a time-delayed IR pump beam from the driving laser in order to perform time-resolved measurements.

O 41.70 Tue 18:30 Poster B1

Exploiting the quantum confinement of electrons for studying and engineering of magnetic properties of nanostructures at surfaces: an *ab Initio* study — •Oleg O. Brovko and Valeri S. Stepanyuk — Max-Planck-Institut für Mikrostrukturphysik, Weinberg 2, D-06120 Halle, Germany

In the presented contribution we demonstrate, that the quantum confinement of electrons might just prove to be a universal tool for both studying and engineering magnetic properties of surface-bound nanostructures.

We demonstrate that it is possible to resolve magnetic properties and coupling of small clusters buried up to 1.5 nm deep beneath a metallic surface by studying the electrons confined between the nanostructure and the vacuum barrier [1]. We also demonstrate, that the exchange coupling of adatoms and addimers adsorbed at the surface to buried magnetic structures is strongly dependent on the local confinement of electrons in the host metal and can be manipulated by a deliberate variation of the nanostructure's burying depth [2]. Finally we point out the possibility to utilize the quantum confinement of electrons on nanoscale islands in order to tune the coupling of single spins [3].

[1] O. O. Brovko, V. S. Stepanyuk, W. Hergert, and P. Bruno, Phys. Rev. B **79**, 245417 (2009).

[2] O. O. Brovko, P. A. Ignatiev, V. S. Stepanyuk and P. Bruno, Phys. Rev. Lett. **101**, 036809 (2008).

[3] O. O. Brovko, W. Hergert, and V. S. Stepanyuk, Phys. Rev. B **79**, 205426 (2009).

O 41.71 Tue 18:30 Poster B1

Oxidative properties of Co$_m$Pt$_n$ clusters — •Ivan Baev, Kai Chen, Steffen Fiedler, Michael Martins, and Wilfried Wurth — Universität Hamburg, Institut für Experimentalphysik

From investigations of the magnetic properties of Co$_m$Pt$_n$ clusters with XMCD it could be seen that the presence of Pt in these clusters can enhance their probability to oxidize. Now these oxidative properties are studied systematically.

It is possible to create small, mass-selected clusters with the size of several atoms with the "ICARUS" cluster source. The created clusters are landed onto a Cu(100) surface with a surface coverage of approximately 5% and investigated with XPS. We measure the Co-2p photoemission lines of Co, Co$_2$, CoPt and Co$_2$Pt clusters to gather information about their oxidative properties. The goal is to measure the change in shape and position of the 2p-lines if the clusters are exposed to a particular oxygen atmosphere and temperature. For comparison CoO and Co$_2$O clusters can also be created directly with "ICARUS".

A proof of the oxidative properties of Pt in Co$_m$Pt$_n$ clusters is a starting point to search for other reactions that are mediated by Co$_m$Pt$_n$.

The small size of Co$_m$Pt$_n$ clusters allows in principle to conduct in depth theoretical calculations. This can lead to new predictions of catalytic active clusters.

This work is supported by the DFG through the collaboration research center SFB 668.

O 41.72 Tue 18:30 Poster B1

Ab initio investigations of Co and Ni adlayers on wide-band-gap semiconductors — •Bernd Stärk, Peter Krüger, and Johannes Pollmann — Westfälische Wilhelms-Universität, Münster

Metal-semiconductor hybrid systems feature novel functionalities which are not feasible with metals or semiconductors alone, combining, e.g., the high conductivity and spin-polarization of ferromagnets with the controllability of semiconductors. In this contribution, we present the results of a comparative study of Co and Ni multilayers on diamond as well as SiC surfaces employing the generalized-gradient approximation of density-functional theory.

Adsorption of Co/Ni adlayers on the C(001)/C(111)-(1x1) surface is distinguished by a very small lattice mismatch. For one adlayer the metal adatoms are found to be located in a position where all surface dangling bonds are saturated. They form covalent *pd* bonds giving rise to characteristic bonding and antibonding bands which exhibit no significant spin splitting. These bonds markedly reduce the magnetic moment at the interface. Adding further adlayers reveals that this effect is very localized and does hardly affect neighboring metal layers. Spin polarization at the Fermi level is quite large amounting to about 50% which is a prerequisite to spintronic applications.

Furthermore, we compare this behaviour to Co/Ni-deposited 6H-SiC(0001) surfaces. They show complex $2\sqrt{3} \times 2\sqrt{3}$ reconstructions due to a large lattice mismatch between the substrate and the adlayers. We discuss implications on the structural and electronic properties and compare our results to experimental findings.

O 41.73 Tue 18:30 Poster B1

Ab initio Insight on Magnetism and Electronic Properties of Fe(001)-p(1x1)O Surface — •Corina Etz[1], Arthur Ernst[1], Serghei Ostanin[1], Wolfram Hergert[2], and Ingrid Mertig[2] — [1]Max Planck Intitute of Microstructure Physics, Halle, Germany — [2]Martin Luther University, Halle, Germany

Besides the electronic structure changes and the enhanced magnetism, the surfaces can undergo further intriguing changes due to relaxations, impurities, oxidation etc.

In the present contribution we chose to present an *ab initio* study of the electronic structure and the magnetic properties of the bcc Fe(001) surface. In order to be able to correlate our results with the latest experimental observations, we have investigated the pure Fe(001) surface taking into account the effect of structural relaxations on its magnetic properties. Since Fe reacts strongly with oxygen, we also studied the iron surface in the presence of oxygen, i.e. Fe(001)-p(1×1)O. The comparison between the magnetic and electronic properties between the clean Fe surface and the oxygen covered one, revealed that the oxygen layer leads to a stabilization of the magnetism in the system. Furthermore, the Fe(001)-p(1×1)O presents a spin–filter capability, which provides the system a great potential for practical applications.

This first principles study was performed using a multi–code approach. The structural relaxations were investigated using VASP. While by means of the Korringa–Kohn–Rostocker Green's function method, including the self interaction corrections (KKR–SIC), the electronic and magnetic properties were studied.

O 41.74 Tue 18:30 Poster B1

XMCD of ultrathin magnetite (Fe$_3$O$_4$) films on titanates (BaTiO$_3$, SrTiO$_3$) — Remya Govind[1], •Martin Trautmann[1], Franziska Steudel[1], Michael Huth[1], Stephan Borek[1], Liudmilla Makhova[2], Joachim Gräfe[2], Daniel Wett[2], Vasili Hari Babu[2], Angelika Chassé[1], Karl-Michael Schindler[1], and Reinhard Denecke[2] — [1]Institute of Physics, Martin-Luther-University Halle-Wittenberg, Germany — [2]Wilhelm-Ostwald-Institute for Physical and Theoretical Chemistry, University Leipzig, Germany

Coupling ferromagnetism to ferroelectricity in multiferroic systems raises interesting fundamental and application related questions. Within the framework of the SFB 762 all-oxide systems (magnetite on titanates) have been investigated using x-ray absorption spectroscopy (XAS) and x-ray magnetic circular dichroism (XMCD) at BESSY II. Thin and ultrathin films of magnetite (Fe_3O_4) have been prepared by reactive metal evaporation of iron in an O_2 atmosphere and characterized using XAS. The controversy about published assignments of XAS spectra to $SrTiO_3$ and $BaTiO_3$ could be resolved on the basis of experimental O K-edge and Ti L-edge spectra and multiple scattering calculations. After in-plane magnetization the XMCD of the films has been determined in grazing incidence at room temperature. Thin films of Fe_3O_4 (30 ML on $SrTiO_3$ and 10 ML on $BaTiO_3$) exhibited an XMCD comparable to published data of bulk and bulk-like systems. However, an ultrathin film on $BaTiO_3$ with a thickness of 3 ML showed no XMCD. Obviously, remanent in-plane magnetization could no longer be achieved.

O 41.75 Tue 18:30 Poster B1

Spin dynamics of Co nano-islands on Cu(111) from first principles — •Danny Böttcher, Arthur Ernst, Ingrid Mertig, and Jürgen Henk — Max Planck Institute of Microstructure Physics, Halle, Germany

Co nano-islands on Cu(111) show a variety of interesting quantum phenomena. Concerning magnetism, the switching of the islands' magnetizations by an external magnetic field has been investigated experimentally by STM [1]. The findings of these experiments can hardly by interpreted satisfactorily in terms of the Stoner-Wohlfarth model because the latter gives disputable numbers (e. g., too large an anisotropy constant). Hence, a microscopic model, with exchange and anisotropy parameters computed reliably from first principles, seems to be necessary.

Here, we present detailed calculations on the spin dynamics of Co nano-islands on Cu(111) within the framework of the Landau-Lifshitz-Gilbert equation with Langevin dynamics. The Heisenberg exchange parameters and the magnetocrystalline anisotropy have been computed from first principles, using our scalar-relativistic and relativistic KKR codes. We address in particular the behaviour of the islands' spins under switching by an external magnetic field and the dependence of the switching fields on the island size.

[1] G. Rodary, S. Wedekind, D. Sander, and J. Kirschner, Jap. J. Appl. Phys. **47**, 9013 (2008).

O 41.76 Tue 18:30 Poster B1

Ultrafast melting of a charge-ordered state in 1*T*-TaS_2 investigated with photoelectron spectroscopy at FLASH — Kai Rossnagel[1], •Christian Sohrt[1], Stefan Hellmann[1], Martin Beye[2], Timm Rohwer[1], Florian Sorgenfrei[2], Michael Bauer[1], Alexander Föhlisch[2], Wilfried Wurth[2], and Lutz Kipp[1] — [1]Institut für Experimentelle und Angewandte Physik, Universität Kiel, 24118 Kiel, Germany — [2]Institut für Experimentalphysik, Universität Hamburg, 22761 Hamburg, Germany

The Free-Electron-Laser in Hamburg (FLASH) generates highly brilliant, ultrashort, and coherent pulses in the XUV regime enabling many fascinating experiments that are not possible at any other source. After various challenges concerning space-charge effects as well as timing and synchronization issues have recently been solved optical pump-XUV probe photoelectron spectroscopy on solid surfaces is now possible over a wide probing photon energy range (∼24 - 570 eV) with time and energy resolutions of ∼700 fs and ∼300 meV, respectively. Our most recent experiments, performed on the correlated layer compound 1*T*-TaS_2 deep in the charge-density-wave (CDW) state, demonstrate that core-level dynamics on the femto-, pico- and nanosecond time scale can be investigated at FLASH. We find that long-range charge order in 1*T*-TaS_2 collapses promptly and that a domain-like CDW state is reached within about 1 ps. The results imply that the CDW and the accompanying periodic lattice distortion, which are strongly coupled in equilibrium, are decoupled after photoexcitation on the time scale for electron-phonon thermalization.

O 41.77 Tue 18:30 Poster B1

Surface and Image-Potential States of Gadolinium Investigated with Spin- and Time-Resolved 2PPE — •Beatrice Andres[1,2], Kristian Döbrich[1], Andreas Goris[1,2], Anke B. Schmidt[3], Markus Donath[3], and Martin Weinelt[1,2] — [1]Max-Born-Institut, 12489 Berlin — [2]Fachbereich Physik, Freie Universität Berlin, 14195 Berlin — [3]Physikalisches Institut, Westfälische Wilhelms-Universität Münster, 48149 Münster

It is still an open question which microscopic processes are responsible for the laser-induced ultrafast demagnetization in ferromagnetic materials. Most of the experiments performed so far lack spin-resolution. Our first goal is to investigate the occupied majority and unoccupied minority $5d_{z^2}$ surface state (SS) of Gd, following the work of Ref. [1]. We will investigate exchange splitting ΔE_{ex}, binding energy and spin polaristion of the SS and their dependence on the temperature. Here the fundamental of our Ti:Sa laser serves as IR pump and the frequency tripled UV as probe pulse (photon energies 1.5 and 4.5 eV, respectively, pulse durations ≈ 40 fs).

In a second step we will focus on the image-potential states which are also expected to show ΔE_{ex} and spin dependent lifetimes (frequency doubled photons at $h\nu = 3$ eV will serve as pump and 1.5-eV-photons as probe). As samples we use 100-Å-thick Gd(0001) films grown *in situ* on W(110).

[1] M. Lisowski *et. al.*, *Phys. Rev. Lett.* **95**, 137402 (2005).

O 41.78 Tue 18:30 Poster B1

Influence of Neon Spacer Layers on Image-Potential States on Cu(100) — •Nico Armbrust[1], Jens Güdde[1], Peter Feulner[2], and Ulrich Höfer[1] — [1]Fachbereich Physik und Zentrum für Materialwissenschaften, Philipps-Universität, D-35032 Marburg — [2]Physik-Department E20, TU München, D-85748 Garching, Germany

The binding energy and lifetime of image-potential states on metal surfaces can be drastically altered by the presence of insulating spacer layers. Previous investigations of Xe, Kr or Ar on Cu(100) showed that the effect of the decoupling depends systematically on the electron affinity of the rare-gas. Here we present an investigation of the influence of Ne spacer layers on the image-potential states on Cu(100) using time-resolved two-photon photoemission (2PPE). Neon represents a particularly interesting case because its large negative electron affinity of −1.3 eV should result in a large tunneling barrier even for very thin Ne adlayers. Experimental challenges are posed by the requirement of a low sample temperature (≤ 7 K) in combination with the optical experiment which requires an unshielded sample. Furthermore the optical excitation leads to unwanted desorption of the Ne adlayers. We find that the binding energies of the first two image-potential states are reduced by about 30% to $E_1 = 438$ meV and $E_2 = 139$ meV and that the lifetime of the $n = 1$ state increases from 40 fs on the clean surface to 300 fs for only one monolayer of Ne coverage. This is an almost three times larger increase of the lifetime than that caused by one monolayer of Ar/Cu(100). With Kr or Xe layer thicknesses of more than 4 ML are required to achieve a similar degree of decoupling.

O 41.79 Tue 18:30 Poster B1

Surface resistivity of Cu ultrathin films due to impurity scattering — •Swantje Heers, Phivos Mavropoulos, Samir Lounis, and Stefan Blügel — Institut für Festkörperforschung and Institute for Advanced Simulation, Forschungszentrum Jülich, 52425 Jülich

In order to understand resistivity measurements on an atomic scale in ultrathin films, it is of crucial importance to investigate the influence of scattering at surface defects on the surface resistivity, especially in the presence of surface bands. Using the Korringa-Kohn-Rostoker Green function method [1] and solving the Boltzmann-equation self-consistently, the surface resistivity can be calculated for adatoms, impurities and vacancies in and below the surface. We have performed density-functional calculations for the Cu(111) surface of finite-thickness slabs with 3d and 4sp atoms as impurities. The thickness of the slab is varied, ranging from six to forty atomic layers. Our formalism allows us to separate the contribution by scattering to bulk states from the one by scattering to surface states. We show that trends are qualitatively different for adatoms, compared to impurities in the surface. This work was supported by the ESF EUROCORES Programme SONS under contract N. ERAS-CT-2003-980409 and the Priority Programme SPP1153 of the DFG grand Bl 444/8-1.

[1] N. Papanikolaou, R. Zeller, P. H. Dederichs *J. Phys.: Condens. Matter* **14**, 2799 (2002).

O 41.80 Tue 18:30 Poster B1

Electronic structure and spin dynamics in Rashba-split quantum-well electron states — •Sebastian Jakobs[1], Felix Jünger[1], Andreas Ruffing[1], Sabine Neuschwander[1], Indranil Sarkar[1], Mirko Cinchetti[1], Stefan Mathias[1,2], and Martin Aeschlimann[1] — [1]Department of Physics and Research Center OPTIMAS, University of Kaiserslautern, 67663 Kaiserslautern, Germany

— [2]JILA and Department of Physics, University of Colorado, Boulder, CO 80309-0440, USA

In the last few years, methods that allow manipulating and measuring the spin of electrons have received lot of attention. For instance, in a two-dimensional electron gas spin-split energy bands can appear, because of spin-orbit interaction and asymmetric confinement of the electron gas (Rashba splitting). Recently, we found quantum-size induced giant Rashba splitting for quantum-well states in Pb and Bi overlayers on Cu(111). These quantum-well systems present ideal model systems to further explore the electron and spin structure as a function of quantum-well film thickness. We carried out first time-, angle- and spin-dependent photoemission experiments, which will be presented in this contribution.

O 41.81 Tue 18:30 Poster B1

Spin-resolved Inverse Photoemission on Rashba-Systems — •Sune Wissing, Christian Eibl, Anke B. Schmidt, and Markus Donath — Physikalisches Institut, Westfaelische Wilhelms-Universitaet, Wilhelm-Klemm-Str. 10, 48149 Muenster, Germany

The possibility to create spin currents without using external magnetic fields could result in useful applications to spintronics. Therefore, the discovery of the spin-orbit splitting on a Au(111) surface by LaShell *et al.* [1] gave rise of a highly interesting and rapidly growing field of research. Many different systems have been investigated by using angle-resolved photoemission in order to find a "giant" Rashba splitting. Yet it was not possible to follow the splitting of the dispersion within the Brillouin zone above the Fermi level.

We present an experimental setup for spin and angle-resolved inverse photoemission for measurement of the Rashba spin splitting in the unoccupied states. In order to observe a Rashba splitting, it is necessary that the in plane wave vector of the electrons is perpendicular to their spin-quantization axis. Therefore we turned our spin-polarized electron source by 90 degrees with the result that the spin-quantization axis is parallel to the rotation axis of our sample. By measuring the Cu(111) L-gap surface state we can show that the angle and energy resolution of our experiment conforms to the requirements for measuring the Rashba splitting.

[1] S. LaShell *et al.*: Phys. Rev. Lett. **77**, 3419 (1996)

O 41.82 Tue 18:30 Poster B1

Electron coincidence spectroscopy of the neutralization of slow Helium ions above metal surfaces — •Christian Tusche and Jürgen Kirschner — Max-Planck-Institut für Mikrostrukturphysik, Weinberg 2, 06120 Halle, Germany

The neutralization of highly charged ions, scattered at a single-crystal metal surface with kinetic energies of a few 10 eV, is usually accompanied by a number of electrons ejected from the target or from the projectile. For instance, neutralization of ground state He^{+} ions proceeds by Auger neutralization, emitting an Auger electron from the metal. In contrast, He^{2+} neutralization can proceed along several paths. E. g. a double electron capture into the outer He-2s and -2p shells is followed by the emission of a He-KLL Auger electron.

The experimental observation that almost all of the scattered ions leave the surface in the neutral ground state requires that a couple of electron-capture and -emission processes take place on each scattering event. Using electron coincidence spectroscopy, we detect electrons emitted form two such steps in the neutralization cascade of 30 eV He^{2+} ions. The experiment employs two separate electron analyzers. The first one triggers the detection, while the second analyzer records all electrons that arrive within a time window of a few ns. Our results suggest that each ion neutralized at the surface emits two electrons – one in the high energy part of the spectrum (20 eV - 40 eV) and one in the low energy part – with a high probability.

O 41.83 Tue 18:30 Poster B1

Electronic structure of $RScO_3$ from x-ray spectroscopies and first–principles calculations — •Christine Derks[1], Karsten Kuepper[2], Michael Raekers[1], Andree Postnikov[3], Reinhard Uecker[4], and Manfred Neumann[1] — [1]Department of Physics, University of Osnabrück, D-49069 Osnabrück — [2]Departement of Solidstate Physics, Univeristy of Ulm, D-89069 Ulm — [3]Laboratoire de Physique des Milieux Denses, Universite Paul Verlaine, F-57078 Metz — [4]Institute for Crystal Growth, D-12489 Berlin

Perovskites of the type RScO3, where R represents a trivalent rare-earth metal, exhibit an enormous variety of physical properties and can be used for different applications. They are high k materials and belong to the best available thin film substrates for the epitaxial growth of high quality thin films. This allows a so called strain tailoring of ferroelectric, ferromagnetic, or multiferroic perovskite thin films by choosing different RScO3.

The electronic structures of a series of RScO3 single crystalls are investigated by means of x-ray photoelectron spectroscopy (XPS), x-ray emission spectroscopy (XES), x-ray absorption spectroscopy (XAS) and band structure calculations. By combining XES and XAS measurements together with theoretical calculations the band gaps of the compounds can be accurately determined. The presented results will broaden the complete experimental and theoretical picture of the valence bands of RScO3 series.

O 41.84 Tue 18:30 Poster B1

Electronic structure of $LaAg_5$ alloy films on Ag(111) — •Christoph Seibel[1], Hendrik Bentmann[1], Luca Moreschini[2], Gustav Bihlmayer[3], Frank Forster[1], and Friedrich Reinert[1,4] — [1]Universität Würzburg, Experimentelle Physik VII, Am Hubland, D-97074 Würzburg, Germany — [2]Ecole Polytechnique Fédérale de Lausanne (EPFL), Institut de Physique des Nanostructures, CH-1015 Lausanne, Switzerland — [3]Institut für Festkörperforschung, Forschungszentrum Jülich, D-52425 Jülich, Germany — [4]Forschungszentrum Karlsruhe, Gemeinschaftslabor für Nanoanalytik, D-76021 Karlsruhe, Germany

We have characterized the growth of La on Ag(111) by UPS, XPS and LEED. At La coverages of about 4 ML or higher and subsequent annealing we observe an ordered (2x2) surface structure that is rotated by 30° with respect to the substrate. In analogy to the well-studied system $CePt_5$, we identify our system as a $LaAg_5$ alloy in a $CaCu_5$-type structure.

Employing angle-resolved photoelectron spectroscopy (ARPES) we measured the band structure along high symmetry lines and the Fermi surface (FS) of the $LaAg_5$ films. We find several sharp bands near the Fermi level and a high anisotropy in the FS. Our results are compared to ARPES results on $CePt_5$ and $LaPt_5$ as well as first-principles calculations. The system shall serve as a reference for iso-structural alloys composed of other lanthanoids, such as Ce or Gd, potentially showing Kondo physics or other magnetic effects.

O 41.85 Tue 18:30 Poster B1

Momentum microscope mapping of electronic states at Cu(111) surfaces by two- and three-photon photoemission — •Ahmet Akin Ünal, Christian Tusche, Cheng-Tien Chiang, Aimo Winkelmann, and Jürgen Kirschner — Max-Planck-Institut für Mikrostrukturphysik, Weinberg 2, 06120 Halle, Germany

We investigate occupied and unoccupied electronic states of Cu(111) using multi-photon photoemission experiments. The frequency-doubled linear-polarized output of a Ti:sapphire oscillator with photon energy of $h\nu = 3.1\,eV$ is used as the excitation source. The electronic dispersions of the unoccupied Shockley surface state and $n = 1$ image potential state of Cu(111) are obtained by two- and three-photon photoemission using a momentum microscope, which comprises a photoelectron emission microscope (PEEM) in combination with two hemispherical imaging energy analyzers. In the case of three-photon photoemission, a one-photon resonance between the unoccupied surface and image-potential states is observed at $k_{\|} \approx \pm 0.66\,\text{Å}^{-1}$. We also investigate the space-charge effects in the momentum microscope as a function of laser intensity and electron optical conditions in the instrument. As a measure of the space-charge effects, the broadening in the energy and momentum distributions of the observed electronic transitions is analyzed.

O 41.86 Tue 18:30 Poster B1

Electronic Properties of Gold Chains on Ge(001) by Angle-resolved Photoemission — •Andreas Dollinger[1], Thorsten Umbach[1], Sebastian Meyer[1], Jörg Schäfer[1], Christian Blumenstein[1], Philipp Höpfner[1], Xiaoyu Cui[2], Luc Patthey[2], and Ralph Claessen[1] — [1]Experimentelle Physik 4, Universität Würzburg, 97074 Würzburg, Germany — [2]Swiss-Light-Source, Paul-Scherrer-Institut, 5232 Villigen, Switzerland

Metallic nanowires formed by adatom adsorption on semiconductor surfaces have established themselves as playground for studying phenomena in low dimensions. A key requisite is their spatial confinement where charge is mostly maintained within the chain architecture. Examples known are, e.g., Au and In on silicon surfaces, where a charge density wave (CDW) is discussed as the low-temperature ground state. Here finite interchain coupling stabilizes the Peierls state and seemingly hinders a stricter one-dimensional regime. In contrast, Au nanowires on Ge(001) are an alternative system where the chains are well separated by several substrate lattice constants. The electronic band structure from angle-resolved photoemission (ARPES) reveals metallic states, persisting down to low temperatures. No structural change, such as a CDW, is observed when cooling to liquid helium temperatures, which allows the search for deviations from the Fermi liquid picture. Variation of photon energies reveals a great variety of bands within the periodicity of the surface reconstruction. We will present high-resolution data on the band topology, as well as an analysis of the spectral properties near the Fermi level.

O 41.87 Tue 18:30 Poster B1

(SP)VLEED: A spin-polarized very-low-energy electron-diffraction experiment — •Kathrin Wulff, Ulrich Burgbacher, Anke B. Schmidt, and Markus Donath — Physikalisches Institut, Westfälische Wilhelms-Universität Münster, 48149 Münster

This poster has been withdrawn.

O 41.88 Tue 18:30 Poster B1

Paramagnetic Y(0001) as a model for ferromagnetic Gd(0001) — •Sebastian D. Stolwijk, Anke B. Schmidt, and Markus Donath — Physikalisches Institut, Westfälische Wilhelms-Universität Münster, Wilhelm-Klemm-Str. 10, 48149 Münster, Germany

Yttrium and gadolinium are isoelectronic elements with respect to their valence bands but differ in their magnetic properties due to the additional 4f electrons in Gd. Therefore, Y may be viewed as paramagnetic model for ferromagnetic Gd. A comparative study of the electronic structure of Y and Gd promises to reveal electronic properties that are directly linked to ferromagnetism.

We determined the surface electronic structure in the vicinity of the Fermi level E_F by a combined direct (PE) and inverse photoemission (IPE) experiment. Our study on clean Y(0001) films on W(110) reveals a surface state right at E_F, which is observed both below and above the Fermi level. High-resolution IPE measurements and results on the stable $p(1\times1)$O/Y(0001) surface oxide expose an additional spectral feature at about 0.6 eV above E_F. Based on bulk-band structure calculations this emission is ascribed to the band edge of Y(0001). The possible observation of a band-edge emission for Gd(0001) sheds new light on the interpretation of its spin-dependent electronic structure [1]. Implications for the understanding of the ferromagnetic Gd(0001) surface will be discussed.

[1] M. Donath et al., Phys. Rev. Lett. 77, 5138 (1996).

O 41.89 Tue 18:30 Poster B1

A Study of band-gap-engineering in ZrS_2Se_{2-x} by means of ARPES — •Alexander Paulheim, Stephan Thürmer, Mohamed Moustafa, Christoph Janowitz, and Recardo Manzke — Institut für Physik, Humboldt-Universität zu Berlin, Newtonstr. 15, D-12489 Berlin, Germany

The layered Zirconium dichalcogenide semiconductors ZrS_2Se_{2-x} allow to adjust the band gap depending on the parameter x [1]. Therefore, they are candidates for third generation solar cell applications. The ternary compounds of ZrS_xSe_{2-x} have been successfully grown with high control of the parameter x by means of the chemical vapor transport technique (CVT) [2]. In an attempt to understand the mechanism of this band-gap-engineering and the underlying band structure variations, the electronic structure of various ZrS_xSe_{2-x} crystals were measured by angle resolved photoemission spectroscopy (ARPES). In great detail the x-dependent behavior of the upper valence band has been studied along all high-symmetric directions of the Brillouin zone. The results reveal a smooth transition of the energetic positions and splitting of the bands from ZrS_2 to $ZrSe_2$.

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[2] R. Nitsche, H.U. Bölsterli, and M. Lichtensteiger, J. Phys. and Chem. of Solids 21, S.199-205, (1961)

O 41.90 Tue 18:30 Poster B1

***In situ* real-time investigations during the formation of a magnetoelectric Fe/ZnO nanocomposite** — •Erik Kröger[1], Matthias Kalläne[1], Kai Rossnagel[1], Hendrik Bentmann[2], Frank Forster[2], Friedrich Th. Reinert[2], and Lutz Kipp[1] — [1]Institut für Experimentelle und Angewandte Physik, Universität Kiel, 24098 Kiel, Germany — [2]Experimentelle Physik II, Universität Würzburg, 97074 Würzburg, Germany

Magnetoelectric materials composed of piezoelectric and ferromagnetic substances have drawn significant interest in recent years due to their multifunctionality and potential technological applications. In order to investigate the geometric, chemical, and electronic structure of such complex materials, we have designed an experimental station for the new storage ring PETRA III in Hamburg for angle-resolved photoelectron spectroscopy. The instrument was used for *in situ* real-time investigations during the formation of the magnetoelectric Fe/ZnO interface. The ZnO substrate was sputtered and annealed under UHV conditions to guarantee high surface quality. LEED and EXAFS studies showed a relaxation of the hexagonal unit cell. Real-time XPS measurements were done on the polar oxygen surface of the ferroelectric ZnO compound during Fe deposition. A charge transfer from the iron adatoms to the ZnO substrate was observed and quantified. The resulting enhanced conductivity of the ZnO surface enabled very high resolution ARPES measurements of the electronic structure over the full 3D Brillouin zone. This work was supported by the BMBF.

O 41.91 Tue 18:30 Poster B1

Electron-Phonon Coupling in a Thin Epitaxial Bi(111) Film on Si(111) studied by ARPES — •Holger Schwab, Hendrik Bentmann, Frank Forster, and Friedrich Reinert — Universität Würzburg, Experimentelle Physik VII, Am Hubland, D-97074 Würzburg, Germany

Employing angle-resolved photoelectron spectroscopy (ARPES) we have studied the electronic structure in thin films of Bi(111) on the Si(111) substrate. The film growth was characterized by low energy electron diffraction (LEED). We present Fermi surfaces and band structures in the high symmetry directions for different film thicknesses. Quantum well states (QWS) as well as the Bi(111) surface state (SS) are observed. The variation of the line width of the SS was measured over a broad temperature range from 40K to 200K. This allows for the determination of the electron-phonon coupling constant λ. The result agrees with previous measurements for the bulk crystal.

O 41.92 Tue 18:30 Poster B1

Comparison of topography and electronic structure of Gd/W(110) and Gd/Y(0001) — •Karen Zumbrägel, Henry Wortelen, Anke B. Schmidt, and Markus Donath — Physikalisches Insitut, Westfälische Wilhelms-Universität Münster, Germany

In Gd the $4f$ electrons are the main carriers of the magnetic moment. In contrast to the $3d$ ferromagnets Fe, Co and Ni, whose ferromagnetic coupling occurs via direct exchange, in Gd the polarisation of the $5d$ and $6s$ valence electrons mediates the ferromagnetic coupling (RKKY interaction). Hence the investigation of Gd is of fundamental relevance for understanding the nature of ferromagnetism.

The electronic structure of thin Gd films is studied as a function of film thickness, topography and substrate. We compare Gd films grown on W(110), the substrate prevalent in literature, with films grown on Y(0001). The high lattice mismatch between W and Gd of up to 15% leads to layer-island growth, while Gd grows layer-by-layer on the well fitting Y (mismatch 0.4%). Combined with varying annealing temperatures, films with different degrees of roughness and impurity could be investigated. For characterising the film quality we employ low energy electron diffraction, Auger electron spectroscopy and scanning tunnelling microscopy. Spin- and angle-resolved direct and inverse photoemission provide information about the spin-dependent electronic structure below and above the Fermi level. The surface state close to the Fermi energy is used as criterion for the quality of the preparation.

O 41.93 Tue 18:30 Poster B1

Splitting of quantum well states in Pb films induced by spin dependent confinement — •yingshuang fu, germar hoffmann, and roland wiesendanger — Institute of Applied Physics, University of Hamburg

The electronic structure of Pb(111) quantum films epitaxially grown on Fe/W(110) substrate is investigated with a cryogenic scanning tunnelling microscope. Spin averaged scanning tunnelling spectroscopy (STS) measurements show that quantum well states are formed inside the nanometre thick Pb films. Interestingly, quantum well states (QWSs) of Pb films split into double peaks, and the splitting energy can be tuned by changing the quantum number of QWS and thickness of quantum films. The splitting is explained by spin dependent quantum confinement from the magnetic substrate which shifts the binding energy of supported QWSs and effectively removes their spin degeneracy. Thus, the Pb layer inherits the exchange splitting of the magnetic substrate and could provide spin-polarized two dimensional electron gases for both spin directions. Further investigations with spin resolved STS are underway to confirm the spin splitting of QWSs.

O 41.94 Tue 18:30 Poster B1

The Two-Dimensional Electron System Sn/Si(111) Investigated by Scanning Tunneling Microscopy — •Thomas Schramm, Philipp Höpfner, Maximilian Herpich, Jörg Schäfer, and Ralph Claessen — Experimentelle Physik 4, Universität Würzburg, 97074 Würzburg

The confinement of electrons to two dimensions may lead to strong electron correlation effects, including a Mott transition. Such two-dimensional electron systems (2DES) can be realized by adsorbing layers of metal adatoms with less than 1 monolayer thickness on (111) semiconductor surfaces. Examples include Pb and Sn on Ge(111) and Si(111) which form a $\sqrt{3} \times \sqrt{3}$-reconstruction upon deposition of 1/3 monolayer of metal. Recent results from scanning tunneling microscopy (STM) and angle-resolved photoelectron spectroscopy provide evidence of a phase transition to a Mott-insulating ground state [1]. Moreover, the triangular lattice in the presence of correlations leads to magnetic frustrations. We have studied the formation of the $\sqrt{3} \times \sqrt{3}$-Sn/Si(111) structure by (STM) and scanning tunneling spectroscopy experiments. Our refined surface preparation leads to perfectly $\sqrt{3} \times \sqrt{3}$-reconstructed surfaces with low defect densities and long range order. The understanding of defect formation is of foremost importance, as this may lead to unintentional doping effects that influence a potential Mott transition. Current studies are underway, and will give a more defined insight into the correlation effects at low temperature.

[1] Modesti *et al.*, Phys Rev. Lett. **98**, 126401 (2007).

O 41.95 Tue 18:30 Poster B1

Liquid and solid lubrication for nanopositioning and nanomeasuring systems — Thomas Haensel[1], Xiangjun Zhang[2], Xiaohao Zhang[2], Angela Keppler[1], Stefan Krischok[1], and •Syed Imad-Uddin Ahmed[1] — [1]Institut für Physik and Institut für Mikro- und Nanotechnologien, TU Ilmenau, P.O. Box 100565, 98684 Ilmenau, Germany — [2]State Key Laboratory of Tribology, Tsinghua University, P.O. Box 100084, Beijing, P.R. China

One of the biggest challenges in the 21^{st} century is to handle the decreasing structure sizes in the low nanometer range. A nanopositioning and nanomeasuring system developed at the TU Ilmenau is an enabling technology that makes this possible. For optimum operation of the positioning tool, it is necessary to have stable and controlled friction as well as low wear. This can be achieved by a combination of solid lubricants like diamond-like carbon (DLC) and liquid lubricants like ionic liquids (ILs). This contribution reports on friction and wear experiments made with tribometers. To implement this machine in vacuum, preliminary friction measurements in high vacuum were performed to ensure that a vacuum application is possible. Especially the liquid film lubrication with ILs might be very suitable as the IL vapor pressure is very low. The results show that in the combination of solid and liquid film lubrication, effects like polarity, viscosity and the force regime play an important role. The results and aspects, which are related with the achieved friction and wear, are discussed under the aspect of stable and low friction.

O 41.96 Tue 18:30 Poster B1

Tribological self-repair mechanisms investigated under medium load conditions — •Mathias Biester[1], Xinlei Gao[2], Jian Li[3], Syed Imad-Uddin Ahmed[1], and Matthias Scherge[1] — [1]Institut für Physik und Institut für Mikro- und Nanotechnologien, TU Ilmenau, P.O. Box 100565, 98684 Ilmenau, Germany — [2]Department of Chemical and Environmental Engineering, Wuhan Polytechnic University, Wuhan, P.O. Box 430023, P. R. China — [3]Wuhan Research Institute of Materials Protection, Wuhan, P.O. Box 430030, P.R. China

Wear is the main effect for the limited life-time of most mechanical systems and causes very cost-intensive repair and replacement activities. Therefore, a lot of efforts are made to reduce wear and to increase the life-time of modern mechanical systems. Cu (II) chelate of bissalicylaldehyde-ethylenediamine was chosen as additive for liquid lubricants, which is investigated as it has a big self-repair potential. This Schiff base copper complex is a metal-organic chelate complex, which is able to create negative wear as well as to reduce friction due to the self-assembling of a protective layer. Under high temperatures and high contact pressures, which occur during the friction processes, the copper is released from the complex and attaches at the surface. This process is investigated using a micro-tribometer in the milli Newton range to create applicational friction conditions. Additional characterisations are performed with AFM, SEM and spectroscopic methods to analyse the self-repair effects and display tendencies for future applications.

O 41.97 Tue 18:30 Poster B1

Velocity Dependence of the Kinetic Friction of Nanoparticles — •Michael Feldmann, Dirk Dietzel, and André Schirmeisen — Institute of Physics and Center for Nanotechnology, University of Münster, Germany

The velocity dependence of interfacial friction is of high interest to unveil the fundamental processes in nanoscopic friction. So far, different forms of velocity dependence have been observed for contacts between friction force microscope (FFM) tips and a substrate surface. In this work we present velocity-dependent friction measurements performed by nanoparticle manipulation of antimony nanoparticles on atomically flat HOPG substrates under UHV conditions. This allows to analyze interfacial friction for very well defined and clean surface contacts. A novel approach to nanoparticle manipulation, the so called 'tip-on-top' technique [1], made it possible to manipulate the same particle many times while varying the velocity. The antimony particles exhibit a qualitatively different velocity dependence on friction in comparison to direct tip-HOPG contacts. A characteristic change in velocity dependence was observed when comparing freshly prepared particles to contaminated specimen, which were exposed to air before the manipulation experiments.

[1] Dietzel et al., Appl. Phys. Lett. 95, 53104 (2009)

O 41.98 Tue 18:30 Poster B1

Dynamische Topographieveränderung einer Kupferoberfläche in einem geschmierten Tribosystem mittels eines neuartigen Tribometers — •Spyridon Korres[1,2] und Martin Dienwiebel[1,2] — [1]Fraunhofer IWM, Joseph-von-Fraunhofer-Straße 7, 76327 Pfinztal, Deutschland — [2]Karlsruhe Institute of Technology - izbs, Kaiserstraße 12, 76131 Karlsruhe, Deutschland

In diesem Beitrag werden experimentelle Ergebnisse topographischer Veränderungen einer Kupferoberfläche in einem geschmierten Tribosystem gezeigt. Um dies zu erreichen, wurde ein neuer experimenteller Versuchsaufbau entwickelt. Dieser erlaubt eine gleichzeitige on-line Messung der Reibung, Topographie und des Verschleißes mit hoher Auflösung. Die Topographie der Kupferoberflächen wurde mittels Holographiemikroskopie aufgenommen, Sub-mikrometer Lateralauflösung wurde mit einem Rasterkraftmikroskop erreicht und eine Radionuklidtechnik-Anlage ermöglicht das Online Messen von Verschleißwerten.Die Änderungen der Topographie wurden mit den Reibkräften korreliert. In dem Versuch wurde ein Eisenstift als Gegenkörper und Poly-alpha Olefin als Schmierstoff eingesetzt. Für das vorliegende System konnte gezeigt werden, dass ein Großteil der Oberflächenstrukturen plastisch verformt bzw. an den Gegekörper transferiert wurde. Zusätzlich wurde die Änderung der Zusammensetzung beider Reibpartner mittels XPS nach der tribologischen Belastung durchgeführt.

O 41.99 Tue 18:30 Poster B1

Energy Dissipation in Dynamic Force Microscopy: The Effect of Temperature — •Gernot Langewisch, Harald Fuchs, and Andre Schirmeisen — CeNTech (Center for Nanotechnology) and Institute of Physics, University of Muenster, Germany

Since its development dynamic force microscopy has proven to be a powerful tool for surface imaging and mapping of tip-sample interactions down to the atomic scale. Conservative as well as dissipative tip-sample forces can be distinguished by dynamic force spectroscopy. Conservative tip-sample forces have been readily described by classical force laws. The exact origin of the dissipative forces is still under discussion, but current theories predict an explicit temperature dependence of the energy dissipation. Therefore, we performed systematic temperature dependent studies to better understand the interaction processes leading to dissipation in dynamic force microscopy. The dissipative tip-sample interactions were measured by dynamic force spectroscopy for silicon tips on NaCl(001) in ultrahigh vacuum in the attractive and repulsive force regimes. Force and dissipation versus distance curves were obtained for different surface temperatures ranging from 35 K to room temperature. Detailed comparison in different distance regimes shows that neither the force nor energy dissipation exhibits a systematic variation with sample temperature.

O 41.100 Tue 18:30 Poster B1

Ab initio based simulations of atomic force and friction force microscopy of KBr(001) — •Christine Broelemann, Peter Krüger, and Johannes Pollmann — Institut für Festkörpertheorie, Universität Münster

Atomic force microscopy offers the capability to investigate surface structure with atomic resolution. In addition, it allows one to study frictional phenomena of single contacts. To analyse the information that can be extracted from such experimental studies theoretical explorations are essential.

We report on ab initio based simulations of noncontact AFM images, corresponding force fields and friction force line profiles. The short range part of the tip-sample interaction potential is calculated within the local-density approximation of density-functional theory and is supplemented by the long range van-der-Waals interaction due to the macroscopic part of the tip. The microscopic part is modeled by K^+ and Br^- terminated tips.

We use an extended Tomlinson model employing the van-der-Waals interaction together with the DFT derived interaction potential to simulate the sliding friction on the surface. Solving the equations of motion within this framework, we obtain lateral force line profiles with typical stick-slip characteristics. The dependance of the results on different tip types as well as on the spring constant and loading force is discussed.

O 41.101 Tue 18:30 Poster B1

Influence of adhesion interaction between rough surfaces on real contact area formation — •Alexander Kovalev[1,2], Nikolai Myshkin[2], and Heinz Sturm[1] — [1]Federal Institute of Materials Research and Testing (BAM), D-12200 Berlin, Germany — [2]Metal-Polymer Research Institute (MPRI), 246050 Gomel, Belarus

Friction units used in the micromechanical systems have a very high surface to volume ratio, so there are high contact adhesion and friction, leading to low operational reliability. For reliable estimating of the adhesion effect is necessary to take into account the local physical-mechanical properties of the asperities and the real geometry of rough surfaces in micro- and nanoscale. The aim of work was to study formation of the real contact area (RCA) between rough surfaces taking into account the action of adhesion force. The contact simulation was carried out involving the well-known contact models of Hertz, JKR, and DMT at micro/nanoscale of forces and deformations level transformed to the Winkler foundation. The DLC coating used for this study was deposited on the silicon plate using a pulsed vacuum arc deposition system. The surface topography of DLC coating was measured with typical AFM. It was found the adhesion force has obvious action at the external load up to 100 *N. At the external load about 100 mN deformation is comparable with basic roughness and adhesion interaction has insignificant effect on RCA. Using the JKR theory has been shown that the dependence between the adhesion force and deformation has S-shaped pattern like the bearing surface curve.

O 41.102 Tue 18:30 Poster B1

Ordered structure of viologen monolayers on a Copper electrode surface — •Emilia Sak[1,3], Min Jiang[1], Knud Gentz[1], Ralf Troff[2], Christoph Schalley[2], Aleksander Krupski[3], and Klaus Wandelt[1] — [1]Institute of Physical and Theoretical Chemistry , University of Bonn , Wegelerstr. 12, 53115 Bonn , Germany — [2]Institute Chemistry and Biochemistry , Free University of Berlin,Taknstr.3, 14195 Berlin,Germany — [3]Institute of Experimental Physics, University of Wroclaw , pl.Maksa Borna 9 , 53-204 Wrocław, Poland

As a typical molecule in the redox-active viologen family, dibenzylviologens (DBV) has been studied by means of EC-STM on a Cu(100) electrode. DBV^{2+} dications adsorb on a chloride modified Cu(100) electrode surface forming a laterally well ordered 2D array of supramolecular cavitand ensembles. Based on these observations we designed new molecules, such as dimetyl-DBV (DMDBV) and tetrametyl-DBV (TMDBV) in order to study in influence of extra substituents. So far, we found two redox peaks P1/P1'(P1 - 305 mV, P1' -240 mV) in the cyclic voltammogram of Cu(100) in a mixture of 10mM HCl and 0,1mM DMDBV for values of Ework > - 420 mV vs RHE. STM images, show that DMDBV molecules form a stable and ordered adlayer structure which also looks like a chessboard with two kinds of mirror domains. When the applied potential is decreased to -400 mV, no obvious structural changes are visible.

O 41.103 Tue 18:30 Poster B1

Structure of water-metal interfaces studied from first principles — •Xiaohang Lin, Sebastian Schnur, and Axel Gross — Institute for Theoretical Chemistry, Ulm University, D-89069 Ulm, Germany

In spite of numerous studies, it is fair to say that the exact atomistic structure of water layers at metal surfaces is not fully clarified yet. We have used density functional theory calculations to address the structure of water layers on different flat and stepped metal substrates which is for example important for an understanding of processes in electrocatalysis and electrodeposition. In order to account for thermal effects, we have performed ab initio molecular dynamics (AIMD) simulations. The simulations indicate that at room temperature water becomes liquid-like on noble metal surfaces such as Au or Ag whereas on more strongly interacting substrates such as Pt and Ru an ice-like hexagonal structure persists, however, the orientation of the single water molecules is disordered [1]. Additional information on the water layers has been obtained by evaluating the vibrational spectra of the water molecules at the metal surface which reflect the water-metal interaction strength.

[1] S. Schnur, A. Groß, New J. Phys., in press.

O 41.104 Tue 18:30 Poster B1

Surface electronic structure of imidazolium-based ionic liquid films on Au(111)/Mica — •Marcel Marschewski[1], Tomonori Ikari[2,3,4], Angela Keppler[3], Oliver Höfft[4], Markus Reinmöller[3], Wichard J. D. Beenken[3], Wolfgang Maus-Friedrichs[1], Stefan Krischok[3], and Frank Endres[4] — [1]Institut für Physik und Physikalische Technologien, TU Clausthal, Leibnizstr. 4, 38678 Clausthal-Zellerfeld — [2]Ube National College of Technology, Department of Electrical Engineering 2-14-1 Tokiwadai, Ube, Yamaguchi 755-8555, Japan — [3]Institut für Physik and Institut für Mikro- und Nanotechnologien der TU Ilmenau, P.O. Box 100565, 98684 Ilmenau — [4]Institute of Particle Technology, TU Clausthal, Arnold-Sommerfeld-Str. 6, 38678 Clausthal-Zellerfeld

Room temperature Ionic Liquids (RT-ILs) are a class of materials, which has recently gained enormous interest. Here we present our results for the surface electronic structure of very thin imidazolium-based ionic liquid (ILs) films on Au(111)/Mica and thick IL films. This was studied by electron spectroscopy using ultraviolet photoelectron spectroscopy (UPS, HeI and HeII) and metastable induced electron spectroscopy (MIES). We have prepared monolayers of four different types of imidazolium-based ILs ($[RMIm]Tf_2N$; R stands for Ethyl-, Butyl-, Hexyl- and Octyl-chains) on Au(111)/Mica by vapour deposition. By comparing these results with our data for the thick IL films we find evidence for ordered growth of the ILs in the monolayer regime. For better understanding of the electronic structure of the ILs, we compare the experimental data with corresponding DFT calculations.

O 41.105 Tue 18:30 Poster B1

Invetigatins on the self assembly process of Octacosan-1-ol and its derivates on artificial surfaces — •Alexander Hommes and Klaus Wandelt — Institut für Theoretische und Physikalische Chemie, Wegelerstr. 12, 53115 Bonn

Waxes occur on the surfaces of all land plants. That the structure of epicuticular wax crystallites is predominantly a process of self-assembly, is now well established both from correlative and generic observations. The waxes are embedded into the 3D matrix of the cuticle and also cover the surface where they build plant specific microcrystalline structures. Dominant wax components are normally considered to be responsible for the formation of wax crystallites. In general, across a wide variety of waxy components like alkanes, alcohols, ketons and aldehyds, several different crystal structures on plant cuticles can be observed.

Long chained alkanes and alcohols were some of the first hydrocarbons to be imaged at solution/solid interface with AFM and STM since they form well ordered films on graphite near room temperature. Investigations on the physisorbed monolayers of Octacosan-1-ol, Hentricontan-16-on (Palmiton), Octacosanoicacid and Triacontan-1-ol at the solution/solid interface on HOPG, Mica and Siliconoxid show an order, e.g. strictly follow the hexagonal arrangement of the carbon atoms of the HOPG.(studied with STM and AFM) The good lattice match between the alkyl backbone and the graphite lattice favours commensurate packing of the hydrocarbon film with the underlying substrate.

O 41.106 Tue 18:30 Poster B1

Self-Assembly of 3D-molecule: Benzene 1,3,5 Triphosphonic acid (BTP) studied by Scanning Tunneling Microscopy

(STM) at the Liquid-Solid Interface — •Nguyen Thi Ngoc Ha[1], Michael Dieblich[1], Michael Mehring[2], and Michael Hietschold[1] — [1]Institute of Physics, Solid Surfaces Analysis Group, Chemnitz University of Technology, Chemnitz, Germany. — [2]Institute of Chemistry, Coordinations Chemistry Group, Chemnitz University of Technology, Chemnitz, Germany.

During the last two decades, there has been major effort toward metal phosphate chemistry due to their endearing properties and their potential for supramolecular assembly[1]. Crystal engineering is a relatively new field of chemical research used to control or predict types of metal phosphonate structure[1,5]. Surprisingly, the phosphonic acids have not been the subject of scanning tunneling microscopy (STM) to our knowledge so far. Here we report a very first STM studying of the benzene triphosphonic acid (BTP) [1,3,5-[(HO)2(O)P]3C6H3] dissolved in an alkanoic acid solvent (octanoic acid). The three-dimensional network formed by self-assembly of this triphosphonic acid on a HOPG(0001) substrate exhibits a ladder-like appearance and agrees very well with other crystallographic studies[2,4,5]. BTP in this structure adsorbed opposite to each other as viewed along an axis orthogonal to the plane defined by the aromatic rings. The brightest features in regular patterns should be reported phosphonic end-groups.

O 41.107 Tue 18:30 Poster B1

Modification of graphene by ion irradiation — •Hanna Bukowska[1], Sevilay Akcöltekin[1], Mourad El Kharrazi[1], Orkhan Osmani[1,2], and Marika Schleberger[1] — [1]Universität Duisburg-Essen, Fakultät für Physik, Lotherstraße 1, 47057 Duisburg, Germany — [2]Technische Universität Kaiserslautern, Fachbereich Physik, Gottlieb-Daimler-Straße, Gebäude 47, 67663 Kaiserslautern, Germany

Ion irradiation can be used to modify surfaces on the nanometer scale. We investigate graphene on different insulator ($SrTiO_3$, TiO_2, and Al_2O_3) and semiconductor (SiO_2) substrates. The bombardment of those target surfaces with swift heavy ions under grazing angle of incidence creates chains of nanodots on the substrate and folds graphene to typical origami-like structures. The shape of the folded graphene seems to depend on the length of the tracks. The length can be controlled by the angle of incidence. From the analysis of atomic force microscopy measurements, we classify the different types of modifications, with the aim to determine the relationship between chain length and origami shape. Further more we want to develop a theoretical understanding of the physical processes leading to the folding.

O 41.108 Tue 18:30 Poster B1

Electronic structure of a monolayer graphene on Ir(111) probed by ARPES — •Marko Kralj[1], Ivo Pletikosić[1], Milorad Milun[1], Petar Pervan[1], Alpha N'Diaye[2], Carsten Busse[2], Thomas Michely[2], Jun Fujii[3], Ivana Vobornik[3], and Tonica Valla[4] — [1]Institut za fiziku, Zagreb — [2]II. Physikalisches Institut, Köln — [3]TASC Laboratory, Trieste — [4]BNL, New York

Amongst realized examples of epitaxial growth on metal substrates, graphene on iridium is an exceptional case of long range structural quality and weak (electronic) bonding to a metal surface. These properties make this system very appealing for experimental studies of the electronic structure of graphene. Our recent ARPES study focused on the K point of graphene revealed that the weak electronic interaction of graphene with Ir(111) is reflected through the 0.1 eV hole doping and a minigap opening in the Dirac cone which is due to the 2.5 nm superperiodic potential originating from the about 10 % mismatched iridium and graphene [1]. In this work, ARPES is used to further investigate electronic properties and quality of graphene on Ir(111). For that purpose, we scan a wide portion of the Brillouin zone, use variable photon energy and different light polarization, and also perform photoemission of the adsorbed Xe.

[1] I. Pletikosić et al., Phys. Rev. Lett. 102, 056808 (2009).

O 41.109 Tue 18:30 Poster B1

Theory of ultrafast carrier relaxation dynamics in graphene — •Torben Winzer, Stefan Butscher, Frank Milde, Andreas Knorr, and Ermin Malić — Institut für Theoretische Physik, Nichtlineare Optik und Quantenelektronik, Technische Universität Berlin, 10623 Berlin, Germany

We present a microscopic calculation of the relaxation dynamics of photoexcited hot electrons and phonons in graphene.

Using a density matrix formalism, the combination with a tight binding approach for the band-structure and a Born-Markov approximation yields Boltzmann-like equations for interacting electrons and phonons.

In the case of electron-phonon coupling, we find an initial fast carrier cooling on the femtosecond timescale followed by slowed down relaxation dynamics due to the generation of non-equilibrium hot phonons.[1][2]

Even though the relaxation of excited carriers into thermal equilibrium occurs predominantly by energy dissipation through phonons, electron-electron scattering thermalizes the system at the time scale of the electron-phonon interaction.

[1] S. Butscher, F. Milde, M. Hirtschulz, E. Malić, and A. Knorr, Appl. Phys. Lett. 91, 203103 (2007). [2] T. Kampfrath, L. Perfetti, F.Schapper, C. Frischkorn, and M. Wolf, Phys. Rev. Lett. 95, 187403 (2005).

O 41.110 Tue 18:30 Poster B1

Scanning tunneling microscopy (STM) studies of microsoldered graphene — •Alexander Georgi[1], Anne Majerus[1], Viktor Geringer[1], Bart Szafranek[2], Daniel Neumaier[2], Marcus Liebmann[1], and Markus Morgenstern[1] — [1]II. Physikalisches Institut, RWTH Aachen and JARA-FIT, Otto-Blumenthal-Straße, 52074 Aachen — [2]Advanced Microelectronic Center Aachen (AMICA), Otto-Blumenthal-Straße 25, 52074 Aachen

Since STM is very susceptible to dirt, it is important to avoid contamination by prior processing. For graphene, we show that microsoldering [1] avoids dirt as resist, which has been found on lithographic samples. However, both samples show intrinsic corrugation with wavelength of 15 nm as previously reported for lithographically contacted graphene [2]. Ni deposition on the surface leads to clusters exhibiting spectroscopic features comparable to theoretical predictions [3]. Further measurements probing the properties of freely suspended graphene layers are presented.

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[2] V. Geringer, M. Liebmann, T. Echtermeyer, S. Runte, M. Schmidt, R. Rückamp, M. C. Lemme and M. Morgenstern, Phys. Rev. Lett. 102, 76102 (2009).
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O 41.111 Tue 18:30 Poster B1

Adsorption of diatomic halogen molecules on graphene — •Alexander N. Rudenko[1,2], Frerich J. Keil[1], and Alexander I. Lichtenstein[2] — [1]Technische Universität Hamburg-Harburg, Institut für Chemische Reaktionstechnik, Eißendorfer str. 38, 21073 Hamburg, Germany — [2]Universität Hamburg, Institut für Theoretische Physik, Jungiusstraße 9, 20355 Hamburg, Germany

We investigate the adsorption of fluorine, chlorine, bromine, and iodine diatomic molecules on graphene using density-functional theory taking into account nonlocal correlation effects by means of vdW-DF approach. It is shown that the van der Waals interactions play a crucial role in the formation of chemical bonding between graphene and halogen molecules, and therefore important for a proper description of adsorption in this system. Adsorption energies are found to be up to an order of magnitude larger than the values obtained using standard semilocal functionals without vdW corrections. In the cases of F_2 and I_2 we also found a considerable ionic contribution to the binding energy, slowly vanishing with the distance. The analysis of the electronic structure shows that ionic interaction arises due to the charge transfer from graphene to the molecules. In addition, graphite intercalation by halogen molecules have been investigated. It is found that the binding energy of graphite layers becomes significantly weaker in the presence of halogen molecules, which agrees with the results of recent experiments on sonochemical exfoliation of intercalated graphite.

O 41.112 Tue 18:30 Poster B1

Gas permeation in graphenoid nanomembranes — •Nils Mellech, Elina Oberländer, Xianghui Zhang, André Beyer, and Armin Gölzhäuser — Universität Bielefeld, Postfach 10 01 31, 33501 Bielefeld, Germany

Permeation and selectivity measurements with Helium and Argon were carried out on freestanding nanomembranes of crosslinked self-assembled biphenylthiol and nitrobiphenylthiol monolayers. An ultrahigh vacuum permeation measurement system based on a quadrupole mass spectrometer was used to determine the permeation properties. The monolayers of biphenylthiol and nitrobiphenylthiol are prepared on gold on mica and crosslinked by electron irradiation. After preparation the nanomembranes which have a thickness of approximately 1 nm are transferred onto a micron-sized opening in a silicon nitride window of a silicon substrate. The nanomembrane seals the UHV chamber from the high pressure feed gas side of the system. Despite its thinness, the membranes remain stable under pressures of up to 30 kPa, even for days. The permeability of nitrobiphenylthiol nanomembranes was found to be substantially lower as compared to biphenylthiol membranes. This is accompanied by a significant increase in the permeation selectivity of He to Ar gas.

O 41.113 Tue 18:30 Poster B1

Graphite and multigraphene based Gas sensor — •Ana Ballestar, Jose Barzola-Quiquia, and Pablo Esquinazi — Division of Superconductivity and Magnetism, Universität Leipzig, 04103 Leipzig

The research and development of solid state gas sensors have widely advanced in recent years. Sensing gas molecules is critical to environmental monitoring, control of chemical processes, space missions and medical applications. In order to judge whether or not a sensor is likely to be commercially successful, the sensitivity, selectivity, stability, speed of response and low cost manufacturing are the parameters to be taken into account. Graphite, considered a semi-metal or zero-gap semiconductor, is a good electrical conductor at 300K. The operational system proposed here is based on the changes of the electrical resistivity produced in mm- and μm-sized samples of graphite and multigraphene while being exposed to different gas molecules. By means of low noise measurements and high sensitivity concerning the variations in the resistivity of graphite samples, we are able to detect the adsorption and desorption of the gas molecules on graphite surface. Depending on the gas molecules we get different variations in the signal, so we have selectivity in the device as well.

O 41.114 Tue 18:30 Poster B1

Automated preparation of high-quality epitaxial graphene on 6H-SiC(0001) — •Markus Ostler, Florian Speck, Markus Gick, and Thomas Seyller — Lehrstuhl für Technische Physik, Universität Erlangen-Nürnberg, Germany

Thermal decomposition of silicon carbide is a viable route for preparing graphene films. In contrast to other methods it has the potential for upscaling graphene synthesis to a wafer scale and the advantage of providing an insulating substrate at the same time. In particular, graphenization of SiC(0001) surfaces in Ar atmosphere has been shown to yield graphene films superior to UHV-grown epitaxial graphene. In this contribution we present details on a recently installed hot-wall reactor for graphene growth on SiC in Ar. Both preparation steps, i.e. the preconditioning of the SiC substrate by hydrogen etching and the graphene growth are performed in this setup in a fully automated manner thus ensuring the preparation of high-quality graphene on an everyday basis. Samples prepared in the new setup were characterized by atomic force microscopy (AFM) and x-ray induced photoelectron spectroscopy (XPS). We present results on the optimization of the hydrogen etching procedure by varying gas flow and temperature. The thickness distribution of graphene samples grown in the automated process is Gaussian with a mean value of 1.1 monolayers and a standard deviation of 0.15 monolayers. This indicates a highly controlled process.

O 41.115 Tue 18:30 Poster B1

Band structure engineering of mono- and bilayer Graphene on SiC(0001) via molecular functionalization — •Camilla Coletti[1], Christian Riedl[1], Dong Su Lee[1], Luc Patthey[2], Benjamin Krauss[1], Klaus von Klitzing[1], Jurgen Smet[1], and Ulrich Starke[1] — [1]Max-Planck-Institut für Festkörperforschung, Heisenbergstr. 1, D-70569 Stuttgart, Germany — [2]Paul-Scherrer-Institut, CH-5234 Villigen-PSI, Switzerland

Although epitaxial graphene on SiC(0001) is a realistic candidate for the implementation of graphene-based electronic devices a drawback might sensibly limit its perspectives. Epitaxial graphene on SiC is in fact electron doped and consequently displays a metallic nature. Hence, the need to tailor its electronic band structure in such a way that the excess of electrons is compensated precisely to the point of charge neutrality. Noncovalent functionalization of epitaxial graphene surfaces with the strong acceptor molecule tetrafluorotetracyanoquinodimethane (F4-TCNQ) allows for a fine tuning of the doping level. Charge neutrality can be achieved for mono- and bilayer graphene as shown from ARPES and Raman spectroscopy. On bilayer samples the magnitude of the existing bandgap can be increased up to more than double of its initial value. Core level analysis and valence band investigations are used to provide a structural characterization of the charge transfer complex. The molecules are stable to air exposure, temperature resistant and can be applied via wet chemistry. Hence surface functionalization via F4-TCNQ appears to be a technologically relevant method to successfully engineer the band structure of graphene.

O 41.116 Tue 18:30 Poster B1

Preparation and characterization study of graphene on SiC(0001) — •Thomas Druga, Martin Wenderoth, and Rainer G. Ulbrich — IV. Physikalisches Institut, Georg-August-Universität Göttingen

We present a preparation and characterisation study of graphene on the silicon-terminated 6H-SiC(0001) surface. The untreated crystals were electrically contacted and transferred in UHV. After annealing at base pressure of $1*10^{-10}$ mbar at 500°C for several hours the samples were graphitized between 1250 and 1300°C by direct current heating. The temperature during preparation was controlled by an optical pyrometer. The surfaces were investigated by low energy electron diffraction (LEED) and scanning tunnelling microscopy (STM) at room temperature. The graphitized surfaces show different step heights resulting from coexisting mono- and bilayer graphene films. Atomically resolved topographies show the typically honeycomb structure of the graphene layer and the 6×6 periodicity resulting from the underlying buffer layer. Lateral resolved scanning tunnelling spectroscopy data indicate finite conductivity around zero bias and lateral variations in the local density of states. This work was supported by the DFG as part of SFB 602 Tp A7.

O 41.117 Tue 18:30 Poster B1

Growth and Chemical Modification of Graphene on Ni(111) — •Wei Zhao, Oliver Höfert, Christian Papp, and Hans-Peter Steinrück — Lehrstuhl für Physikalische Chemie II, Universität Erlangen-Nürnberg, Egerlandstr. 3, 91058 Erlangen

The outstanding electronic properties of graphene make it a promising candidate for future spintronic applications in electronic devices and setups as well as gas sensors. Therefore, we first studied the growth of graphene on Ni (111) under different temperatures (773-950 K) and with different carbon sources such as ethylene and propylene, by in situ X-ray photoelectron spectroscopy (XPS). After cooling to room temperature, a second contribution showed up in C 1s region of graphene on Ni (111), enabling a better understanding of the structure of graphene on this surface.

For potential use in chemical gas sensors, functionalized graphene needs to be. Doping with hetero atoms like N might be one way to introduce sensitivity towards different gases. Our approach to achieve what gentle sputtering chemical modification of the graphene sheets on Ni (111) with molecular nitrogen. To reveal changes in chemical properties due to the sputtering process, we used benzene as probe molecule and studied its interaction with pristine and modified graphene layers by XPS and TPD.

This work was supported by BMBF (05 ES3XBA / 5) and the DFG through the Cluster of Excellence"Engineering of Advanced Materials".

O 41.118 Tue 18:30 Poster B1

Influence of charge on the Raman Spectrum of Epitaxial Graphene on Silicon Carbide — •Stephan Wittmann[1], Jonas Röhrl[1], Daniel Waldmann[2], Johannes Jobst[2], Florian Speck[1], Markus Ostler[1], Heiko Weber[2], Martin Hundhausen[1], and Thomas Seyller[1] — [1]Lehrstuhl für Technische Physik, Universität Erlangen-Nürnberg, Germany — [2]Lehrstuhl für Angewandte Physik, Universität Erlangen-Nürnberg, Germany

Epitaxial graphene prepared on the surface of SiC wafers might be mechanically strained and electrically charged due to doping from the substrate. Raman spectroscopy can be employed for characterization of graphene layers due to influence of strain and charge on the frequencies of the Raman-active phonons. In order to differentiate between both effects on the prominent features in the Raman spectra (G-peak and 2D-peak) we employ a 6H-SiC wafer with an integrated back gate. By varying the electric field, applied on the graphene layer via a back gate, we change the charge state and accordingly some phonon frequencies. We show, that the variation of the back gate voltage influences the zone-center optical phonon (G-peak).

O 41.119 Tue 18:30 Poster B1

Electronic structure of graphene on SiC produced via low-

T synthesis — •Martin Weser, Carsten Enderlein, Karsten Horn, and Yuriy Dedkov — Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, Germany

The graphitization of the SiC(0001)-surface, by annealing at temperatures above 1150° C under UHV conditions, has been known since a long time and became one of the dominating methods for graphene fabrication in the field of experimental physics in the last ten years. Here the LEED, core-level PES, and ARPES-results of a graphene layer produced by nickel diffusion on SiC are presented. The band maps show clear graphene π-bands with an unusual band splitting at the border of the Brillouin zone that is, up to our knowledge, not comparable to any graphene-based system known so far. This band splitting, as well as a number of unusual features in the spectral function, are ascribed to the formation of a Ni_2Si-interlayer that locally breaks the symmetry of the two sublatices, by hybridization of only one of them, which leads to an electronically separated second sublattice.

O 41.120 Tue 18:30 Poster B1

Analysis of model interfaces for Li ion batteries — •Andreas Seemayer, Aparna Pareek, Dirk Vogel, Michael Rohwerder, and Frank Renner — Max-Planck-Institut für Eisenforschung GmbH, Düsseldorf, Germany

Lithium ion batteries are the most promising power source for future electromobility applications. Therefore a better understanding of the basic processes in Lithium ion batteries is needed. Especially nowadays research projects aim to improve real systems in terms of higher rate capability, cycle life, safety and operating temperature.

Following the surface science approach we focus on the investigation of single crystal model systems of possible anode and cathode materials and electrode / solid electrolyte interfaces prepared by electrochemical deposition, molecular beam epitaxy or pulsed laser deposition.