O 58: Poster Session III (Solid/liquid interfaces; Metals; Semiconductors; Oxides and insulators)

Time: Wednesday 18:15–21:45 Location: Poster B

O 58.1 Wed 18:15 Poster B

Dye-sensitized Zinc Oxide on Tungsten Wire Electrodes — •Tim Helbig, Melanie Rudolph, and Derck Schlettwein — Justus-Liebig-Universität Gießen, Institut für Angewandte Physik, Heinrich-Buff-Ring 16, D-35392 Gießen

Thin films of Zinc Oxide/Eosin Y were deposited on tungsten wires via electrochemical deposition from aqueous solutions by using the dye Eosin Y as a structure-directing agent (SDA). After deposition the SDA was removed by an aqueous alkaline solution, leaving behind a porous zinc oxide film. As a sensitizer, the dye D149 was adsorbed to the surface of the porous zinc oxide. The films were studied as photo anodes in dye-sensitized solar cells (DSC) using the tungsten wire as back contact. The photoelectrochemical performance was measured in an iodide-containing electrolyte and a platinum wire as counter electrode. As light source a xenon arc lamp with an energy output of $100mW/cm^2$ was used. A photovoltaic efficiency of such cells of up to 1.4 % was reached but the films could not be stabilized under the present conditions. Degradation mechanisms and optimization strategies will be discussed.

O 58.2 Wed 18:15 Poster B

Measuring hydrodynamic force on soft materials — •Farzaneh Kaveh, Michael Kappl, and Hans-Jürgen Butt — Max-Planck Institute for Polymer Research, Mainz, Germany.

Hydrodynamic drainage occurs when two surfaces approach each other in liquid. When the distance between the surfaces becomes small, the confined liquid in the gap is squeezed out. At high approaching velocity, the shear rate is high, causing a hydrodynamic force. Recent measurements have shown that at such a high shear rate, the no slip boundary condition may break down, even in the case of complete wetting. Hydrodynamic force at the nanometre scale has been measured on hard substrates and on bubbles in other works [1]. We aim to measure hydrodynamic force on soft substrates and apply a model which has been developed for deformable interfaces [2]. The goal is to understand the influence of soft substrates on hydrodynamic boundary condition at different velocities. The measurements are carried out by atomic force microscopy (AFM) using fresh cured polydimethylsiloxane (PDMS) as a soft substrate and 10 μm borosilicate glass spheres attached to a tip-less cantilever (colloidal probe technique). We record forces at approaching velocities of 0.5-120 μm/s. At low velocities, i.e., low shear rates no slip will occur. At high approaching velocities, slip may occur and should be visible in the hydrodynamic force.

[1] Bonaccurso E., Butt H.-J., Craig V.S., *Phys. Rev. Lett.* **90**, 144501 (2003).

[2] Carnie S.L., Chan D.Y.C., Lewis C., Manica R., Dagastine R.R., *Langmuir* **21** (7), 2912 (2005).

O 58.3 Wed 18:15 Poster B

GIXD and X-ray reflectivity studies on the mercury-electrolyte interface under potential control — •Sven Festersen[1], Annika Elsen[1], Benjamin Runge[1], Oliver H. Seeck[2], Moshe Deutsch[3], Olaf M. Magnussen[1], and Bridget M. Murphy[1] — [1]Institute for Experimental and Applied Physics, Christian-Albrechts-Universität, Kiel, Germany — [2]PETRA III, DESY, Hamburg, Germany — [3]PD, Bar-Ilan University, Ramat-Gan, Israel

The interface between mercury and electrolyte solutions has been subject of extensive electrochemical studies, but structural information is largely lacking up to now. To investigate the interface structure on atomic scales, in situ GIXD and X-ray reflectivity measurements on a mercury electrode in aqueous solution, containing NaF, NaBr and PbBr$_2$, have been performed. Experiments were carried out at different potentials applied using the LISA liquid surface diffractometer at PETRA III (DESY, Hamburg). Using in situ x-ray reflectivity studies a potential dependent reversible adlayer formation at the mercury-electrolyte interface has been observed. Additional peaks in the reflectivity data also suggested electrochemical growth of 3D crystallites at the interface. The existence of the latter was confirmed by grazing incidence diffraction. The existence of partial powder rings indicates a preferred orientation of these crystallites with respect to the interface.

O 58.4 Wed 18:15 Poster B

Charge transfer processes in platinum-silicon-diodes induced by electrochemical surface reactions at the platinum-sulfuric acid interface — •Damian Bürstel and Detlef Diesing — Fakultät für Chemie, Universität Duisburg-Essen, D-45117 Essen, Germany

Schottky diodes consisting of a 16 nm platinum film as electrochemical working electrode and a n-doped Si<111>-substrate as back electrode are used to study the energy dissipation and charging effects of the platinum film induced by electrochemical surface reactions. For this purpose cyclovoltammetric experiments are carried out in 1 M sulfuric acid and the charge transfer processes between the platinum and the silicon back electrode is measured as a current j_{dev} during this experiments. Furthermore these processes are studied as a function of the internal barrier height varied by applying a bias U_{bias} at the silicon back electrode. The current j_{dev} may monitor excitations and also heating effects of the platinum film since diodes with a low internal barrier are sensitive for excitations with very small energies. It is shown that j_{dev} depends significantly on U_{bias} which is comparable with results from photo excitation experiments for these devices. An additional current in j_{dev} is measured in the $\mathrm{H}_{\mathrm{upd}}$ region. This effect can be explained by a modification of the internal field of the diode due to a shift in the chemical potential caused by the adsorption of hydrogen. This shift can achieve values of 20 mV for the whole $\mathrm{H}_{\mathrm{upd}}$ region. Sulfate and oxygen adsorption have a much smaller effect on the chemical potential of the film.

O 58.5 Wed 18:15 Poster B

Variations in backbone morphology of MnO$_x$ infiltrated carbon xerogels — •Christian Weber[1], Volker Lorrmann[1], Gudrun Reichenauer[1], and Jens Pflaum[1,2] — [1]Bavarian Center for Applied Energy Research e.V. (ZAE Bayern), D-97074 Würzburg — [2]Julius-Maximilians-University of Würzburg, Institute of Physics, Experimental Physics VI, D-97074 Würzburg

Electrochemical capacitors (EC) bridge the gap between conventional capacitors with high power but low energy density and batteries with high specific energy density but rather low power density. In this contribution we analyzed hybrid capacitor structures relying on charge storage by the electrochemical double-layer between electrolyte and porous carbon electrode and an additional pseudocapacitance caused by redox processes of manganese oxide (MnO$_x$) with the electrolyte's ions. Variations in the structure of the carbon xerogel backbone and the amount of deposited MnO$_x$ were characterized electrochemically and structurally. From MnO$_x$-mass uptake and its correlation with carbon particle size, we can conclude that the deposition of MnO$_x$ preferably takes place on the external surface area of the carbon particles. As the amount of deposited MnO$_x$ scales with the external surface area, a thinner layer will provide a more efficient use of the active material and lead to better electrode performance.

Financial support by Deutsche Bundesstifung Umwelt is thankfully acknowledged.

O 58.6 Wed 18:15 Poster B

Dilatation measurements of porous carbon electrodes during charging — •Anja Keckeisen[1], Christian Weber[1], Volker Lorrmann[1], Gudrun Reichenauer[1], and Jens Pflaum[1,2] — [1]Bavarian Center for Applied Energy Research e.V. (ZAE Bayern), D-97074 Würzburg — [2]Julius-Maximilians-University of Würzburg, Institute of Physics, Experimental Physics VI, D-97074 Würzburg

Electrochemical double layer capacitors, also known as "supercapacitors" are high power energy storage devices. Due to purely electrostatic charge storage, they achieve very long cycle lifetimes. A suited model system for investigating porous electrodes are carbon xerogels since their properties like particle size or micropore distribution can be tuned in a controlled fashion. We present a method to measure the length variation of supercapacitor carbon electrodes upon charging. While performing cyclic voltammetry measurements we observe changes of the electrode dimensions as a consequence of ion loading into the carbon micropores. By varying the ratio between pore and ion size as well as the particle size of the carbon xerogel backbone we can draw conclusions on the influence of the carbon structure on the charging process, which provides a microscopic model of charging with respect to anions and cations.

O 58.7 Wed 18:15 Poster B

Shape-persistent linear oligomers. — •Robert May, Stefan-Sven Jester, and Sigurd Höger — Rheinische Friedrich-Wilhelms-Universität Bonn, Kekulé-Institut für Organische Chemie und Biochemie, Gerhard-Domagk-Str. 1, 53121 Bonn, Germany

Conjugated shape-persistent arylene-alkynylene oligomers are discussed as one-dimensional molecular wires and as building blocks for supramolecular materials as well as for two-dimensional adlayers on surfaces. Oligomerization reactions and subsequent recycling gel permeation chromatography for separation of the crude products allow an efficient acces to monodisperse oligomers of distinct oligomerization degree in sufficient quantities. Here we present an approach towards monodisperse shape-persistent oligo(phenylene-butadiynylene)s of up to 38 nm length. Self-assembled monolayers of these molecules at the liquid/solid interface (here: 1,2,4-trichlorobenzene/HOPG) are investigated by scanning tunneling microscopy.

O 58.8 Wed 18:15 Poster B

The crystal-fluid interface in a hard sphere system — •Andreas Härtel[1], Mohammad Hossein Yamanai[2], Martin Oettel[2], Roberto E. Rozas[1], Jürgen Horbach[1], Kirill Sandomirski[3], Stefan U. Egelhaaf[3], and Hartmut Löwen[1] — [1]Theoretische Physik II: Weiche Materie, Heinrich-Heine-Universität Düsseldorf, Germany — [2]Institut für Physik, WA 331, Johannes-Gutenberg-Universität Mainz, Germany — [3]Condensed Matter Physics Laboratory, Heinrich-Heine-Universität Düsseldorf, Germany

Properties of bulk crystals and the crystal-fluid interface in a system of hard spheres are studied by density functional theory using unconstrained minimization [1] of accurate fundamental measure functionals [2]. Results for free energies, density distributions and vacancy concentrations of bulk crystals compare very well to data from Monte Carlo simulations [3]. For the equilibrium hard-sphere crystal-fluid interface we combine fundamental measure density functional theory, Monte-Carlo computer simulation [4] and confocal microscopy experiments [5] on sterically-stabilized colloids to determine the orientation-resolved interfacial tension and stiffness.

[1] R. Ohnesorge et al, Phys. Rev. E **50**, 4801 (1994)
[2] H. Hansen-Goos and R. Roth, JPCM **18**, 8413 (2006)
[3] M. Oettel et al, Phys. Rev. E **82**, 051404 (2010)
[4] R. E. Rozas and J. Horbach, Europhys. Lett. **93**, 26006 (2011)
[5] K. Sandomirski et al, Soft Matter **7**, 8050 (2011)

O 58.9 Wed 18:15 Poster B

Molecular Scale Structure of Ionic Liquids near Electrodes — •Peter Reichert[1], Jannis Ochsmann[1], Kasper Skov Kjaer[2], Tim Brandt van Driel[2], Martin Meedom Nielsen[2], Harald Reichert[3], Diego Pontoni[3], and Markus Mezger[1] — [1]Max-Planck-Institut für Polymerforschung, Mainz, Germany — [2]Technical University of Denmark and Risø National Lab, Roskilde, Denmark — [3]European Synchrotron Radiation Facility, Grenoble, France

To understand and optimize electrochemical processes in ionic liquids (ILs), information on their molecular-scale structure near electrodes is essential. Recent high-energy x-ray reflectivity experiments on dielectric substrates revealed interfacial layering comprised of alternating anion and cation enriched regions with this modulation decaying into the bulk liquid. To investigate the molecular-scale arrangement of ions near electrodes under electrochemical control, a novel sample chamber was developed. For the in-situ experiments at the High-Energy Micro Diffraction instrument at ID15, ESRF we selected two hydrophobic ILs based on butyl-1-methylpyrolidonium and tetrabutylammonium cations with the tris(pentafluoroethyl)trifluorophosphate anion that exhibit an exceptional wide electrochemical window. The solid-liquid interface between the ILs and a boron doped diamond substrate was studied at electrochemical potentials between -2.5 V and +1.6 V vs. platinum quasi reference electrode. Quantitative analysis of the experimental x-ray reflectivity data revealed distinct changes in the ion distribution near the interface, induced by the applied potentials.

O 58.10 Wed 18:15 Poster B

Determination of single crystal emissivity by comparison with black-body radiation — •Fabian Scheepers, Sara Wanjelik, and Mathias Getzlaff — Institute of Applied Physics, University Duesseldorf

Contactless determination of temperature provides advantages towards traditional thermometers. Pyrometers allow a quick measurement up to several thousand degrees Celsius even in physically and chemically aggressive environment. Based on Planck's law, nowadays used devices are mostly limited by the knowledge of surface conditions. Ecspecially high reflective metals are the actual challenge. Their emissivity can vary over a large range. Therefore, the temperature and surface dependent correction coefficient must be known. Here we report concerning this correction for a tungsten surface; it was obtained by a spot infrared pyrometer that compared the apparent and their associated black-body radiation.The black-body was realised in the form of a cylindrical bore in the tested material and heated by electron impact. Additionally, a tungsten-based thermocouple was used for a second independent temperature determination.

O 58.11 Wed 18:15 Poster B

Removal of carbon impurities in tungsten by extended annealing — •Sven Kalka — Heinrich Heine Universität, Düsseldorf

In order to carry out experiments in the field of surface science, atomically clean surfaces have to be prepared. A clean surface on the atomic scale is also important when used as a substrate for further experiments, like deposition of thin films. In the case of W(110) surfaces, most of the adsorbates can easily be removed by heating the crystal to about 2000K. Tungsten carbides however are stable even at high temperature and need to be removed separately. Carbon is an impurity within the bulk and diffuses to the surface again, so the cleaning procedure needs to be repeated. Thus, the removal of the carbon impurities within the bulk or at least the near surface region is desirable. We exposed the crystal to an oxygen atmosphere of 10^{-6}mbar, while heating it for several days. With this approach, we reduce the carbon content within the crystal and the subsequent diffusion of carbon to the surface. By STM imaging and LEED, we can evaluate the remaining impurities on the surface directly. Comparison of STM images at different stages of the annealing process indicates a reduction of carbon within the bulk.

O 58.12 Wed 18:15 Poster B

Investigation of the laser-cleaning process on Lead photocathodes — •Susanne Schubert[1], Roman Barday[1], Thorsten Kamps[1], John Smedley[2], Robert Nietubyc[3], Andrei Varykhalov[1], and Giesela Weinberg[4] — [1]HZB, Berlin, Germany — [2]BNL, Upton, USA — [3]NCBJ, Swierk, Poland — [4]FHI, Berlin, Germany

Metal photocathodes are widely used in electron injectors due to their stability and long life time. Due to adsorption of contaminants the work function increases and thus the quantum efficiency is reduced. In order to increase the quantum efficiency of our Pb cathode we performed a cleaning procedure by means of a high power excimer laser as suggested by Smedley [1]. We present the results of a combined photo emission, SEM and quantum efficiency measurement study on witness samples. Thin Lead films were arc-deposited on optical polished Mo-substrates [2]. Before and after irradiation the sample was analyzed at 140 eV photon energy at a XPS/ARPES end station at the synchrotron radiation source Bessy II. Since the surface roughness is of concern for the injector performance it was examined before and after the irradiation procedure with white-light-interferometry and the surface morphology by means of SEM.

[1]J. Smedley et al, PRST-AB 11, 013502 (2008) [2]Rao, T. et al., IPAC 2010, THPEC020 (2010)

O 58.13 Wed 18:15 Poster B

Anisotropic Change in Surface Resistance upon Adsorption of Oxygen on Cu(110) as observed by IRRAS — •Jan Pischel, Olaf Skibbe, and Annemarie Pucci — Kirchhoff-Institut für Physik, Im Neuenheimer Feld 227, D-69120 Heidelberg

Adsorbate induced changes in the electrical conductivity of thin metal films are of great interest because of their importance in technological applications, e.g. microelectronic devices. By developping the concept of surface friction between conduction electrons and adsorbate, Persson showed that changes in surface resistance will result in a broadband infrared absorption feature in the case of reflection experiments with p-polarized radiation [1]. Taking advantage of that fact, Otto et al. showed that on the highly anisotropic Cu(110) surface, interaction between conduction electrons and adsorbates settling on top of the close-packed rows of the surface is restricted to the case where the plane of incidence is parallel to these rows [2].

Tying in with these findings, we investigated the anisotropic change in surface resistance induced by formation of the (2×1)O-Cu(110) *Added-Row* reconstruction, where involvement of the second layer lead to a non-vanishing change in surface resistance also in the case of perpendicular orientation of the plane of incidence with respect to the rows.

[1] B. N. J. Persson. Phys. Rev. B, **44**:3277-3296, 1991.

[2] A. Otto et al. New J. Phys., **9**:288, 2007.

O 58.14 Wed 18:15 Poster B

Adsorption geometry and phase diagram of Br/Pd(110) — •Alexander Menzel, Peter Amann, Michael Cordin, and Erminald Bertel — Institute for Physical Chemistry, University of Innsbruck, Austria

As the adsorbate system Br/Pt(110)-c(2x2) at 0.5ML Bromine coverage can be used as a low-dimensional model system [1], we were interested in the phase diagram of Br and Cl on the isoelectronic Pd(110) surface.

The electronic surface resonances, which are responsible for the low-dimensional behavior in the case of Pt(110), can be found in ARPES spectra at Pd(110), too. The phase diagram of Br- and Cl-covered Pd(110) was studied for coverages below 1ML. Using LEED, well ordered c(2x4) and c(4x2) Br/Pd(110) phases were found for a coverage of 0.25ML and 0.75ML, respectively. A continuous spot splitting of fractional order spots is observed for coverages in between. As shown by STM, the spot splitting below 0.5ML is due to anti-phase domains in [001]-direction, whereas above 0.5ML, the splitting is caused by continuous compression along [110]-direction. Interestingly, the c(2x2) phase expected for 0.5ML cannot be observed in the temperature range of the experiments (above 100K). A diagram of the observed phases is presented.

[1] P. Amann et al., Eur. Phys. J B 10, 15 (2010).

O 58.15 Wed 18:15 Poster B

DFT Studies on the Adsorption of *R,R*-Tartaric Acid at Copper Surfaces — •Felix Hoffmann and Jörg Behler — Lehrstuhl für Theoretische Chemie, Ruhr-Universität Bochum, D-44780 Bochum

The adsorption of organic molecules at metal surfaces has a wide range of applications, e.g. in corrosion protection, surface functionalization and heterogeneous catalysis. Typically, the products in heterogeneous catalysis are a mixture of enantiomers, but there are some systems yielding an excess of one species. Such enantioselective processes at surfaces have received a lot of attention in recent years. An important aspect of these systems is the modification of the bare metal surface by chiral modifier molecules. An important model system for the formation of globally chiral phases at surfaces is the adsorption of *R,R*-tartaric acid at the Cu(110) surface. Using density-functional theory, we investigate the structural and energetic properties of a variety of phases. Further, the influence of surface defects on the adsorption energy is studied.

O 58.16 Wed 18:15 Poster B

Co-Phtalocyanine on Au(100) Surfaces — •Eva Rauls and Wolf Gero Schmidt — Theoretische Physik, Universität Paderborn, Warburger Str. 100, 33100 Paderborn

For several reasons, phtalocyanines (Pc) with or without metal center are currently under intense investigation in surface physics. The biocompatibility of these molecules together with their electronic structure makes them highly interesting for energy transfer processes in medical applications. In nanotechnology, they are especially useful due to their flexibility, since the basis of these molecules can easily be varied with different functional groups substituting parts of the molecule or simply attached to the core of the molecule. But already upon exclusively exchanging the center atom, the binding energy to a substrate, the molecular deformation or the spin state can be tailored.

In this work, we present our first principles investigations of Co-Pc on Au(100)-surfaces. In contrast to our previous studies of similar porphyrins on Au(111) [1] or Au(110), the flat surface geometry does not induce the strong deformation observed in these cases. A comparatively strong interaction of the complete molecule with the substrate is observed.

[1] S. Müllegger, E. Rauls, et al. ACS Nano 5, 6480 (2011).

O 58.17 Wed 18:15 Poster B

Adsorption dependent charge state of self-assembled donor-acceptor complexes on Au(111) — •Tobias R. Umbach, Isabel Fernández-Torrente, Jose I. Pascual, and Katharina J. Franke — Institut für Experimentalphysik, Freie Universität Berlin, Arnimallee 14, 14195 Berlin, Germany

The redistribution of charge between organic species and surfaces plays a key role for tuning the electronic functionality of molecular organic compounds on metal surfaces. We investigate self-assembled monolayers of 11,11,12,12-tetracyanonaphtho-2, 6-quinodimethane (TNAP) mixed with sodium (Na) on a Au(111) surface by low temperature scanning tunneling microscopy and spectroscopy (LT-STM, LT-STS). Successive deposition of TNAP and Na leads to the formation of an ordered windmill structure of TNAP and Na. The molecules close to the soliton lines are single charged accompanied by a Kondo resonance observed in STS transport experiments. In contrast, all other TNAP molecules show no Kondo resonance. The adsorption site dependent charge state of the TNAP molecules in the Na-TCNQ layer is an indication for different alignments of the molecular orbitals and therefore variations of the charge transfer process.

O 58.18 Wed 18:15 Poster B

Adsorption of Diindenoperylene on Cu(111) Surfaces — •Hazem Aldahhak, Eva Rauls, and Wolf Gero Schmidt — Theoretische Physik, Universität Paderborn, Warburger Str. 100, 33100 Paderborn

Thin films of organic molecules like diindenoperylene (DIP) on metal substrates are of great interest for the further miniaturization of organic optoelectronic devices. As recently reported, films of DIP molecules on Cu(111) surfaces behave ambipolarly. In contrast to deposition on largely extended terraces, deposition of DIP molecules on narrow terraces (<15 nm) of Cu(111) leads to an interesting structure with co-directionally oriented molecules, the symmetry of which is not dictated by the hexagonal substrate symmetry [1].

In order to clarify this behavior, we investigated the balance between intermolecular and molecule-substrate interactions in this system. We performed first principles density functional theory calculations for various adsorbate structures. For isolated DIP molecules, the calculation of the potential energy surface (PES) allows us to determine the activation energy for the mobility of the molecules as a prerequisite for self organisation. At higher coverages, the molecules are found to organise in adsorbate structures which agree well with the experimental findings in [1].

[1] De Oteyza et al., Phys. Chem. Chem. Phys. 11, 8741 (2009).

O 58.19 Wed 18:15 Poster B

Observing Structural Phase Dynamics and Molecular Aggregation in Real Time: Dispersive NEXAFS Applied to Organic Films — •Markus Scholz[1,2], Christoph Sauer[1,2], Michael Wiessner[1,2], Holger Wetzstein[1,2], Achim Schöll[1,2], and Friedrich Reinert[1,2] — [1]Physikalisches Institut, Experimentelle Physik VII und Wilhelm Conrad Röntgen Research Center for Complex Material Systems (RCCM), Universität Würzburg, D-97074 Würzburg — [2]Gemeinschaftslabor für Nanoanalytik, Karlsruher Institut für Technologie KIT, D-76021 Karlsruhe

We present a novel experimental approach which allows following structural and electronic changes in organic films by quick near edge X-ray absorption fine-structure spectroscopy (QNEXAFS). This technique utilizes the energy-dispersive mode of the BESSY UE52-PGM beamline[1] and allows NEXAFS with about one second time resolution. We show the potential of the method on the example of thin films of the organic molecule 1,4,5,8-naphthalene-tetracarboxylicacid-dianhydride (NTCDA). The time-evolution of the NEXAFS signal recorded at different temperatures allows distinguishing between different processes that are involved in the reorganization of the film. Moreover, since the technique also monitors spectroscopic details we are able to observe changes within the signature of the NEXAFS spectra during the phase transition.

[1] Batchelor, Schmidt, Follath, Jung, Fink, Knupfer, Schöll, Noll, Siewert, Büchner, Umbach, Nuclear Inst. And Methods in Physics Research Section A, Volume 575, Issue 3 (2007), 470

O 58.20 Wed 18:15 Poster B

Chemisorptive bonding of Pyrenetetraone on Cu(111) and Ag(111) measured with XSW — •Christoph Bürker[1], Jens Niederhausen[2], Steffen Duhm[3], Takuya Hosokai[4], Jörg Zegenhagen[5], Ralph Rieger[6], Joachim Räder[6], Klaus Müllen[6], Alexander Gerlach[1], Norbert Koch[2], and Frank Schreiber[1] — [1]Universität Tübingen, Germany — [2]Humboldt-Universität zu Berlin, Germany — [3]Chiba University, Japan — [4]Iwate University, Japan — [5]ESRF, France — [6]Max-Planck-Institut für Polymerforschung Mainz, Germany

The X-ray Standing Wave (XSW) technique [1] is a high precision method to obtain the vertical bonding distance for each chemical element of the molecule. In recent years it was shown that the bonding distance may be dependent on the substrate and correlated with the interaction strength [2].

We present the adsorption geometry of PYTON (4,5,9,10-Pyrenetetraone, $C_{16}H_6O_4$) on Cu(111) and Ag(111). Our results show a significant bending of the oxygen atoms towards the substrate, both for Cu(111) and for Ag(111). Furthermore, for both metals the bonding distance of PYTON is relatively small, indicating a strongly interacting, chemisorbed system with a possible charge transfer between PYTON and substrate. Comparing these results with PTCDA ($C_{24}H_8O_6$) adsorbed on the same metals [2,3] we see a stronger and almost substrate independent interaction of PYTON with Cu(111) and Ag(111). [1] J. Zegenhagen, Surf. Sci. Rep. **18** (1993),199 [2] S. Duhm et al., Org. Electr. **9** (2008),111 [3] A. Gerlach et al., Phys. Rev. B **75** (2007)

O 58.21 Wed 18:15 Poster B

Pentacene/Ag(110): A comparison of DFT and GW results with photoemmision data — •Daniel Lüftner[1], Thomas Ules[2], Georg Koller[2], Michael G. Ramsey[2], and Peter Puschnig[1] — [1]Lehrstuhl für Atomistic Modelling and Design of Materials, Montanuniversität Leoben, Franz-Josef-straße 18, A-8700 Leoben, Austria — [2]Institut für Physik, Karl-Franzens-Universität Graz, Universitätsplatz 5, A-8010 Graz, Austria

We have prepared a monolayer of pentacene on Ag(110) and studied its valence electronic structure by angle-resolved photoemission spectroscopy. Thereby, an extensive data set of the photocurrent I as a function of parallel momenta (k_x, k_y) and binding energy E_b has been obtained. By comparing this data cube with simulated momentum maps of various pentacene molecular orbitals, we unambiguously identify four molecular states between the Fermi level and the top of the Ag *d*-band. This allows us to investigate in detail their energetic positions, broadenings, and modifications in orbital shapes upon adsorption. Moreover, we have calculated the electronic structure of different geometric arrangements of pentacene molecules within the framework of density functional theory (DFT) and – on top of that – the G_0W_0 approximation. We show that G_0W_0 corrections greatly improve DFT band gaps and demonstrate that the G_0W_0 gaps are strongly dependent on the local environment of the pentacene molecule, an effect which is absent in DFT orbital energies. Finally, we compare the orbital energies from DFT and G_0W_0 calculations to the experimental values obtaiend for the pentacene monolayer on Ag(110).

O 58.22 Wed 18:15 Poster B

Spin crossover effect in single aza-BODIPY molecule — •Jörg Meyer, Anja Nickel, Robin Ohmann, Cormac Toher, Francesca Moresco, and Gianaurelio Cuniberti — Institute for Materials Science and Max Bergmann Center of Biomaterials, TU Dresden, 01062 Dresden, Germany

Aza-BODIPY are a class of organic fluorescent dyes which have recently become interesting for organic photovoltaics because of their strong tuneable infrared absorption and their high stability. We investigated two molecular species consisting of two aza-BODIPY core units bound to one central metal atom by low temperature STM/STS and ab initio DFT calculations. The aim of this study was to find out how the different metal atoms (Co, Zn) influence the properties of the organic molecules. Because of steric hindrance among the aza-BODIPY ligands these molecules have a three dimensional structure. That is why the inner structure of the molecule could not be imaged by STM. We evaporated the aza-BODIPY onto a Ag(110) surface, separately. Both molecular species show two different adsorption geometries and are topographically identical. In the STS measurements of the Co-aza-BODIPY different spectra were obtained for the same position on the same molecule. One part of the spectra was very similar to those measured on Zn-aza-Bodipy, while the other spectra showed additional states near the Fermi level. DFT calculations indicate that the changes in these spectra are related to the spin crossover effect.

[1]J. Meyer et. al, Phys. Chem. Chem. Phys. 13, 14421 (2011).

O 58.23 Wed 18:15 Poster B

Self-assembled monolayers of phthalocyanines on gold substrates — •Nadezda Lilicenko[1], Florian Vogel[1], Ulrich Glebe[2], Ulrich Siemeling[2], and Frank Träger[1] — [1]Institur für Physik and Center for Interdisciplinary Nanostructure Scienece and Technology - CINSaT, Universität Kassel, Germany — [2]Institur für Chemie and Center for Interdisciplinary Nanostructure Scienece and Technology - CINSaT, Universität Kassel, Germany

Stable self assembled monolayers (SAMs) of advanced molecules on metal surfaces have attracted considerable attention over the last years. SAMs have found many applications, for example in nanotechnology, as biosensors, for chemical vapour sensing or molecular electronics. In this context, phthalocyanines (PCs) are of great interest, because they exhibit fascinating physical properties, which arise from their delocalized pi-electrons. In our experiments we have used two thioether substituted (sub-)phthalocyanine derivatives for SAM formation, one subphthtalocyanine with boron as central atom and one bis(phthalocyaninato)terbium - single molecular magnet. To study the adsorption of the molecules, we applied optical second harmonic generation (SHG). SHG permits to monitor adsorption process as well as the ordering within the film. The information about monolayer formation kinetics was obtained by fitting the measured SHG data with three kinetic models: first-order, second-order and diffusion limited Langmuir kinetic. As a complementary technique to proof that only monolayer formation takes place, ellipsometric measurements have been performed.

O 58.24 Wed 18:15 Poster B

Plasmonic light emission boosted by the charging of a molecule — Alexander Kabakchiev[1], Theresa Lutz[1], •Christian Dette[1], Christoph Grosse[1], Klaus Kuhnke[1], Uta Schlickum[1], and Klaus Kern[1,2] — [1]Max-Planck-Institut für Festkörperforschung, D-70569 Stuttgart, Germany — [2]Institut de Physique de la Matière Condensée, Ecole Polytechnique Fédérale de Lausanne, CH-1015 Lausanne, Switzerland

The efficiency of light generation in a scanning tunneling microscope (STM) can depend on the accumulated charge on an individual organic molecule. We employ STM in ultra-high vacuum at liquid helium temperature to study tunnel-current-induced luminescence on the single molecule level. *fac*-$Ir(ppy)_3$ molecules deposited on a C_{60} double layer on Au(111) are investigated by spatially resolved differential conductance spectroscopy and luminescence spectroscopy. We observe that individual $Ir(ppy)_3$ molecules are surrounded by an extended area in which the light emission is boosted by up to two orders of magnitude above the emission on the C_{60} layer. This area increases with the applied bias voltage. Optical spectroscopy reveals that the luminescence is not intrinsic to $Ir(ppy)_3$ but is due to locally excited tip-induced plasmons. Differential conductance maps exhibit a strong ring-like feature which coincides with the margins of the area of enhanced luminescence. We demonstrate that the efficiency of plasmon generation can thus be controlled by a reversible electric-field-induced elementary charge transfer.

O 58.25 Wed 18:15 Poster B

Deposition and investigation of Mn_{12} single molecule magnets on surfaces — •Philipp Erler[1], Stefan Ambrus[2], Sebastian Höll[1], Samuel Bouvron[1], Sönke Voss[1], Michael Burgert[2], Ulrich Groth[2], Elizabeta Cavar[1], and Mikhail Fonin[1] — [1]Fachbereich Physik, Universität Konstanz, 78457 Konstanz — [2]Fachbereich Chemie, Universität Konstanz, 78457 Konstanz

Single molecule magnets (SMMs) represent a class of metalorganic compounds which show magnetic bistability of purely molecular origin and a rich quantum spin behavior below a certain blocking temperature. Because of their superparamagnetic properties and the additional benefits of a monodisperse size distribution, an inexpensive fabrication through self-assembly and the chemical tunability of their molecular ligand shell, SMMs are particularly interesting for applications in spin-based data storage and quantum-computing technologies.

Here we present a detailed study of several Mn_{12} derivatives chemically bound to a gold surface. We investigated the structural and electronic properties of the Mn_{12} molecules in a self-assembled monolayer by means of scanning tunneling microscopy (STM) and spectroscopy (STS) and X-ray photoelectron and absorption spectroscopy (XPS, XAS). Low temperature STM images are shown, revealing a submolecular resolution. Furthermore, we implemented electrospray ionization (ESI) for the deposition of Mn_{12} molecules in ultra high vacuum. In contrast to a wet chemical preparation procedure, this method offers the advantages of a control over the surface coverage and a free choice of the substrate and the molecular ligand.

O 58.26 Wed 18:15 Poster B

Characterizing a Charge Transfer Complex by nc-AFM/STM — •Fabian Schulz, Isabel Fernandez-Torrente, Adrian Oliv-

era, Christian Lotze, Martina Corso, Katharina Franke, and Jose Ignacio Pascual — Freie Universität Berlin, Institut für Experimentalphysik, Arnimallee 14, 14195 Berlin, Germany.

The F4-TCNQ/Au(111) metal-organic interface is a promising candidate for the design of molecular organic electronics, due to its potential regarding Fermi level alignment and facilitation of charge-carrier injection. Therefore, much experimental and theoretical effort has been made to understand the charge transfer process taking place upon adsorption of F4-TCNQ on Au(111). Still, the results remain controversial [1], making more in-depth investigations necessary [2].

By combined qPlus noncontact-AFM/STM measurements - in both imaging and spectroscopy mode - we find the co-existence of two different ordered submonolayer F4-TCNQ/Au(111) phases, yielding also two different charge states. One of them shows a Kondo resonance in conductance experiments, indicating the existence of a single occupied molecular orbital and thus, charge transfer of one electron from the substrate to the molecule. Measurements of the local contact potential difference (LCPD) on different molecular sites reveal that the different charge states can be correlated with different LCPD values [3].

[1] Z.G. Soos *et al.*, Organic Electronics **12**, 39 (2011).
[2] G.M. Rangger *et al.*, Physical Review B **79**, 165306 (2009).
[3] L. Gross *et al.*, Science **324**, 1428 (2009).

O 58.27 Wed 18:15 Poster B

Triazatriangulenium on Ag(111) investigated with scanning tunneling and atomic force microscopy — •Katharina Scheil[1], Nadine Hauptmann[1], Christian Hamann[1], Thiruv. Gopakumar[1], Franziska Otte[2], Rainer Herges[2], and Richard Berndt[1] — [1]Institut für Experimentelle und Angewandte Physik, Christian-Albrechts-Universität zu Kiel, 24098 Kiel, Germany — [2]Otto-Diels-Institut für Organische Chemie, Christian-Albrechts-Universität zu Kiel, 24098 Kiel, Germany

Triazatriangulenium (TATA) has been proposed as a platform to controllably attach functional molecules to metallic surfaces. We used a combined low-temperature scanning tunneling and atomic force microscope in ultra high vacuum to investigate this platform on Ag(111) surfaces. The molecule TATA was deposited using electrospray ionization. TATA molecules arrange in a complex pattern comprising ring-like subunits. The underlying intermolecular interactions will be discussed. Financial support by the Deutsche Forschungsgemeinschaft via the SFB 677 is gratefully acknowledged.

O 58.28 Wed 18:15 Poster B

Mixing Chromophores in SAMs of Azobenzene Derivatives — •Daniel Brete[1,2], Daniel Przyrembel[2], Wolfgang Freyer[1], Robert Carley[1,2], Cornelius Gahl[1,2], and Martin Weinelt[1,2] — [1]Max-Born-Institut Berlin — [2]Freie Universität Berlin

Since photoisomerisation of azobenzene-functionalised alkanethiols in self-assembled monolayers (SAMs) on gold is generally suppressed, controlled dilution of the switching moieties is desirable.

In a solution of dissimilar thiols in general one component is preferentially adsorbed leading to a single component SAM. From a solution of two similar azobenzene-functionalised alkanethiols differing only by their tail group, 6-(4-trifluoromethyl-4'-azobenzeneoxy)-hexane-1-thiol and 6-(4-cyano-4'-azobenzeneoxy)-hexane-1-thiol, we obtained mixed SAMs. HR-XPS measurements show that the composition of the SAM reflects the concentrations of the two components in solution. Shifts in the XPS peak positions indicate that real mixing and not the formation of uniform islands occurs at the surface while NEXAFS data demonstrate that the orientation of the molecules in the mixed SAM is identical to that of the single component SAMs. This is a first step towards decoupling of the chromophores.

O 58.29 Wed 18:15 Poster B

Adsorption of fluorinated and non-fluorinated CuPc on Ag(111) — •Christoph Kleimann, Sonja Schröder, Benjamin Stadtmüller, Ingo Kröger, Christa Elsaesser, and Christian Kumpf — Peter Grünberg Institut (PGI-3), Forschungszentrum Jülich, 52425 Jülich, Germany and Jülich-Aachen Research Alliance (JARA) - Fundamentals of Future Information Technology

Organic thin films usually exhibit a variety of different structures when they adsorb on metal surfaces, depending on the particular interface properties. It is our goal to obtain a fundamental understanding of molecular assembly and the interaction characteristics for both, organic-metal contacts and hetero-organic interfaces.

Here we present results on the adsorption of copper(II)-hexadecafluoro-phthalocyanine (F16CuPc) on Ag(111). We have used spot-profile-analysis LEED (SPA-LEED) for identifying different phases, and scanning tunneling microscopy (STM) as well as x-ray standing waves (XSW) for further characterization.

At low coverages and room temperature a disordered phase is observed. When the first monolayer is closed, the molecules arrange themselves in long rows. Along the rows the molecules are very well ordered, but neighboring rows are often slightly shifted with respect to each other, which is reflected by well defined streaks in the SPA-LEED images.

We also present first results obtained for mixed layers of fluorinated and non-fluorinated molecules (F16CuPc and CuPc).

O 58.30 Wed 18:15 Poster B

Revealing molecular dynamics through Scanning Noise Microscopy and Spectroscopy — •Johannes Schaffert[1], Maren C. Cottin[1], Andreas Sonntag[1], Hatice Karacuban[1], Christian A. Bobisch[1], Nicolás Lorente[2], Jean-Pierre Gauyacq[3], and Rolf Möller[1] — [1]Faculty of Physics, Center for Nanointegration Duisburg- Essen, University of Duisburg-Essen, 47048 Duisburg, Germany — [2]Centre d'Investigació en Nanociència i Nanotecnologia (CSIC-ICN), Campus UAB, E-08193 Bellaterra, Spain — [3]Institut des Sciences Moléculaires d'Orsay, CNRS-Université Paris-Sud 11, UMR 8214, Bâtiment. 351, Université Paris-Sud, F-91405 ORSAY Cedex, France

We show how by adding the real-time characterization of the tunnelling current noise to the standard operation of Scanning Tunneling Microscopy (STM), switching processes on surfaces can be analyzed. This kind of Scanning Noise Microscopy (SNM) was applied for individually adsorbed organic CuPc molecules on Cu(111). It reveals excitation spectra as well as excitation maps with Angstrom spatial resolution. The Noise Spectroscopy clearly exhibits the molecular orbitals LUMO, HOMO and HOMO-1, which could be observed by conventional Scanning Tunneling Spectroscopy only faintly. The mechanism of the molecular switch could be identified as an in-plane libration between the ground state and two transiently occupied states. The findings are confirmed by Density Functional Theory calculations.

O 58.31 Wed 18:15 Poster B

Binary donor acceptor films of TTT and TNAP on Au(111) investigated by LEED and STM — •Benjamin Fiedler[1], Elena Rojo-Wiechel[1], Julia Simon[2], Johannes Beck[2], and Moritz Sokolowski[1] — [1]Institut für Physikalische und Theoretische Chemie der Universität Bonn — [2]Institut für Anorganische Chemie der Universität Bonn

We prepared pure and mixed monolayers of electron accepting and electron donating molecules, namely Tetrathiotetracene (TTT) and Tetracyanonaphthoquinodimethane (TNAP), on Au (111) under ultrahigh vacuum conditions. The films were studied by LEED and STM. Pure TTT shows a complex film growth with a disordered phase at low coverage and an ordered phase at high coverage. In addition, the deposition of TTT leads to a lifting of the Au (111) surface reconstruction. For TNAP the Au(111) surface reconstruction is preserved after deposition. The unit cells of the ordered monolayers of TTT and TNAP are orientated differently with respect to Au(111) surface, but exhibit similar size and shape. Both molecules arrange in brick wall type structures. Quite differently, in the mixed film the molecules are arranged in alternating parallel rows of one type of molecule. Interestingly, the two dimensional arrangement of TTT and TNAP is rather similar to that in alternating stacks of TTF/TCNQ bulk charge transfer crystals.

This work was supported by the DFG through SFB 813.

O 58.32 Wed 18:15 Poster B

HREELS Investigation of Ethene Chemisorption on Cu(110) — •Emanuel Welsch, Olaf Skibbe, Jan Pischel, and Annemarie Pucci — Kirchhoff-Institut für Physik, Im Neuenheimer Feld 227, D-69120 Heidelberg

Nowadays, the adsorption of ethene has been studied extensively and is well understood on a large number of the many possible single crystal metal subtrates. However, the properties of the chemisorption systems C_2H_4 on Cu(110) and on roughened copper substrates have always been discussed controversially [1-3], comprising the questions of adsorption geometry and of the anomalous IRRAS intensity of the observed gas phase Raman active vibrational modes. Whilst the former has implications on the issue whether a certain mode is dipole allowed or not, the explanation of the latter demanded a new excitation mechanism. Such a mechanism, based on the creation of electron hole pairs, has been established for the case of roughened copper substrates [4].

In this work we present the results of recent HREELS measurements which clearly demonstrate that the abovementioned model cannot explain the activation of the Raman active modes in the case of C_2H_4/Cu(110). Furthermore the selection rules of impact scattering are applied in order to discuss the compatibility of the spectra with several of the possible adsorption geometries.

[1] C. J. Jenks et al. Surf. Sci. Lett., **277**:L89-L94, 1992.
[2] J. Kubota et al. Phys. Chem., **98**:7653-7656, 1994.
[3] R. Raval. Surf. Sci., **331-333**:1-10, 1995.
[4] A. Priebe et al. J. Phys. Chem. B, **110**:1673-1679, 2006.

O 58.33 Wed 18:15 Poster B

Chemical transformations drive complex self-assembly of uracil on close packed coinage metal surfaces — •Anthoula C. Papageorgiou, Sybille Fischer, Joachim Reichert, Katharina Diller, Florian Blobner, Florian Klappenberger, Francesco Allegretti, and Johannes V. Barth — Physik Department E20, Technische Universität München, 85748 Garching, Germany

We address the interplay between adsorption, chemical nature and self-assembly of uracil on Ag(111) and Cu(111) surfaces as a function of molecular coverage and temperature. We find that the metal surface acts both as a template and a catalyst for the resulting self-assembled structures. With a combination of STM, synchrotron XPS and NEXAFS studies, we unravel a molecular phase map on Cu(111) consisting of three phases, in stark contrast to what is observed for the case of uracil on the more inert Ag(111) surface. On Ag(111) uracil adsorbs flat, intact and forms close packed two-dimensional islands. The self-assembly is driven by stable hydrogen bonded dimers with poor two-dimensional order. On Cu(111) complex structures are observed and we determine these phase transformations to be driven by gradual deprotonation of the uracil molecules. Our XPS study reveals the tautomeric signature of uracil in the contact layer and its deprotonation site. Our data show a dependence between molecular coverage and molecule-metal interaction, as the molecules tilt at higher coverages in order to accommodate for a higher packing density. After deprotonation of both uracil N atoms, the observed adsorption geometry can be understood only with significant charge redistribution in the molecule.

O 58.34 Wed 18:15 Poster B

Evolution of metallophthalocyanine multilayers on Cu(111) during thermal treatment depends on the type of metal center — •Jie Xiao[1], Min Chen[1], Hans-Peter Steinrück[1], and J. Michael Gottfried[2] — [1]Lehrstuhl für Physikalische Chemie II, Universität Erlangen-Nürnberg, 91058 Erlangen, Egerlandstrasse 3, Germany — [2]Fachbereich Chemie, Universität Marburg, 35032 Marburg, Hans-Meerwein-Strasse, Germany

Vapor deposited multilayer (> 20 ML) Co-phthalocyanine (CoPc) on Cu(111) behaves differently than other transition metal phthalocyanines (MPcs) with the same coverage, such as ZnPc, CuPc and NiPc, when the respective multilayers are heated to a temperature well above their multilayer desorption temperature. For CoPc, the residual coverage is about 6 monolayers after annealing to 650 K, compared to 1-2 monolayers for the other MPcs. This has been found by X-ray and ultraviolet photoemission measurements. Transition metal phthalocyanines, including CoPc, have been demonstrated to adopt a flat-lying orientation on metal substrates, at least at submonolayer and monolayer coverages. However, the residual layer after CoPc desorption shows a different UP spectrum than a directly deposited film of the same coverage, suggesting that the post-heating step causes a different molecular orientation. Possible origins of this effect, including partial reaction of the peripheral C-H bonds with the Cu substrate, will be discussed. Support by the DFG through SFB 583 and the Alexander-von-Humboldt Foundation is gratefully acknowledged.

O 58.35 Wed 18:15 Poster B

STM Signatures of C60 and C58 on Au(111) Surfaces: a DFT Study — •Melanie Stendel[1,2], Alexej Bagrets[2], Christian Seiler[1,2], and Ferdinand Evers[1,2] — [1]Institut für Theorie der Kondensierten Materie, Karlsruhe Institute of Technology (KIT), 76131 Karlsruhe, Germany — [2]Institut für Nanotechnologie, Karlsruhe Institute of Technology (KIT), 76344 Karlsruhe, Germany

Recent STM-experiments [1] have measured the surface topography of C60 molecules and two isomers of C58 adsorbed on a Au(111) surface. This topography exhibits a pronounced variation for the C60-fullerene and the C58 derivates, which highlights the significantly different electronic structure of the underlying species. Hence, the functionality of a putative fullerene-based thin film technology would be very sensitive to the use of the constituting molecule, C60, C58 and others.

Here, we present a systematic study of the possible adsorption geometries of C60 and C58 on Au(111) within the density functional theory (DFT). Further, we calculate a map of the local density of states in the tip-plane above the molecule for each geometry. Based on this map a qualitative comparison with experimentally determined topographies will be given.

[1] AG Kappes and AG Wulfhekel, Karlsruhe Institute of Technology (KIT), 76131 Karlsruhe, Germany, measurements to be published.

O 58.36 Wed 18:15 Poster B

Scanning tunneling microscopy and spectroscopy of TMP-TCNQ — •Sandra Perkert[1], Katerina Medjanik[1], Shahab Naghavi[2], Milan Rudloff[3], Vita Solovyeva[3], Dennis Chercka[4], Torsten Methfessel[1], Sergej Nepijko[1], Michael Huth[3], Claudia Felser[2], Martin Baumgarten[4], Klaus Müllen[4], Gerd Schönhense[1], and Hans-Joachim Elmers[1] — [1]Institut für Physik, Johannes Gutenberg-Universität, 55099 Mainz, Germany — [2]Institut für Analytische und Anorganische Chemie, Johannes Gutenberg-Universität, 55099 Mainz, Germany — [3]Physikalisches Institut, Goethe-Universität, 60438 Frankfurt am Main, Germany — [4]Max-Planck-Institut für Polymerforschung, 55128 Mainz, Germany

Organic charge transfer (CT) salts are promising new materials for electronic devices. For a better understanding of their interaction with metal substrates we investigate thin films of the well-known acceptor 7,7,8,8-Tetracyanoquinodimethane (TCNQ) and the new synthesized donor Tetramethoxypyrene (TMP) on a W(110) and an Au(111) surface with scanning tunneling microscopy (STM) and spectroscopy (STS). The topographic images show a self-organized structure of TMP and TCNQ on both substrates. On the Au(111) surface TCNQ assembles in an oblique Bravais lattice with different orientational domains. STS measurements reveal the electronic structure of the molecules and the energetic position of HOMO and LUMO. The measured energy gap between HOMO and LUMO is much smaller for the CT-salt TMP-TCNQ than for the pure donor TMP and the pure acceptor TCNQ. These results fit well to theoretical calculations.

O 58.37 Wed 18:15 Poster B

Planar gold nano crystals as photonic substrate for single-molecule mechano-optical investigations — •Sören Grannemann, Tamara Münnich, Volker Walhorn, and Dario Anselmetti — Biophysics and Applied Nanoscience, Faculty of Physics, Bielefeld University, Germany

The combination of scanning probe microscopy and optical microscopy techniques is a valuable tool for biological and biomedical investigations at the single molecule level. For these investigations transparent substrates are needed that allow easy sample immobilization. Thin (approx. 20nm) gold films are (quasi) transparent materials whose surface modification by thiol-chemistry is easy and well established. Planar gold nano crystals (PGNC) grown via the thermal aqueous solution method [1] exhibit sizes ranging from some 100 nm to several microns while their thickness lies in the range of roughly 20 nm. Furthermore, the Gold (111) surface is atomically smooth and ideally allows for the immobilization of self-assembled monolayers. We synthesized PGNC and immobilized them on indium tin oxide (ITO) coated glass cover slips. The nano-crystals were investigated by atomic force microscopy (AFM) to characterize their size, thickness and surface roughness. Furthermore, the excitation and detection of single molecule fluorescence through the PGNC by total internal reflection fluorescence (TIRF) microscopy is demonstrated. Therefore, we modified the immobilized PGNC with a mercapto-alkyl self-assembled monolayer exhibiting sparsely distributed amino moieties for dye attachment. [1] H.-C. Chu, C.-H. Kuo and M. H. Huang, Inorg. Chem., 808, 2006.

O 58.38 Wed 18:15 Poster B

UV-Vis spectroscopy studies of photoswitching of azobenzene-containing molecular platform adlayers on Au — •Nicolai Krekiehn[1], Ulrich Jung[1], Mathias Müller[1], Jens Kubitschke[2], Sandra Ulrich[2], Rainer Herges[2], and Olaf Magnussen[1] — [1]Institut für Experimentelle und Angewandte Physik der Christian-Albrechts-Universität, Kiel, Deutschland — [2]Otto-Diels-Institut für Organische Chemie Christian-Albrechts-Universität, Kiel, Deutschland

Photofunctional self-assembled monolayers (SAMs) on solid substrates are of current interest for the preparation of functional nanosystems. These SAMs, however, often exhibit inherent disadvantages as reduced structural order or strong electronic coupling with the substrate (in particular pronounced for metals), which may cause an efficient quenching of the desired functions. We recently introduced a novel aproach for formation of such SAMs basing on molecular platforms, whose structural properties (orientation of the function, lateral and vertical distances of the platforms) can be precisely controlled and verified this concept by STM[1] and various spectroscopies[2].

Here, we present preliminary spectroscopic studies of photoswitching in platform SAMs containing azobenzene, a prototypical molecular switch. Measurements were performed in either transmission or reflection geometry. The photoswitching reactions were found to obey 1st order kinetics and exhibit high quantum efficiencies.

[1] Kuhn et al. PCCP (2010), 12, 4481,[2] Jung et al., Langmuir (2011), 27, 5899

O 58.39 Wed 18:15 Poster B

Ultrathin films of NTCDA on Ag(111): Growth and thermal evolution beyond the monolayer — •Carolin R. Braatz, Gregor Öhl, and Peter Jakob — Fachbereich Physik, Philipps-Universität Marburg

The growth of well defined thin films of large organic molecules using molecular deposition techniques depends critically on the structural properties of the substrate and/or the contact layer between organic film and the substrate. A comprehensive characterization of these is therefore vital to arrive at an improved understanding of the growth mechanisms of organic layers with destined properties. In this contribution the growth and the thermal evolution of NTCDA layers on Ag(111) have been studied in the temperature range 80 – 550 K using FT-IRAS, SPA-LEED, and TPD. Particular attention is devoted to phase transformations of monolayer and bilayer NTCDA/Ag(111) under different growth conditions and their effect on the initial growth of multilayer films. The potential of IRAS as an in-situ analytical technique to characterize organic film growth is discussed.

O 58.40 Wed 18:15 Poster B

STM investigation on the adlayer structures of the ionic liquids EMIM-TFSA and BMP-TFSA on Au(111) in the submonolayer regime — •Benedikt Uhl, Michael Roos, and Rolf Jürgen Behm — Ulm University, Institute of Surface Chemistry and Catalysis, D-89069 Ulm, Germany

The adlayer structures of the ionic liquids (IL) 1-butyl-1-methylpyrrolidinium-bis(trifluoromethylsulfonyl)imide (BMP-TFSA) and 1-ethyl-3-methylimidazolium-bis(trifluoromethylsulfonyl)imide (EMIM-TFSA) on Au(111) have been investigated by scanning tunneling microscopy (STM). Especially the structure of the first layer of adsorbates on the metal surface is under investigation. The measurements were performed in ultra high vacuum (UHV) at temperatures between 100 K and 298 K, with coverages in the submonolayer and the monolayer regime. At temperatures around 100 K the BMP-TFSA as well as the EMIM-TFSA adsorbates appear as round shaped protrusions in the STM pictures. The nature of these protrusions, which may represent cations, anions or both of them, is discussed. Depending on the preparation process, the adsorbates form different structures, a 2D glass-like phase as well as 2D crystalline structures with long-range order. The different structures are presented in detail (2D density, unit cell) and their dependence on surface coverage is elucidated. The 2D crystalline structures show strong dependence on the Au(111) reconstruction pattern. In this context the influence of the substrate on the structure formation is discussed.

O 58.41 Wed 18:15 Poster B

STM investigation of PbPc adsorbed on Ag(111) — •jiang peng and hietschold michael — Chemnitz University of Technology, Institute of Physics, Solid Surfaces Analysis Group, D-09107 Chemnitz, Germany

We have investigated the adsorption of PbPc on Ag(111). Using OMBE, an ultrathin film of PbPc (a little more than one monolayer) has been deposited on Ag(111) and annealed for 20min to 250°C. Two different adsorption structures have been found. The molecular unit cells characterise A=1.59nm, B=1.84nm with a angle of 87°, and A=1.75nm, B=1.626nm with a angle of 79°, respectively. On the Ag(111) surface we found all of the shuttle-cock shaped molecules in the Pb-down adsorption configuration, no molecules have been adsorbed with the Pb atom up. PbPc molecules on the second layer lie directly on top of the first layer making a direct stack. The molecular adsorption structures found suggest at relatively strong interaction between Pb and Ag substrate, which forces central Pb atom in the down position.

O 58.42 Wed 18:15 Poster B

Ultraviolet photoemission from ionic liquids — •Rebecca Pöschel and Thomas Fauster — Friedrich-Alexander Universität Erlangen, Lehrstuhl für Festkörperphysik, Staudtstr. 7, 91058 Erlangen, Germany

Room-temperature ionic liquids entirely consist of molecular ions. Due to their very low vapor pressure they can be used and studied under ultrahigh vacuum conditions on single-crystal surfaces.

In this study we used two ionic liquids containing the same cation 1-ethyl-3-methylimidazolium $[\mathrm{EMIM}]^+$ and two different anions bis(triflouromethylsulfonyl)amide $[\mathrm{Tf_2N}]^-$ and tetracyanoborate $[\mathrm{TCB}]^-$. Films of different thicknesses between 0.3 and 20 monolayers were deposited on a well-defined Cu (100) single-crystal surface via evaporation. The samples were measured by vacuum ultraviolet (VUV) photoelectron spectroscopy (21.2 eV) under normal emission. The molecular orbitals were studied as a function of layer thickness and a strong radiation damage was observed.

O 58.43 Wed 18:15 Poster B

Ultrathin samaria films on Pt(111) studied by PES and LEED — •J.H. Jhang[1], A. Schaefer[1], D. Ragazzon[2], L.E. Walle[3], M.H. Farstad[3], A. Borg[3], A. Sandell[2], and M. Bäumer[1] — [1]Institute for Applied and Physical Chemistry, Universität Bremen, Germany — [2]Department of Physics and Astronomy, Uppsala University, Sweden — [3]Department of Physics, NTNU, Trondheim, Norway

Rare earth oxides (REOs) exhibit high potential as catalysts due to the ability to easily switch between oxidation states. Their catalytic capability depends strongly on the storage and release of oxygen. The tendency to promote partial or total oxidation reactions is influenced by the existing oxidation states and oxygen mobility: While ceria (3+ and 4+ as stable oxidation states) is a good catalyst for total oxidation, samaria (only 3+ as stable oxidation state) seems to be the most effective REO for partial oxidation of methane, to just name one example. Therefore, in order to look into the atomic details of oxygen transport and transfer a simplified two dimensional model system may be prepared and studied under controlled conditions in ltra-high vacuum (UHV). Studies of REO films other than ceria are however very limited. This makes the exploration of other REOs highly motivated. We present first results on samaria growth on Pt(111) by using physical vapour deposition (PVD) in UHV. Two methods will be presented for samaria growth: oxidation of a surface alloy and deposition in elevated oxygen background pressure. The generated oxide layers are investigated by synchrotron radiation based photoelectron spectroscopy (PES) and low energy electron diffraction (LEED).

O 58.44 Wed 18:15 Poster B

STM investigation of ultra thin silver films on Nb(110) — •Matthias Stocker, Holger Pfeifer, Berndt Koslowski, and Paul Ziemann — Institut für Festkörperphysik, Universität Ulm, D-89081 Ulm

Thin silver films (in the monolayer range) were thermally evaporated onto Nb(110) at approximately 100 °C and analyzed by scanning tunneling microscopy (STM) and spectroscopy (STS) at 5.3 K. The Ag/Nb(110) forms islands of 2ML height which coalesce to form a contiguous layer at a nominal coverage of 2ML. On the islands we find quasi-periodic depressions of depth ~0.1 nm and period ~2 nm pointing to a significant stress within the Ag layer. Spectroscopy reveals a marked difference between the DOS off and on the island with strong resonances at (-1.4, -1.0, 0.0, 0.7) eV which cannot be attributed to quantum well states in the silver. The origin could be hybridization of Ag with Nb states at the interface. On the island, the DOS is strongly reduced above the Fermi energy indicating the development of the L gap in the Ag layer. The stress in the Ag layer with the locally varying strain leads to prominent changes in the DOS as revealed by dI/dV maps.

O 58.45 Wed 18:15 Poster B

Adsorption of CO on $\mathrm{Rh_N}$/Ru(0001) Films — •Sebastian Thussing, Pawel Gazdzicki, and Peter Jakob — Fachbereich Physik, Philipps-Universität Marburg, 35032 Marburg, Germany

The growth of thin ($\leq$ 3 ML) Rh/Ru(0001) films and the adsorption of CO on these films have been investigated in the temperature range

85 – 1350 K using IRAS, TPD, and LEED. Specifically, the shifts of the CO stretching vibration due to lateral interactions, lattice strain and influence by the substrate were investigated. Furthermore, the dependence of CO adsorption energies and coverages on the Rh-film thickness were explored. A minimum in CO desorption energy was thereby found for the first Rh monolayer. For these layers four distinct long-range ordered phases of CO, with characteristic occupation of the various CO adsorption sites, have been observed. Based on our ability to discriminate the various CO species according to their local binding geometry, morphological changes in the island size distribution (ranging from single Rh atoms to extended Rh islands and Rh/Ru surface alloys) have been analyzed. The findings are discussed in the context of recent work on Pt_N/Ru(0001) layers [1, 2].

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[2] Jakob, P. and Schlapka, A., Surf. Sci. 601, 3556 (2007).

O 58.46 Wed 18:15 Poster B

Preparation and in-situ analysis of MOVPE-prepared Si(111) surfaces — •Thomas Haensel[1], Weihong Zhao[1], Henning Döscher[1,2], Sebastian Brückner[1], Peter Kleinschmidt[3], Oliver Supplie[2], Matthias M. May[2], and Thomas Hannappel[1,3] — [1]Technische Universität Ilmenau, Institut für Physik, Fachgebiet Photovoltaik, Gustav-Kirchhoff-Straße 5, D-98684 Ilmenau — [2]Helmholtz-Zentrum Berlin für Materialien und Energie, Hahn-Meitner-Platz 1, D-14109 Berlin — [3]CiS Forschungsinstitut für Mikrosensorik und Photovoltaik GmbH, Konrad-Zuse-Straße 14, D-99099 Erfurt

III-V nanowires are one example for new solar cell concepts aiming at high efficiency. Compared to III-V wafers, silicon substrates benefit from low cost and mature high quality manufacturing. Generally, III-V nanowires are prepared on {111} surfaces. While the preparation of pristine Si(111) is well-established in ultra-high vacuum (UHV), little is known about the preparation of Si(111) surfaces grown in metal organic vapor phase epitaxy (MOVPE) ambient. A contamination-free transfer system enables us to relate in situ reflection anisotropy spectroscopy (RAS) and UHV based techniques such as scanning tunneling microscopy (STM), low energy electron diffraction (LEED) and X-ray photoelectron spectroscopy (XPS). Similarly, we analyzed the nucleation of GaP on Si(111).

O 58.47 Wed 18:15 Poster B

Double layer steps on Silicon(100) prepared in H_2 ambient — •Wei Hong Zhao[2], Johannes Luczak[1], Peter Kleinschmidt[1,3], Sebastian Brückner[1,2], Henning Döscher[1,2], Oliver Supplie[1], and Thomas Hannappel[1,2,3] — [1]Helmholtz-Zentrum Berlin, Institut Solare Brennstoffe und Energiespeichermaterialien, D-14109 Berlin — [2]TU Ilmenau, Institut für Physik, Fachgebiet Photovoltaik, D-98693 Ilmenau — [3]CiS Forschungsinstitut für Mikrosensorik und Photovoltaik, D-99099 Erfurt

Preparation of double-layer steps is important for heteroepitaxial growth of III-V semiconductors on Si(100). Single-layer steps on Si(100) are associated with the presence of two domains with different dimer orientations on the reconstructed surface, leading to the initiation of anti-phase domains (APDs) in the epitaxial III-V layer. Our process consists of deoxidation, homoepitaxial growth employing silane, annealing and cooling in hydrogen ambient. We studied the surface structure using Fourier-transform infrared spectroscopy, low-energy electron diffraction and scanning tunneling microscopy (STM). STM measurements on Si(100) show the formation of D_A and D_B - double-steps on a surface with an intermediate offcut of 2° in [011] direction dependent on cooling procedere. The STM images on 6° misoriented samples revealed a preference for D_B double layer steps.

O 58.48 Wed 18:15 Poster B

Adsorption of Organic Molecules on Potassium Chloride — •Hazem Aldahhak, Eva Rauls, and Wolf Gero Schmidt — Theoretische Physik, Universität Paderborn, Warburger Str. 100, 33100 Paderborn

The ability to grow self-assembled supramolecular nanostructures on solid surfaces has important implications in both basic science and nanotechnology. The constraint to two dimensions enables us to reduce the molecular mobility and study the various interactions between the adsorbed molecules on the one hand and between molecule and surface on the other hand, separately. In recent years, metal surfaces were used as the most common substrate. However, the surfaces of alkali salts like sodium or potassium chloride, open up new possibilities. Surface symmetry and ionicity as well as technological reasons, like e.g. simple mechanisms for the desorption of grown supramolecular assemblies, make these surfaces a worthwile alternative to metal substrates.

We present our investigations of the adsorption of organic molecules like PTCDA on KCl and NaCl surfaces. To this aim, we have performed first principles density functional theory calculations and focussed on both the geometric and electronic structure of single molecules as well as molecular layers at higher coverages.

O 58.49 Wed 18:15 Poster B

Charge Localization Dynamics Induced by Oxygen Vacancies on the TiO2(110) Surface and Titania and Gold-promoted Titania Surfaces Interaction with small molecules — •Matteo Farnesi Camellone — Ruhr-Universität Bochum D-44780 Bochum

We use ab initio molecular dynamics to investigate the dynamics of an F–center created by an oxygen vacancy on the TiO2(110) rutile surface. The simulations uncover a truly complex, time-dependent behavior of fluctuating electron localization topologies in the vicinity of the oxygen vacancy. Although the two excess electrons are found to populate preferentially the second subsurface la<x>yer, they occasionally visit surface sites and also the third subsurface layer [1]. We then study the interaction of CO with the (110) Au supported (110) TiO2 surface catalysts. The structural, electronic, dynamical and thermodynamic properties of the gold promoted titania surfaces are investigated by means of density functional theory calculations that account for the on site Coulomb interaction via the inclu sion of a Hubbard term (GGA+U). The interaction between gold and substrate is accompained by an extensive charge reorganization at the metal-oxide contact wich leads to Au oxidation and the reduction of the titanum dioxide substrate. It is shown that the catalytic activity of the (110) TiO2 substrate is efficiently improved by supported and dispersed Au adatoms on the same substrate. [2]

[1] P. M. Kowalski, M. Farnesi Camellone, N. N. Nair, B. Meyer, and D. Marx, Phys. Rev. Lett. , 146405 (2010). [2] M. Farnesi Camellone, P. M. Kowalski, and D. Marx, Phys. Rev. B 84, 035413 (2011)

O 58.50 Wed 18:15 Poster B

Density functional calculation of interface structure of Fe/ZnO — •Sougata Pal and Eckhard Pehlke — Institut für Theoretische Physik und Astrophysik, Universität Kiel, Germany

Interfaces between magnetic and piezoelectric materials bear the possibility of magnetoelectric coupling phenomena which occur at the interface, in addition to coupling via long range strain fields [1]. As a model system, we have started to investigate the adsorption of 1/4 – 1 ML Fe on both the unreconstructed and the (2×2) vacancy-reconstructed ZnO(000$\bar{1}$) surfaces by means of density functional calculations. First, the lowest-energy structures have to be identified. Among the calculated adsorption sites, the *fcc* hollow position is energetically favorable. At sufficiently large oxygen chemical potential, the energy can be further lowered by substituting the top layer Zn-atoms with Fe atoms. In this case the Zn-atoms created by the Zn-Fe exchange are assumed to become oxidized and included into the ZnO bulk. It has turned out be energetically unfavorable, however, to exchange Zn-atoms in deeper layers with Fe-atoms. The interface between ZnO and the locally formed Fe-oxide is thus expected to be sharp. The findings are consistent with Fe-oxidation observed experimentally [2,3].

[1] J.M. Rondinelli, *et al.*, Nature Nanotechnology **3**, 46 (2008).

[2] A. Demund *et al.*, Surf. Interface Anal. **40**, 27 (2008).

[3] Guo-Dong Wang *et al.*, Surf. Review and Lett. **15**, 295 (2008).

O 58.51 Wed 18:15 Poster B

III-V on Si(100) for photoelectrocatalysis — •Matthias M. May[1,2], Oliver Supplie[1,2], Henning Döscher[1], Sebastian Fiechter[1], Hans-J. Lewerenz[1,3], Klaus Schwarzburg[1], and Thomas Hannappel[1,4,5] — [1]Helmholtz-Zentrum Berlin, Institut Solare Brennstoffe und Energiespeichermaterialien, D-14109 Berlin — [2]Humboldt-Universität zu Berlin, Institut für Physik, D-12489 Berlin — [3]California Institute of Technology, Pasadena, USA — [4]TU Ilmenau, Institut für Physik, Fachgebiet Photovoltaik, D-98693 Ilmenau — [5]CiS Forschungsinstitut für Mikrosensorik und Photovoltaik, D-99099 Erfurt

III-V semiconductors on Si(100) represent possible candidates for photoelectrochemical splitting of H_2O. InP grown by MOVPE has proven to be a promising photocathode for H_2 evolution [1]. GaP is closely related to InP and can be grown on Si(100) [2] combining a III-V semiconductor with the inexpensive Si substrate. Lattice match and band gap engineering can be achieved via incorporation of e.g. N [3].

This heteroepitaxial system also opens the possibility of a monolithically integrated photoelectrochemical tandem device addressing both hydrogen and oxygen evolution. First experiments investigating the fundamental properties regarding surface chemistry and topography of these III-V systems on Si are presented.
[1] Lewerenz et al., *Energy Environ. Sci.* **3** (2010)
[2] Döscher et al., *J. Appl. Phys.* **107**, 123523 (2010)
[3] Shan et al., *Phys. Status Solidi B* **223**, (2001)

O 58.52 Wed 18:15 Poster B

Laser interferometric observations of capillary rise in arrays of silicon nanochannels — •Mark Busch[1] and Patrick Huber[1,2] — [1]Experimental Physics, Saarland University, Saarbrücken, Germany — [2]Faculty of Physics and Astronomy, Pontifical Catholic University, Santiago, Chile

We present measurements on the capillary rise of liquids in mesoporous silicon films. The time-dependent rise level of the liquid within the pores has been determined with laser interferometry [1]. The measurements are based on the change of refractive index during the filling of the pores. Such measurements allow one to explore the initial stages of nanochannel filling.

In particular we focus on the orientation and temperature dependence of the filling process. The presented measurements were taken with 2-Propanol and 1-Decanol.

[1] Acquaroli, L. N. *et al.* Capillary Filling in Nanostructured Porous Silicon, *Langmuir* **2011**, *27(5)*, 2067-2072

O 58.53 Wed 18:15 Poster B

On the GaN crystal growth in the MOCVD method: a DFT study — Maria Ptasińska[1], •Jacek Piechota[1], Jakub Sołtys[1], and Stanisław Krukowski[1,2] — [1]Interdisciplinary Centre for Materials Modelling, University of Warsaw, Pawińskiego 5a, 02-106 Warsaw, Poland — [2]Institute of High Pressure Physics (UNIPRESS), Polish Academy of Sciences, Sokołowska 29/37, 01-142 Warsaw, Poland

The purpose of this study is to construct the GaN (gallium nitride) crystal growth model of MOVPE (Metal Organic Vapor Phase Epitaxy) method employing TMG (trimetylogallium) and NH3 (ammonia) as reaction precursors. Two possible reaction paths are taken into consideration. The first one is the decomposition of TMG in the gas phase under high temperature and pressure in the MOVPE chamber and the atomic Ga adsorption on the GaN crystal surface. The second one is TMG decomposition at GaN crystal surface. Calculations indicate that there is charge transfer from the TMG molecules to the GaN surface during approach of TMG molecules to the GaN surface. This may result in bonds breaking in the TMG molecule and Ga adsorption at the surface. Two cases were examined: First the adsorption on the GaN(000-1) surface with broken bonds and second the adsorption on the GaN(0001) surface covered with NH2. Under some special conditions the TMG decomposition was observed close to the GaN surface which is preliminary step to construct general theory of decomposition of various molecules during the GaN crystal growth in the MOCVD method.

O 58.54 Wed 18:15 Poster B

Theoretical investigation of the Zn, O, O2, and H2O adsorption on the polar ZnO(0001) and ZnO(000-1) surfaces — Jakub Sołtys[1], •Jacek Piechota[1], and Stanisław Krukowski[1,2] — [1]Interdisciplinary Centre for Materials Modelling, University of Warsaw, Pawińskiego 5a, 02-106 Warsaw, Poland — [2]Institute of High Pressure Physics (UNIPRESS), Polish Academy of Sciences, Sokołowska 29/37, 01-142 Warsaw, Poland

Performed density functional theory simulations of adsorption of the Zn and O atoms, as well as O2 and H2O molecules on the polar ZnO(0001) and ZnO(000-1) surfaces clarify the principal processes, important for growth of ZnO from the vapor. Demonstrated results indicate that Zn atom is adsorbed at both ZnO surfaces without any energy barrier, but with ultimately different adsorption energies: 0.34 eV for the metallic, and 3.37 for the nonmetallic surface, respectively. In contrast, O atoms are attached very strongly at both polar surfaces, with energies equal to 5.47 eV for the metallic and 2.47 eV for the nonmetallic surface, respectively. The difference between both polar surfaces is the highest for adsorption of molecular oxygen, the O2 molecule is adsorbed on the Zn-face with the energy of 2.45 eV, while in contrast is not adsorbed at the oxygen face of ZnO at all. Some results of adsorption of H2O at both ZnO surfaces are also presented.

O 58.55 Wed 18:15 Poster B

Scanning Tunneling Microscopy study of single-crystalline $Sr_3Ru_2O_7$ — •Bernhard Stöger[1], Zhiming Wang[1], Michael Schmid[1], Ulrike Diebold[1], David Fibes[2], and Zhiqiang Mao[2] — [1]Institute of Applied Physics, Vienna University of Technology, Vienna, Austria — [2]Department of Physics and Engineering Physics, Tulane University, New Orleans, LA, USA

Perovskite oxides play an important role as cathodes in solid oxide fuel cells (SOFC) and in catalysis. Investigating surface defects such as oxygen vacancies and the adsorption of relevant molecules helps gaining more insight into the physics behind SOFCs and catalytic processes.

High quality $Sr_3Ru_2O_7$ (SRO) single crystals were grown using the floating zone technique. $Sr_3Ru_2O_7$ is part of the ruthenate Ruddlesden-Popper series $Sr_{n+1}Ru_nO_{3n+1}$, which have a layered structure. We investigated the surface of SRO, by means of Scanning Tunneling Microscopy (STM) at 78 K. The single crystals were cleaved in ultra-high vacuum at 150 K, which results in rather large terraces. We have characterized the defects that are present at as-cleaved surfaces, and how their appearance changes with applied STM tunneling parameters. Adsorption of carbon monoxide dosed at 105 K, results in asymmetric cross-like features that span several surface unit cells.

This work was supported by the Austrian Science Fund (FWF project F45)

O 58.56 Wed 18:15 Poster B

Vibronic states of Br_4TPP porphyrines on a Cu_3N insulating film — •Martina Corso[1], Jingcheng Li[1], Zechao Yang[1], Christian Lotze[1], Anna Strozecka[1], Lena Kaufmann[2], Max Kerbs[2], Arno Wiehe[2], Christoph A. Schalley[2], Katharina Franke[1], and Jose Ignacio Pascual[1] — [1]Institut für Experimentalphysik, Freie Universität Berlin, Arnimallee 14, 14195 Berlin, Germany — [2]Institut für Chemie und Biochemie, Freie Universität Berlin, Takustr. 3, 14195 Berlin, Germany

Insulating thin films grown on metal surfaces decouple adsorbates from the electron density of the underlaying substrate. In this work we use low temperature STM to study the vibronic states of tetra(4-bromophenyl)porphyrin (Br_4TPP) molecules decoupled from a Cu(110) surface by a single copper nitride layer (Cu_3N). Differential conductance spectra (dI/dV) taken on isolated Br_4TPP show that two types of molecules coexist on the surface, probably due to a different local adsorption environment. They preserve the same electronic structure but shifted of 350 meV. A series of equally spaced peaks ($\sim$ 170 meV) corresponding to vibronic states appears in the LUMO of Br_4TPP measured in dI/dV spectra. The detection of this vibronic progression, not observed on Cu(110), is enabled by the extended lifetime of the transient charged states of individual Br_4TPP which is seven times larger on copper nitride than on the bare metal.

O 58.57 Wed 18:15 Poster B

LEED and PIRS study of SF_6 physisorption on NaCl(100) — •Mirko Langer, Stephan Härtel, Jochen Vogt, and Helmut Weiss — Chemisches Institut der Universität Magdeburg, Universitätsplatz 2, 39106 Magdeburg, Germany

The interaction of the antropogenic greenhouse gas SF_6 with the NaCl(100) surface was investigated using low-energy electron diffraction (LEED) and polarization infrared spectroscopy (PIRS) under ultrahigh vacuum conditions and cryogenic temperatures. Consistent with the results of a previous study of SF_6 adsorption on NaCl thin films [1], SF_6 exhibits a complicated Stranski-Krastanov film growth behavior on NaCl(100): pronounced 3D nano crystal formation occurs at a substrate temperature of 64 K, indicated by strong absorptions in the region of the asymmetric S-F stretch mode. The observed characteristic Davydov splitting of about 100 cm^{-1} is consistent with the large vibrational polarizability of SF_6 and its bcc bulk structure. In contrast to many other physisorption systems, a 2D adsorbate of SF_6 is formed only at lower temperatures below 45 K, indicated by the appearance of superstructure spots in the LEED patterns. The unusual growth behavior is attributed to the strong lattice mismatch between adsorbate and substrate.
[1] A. Klekamp, E. Umbach, Surf. Sci. Lett. 284 (1993), 291

O 58.58 Wed 18:15 Poster B

Growth and characterisation of Fe thin films on MgO(100) — •Hendrik Bettermann, Wolfgang Rosellen, Torsten Veltum, and Mathias Getzlaff — Institute of Applied Physics, University Duesseldorf

This investigation focuses on Fe films on commercially available MgO substrates. MgO as an insulating material is an interesting substrate for the deposition of thin films. It can provide a cost-efficient one-time alternative to W(110)-substrates.

One possible application for Fe films is the use of it as a supporting and magnetically conducting material for the deposition of magnetic nanoparticles consisting of Ni, Co, or alloys thereof. These are interesting from a technological point regarding data storage due to their size dependent electronic and magnetic properties.

The Fe thin films are investigated and characterised in-situ by LEED (low energy electron diffraction), AES (Auger electron spectroscopy), and STM (scanning tunneling microscopy). XRF (X-ray fluorescence spectroscopy) is also available to perform ex-situ investigations.

We focus on optimized parameters during deposition to produce flat films and wide terraces by variation of both film thickness and annealing temperature.

O 58.59 Wed 18:15 Poster B

Ferrocene ultrathin films on NaCl(100) – a high resolution FTIR study — Birgit Vogt and •Jochen Vogt — Chemisches Institut der Universität Magdeburg, Universitätsplatz 2, 39106 Magdeburg, Germany

Ferrocene $(C_5H_5)^-Fe^{2+}(C_5H_5)^-$ is a prototype of an organometallic sandwich complex. The thin film properties of ferrocene are of interest in many respects, e. g. due to its potential use as a precursor for the deposition of iron or iron oxide films on surfaces [1]. We report on the preparation of ultrathin films of ferrocene on the NaCl(100) surface below 30 K and ultrahigh vacuum conditions. The films were characterized using polarization fourier transform infrared spectroscopy (PIRS). Upon cooling the films from 180 K to 25 K, pronounced reversible frequency shifts and splittings of the distortion modes of the cyclopentadienyl rings are observed. The bending mode at 818 cm^{-1} splits into at least six narrow components between 810 and 830 cm^{-1} with different fractions of absorption in s- and p-polarization, respectively. These are consistent with different orientations of the associated dipole moments with respect to the substrate surface, and a high degree of film crystallinity. Coadsorption experiments with CO_2 reveal that the applied method of preparation results in ferrocene films which cover 60 to 80 percent of the substrate surface.

[1] A. B. F. Martinson et al., J. Phys. Chem. C 115 (2011), 4333

O 58.60 Wed 18:15 Poster B

Morphology and structure of epitaxial films of TiO_x, BaO_x, and $BaTiO_3$ on Pt(100) — •Klaus Meinel[1], Stefan Förster[1], Henning Neddermeyer[1], and Wolf Widdra[1,2] — [1]Institute of Physics, Martin-Luther-Universität Halle-Wittenberg, D-06099 Halle, Germany — [2]Max-Planck Institut für Mikrostrukturphysik, D-06120 Halle, Germany

Interesting applications are expected for films of ternary oxides with perovskite structure such as $BaTiO_3$ which display ferroelectric behavior. In previous work of epitaxial $BaTiO_3$ films on Pt, magnetron sputtering from a $BaTiO_3$ target has been used for film deposition [1]. In the present work, the more gentile reactive vapor deposition of Ti and BaO in an O_2 atmosphere is used for film preparation. STM, SPA-LEED, AES, and XPS have been applied for investigating morphology, structure, thickness, and composition of the binary oxide (TiO_x and BaO_x) films on Pt(100). After carefully adjusting the deposition rates, the simultaneous growth of both materials yields high quality $BaTiO_3$(100) films. With respect to Pt(100), their unit mesh is rotated by 45° yielding a misfit of only 2%. Several superstructures develop which are induced by O vacancies. With the calibrated deposition of the oxides of Ti and Ba, in principle, also a layer by layer construction of $BaTiO_3$ films is possible which allows a deliberate assessment of the interface and surface terminations.

[1] S. Förster, W. Widdra, Surf. Sci. 604, 21631 (2010).