

O 14 Poster session I (Adsorption, Epitaxy and growth, Phase transitions, Surface reactions, Organic films, Electronic structure, Methods) (sponsored by Omicron Nanotechnology GmbH)

Time: Monday 18:00–21:00

Room: P2

O 14.1 Mon 18:00 P2

A Kinetic Monte Carlo Simulation Toolkit for Modelling Processes at Surfaces — ●MICHAEL HOHAGE, ALEXANDER DORNINGER, BERNHARD LEHNER, and PETER ZEPPENFELD — Institute of Experimental Physics, Johannes-Kepler-University Linz, A-4040 Linz

We developed a Kinetic Monte Carlo (KMC) Simulation Tool, capable of studying adsorption, growth, diffusion, desorption and reactions on solid surfaces. The comprehensively tested simulation kernel [1-3] has been successfully used in various recent studies [2-6]. It has been extended by a state-of-the-art graphical user interface, which allows an intuitive definition of the simulation model: Several editors assist in generating surface models, specifying interaction models and reaction pathways, declaring the sequence of operations performed with the virtual sample and choosing the observables. Additional tools assist in data evaluation and visualization. We present this Windows32 compatible KMC simulation tool and show its application to selected growth and desorption phenomena.

[1] B. Lehner, M. Hohage and P. Zeppenfeld, *Surf. Sci.* 454-456 (2000) 251. [2] B. Lehner, M. Hohage and P. Zeppenfeld, *Chem. Phys. Lett.* 336 (2001) 123. [3] B. Lehner, *Non-Ideal Desorption Phenomena in Experiment, Theory and Computersimulation*, Universit^{ts}verlag Rudolf Trauner, Linz, 2003. [4] B. Lehner, M. Hohage and P. Zeppenfeld, *Phys. Rev. B* 65 (2002) 165407. [5] B. Lehner, M. Hohage and P. Zeppenfeld, *Chem. Phys. Lett.* 369 (2003) 275. [6] B. Lehner, M. Hohage and P. Zeppenfeld, *Chem. Phys. Lett.* 379 (2003) 568.

O 14.2 Mon 18:00 P2

DFT study of molybdenum sulfide clusters on the Au(111) surface — ●IGOR POPOV, SIBYLLE GEMMING, and GOTTHARD SEIFERT — Physikalische Chemie und Elektrochemie, TU Dresden, D-01062 Dresden

Understanding of physics and chemistry of the Schottky contact plays an important role in proper functioning of present electronic devices. Molybdenum sulfide clusters deposited on the gold (111) surface provide an example of such contacts. We investigated atomic and electronic properties of the structure, using a DFT method with a plane wave basis set. In addition, speed and reliability of the density functional based tight binding method (DFTB) allows studying of the self landing of the clusters on the surface, using molecular dynamics simulations. Calculations showed that these clusters can be well bonded on the surface at the certain high symmetry points, despite the fact of negligible electron transfer between the two subsystems. Sulfur atoms at bridge sites have the largest contribution to the binding, but also "core" molybdenum atoms in the neighbourhood of the surface have appropriate influence. The existence of a well-defined binding site may allow a self-organised deposition of the clusters and thus provide a suitable contact basis for molecular wires.

O 14.3 Mon 18:00 P2

H/Pt(110) (1x4): Hydrogen induced row pairing on the missing row reconstructed surface. — ●ALEXANDER MENZEL¹, ENRICO DONÀ¹, MARIANA MINCA¹, ERMINGALD BERTEL¹, RINALDO ZUCCA², and JOSEPH REDINGER² — ¹Institut für Physikalische Chemie, Innrain 52a, A-6020 Innsbruck, Austria — ²Center for Computational Materials Science, Gumpendorferstraße 1A, A-1060 Vienna, Austria

Various phases of hydrogen on Pt(110) are investigated by temperature programmed desorption spectroscopy (TPD), quantitative low-energy electron diffraction (LEED) and variable-temperature scanning tunneling microscopy (VT-STM). H is initially taken up with a sticking coefficient of almost one into the short-bridge sites of the close-packed rows of the Pt(110)-(1x2) missing-row reconstructed surface. After saturation of these sites the sticking coefficient drops significantly and further uptake of up to 1.5 monolayers (ML) into lower-binding energy sites is observed. Beyond 1.5 ML extensive H exposures give rise to an autocatalytic desorption feature similar to Ni(110){1}. LEED shows the formation of a (1x4) structure, which is only seen at low primary energies. VT-STM reveals that this structure is due to a row pairing. Again this parallels findings on Ni(110), where at low temperatures also a pairing row recon-

struction is observed [1]. Surprisingly, however, the row pairing in the present case involves rows which are separated by almost 0.8 nm due to the missing row reconstruction. \Zitat{1} {K. Christmann, *Surf. Sci. Rep.* 9, 1 (1988)}

O 14.4 Mon 18:00 P2

Electronic and Structural Properties of Ferrocene-based Molecules on Ag(111) — ●JÖRG MEYER¹, CHRISTOPH TEGENKAMP¹, THOMAS BREDOW², and HERBERT PFNÜR¹ —

¹Institut für Festkörperphysik, Universität Hannover, Appelstraße 2, D-30167 Hannover, Germany — ²Institut für Theoretische Chemie, Universität Hannover, Am Kleinen Felde 30, D-30167 Hannover, Germany

The combination of appropriate electronic properties and structural flexibility makes ferrocene-based (organometallic) molecules suitable candidates for molecular electronics. In addition to the thermal stability, high electron mobility and the possibility to use ferrocene units as building blocks for molecular wires, one further unique property of these structures is the supposed low energetical barrier allowing relaxed adsorption geometries between given metal contacts [1].

Ferrocenedithiol (FDT) is one of the simplest members of this class of molecules. Indeed, the energy cost for conformational changes between (local) D5h and D5d symmetry has been calculated to 4kJ/mol. To get a first insight into adsorption geometry and electronic properties of FDT on Ag(111) surfaces we performed theoretical studies by means of DFT-GGA as implemented in the software package VASP [2]. Models for different adsorption sites, local chemical bonding and results describing the electronic structure of the adsorbed molecule will be shown and compared to experimental results.

[1] M. Vollmann, H. Butenschön, *C. R. Chimie* 8 (2005) 1282

[2] G. Kresse, J. Furthmüller, *J. Comput. Mater. Sci.* 6 (1996) 15

O 14.5 Mon 18:00 P2

Influence of Ag on the CO adsorption and desorption behavior on Pt(644) — ●REGINE STREBER, BARBARA TRÄNKENSCHUH, JOHANNES SCHÖCK, CHRISTIAN PAPP, REINHARD DENECKE, and HANSPETER STEINRÜCK — Lehrstuhl für Physikalische Chemie II, Universität Erlangen-Nürnberg, Egerlandstr. 3, 91058 Erlangen

The influence of Ag on the interaction of CO with a stepped Pt(644)=[5(111)x(100)] surface was studied by using in-situ high-resolution X-ray photoelectron spectroscopy. AES studies indicate that the growth of Ag on stepped platinum surfaces follows a Stranski-Krastanov mechanism [1]. For small (< 0.5 ML) Ag coverages, a row-by-row growth mode has been reported for deposition at 300 K [2]. Besides studying the Ag growth by taking XP spectra in the Ag 3d and Pt 4f binding energy regions, we determined its influence on the CO adsorption behavior by quantitative analysis of time-dependent C 1s spectra. For a silver coverage resulting in monatomic chains along the steps, the total CO coverage at 130 K is mainly associated with the Pt terraces but almost as large as for clean Pt(644) terraces, in spite of the Ag decoration; however, the ratio between CO bonded to on-top and bridge sites decreases. Interestingly, when heating the resulting layers, the C 1s signal related to CO step adsorption is reappearing between 300 and 400 K. The desorption behavior of CO and Ag is also studied by TPD.

[1] P.W. Davies et al., *Surf. Sci.* 121 (1982) 290.

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

O 14.6 Mon 18:00 P2

Probing complex adsorption structures: A joint experimental and theoretical study — ●JAN HAUBRICH¹, DAVID LOFFREDA², FRANÇOISE DELBECQ², PHILIPPE SAUTET², ALEXANDER KRUPSKI¹, CONRAD BECKER¹, and KLAUS WANDEL¹ — ¹Inst. f. Phys. u. Theo. Ch., Wegeler. 12, D-53115 Bonn — ²Lab. de Chimie, UMR CNRS 5182, ENS Lyon, 46 Allée d'Italie, F-69364 Lyon Cedex 07

Studies on catalysis such as the selective hydrogenation of α,β -unsaturated aldehydes on transition metal surfaces represent a challenge to both experimentalists and theoreticians. Although numerous studies

have been dedicated to systems like acrolein or prenal on Pt(111) in recent years, the details of the molecule-surface bonding still remain under debate. Yet the selectivities of such processes depend crucially on the adsorption complexes. Their characterization is even more complicated when alloy surfaces are considered because alloying is often used to optimize the properties of the catalyst. We here present a joint experimental and theoretical study on molecule-surface bonding of prenal on Pt(111) and two Pt-Sn surface alloys based on the interpretation of HREEL spectra using ab initio density-functional theory (DFT). HREELS experiments carried out on the three model-catalysts show highly complex spectra of the adsorbed prenal at low temperatures. Combining the HREEL spectra with the results of the vibrational analysis obtained from the DFT calculations, we are able to identify stable adsorption geometries, interpret the normal modes corresponding to the measured loss peaks and to point to likely reaction intermediates.

O 14.7 Mon 18:00 P2

Order on a disordered layer: Dy chain structures on Mo(112) — ●C. TEGENKAMP¹, A. FEDORUS², A. NAUMOVETS², J. ZACHARIAE¹, and H. PFNÜR¹ — ¹Institut für Festkörperphysik, Abteilung Oberflächen, Appelstr. 2, 30167 Hannover, Germany — ²Institute of Physics, Natl. Academy of Sciences, Prospect Nauki 46, UA-03039, Kyiev-39, Ukraine

The formation of atomic chain structures on surfaces by self assembly is inevitably related to a characteristic interaction mechanism between them. Even more, the coupling determines strongly the electronic property of single chains. For a variety of electropositive metals adsorbed on either anisotropic (110)-fcc or (112)-bcc metal surfaces the formation of (nx1) structures (n=5,7,8,9..) have been observed and can be explained by Friedel oscillations along a surface state.

In contrast, the Dy/Mo(112) system shows a less pronounced interaction, because the system forms a 2D glass phase, i.e. surface alloying takes place for annealing temperatures higher than 300K and coverages up to 0.5ML. Interestingly, on top of this disordered phase the growth of ordered chain structures is possible, as revealed by STM and LEED experiments, i.e. the formation of (2x1), (4x1) and (5x1) structures have been found for initial coverages higher than 0.8ML Dy [1]. Furthermore, for coverages between 0.6 and 0.8ML a rectangular (7x1) and a uniaxial incommensurate (5x1) phase have been identified and will be discussed. [1] A. Fedorus et al. Eur. Phys. J.B 24 (2001) 395.

O 14.8 Mon 18:00 P2

Interaction of oxygen and hydrogen with a Pd(110) surface — ●TOBIAS PERTRAM, MARKO KRALJ, ALEKSANDER KRUPSKI, CONRAD BECKER, and KLAUS WANDEL — Institute of Physical and Theoretical Chemistry, University of Bonn, Wegelerstr. 12, D-53115 Bonn, Germany

The clean Pd(110) surface has a tendency towards reconstruction and even small quantities of adsorbed atoms can trigger the process of surface restructuring. In the case of room temperature hydrogen adsorption it is understood that the (1x2) missing-row reconstruction is stabilized by the creation of (111) micro facets, which provide the most stable adsorption sites for hydrogen atoms [1].

In our study we perform in situ scanning tunneling microscopy (STM) and observe the surface restructuring induced by the adsorption of hydrogen or oxygen on clean Pd(110). We are interested in the adsorption of small amounts of the respective adsorbate and study the importance of large terraces and step edges in the initial stages of restructuring. The results indicate that the steps oriented in the [001] direction are of particular significance for the coherent surface restructuring. A statistical analysis shows that the reconstructed surface area for small exposures increases exponentially with exposure. This suggests that equal amounts of adsorbate do not lead to equal increments of restructured area but the accumulated dose plays a crucial role in the kinetics.

[1] V. Ledentu, W. Dong, P. Sautet, G. Kresse, J. Hafner, Phys. Rev. B 57 (1998) 12482.

O 14.9 Mon 18:00 P2

Development of an *in-situ* exchangeable inert Shapal-M-based molecule evaporator — ●KNUD LÄMMLE, ALEXANDER SCHWARZ, and ROLAND WIESENDANGER — Institute of Applied Physics, University of Hamburg, Jungiusstr. 11, D-20355 Hamburg

We describe the development of an *in-situ* exchangeable evaporator

and the required peripheral equipment for the preparation of organic molecules on clean substrates in an UHV environment. The evaporator is mounted on a transfer shuttle compatible with an existing Omicron chamber system. The crucible is made of Shapal-M, a machinable ceramic with a high thermal conductivity as well as a high mechanical stress resistivity and therefore much better suited than other non-metallic materials normally used like alumina, boron nitride or vitreous carbon. It is heated by a tungsten filament, which is wound directly around the Shapal-M cylinder. For precise temperature regulation, a thermocouple is integrated into the crucible. Moreover, the evaporation rate can be monitored by a quartz crystal microbalance. In order to manipulate the growth mode of the molecular thin films, the sample stage is equipped with a thermocouple controlled heating unit.

O 14.10 Mon 18:00 P2

Electrochemical deposition of Cu nanowires on TaS₂ — ●YINXIANG BAI¹, SUJIT KUMAR DORA¹, OLAF MAGNUSSEN¹, RAINER ADELUNG², and MADY ELBAHRI² — ¹Institut für Experimentelle und Angewandte Physik, Christian-Albrecht-Universität zu Kiel, Leibnizstr. 19, 24118 Kiel, Germany — ²Technische Fakultät der Christian-Albrechts-Universität zu Kiel, Kaiserstraße 2, 24118 Kiel, Germany

Metal deposition on transition metal dichalcogenides under vacuum conditions has been shown to result in the formation of metal nanowires for a number of systems [1]. Here we demonstrate that similar nanowires can also be formed by electrochemical deposition, using Cu electrodeposition on TaS₂ as an example. Studies by cyclic voltammetry, ex-situ scanning electron microscopy, and in-situ scanning tunnelling microscopy reveal characteristic differences to Cu nanowires formed by vacuum deposition as well as details on the growth process.

[1] R. Adelung, R. Kunz, F. Ernst, L. Kipp, and M. Skibowski, in: Adv. in Solid State Physics 43, B. Kramer (Ed.), Springer, Heidelberg, 2003, p. 463-476

O 14.11 Mon 18:00 P2

STM-Study of Cu growth and adsorption of atomic hydrogen on the ZnO(0001)-Zn and ZnO(10-10) surfaces — ●MARTIN KROLL, THOMAS LÖBER, and ULRICH KÖHLER — Experimentalphysik / Oberflächenphysik, Ruhr-Universität Bochum, 44780 Bochum, Germany

The growth of Cu on ZnO-surfaces was studied as a model system for a catalyst for the low-temperature synthesis of methanol. Scanning tunneling microscopy (STM) was used to analyse the polar ZnO(0001)-Zn surface and the non-polar, mixed terminated ZnO(10-10) surface. The reaction of atomic hydrogen with both ZnO-surfaces was examined as a function of temperature from room temperature up to 700°C. For higher temperature an etch-attack was found. The influence of temperature and a hydrogen pre-coverage on the morphology of copper clusters was determined. A bimodal distribution of copper-clusters was found after annealing. Additionally, also the adsorption of water was studied.

O 14.12 Mon 18:00 P2

Role of elastic relaxations in reconstructed (2x1) O phase on Cu(110) studied by different coverages at room temperature and 600 K. — ●MARINA MOISEEVA¹, CHRISTIAN BOMBIS², and HARALD IBACH¹ — ¹Institut für Schichten und Grenzflächen ISG 3, Forschungszentrum Julich GmbH, 52425 Julich — ²Department of Physics and Astronomy, Ny Munkegade, Building 520,DK-Aarhus C, Denmark

The surface stress induced by self-assembly of (2x1)O on Cu(110) has been studied using bending bar technique. This technique makes enable to measure a substrate curvature and to characterise the surface by STM simultaneously.

In case of thermal equilibrium, according to the theory of Allerhand et al.[1] the domain wall energy β can be estimated to $-0.16 \text{ meV}/\text{\AA}$ at RT and $0.02 \text{ meV}/\text{\AA}$ at 600 K. At both temperatures, compressive surface stresses decreases in its absolute value when Cu-O coverage increases. The influence of kinetic processes can be seen in an asymmetric shape of a stripe periodicity vs. coverage curve.

[1] O.L.Allerhand et al.Phys.Rev.Lett.61,1973(1988); V.I.Marchenko JETP, 79,257(1980)

O 14.13 Mon 18:00 P2

Local surface potential analysis of vapor phase deposited bifunctional phosphonic acid self-assembled monolayers by means of Kelvin probe force microscopy — ●MATHIAS RODENSTEIN¹, CHRISTIAN LOPPACHER¹, ULRICH ZERWECK¹, EVELYN JÄHNE², SIBYLLE GEMMING³, GOTTHARD SEIFERT³, and LUKAS ENG¹ — ¹Institute of Applied Photophysics, Technische Universität Dresden, D-01062 Dresden, Germany — ²Institute of Macromolecular Chemistry and Textile Chemistry, TU Dresden, D-01062 Dresden, Germany — ³Institute of Physical Chemistry and Electrochemistry, TU Dresden, D-01062 Dresden, Germany

Mono- and bifunctional self-assembly monolayers (SAM) having a phosphonic acid (PA) anchoring group were investigated with respect to their film formation and interface dipolar properties on the nanometer scale. Films were grown by physical vapor phase deposition onto muscovite mica under UHV conditions and compared to liquid phase deposited PA-SAMs formed on mica and oxidic substrates such as SiO₂.

The local growth behavior was analyzed using non-contact scanning force microscopy (nc-SFM). We find a similar growth behavior for the two different deposition methods used here. The layer formation follows three steps: island nucleation, aggregation, and coalescence. Furthermore, we inspected our PA-SAMs with respect to the build-up of an interface and molecular dipole by simultaneously complementing our nc-SFM measurements with frequency modulated Kelvin probe force microscopy (KPFM).

O 14.14 Mon 18:00 P2

Ab initio study of the functionalization stability of the H:Si(001) surface — ●ALESSANDRA CATELLANI^{1,2}, CLOTILDE S. CUCINOTTA^{2,3}, ANDRAS STIRLING^{4,5}, ALICE RUINI^{2,3}, and ELISA MOLINARI^{2,3} — ¹CNR-IMEM, Parco Area delle Scienze 37a, 43010 Parma, Italy — ²CNR-INFN National Center on nanoStructures and bioSystems at Surfaces (S3), Via Campi 213a, 41100 Modena, Italy — ³Dipartimento di Fisica, Università di Modena e Reggio Emilia, Via Campi 213a, 41100 Modena, Italy — ⁴Department of Chemistry and Applied Biosciences, ETHZ, Lugano, CH — ⁵Chemical Research Center, Budapest, H-1525, Hungary

We performed finite-temperature ab initio simulations of water interaction with the functionalized H:Si(001) surface, within the metadynamics approach. Since most of the relevant technological treatments of hybrid systems are performed in wet ambient conditions, this study provides an estimate of the stability of different possible functionalization schemes. In order to understand the role of competing hydrophobic fragments, and probe different chemical environments and bonding properties, we concentrated on the cases of Si-C and Si-O-C bonded monolayers at different coverages: we provide trends as a function of the molecule parameters.

O 14.15 Mon 18:00 P2

Conductance and atomic structure of Pb wires on Si(557) — ●MARCIN CZUBANOWSKI, HERBERT PFNÜR, ZIAD KALLASSY, and CHRISTOPH TEGENKAMP — Institut für Festkörperphysik, Abteilung*Oberflächen, Appelstrasse 2, 30167 Hannover, Germany

The adsorption of Pb on Si(557) substrates leads to the formation of anisotropic metallic structures as revealed by conductivity measurements and STM. In particular, the annealing of at least 1ML Pb to 640K forms an atomic chain structures, which show below $T_c=78K$ a metallic $1/T$ conductance behavior in the direction along the wires $[110]$, whereas in the $[1\bar{1}2]$ direction an insulating behavior is found. As seen by STM, this transition in conductance is associated with an order-disorder transition in form of a tenfold periodicity below T_c [1].

Recent LEED experiments support the model, that the superperiodicity along the atomic wires is induced by domain walls. For annealing temperatures of 620K a Pb induced $\sqrt{3}\times\sqrt{3}$ is found, which is characteristic for Pb on Si(111) and can be explained by the well-known honeycomb structure of triplets of Pb atoms on T_4 positions. The coverage of 1ML is in consistency with Auger and conductivity measurements. The LEED pattern changes dramatically for an annealing temperature of 640K, i.e. where 1D conductance is found and the atomic wire structure is formed. A detailed LEED analysis has shown, that a $\sqrt{31}\times\sqrt{3}$ domain structure along the $[110]$ has formed. Similar results have been obtained for annealing close to the desorption threshold of Pb/Si(111)[2].

[1] C. Tegenkamp et.al. PRL 95, 176804 (2005).

[2] A. Petkova Dissertation Universität Hannover 2003

O 14.16 Mon 18:00 P2

Adsorption of acetylene and ethylene on group-IV semiconductor (001) surfaces: results from ab-initio theory — ●J. WIEFERINK, P. KRÜGER, and J. POLLMANN — Institut für Festkörpertheorie, Universität Münster, Wilhelm-Klemm-Str. 10, 48149 Münster

A detailed understanding of the adsorption of organic molecules on semiconductor surfaces is a key for their future use in semiconductor devices. We have, therefore, carried out a comparative theoretical study of the adsorption of acetylene and ethylene on (001) surfaces of Si, Ge, and SiC. Optimized structures, adsorption energies and electronic properties have been calculated employing density functional theory.

On Si(001)-(2x1), both acetylene and ethylene adsorb in *on top* positions above intact symmetric Si-Si dimers. Acetylene molecules may alternatively bridge two Si atoms on two adjacent dimers. Our electronic structure for ethylene on Si(001) is in very good agreement with ARUPS data. The same obtains for our results for ethylene on Ge(001).

In addition we present the first ab-initio results for acetylene and ethylene on SiC. The adsorption behavior of these molecules on Si-terminated SiC(001)-(2x1) is completely different from the adsorption on Si or Ge(001). This is related to the much smaller lattice constant of SiC, as compared to Si, and to its strong ionicity. For molecular adsorption of ethylene a cross dimer geometry turns out to be most favorable while acetylene prefers a rotated bridge site on SiC(001).

O 14.17 Mon 18:00 P2

Core level photoelectron spectroscopy studies of Au/4H-SiC(0001) surface — ●C. VIROJANADARA^{1,2} and L.I. JOHANSSON¹ — ¹IFM, Linköping University, Linköping, Sweden. — ²Present address: Max-Planck-Institut für Festkörperforschung, Stuttgart, Germany

Studies of Au overlayers on two differently prepared SiC(0001) surfaces are reported. A Si-rich 3x3 surface prepared by Si deposition and subsequent annealing and a $(\sqrt{3}\times\sqrt{3})R30^\circ$ reconstructed prepared by in situ heating only. The effects induced by Au layers deposited on these surfaces were investigated using photoemission and low energy electron diffraction (LEED). The formation of ordered overlayer structures was identified and features developing in the Si 2p, C 1s and Au 4f core level spectra were investigated in detail. After deposition of 4 to 8 Å thick Au layers on the 3x3 surface three new stable reconstructions $2\sqrt{3}\times 2\sqrt{3}R30^\circ$, 3x3 and 5x5 were revealed after annealing at progressively higher temperatures between 500-900°C. The surface related components appearing in the Si 2p and Au 4f core levels indicated silicide formation. The LEED pattern and the intensity variations observed for the different core level components versus photon energy suggested formation of an ordered Au-silicide with some excess Si on the top. For the $(\sqrt{3}\times\sqrt{3})R30^\circ$ surface the evolution of the core level spectra after Au deposition and annealing was found to be distinctly different compared to the Si-rich 3x3 surface. Only one stable reconstruction, a 3x3 phase, was then observed at similar annealing temperatures. These findings will be presented and discussed.

O 14.18 Mon 18:00 P2

Why does molecular hydrogen adsorb on SiC(001)-c(4x2) but not on SiC(001)-(3x2)? An ab-initio investigation — ●X. PENG, P. KRÜGER, and J. POLLMANN — Institut für Festkörpertheorie, Wilhelm-Klemm-Str. 10, 48149 Münster

In recent experiments (V. Derycke et al. PRB 63, 201305) the amazing observation was made that molecular hydrogen readily adsorbs on the SiC(001)-c(4x2) surface while it hardly interacts with SiC(001)-(3x2) although both surfaces are characterized by similar Si dimers.

To elucidate the origin of the very different reactivities of H₂ on these surfaces we have performed ab-initio density-functional calculations for a variety of hydrogenated surface configurations. In general, we find that intradimer adsorption of H₂ on top of a single surface dimer is unlikely due to a significant energy barrier. Instead, interdimer adsorption of H₂ molecules between two neighboring dimers can occur without an energy barrier when the dimers are sufficiently close-by. In that case, the H₂ molecule dissociates by simultaneous adsorption of the two H atoms at the dangling bonds of two neighboring dimers. At the c(4x2) surface, the distance between neighboring dimers is small enough to easily allow for interdimer adsorption of H₂ without any energy barrier. This holds for both the missing row asymmetric dimer (MRAD) as well as the alternating up and down dimer (AUDD) model. Intradimer adsorption on an up dimer in the AUDD model, as conjectured before, turns out to be unlikely due to the energy barrier mentioned above. At the 3x2 surface,

on the contrary, H_2 adsorption is strongly hindered due to a much too large distance between neighboring dimers.

O 14.19 Mon 18:00 P2

Theory of hydrogen-induced surface metallization of 3C-SiC(001)-(3x2) — ●X. PENG, P. KRÜGER, and J. POLLMANN — Institut für Festkörpertheorie, Wilhelm-Klemm-Str. 10, 48149 Münster

Hydrogenation usually passivates semiconductor surfaces. It has never been thought to be a means of making them metallic. Yet, recent experiments have provided clear evidence for the metallization of the SiC(001)-(3x2) surface by hydrogenation [1]. In order to explain this finding it was conjectured [1] that in a first step monohydride units are formed at the top layer Si dimers. Further H adatoms were assumed to break Si dimers in the third layer and to become bonded to one of the two dimer atoms leaving a Si dangling bond at the other.

In order to contribute to a deeper understanding of this surprising metallization we have investigated a rich variety of hydrogen configurations at the SiC(001)-(3x2) surface by calculating their atomic and electronic structure, phonon frequencies and formation energies within density functional theory. Our results show that the dangling bonds in the third layer, supposed to be essential for surface metallization, are highly unstable. Instead, angular Si-H-Si bridge bonds are formed on the third layer with the H atom located at the center above the two Si atoms. The weakly bound Si-H-Si structure gives rise to the surface metallization. Interestingly, our results show that the formation of dihydride instead of monohydride units at the top layer is energetically even more favorable. In addition, we find that H atoms can also form Si-H-Si bridge bonds on the second layer inducing surface metallization, as well.

[1] V. Derycke et al. *Nature Mat. Sci.* 2, 247 (2003)

O 14.20 Mon 18:00 P2

Ellipsometric measurements on HOPG: Layering of 1-Propanol — ●MATTHIAS WOLFF and KLAUS KNORR — Technische Physik, Universität des Saarlandes, 66123 Saarbrücken

We present high resolution ellipsometric measurements on monolayer growth on HOPG. Sorptionisotherms of C_3H_7OH on HOPG show an alternating step height in the ellipsometric signal. This indicates changes in the orientation of the molecules and layer density. The layering is distinct from the FHH model.

O 14.21 Mon 18:00 P2

Hydrogen adsorption on carbon nanoparticles at low temperatures — ●MELANIE HENTSCHÉ¹, HELMUT HERMANN¹, KLAUS WETZIG¹, and GOTTHARD SEIFERT² — ¹IFW Dresden, P.O.Box 27 01 16, D-01171 Dresden — ²TU Dresden, Institute for Physical Chemistry and Electrochemistry, Bergstr. 66b, D-01062 Dresden

Carbon powders with particle size on the nanometre scale are prepared by high energy ball milling. The hydrogen adsorption properties of these materials are investigated in the temperature and pressure range of 40 K to 300 K and 1 Bar to 200 Bar, respectively. The experimental data suggest that the adsorption capacity depends not only on the specific surface area of the powders but also on the morphology of the surfaces. It is also shown that the microstructure of the carbon powders can be modified by changing the preparation conditions including milling under different atmospheres and at low temperatures.

O 14.22 Mon 18:00 P2

Adsorption and dissociation studies of acetylene on steel — ●HESNA HÜLYA YILDIZ ÜNVEREN, REINHARD DENECKE, and HANSPETER STEINRÜCK — Lehrstuhl für Physikalische Chemie II, Universität Erlangen-Nürnberg, Egerlandstr. 3, 91058 Erlangen

Normal steel can be turned into high performance (hard and wear resistant) material by low-pressure carburization. In this process, carbon atoms from dissociation of hydrocarbons diffuse into the surface layer of the steel.

In order to gain a more detailed understanding of this surface process, adsorption and dissociation of acetylene on steel have been investigated utilizing molecular beam techniques and Auger electron spectroscopy. Sticking probabilities were measured by the technique of King and Wells for different surface temperatures between 100 and 950 K and varying kinetic energy of the acetylene molecules, using controlled sample conditions. While no or very small adsorption of acetylene was observed for low kinetic energies of the molecules (~90 meV) at surface temperatures below 800 K, a significant reactive sticking coefficient of approx. 10 % could be found at 900 K. In a second step the kinetic energy of the

molecules is increased (by seeding) to enable dissociation at lower substrate temperatures where no diffusion occurs. By combination of the results, the dissociation step and the diffusion of carbon into the bulk can be disentangled.

This work is supported by BMBF (03X2506C).

O 14.23 Mon 18:00 P2

Simulations of film growth on polymer substrates — ●ROBERTO ROZAS and THOMAS KRASKA — Physical Chemistry, University Cologne, Luxemburger Str. 116, D-50939 Köln, Germany.

The physical properties of thin films on surfaces are different from the properties of the corresponding bulk phase. The study of the growth mechanism and its effect on the properties such as the size, shape and orientation of the deposited grains on a surface is fundamental for the improvement of the quality of thin films required in the development of advanced materials involving nanometer-scale structures. By means of molecular dynamics simulations the growth mechanisms of argon clusters on polyethylene film surfaces is investigated. In this system the weak interactions between the polymer and argon can be approximate by means of Berthelot combination rules. The polymer is modelled by a united atom model. Films in the glass phase are put in contact with a previously equilibrated vapour phase consisting of 5000 argon atoms. A Nosé-Hoover thermostat is applied to the polymeric substrate while the vapour phase is simulated in the microcanonical ensemble. Different regions of the phase diagram of argon are simulated, that means, different degrees of saturation and supersaturation of the vapour phase. Outside the saturation curve for low dense, stable gas phases, the argon atoms adsorb on the polyethylene surface building short-life two-dimensional islands (adsorption). The formation of stable argon clusters on the surface is observed for supersaturated vapour phases (heterogeneous nucleation).

O 14.24 Mon 18:00 P2

PIRS and LEED study of quasi-orthorhombic acetylene thin films on KCl(100) — ●JOCHEN VOGT and HELMUT WEISS — Chemisches Institut der Universität Magdeburg, Universitätsplatz 2, 39106 Magdeburg, Germany

The epitaxial growth of acetylene thin films on KCl(100) single crystal surfaces has been studied by means of low-energy electron diffraction (LEED) and polarization infrared spectroscopy (PIRS) in transmission geometry at 40 K. IR spectra in the regions of the infrared active fundamentals ν_3 and ν_5 were recorded at increasing coverages up to 20 layers. In both cases a triplet structure of the spectra was observed. LEED experiments without extensive adsorbate charging effects were possible up to coverages of 4 layers and indicated a $(\sqrt{2} \times \sqrt{2})R45^\circ$ symmetry, consistent with the results of helium atom diffraction experiments [1]. All experiments support a parallel orientation of the molecules in the layers, as expected for the low-temperature orthorhombic phase of C_2H_2 . Based on the structure model of this phase the PIRS film spectra were analyzed using a dynamic dipole-dipole coupling model. Good agreement between simulated and experimental spectra is obtained for both fundamental modes if the possibility of azimuthal misorientations of adjacent layers by 90° is taken into account.

[1] J. P. Toennies et al., *Phys. Rev. B* 65, 165427 (2002)

O 14.25 Mon 18:00 P2

Structural and Chemical Analysis of Epitactic Rutile $TiO_2(011)$ Films Grown on $Re(10\bar{1}0)$ — ●WILHELMINE KUDERNATSCH, DIRK ROSENTHAL, and KLAUS CHRISTMANN — Institut für physikalische und theoretische Chemie, FU Berlin, Germany

Titanium oxide films were grown on a $Re(10\bar{1}0)$ surface by electron beam deposition. Composition and structure were determined by X-ray photoelectron and Auger electron spectroscopy as well as by low energy electron diffraction (LEED) and X-ray diffraction (XRD) measurements carried out at BESSY. The chemical activity of our films was examined by temperature programmed desorption (TPD) of CO, CO₂ and H₂O. TiO_2 films with a well-defined stoichiometry and surface structure require high temperature deposition ($T = 900$ K) in an O₂ atmosphere as indicated by a unique $pg(2 \times 2)$ LEED pattern with missing spots in $h = n \pm \frac{1}{2}$ and $k = 0$ positions. While this pattern could stem from both a rutile(011)-(2x1) or a brookite(001) surface, XRD and LEED faceting analyses reveal that the actual phase consists of rutile(011). CO-TPD from this phase shows a single TD state at 132 K; the CO saturation coverage could be determined to be $1.15 \times 10^{18} / m^2$ ($= 0.56$ CO molecules per $TiO_2(011)-(2 \times 1)$ unit mesh). Our CO, CO₂ and H₂O data will be discussed and compared

with related work recently published in the literature.

O 14.26 Mon 18:00 P2

GIXRD and XRR Studies on Semiconductor Insulator Multilayers — ●T. WEISEMÖLLER¹, C. DEITER¹, A. GERDES², B. H. MÜLLER³, C. R. WANG³, K. R. HOFMANN³, and J. WOLLSCHLÄGER¹ — ¹Fachbereich Physik, Universität Osnabrück, D-49069 Osnabrück — ²Institut für Festkörperphysik, Universität Hannover, D-30167 Hannover — ³Institut für Halbleiterbauelemente und Werkstoffe, Universität Hannover, D-30167 Hannover

Reducing the size of electronic structures to the nanometer regime it is necessary to grow atomic thin and flat epitaxial films of semiconductors and insulators. Here, CaF₂ and Si are good candidates because of their lattice matched laminar growth. The additional deposition of silicon and germanium at room temperature with successive heating with and without flux of a surfactant material (Sb and B) was investigated by means of grazing incidence x-ray diffraction (GIXRD), x-ray reflectivity (XRR) and atomic force microscopy (AFM). Annealing 10nm thick silicon films up to 630°C under boron atmosphere provides semiconductor layers of the highest quality (roughness <0.34nm).

O 14.27 Mon 18:00 P2

Relaxation of thin CaF₂ Films on Si(111) — ●C. DEITER¹, T. WEISEMÖLLER¹, B. ZIMMERMANN¹, A. GERDES², and J. WOLLSCHLÄGER¹ — ¹Fachbereich Physik, Universität Osnabrück, D-49069 Osnabrück — ²Institut für Festkörperphysik, Universität Hannover, D-30167 Hannover

We investigated the structure of CaF₂ films of various thicknesses (1nm-10nm) at different growth temperatures (500°C and 600°C) by grazing incidence x-ray diffraction (GIXRD). The intensity distribution of the crystal truncation rods was analysed by calculations based on the kinematic approximation. The crystal quality of CaF₂ films on Si(111) depends on the amount of the deposited material and the processing temperature. Above a certain temperature - depending on the film thickness - the insulator starts to relax partially by forming smaller crystallites limited by dislocations and substrate step edges. In contradiction to the classical approach by a model using only one CaF₂ species a simulation of lateral coexisting pseudomorphic and relaxed crystallites perfectly fit the measured data.

O 14.28 Mon 18:00 P2

Growth and Structure of Titanium Dioxide Films on a Rhenium(0001) Surface — ●SUSANNE ROTH, DIRK ROSENTHAL, and KLAUS CHRISTMANN — Institut für Chemie und Biochemie, FU Berlin

Titanium dioxide films of various thickness were grown onto a Re(0001) surface at 800 - 900 K via co-deposition of titanium and oxygen in UHV. Growth, stoichiometry, and surface structure were determined using X-ray photoelectron spectroscopy (XPS), ion scattering spectroscopy (ISS), and low-energy electron diffraction (LEED) as a function of film thickness. XPS unambiguously showed that all films possess TiO₂ stoichiometry. Since the Re substrate ion scattering signal disappeared after deposition of a monolayer equivalent of TiO₂ the thin film growth could be governed by both a Stranski-Krastanov (SK) and a Frank-van der Merwe (FW) mechanism. The TiO₂ phase exhibits a clear hexagonal LEED pattern with running spots indicating faceting phenomena due to island growth. Therefore we favour a SK growth mechanism. Our results are discussed and compared with previous data published in the recent literature on similar systems.

O 14.29 Mon 18:00 P2

Adatom - and vacancy cluster creation on Cu(001) — ●GEORGIANA STOIAN, RAOUL VAN GASTEL, HERBERT WORMEESTER, and BENE POELSEMA — University of Twente, Enschede, The Netherlands

The collision of a noble gas ion with a surface results in a multitude of processes, including the emission of substrate atoms in the vacuum and the creation of adatoms, surface - and bulk vacancies. On the time scale of the ion impact these processes are virtually independent of temperature. Between ion impacts in the same microscopic area, depending on substrate temperature, diffusion processes can dramatically alter the morphology due to the coarsening and annihilation of adatom - and vacancy clusters. The temperature dependence between 200 and 300 K of the resulting morphology of Cu(001) is studied with STM for very low fluences, i.e. the regime in which only about 1% of the surface atoms has been hit by an incoming ion. The use of Ar ions with energy of 800 eV

limits the depth-range of the ion impact to the very surface region.

O 14.30 Mon 18:00 P2

Layer-by-layer growth of C₆₀/Au(111) film studied by scanning tunneling microscopy — ●UNG HWAN PI¹, HAN YOUNG YU², CHAN WOO PARK², MIN KI RYU², ANSOON KIM², and SUNG-YOOL CHOI² — ¹Present address: University of Hamburg, IAP, Jungiusstr. 11, 20355 Hamburg — ²Nanoelectronic device team, Future Technology division, Electronics and Telecommunications research Institute, Daejeon 305-350, South Korea

The surface of C₆₀/Au(111) film has been studied with scanning tunneling microscopy (STM) during layer-by-layer growth. From the first to the fourth layer, the growth behavior, the effect of annealing, and the electrical property of each layer were investigated. Due to the charge transfer from the Au(111) substrate, the first layer showed big difference from the other layers. We could estimate the relative intensity of the molecular interaction at each layer qualitatively. Scanning tunneling spectroscopy performed on each different layer showed the change of the electronic states with film thickness. The substrate-induced effect vanished at the fourth layer.

O 14.31 Mon 18:00 P2

Structure and Composition of Ultra-thin Fe Layers on Pt(111) — ●R. CHOPRA, T.Y. LEE, A. ENDERS, K. KUHNKE, U. STARKE, and K. KERN — Max-Planck-Institut für Festkörperforschung, Stuttgart, Germany

The growth of Fe on vicinal Pt surfaces provides access to magnetic nanostructures with interesting properties. In order to understand the structural properties of the Fe-Pt interface and the alloying process during annealing, ultra-thin epitaxial Fe films were studied on flat Pt(111). Low-energy electron diffraction (LEED) and Auger electron spectroscopy (AES) were used to characterize the film properties after deposition and upon annealing. Fe films between 0.5 ML and 3 ML display a non-pseudomorphic arrangement, although with limited long-range order immediately after deposition at 90 K or room temperature. Yet, a tendency towards a specific epitaxial relationship between the bcc-film and the fcc-substrate is observed in LEED that develops into very well ordered incommensurate superstructures corresponding to a Kurdjumov-Sachs orientation at about 500 to 600 K. At these temperatures, the initial Fe richness after deposition is considerably reduced according to AES. Further annealing to about 700 to 800 K leads to a further reduction of the Fe/Pt composition ratio accompanied by a (2×2) LEED pattern. Detailed inspection of the LEED spots and their intensity reveals the presence of a (2×1) superstructure in three domains. This phase is attributed to a Pt-Fe surface alloy.

O 14.32 Mon 18:00 P2

Structure and Growth of Fe Films on the Ir(100)-(1×1) surface — ●VERENA MARTIN, CHIARA GIOVANARDI, WOLFGANG MEYER, LUTZ HAMMER, and KLAUS HEINZ — FAU Erlangen-Nürnberg, Lehrstuhl für Festkörperphysik, Staudtstr.7, D-91058 Erlangen

The growth of iron on the metastable (1×1) phase of Ir(100) in the coverage regime of 1 - 9 monolayers (ML) was investigated by STM and quantitative LEED. The films were deposited at low sample temperature (100 K) and subsequently annealed to about 420 K in order to improve the film quality. LEED intensity spectra probing the local film structure prove that this annealing procedure has no influence on the structure and stoichiometry of the films. STM shows that rather flat films result in the whole thickness regime. Clear (1×1) LEED patterns without any satellite features indicate pseudomorphic growth despite the large lattice misfit of 5.3% between Ir and bcc Fe. LEED structure determinations performed for films of various thicknesses reveal a tetragonally distorted bcc film structure with a 14% vertical expansion of deeper layer spacings. In contrast and unusual for metal surfaces, the outermost two layer distances are even further expanded, a feature also found for similarly distorted Fe films on Rh(100) [1]. Low temperature hydrogen adsorption induces on the Fe films a surface reconstruction.

[1] A.M. Begley, S.K. Kim, F. Jona, P.M. Marcus, Phys. Rev. B 48 (1993) 1786

O 14.33 Mon 18:00 P2

Subnanosecond dynamics of the liquid-vapor phase transition at interfaces — ●FLORIAN LANG, JOHANNES BONEBERG, and PAUL LEIDERER — University of Konstanz, Postfach M 676, Universitaetsstr. 10, 78457 Konstanz, Germany

When a liquid is heated rapidly, the transition to the vapour phase does not occur at the equilibrium boiling temperature, but the liquid rather remains in a metastable superheated state. Only at a distinctly higher temperature evaporation will take place via nucleation or - at sufficiently large superheating - a spinodal process. We have studied here the evaporation process in a liquid film in contact with a solid substrate, which was heated momentarily by a short Nd:YAG laser pulse. The liquid layer (isopropanol, C₃H₈O) had a thickness of some hundred nanometers. Due to heat transfer, the fluid adjacent to the interface evaporates and the film on top is ejected as an intact liquid layer. The phase transition and the ejection process are monitored by reflectometry with a temporal resolution of about 200 ps and a spatial sensitivity on the nanometer-scale in the direction perpendicular to the substrate. We demonstrate that this approach allows us to determine the generated pressures, the achievable superheating and the relevant timescales of the process and as a consequence provides insights in the nature of the very early stages of the phase transition.

O 14.34 Mon 18:00 P2

AFM Study of Defect-Induced Depressions of the Smectic-A/Air Interface — ●CHRISTIAN BAHR, VINCENT DESIGNOLLE, STEPHAN HERMINGHAUS, and THOMAS PFOHL — Max Planck Institute for Dynamics and Self-Organization, Bunsenstr. 10, 37073 Göttingen

The smectic-A/air interface of liquid-crystal droplets with antagonistic boundary conditions is studied by atomic force microscopy (AFM). The droplets are prepared on coated silicon wafers on which a planar alignment is preferred in contrast to the homeotropic alignment at the air interface. As a result, focal conic defects appear in the smectic-A phase causing a characteristic pattern of depressions in the droplet surface. The dimensions of the defect-induced depressions are measured by AFM as a function of temperature for two different compounds possessing a smectic-A – isotropic and a smectic-A – nematic transition. Whereas the results are independent of temperature in the smectic-A – isotropic case, reflecting the first-order nature of the transition, a pronounced temperature dependence is observed for the second compound, where the depth of the defect-induced depressions decreases continuously with increasing temperature and vanishes at the second-order transition to the nematic phase. These observations can be qualitatively explained through the behavior of the layer compressional elastic constant at the smectic-A – nematic transition.

O 14.35 Mon 18:00 P2

Model reaction studies on ultra-thin vanadium oxide films on Pd(111) — ●MARKUS KRATZER and ADOLF WINKLER — Institute of Solid State Physics, Graz University of Technology, A-8010 Graz

We have investigated the permeation/desorption of deuterium and the water production via reaction of permeating deuterium with gas phase oxygen on specifically prepared vanadium oxide films on Pd(111). Auger spectroscopy and LEED has been used to analyse and characterise the ultrathin vanadium oxide films. It is known that 0.3 ML of vanadium evaporated under oxygen atmosphere produce a stable (2x2) honeycomb like vanadium oxide film of V₂O₃ stoichiometry [1]. This unconventionally coordinated structure has been assumed to exhibit interesting catalytic properties. In this work we have focused on the translational energy distribution of the associatively desorbing deuterium and the water reaction product, using a time-of-flight spectrometer. The deuterium supply proceeds via permeation through a Pd(111) single crystal. On the clean Pd(111) surface both the desorbing deuterium molecules and the water molecules exhibit a thermalised kinetic energy distribution. On the Pd(111) surface covered with a (2x2) V₂O₃ film, however, desorbing deuterium shows a slightly translationally cooled energy distribution under reaction conditions. This demonstrates that the permeating/resurfacing D atoms with higher kinetic energy react preferentially with oxygen to D₂O, rather than to recombine with another D atom.

[1] S. Surnev et al., Surf. Sci. 495 (2001) 91

This work has been supported by the Austrian Science Fund, Project S9006-N02

O 14.36 Mon 18:00 P2

Activated associative desorption: CO recombination driven by hot electrons — ●STEFFEN WAGNER¹, MARCEL KRENZ¹, ALEXANDER KAEBE¹, CHRISTIAN FRISCHKORN¹, MARTIN WOLF¹, and ALAN LUNTZ² — ¹Freie Universität Berlin — ²University of Southern Denmark, Odense

The formation and desorption of molecular CO from atomic carbon and oxygen bound to a Ru(001) surface have been investigated femtosecond-laser irradiation. A strong non-linearity in the desorption yield with respect to the applied laser fluence and a narrow two-pulse correlation (2PC) width indicate an electron-mediated reaction mechanism. Surprisingly, measurements of the translational energy of the desorbing CO molecules show almost no dependence on the applied laser fluence. The origin of these findings is attributed to the shape of the potential energy surface where along the reaction pathway a high barrier (~1.8 eV) and a deep chemisorption well (~0.8 eV) have to be traversed. We assign the fluence independent translational energy to a thermalization of the nascent molecules in the chemisorption well. Experiments employing time-resolved vibrational spectroscopy via sum-frequency generation on the CO stretch vibration are underway and will give further insight into this reaction.

O 14.37 Mon 18:00 P2

CO oxidation on Ir(111) surfaces: consequences of anisotropic diffusion and noise — ●STEFAN WEHNER¹, PATRICK HOFFMANN², DIETER SCHMEISSER², HELMUT R. BRAND³, and JÜRGEN KÜPPERS^{1,4} — ¹Experimentalphysik III, Universität Bayreuth, 95440 Bayreuth, Germany — ²Angewandte Physik II, Brandenburgische Technische Universität Cottbus, 03013 Cottbus, Germany — ³Theoretische Physik III, Universität Bayreuth, 95440 Bayreuth, Germany — ⁴Max-Planck-Institut für Plasmaphysik (EURATOM Association), 85748 Garching, Germany

The CO oxidation reaction on Iridium(111) surfaces shows bistability in a limited range of the CO fraction of the reactant gas flux Y and a wide range of temperatures T . The two branches are characterized by their reactivity for CO₂ formation. The upper rate (high CO₂ formation) rate is related to high oxygen coverage on the surface, the lower rate (little CO₂ formation) to high CO coverage.

Quadrupole mass spectroscopy and PEEM (photoelectron emission microscopy) was employed to study the influence of a noisy reactant gas flux composition on the spatio-temporal pattern development in the CO oxidation reaction on flat Ir(111) and stepped Ir(977) surfaces. PEEM shows nucleation and growth of few oxygen resp. CO islands at small noise amplitudes. Anisotropic diffusion of CO parallel and normal to the steps causes elliptic shapes of large islands. The long axes of the ellipses are aligned along the steps. At increased noise amplitudes the density of islands becomes larger.

2D modeling of the phenomena based on reaction-diffusion differential equations reproduces the experimental findings quite nicely.

O 14.38 Mon 18:00 P2

Oxidation of magnesia-supported Pd-clusters leads to the ultimate limit of epitaxy with a catalytic function — ●BERND HUBER¹, PEKKA KOSKINEN², HANNU HÄKKINEN³, and MICHAEL MOSELER^{1,3} — ¹Freiburg Materials Research Center, University of Freiburg, D-79104 Freiburg, Germany — ²Fraunhofer Institute for Mechanics of Materials, Wöhlerstr. 11, D-79108, Germany — ³Department of Physics, NanoScience Center, FIN-40014 University of Jyväskylä, Finland

Oxide-supported transition metal clusters and nanoparticles have attracted significant attention owing to their important role as components of model-catalysts, sensors and solar-cells. For small clusters, functionality and structure are closely interrelated. However, knowledge of the structure of the bare cluster is insufficient since the interaction with the chemical environment might cause drastic structural changes. Here we show by ab initio simulations based on the density functional theory that the reaction with molecular oxygen transforms small, non-crystalline, magnesia-supported Pd-clusters to crystalline PdO nano-oxide clusters that are in epitaxy with the underlying support. Restructuring of the Pd backbone is controlled by the electrostatic interaction with magnesia leading to a strong reduction of the O₂ dissociation barrier. The supported PdO clusters are likely to serve as Mars-van Krevelen oxygen reservoirs in catalytic oxidation reactions as observed previously for PdO overlayers and demonstrated here for the oxidation of CO molecules

[1] B. Huber, P. Koskinen, H. Häkkinen and M. Moseler, NMat (in press)

O 14.39 Mon 18:00 P2

Hydrogenation of 1,3-butadiene on Pd(111) and PdSn/Pd(111) surface alloys — ●BREINLICH CHRISTIAN, JAN HAUBRICH, CONRAD BECKER, and KLAUS WANDEL — University of Bonn, Institute for Physical and Theoretical Chemistry, Wegelerstr.12, 53115 Bonn

We have investigated the adsorption and hydrogenation of 1,3-butadiene on Pd(111) and PdSn/Pd(111) surface alloys under UHV conditions using TPD and HREELS. The Pd-Sn surface alloys were produced by annealing of tin layers of various thicknesses. Depending on the amount of deposited tin and the annealing temperature this procedure resulted in the formation of ordered surface alloys of $(\sqrt{3} \times \sqrt{3})R30^\circ$ or $p(2 \times 2)$ superstructure, which were characterized by LEED, AES and UPS. The adsorption and reaction of 1,3-butadiene was investigated by TPD. After 1,3-butadiene adsorption at 55 K the desorption of the multilayer was found near 120 K on all surfaces. Further heating lead to desorption of part of the monolayer around 180 K and to partial hydrogenation to butene at 200 - 230 K. At higher temperatures the remaining species decompose into hydrogen and surface carbon. The partial hydrogenation is highly selective since no desorption of butane has been found. The branching ratio of desorption vs. hydrogenation vs. decomposition on the bare surface and the surface alloys is clearly a function of the surface stoichiometry. HREELS investigations reveal the adsorption modes of 1,3-butadiene on these surfaces.

O 14.40 Mon 18:00 P2

STM investigations on ordered monolayers of a large tetralactame macrocycle on single crystal metal surfaces — ●JORDAN KOSSEV and MORITZ SOKOLOWSKI — Institut für Physikalische und Theoretische Chemie, Universität Bonn, Wegelerstr. 12, 53115 Bonn, Germany

Large macrocycles are of interest for investigations on mechanically interlocked molecules, e.g., catenanes and rotaxanes [1]. We have studied macrocycle molecules (905.05 amu) of the tetralactame type under UHV on the Au(111) surface. The molecules were deposited from a home build Knudsen cell and STM images were taken at different coverages at room temperature. Two different long range ordered phases, α and β , were observed after annealing to 400 K. The STM images are explained by a structure with partially overlapping and inclined lying molecules. This model is also supported from DFT calculations which reveal that hydrogen bonds between the molecules are responsible for the observed structures. The macrocycles were kindly supplied by C. A. Schalley and F. Vögtle. DFT calculations were done by W. Reckien and B. Kirchner. This work was supported by the DFG (SFB 624).

[1] C. A. Schalley, K. Beizai, F. Vögtle, Acc. Chem. Res. 34 (2001) 465.

O 14.41 Mon 18:00 P2

Influence of surface defects on the lateral order at metal-organic interfaces — ●PAVO VRDOLJAK¹, LENNART KILIAN¹, DOMINIQUE HÜBNER¹, ACHIM SCHÖLL¹, RAINER FINK², and EBERHARD UMBACH¹ — ¹Universität Würzburg, Experimentelle Physik II — ²Universität Erlangen, Physikalische Chemie II

The adsorption of organic molecules on well-ordered metal surfaces is governed by a complicated interplay between the structural, chemical, and electronic properties of adsorbate and substrate. Thus for many large organic molecule-on-metal systems various structural modifications may occur depending on, e.g., the substrate surface, temperature, or coverage. However, steps and surface defects may have a large influence on the lateral order and on phase transitions between different structural modifications. This is an issue that has not yet been investigated in depth for large organic adsorbates. Our present model system is a monolayer of 1,4,5,8-naphthalene-tetracarboxylic acid dianhydride (NTCDA) on Ag(111) which shows various superstructures with different degrees of long-range order depending on coverage and substrate temperature. We analyse the influence of substrate and surface defects on the order of different structural modifications of the adsorbate layer and on the transitions that occur between these phases.

O 14.42 Mon 18:00 P2

Investigation of structural and vibronic properties of Tetracene phases on Ag(111) — ●SERGUEI SOUBATCH, RUSLAN TEMIROV, and STEFAN TAUTZ — International University Bremen, Bremen, Germany

Recently, two ordered phases of Tetracene on Ag(111) surface have been registered with low energy electron diffraction [1]: The so-called α -phase forms upon deposition at room temperature (RT) and subsequent cooling, while β -phase appears upon cooling, if Tetracene molecules are deposited on the substrate kept at 230K. The β -phase transforms into α -phase upon annealing at RT and subsequent cooling.

Here we report on our microscopic and spectroscopic study of these phases and the process of phase transformation. Unit cells found for

both the phases from scanning tunneling microscopy images agree with good accuracy to those of reported in [1]. An additional ordered transition phase as well as a disordered phase have been observed for annealed films of initial β -phase. The comparison of high resolution electron energy loss spectra with calculated vibrational modes of a free Tetracene molecule reveals, that the α -phase is composed of flat laying molecules, while the β -phase consists of tilted ones, in conformity with [1]. However, STM images suggest that the ordered β -phase forms on top of a disordered layer of molecules.

[1] A. Langner et al., Surf. Sci. 574 (2005) 153.

O 14.43 Mon 18:00 P2

Structure and Reactivity of Metalloporphyrins on a Ag(111) Surface — ●K. FLECHTNER¹, T. LUKASCZYK¹, L. MERTE¹, J. M. GOTTFRIED¹, H.P. STEINRÜCK¹, T. SHUBINA², and T. CLARK² — ¹Universität Erlangen-Nürnberg, Lehrstuhl für Physikalische Chemie II, Egerlandstr. 3, D-91058 Erlangen, Germany — ²Universität Erlangen-Nürnberg, Chemie-Computer-Centrum, Nägelsbachstrasse 2, 91052 Erlangen, Germany

Metalloporphyrins are among the most abundant organometallic compounds in nature and control various biochemical reactions. The decisive step in these reactions is often the attachment of a ligand on the central metal atom. Here, we investigate adsorbate layers of Tetraphenylporphyrin-Co(II) and Tetrakis-(3,5-di-tert-butylphenyl)porphyrin-Co(II) as model compounds for natural porphyrin systems. In particular, we report an XPS and LEED study of the growth of the porphyrins on Ag(111), the preparation of ordered monolayers, and their thermal stability. The Co 2p_{3/2} photoemission signal consists of four peaks corresponding to different final states and/or different oxidation states of the Co ion. Monolayers show an additional Co 2p_{3/2} peak that probably reflects the Co(II)-Ag interaction. Both porphyrins form ordered monolayers. Furthermore, we examined the adsorption of small molecules such as H₂O, NH₃, CO, and NO at the Co ion of the porphyrins. For comparison with our experimental data, we also computed the ligand-to-metal binding energies of these molecules with DFT. Likewise, we studied the properties of Zn(II)-porphyrin layers. This work was supported by the DFG through SFB 583.

O 14.44 Mon 18:00 P2

Thickness dependent NEXAFS study of pentacene/Ag(111) — ●S.K.M. JÖNSSON¹, B. DOYLE², M. PEDIO², S. NANNARONE², and F.S. TAUTZ¹ — ¹School of Engineering and Science, International University of Bremen, P.O. Box 750561, 28725 Bremen, Germany — ²TASC-INFN National Laboratory, Area Science Park, 34012 Basovizza (Trieste), Italy

The thickness dependent orientation and the in-plane order/disorder of pentacene layers on Ag(111) substrates has been investigated with Near-Edge X-ray Absorption Spectroscopy (NEXAFS). Based on previous XPS, STM and HREELS studies, it is known that for RT deposition the first monolayer is a disordered layer in which the pentacene molecules are oriented parallel to the Ag surface. With additional pentacene growth, an ordered layer is formed on top of the first disordered layer. This ordered growth is continued for a few additional layers. The NEXAFS signals, taken at 5 different polar angles for each of the layers, allows us to determine the orientation of the pentacene molecules in each of the layers formed, while the NEXAFS signals taken at 5 different azimuthal (in-plane) angles provides qualitative information concerning the degree of order/disorder within a layer. By comparing the NEXAFS signal of the monolayer, bilayer, etc with the NEXAFS signal of thick pentacene film it is also possible to draw conclusions concerning the bonding of each of the layers.

O 14.45 Mon 18:00 P2

Investigation of pure and plasma treated wood and wood components with surface analytical techniques — ●LOTHAR KLARHÖFER¹, WOLFGANG MAUS-FRIEDRICHS¹, VOLKER KEMPTER¹, and WOLFGANG VIÖL² — ¹Institut für Physik und Physikalische Technologien, TU Clausthal, Leibnizstr. 4, 38678 Clausthal-Zellerfeld — ²HAWK FH Hildesheim/Holzwinden/Göttingen, Fakultät Naturwissenschaften und Technik, Von-Ossietzky-Straße 99, 37085 Göttingen

Surface properties of wood can be changed using a dielectric barrier discharge at atmospheric pressure. Depending on the utilised gas the surface tension and chemical activity can be increased or hydrophobic surfaces can be obtained by plasma-polymerisation. For characterising the altered wood surfaces different electron spectroscopic methods are

used. XPS is a well known technique for analysing the chemical composition of wood surfaces. UPS and MIES are largely unknown methods on cellulosic materials. As UPS reflects the Density Of States (DOS), MIES the Surface Density of States (SDOS) respectively, these methods are useful to characterise changes of wood surfaces based on plasma treatment. It is shown that these techniques indeed yield reproducible results and, in particular, possess the potential to give information on the interaction of molecules with wood surfaces.

For this purpose, fingerprint MIES and UPS spectra of the wood components, lignin, cellulose and extractives are being collected in order to interpret the corresponding wood spectra. Thin films were prepared out of these components under clean conditions. The analysis of the spectra will be presented at the conference.

O 14.46 Mon 18:00 P2

Coadsorption of 1-decanethiol and PTCDA on Ag(111)-surfaces in the submonolayer regime — ●FLORIAN POLLINGER, STEFAN SCHMITT, CHRISTIAN KUMPF, ACHIM SCHÖLL, and EBERHARD UMBACH — Exp. Phys. II, Univ. Würzburg, 97074 Würzburg

Deposited on vicinal Ag(111) the planar molecule 3,4,9,10-perylenetetracarboxylic acid-dianhydride (PTCDA) induces a surface rearrangement by step bunching and subsequent facetting. The resulting supersteps form a grating-like pattern on mesoscopic dimensions by self-organization. As a consequence, one receives a template structure on nanometer scale from both a morphologic and chemical point of view.

One possible application of such a template is the growth of an organic coadsorbate. As a candidate, we chose 1-decanethiol, an often investigated archetype molecule forming self-assembled monolayers (SAMs) on noble metals. The coadsorption behaviour has been investigated on saturated monolayers and submonolayers of PTCDA on Ag(111) surfaces with XPS, STM and TDS.

O 14.47 Mon 18:00 P2

STM study of CuPC molecules on Cu(111) and Au(111) — ●STEFAN KUCK, ANDRE WACHOWIAK, GERMAR HOFFMANN, and ROLAND WIESENDANGER — Institut für Angewandte Physik und Zentrum für Mikrostrukturforschung, Universität Hamburg, 20355 Hamburg, Germany

Local probe techniques have proven to be a powerful tool for investigations of growth phenomena and intermolecular orientational order of thin molecular layers and single molecules on a substrate surface. The delicate balance between substrate temperature, molecules and intermolecular interaction determines varieties of observed structures. Using a homebuilt variable temperature STM (30 K - room temperature) we studied the growth of CuPC molecules on the Cu(111) and Au(111) surfaces. Single CuPC molecules prefer two orientations with respect to the underlying substrate lattice [1]. Scanning tunneling spectroscopy measurements reveal the energetic position of the molecular resonances and show the spatial distribution of molecular orbitals.

[1] P. H. Lippel *et al.*, Phys. Rev. Lett. **62**, 171 (1989).

O 14.48 Mon 18:00 P2

Functional Nanostructures for Electronic Devices — ●FRANK SPERKA¹, ELENA MENA-OSTERITZ², and OTHMAR MARTI¹ — ¹Dept. Experimental Physics, Uni Ulm — ²Dept. Organic Chemistry, Uni Ulm

The aim of this project is to produce nanostructured surfaces on structured substrates adapted to molecular structures. Furthermore we want to study the local electric and optical properties of those surfaces.

Various series of self-assembly-structures of macrocycles Cyclo(terthiophen-diimine) like C[3T-DA]_n, Cyclo(quinquethiophen-diimine), C[5T-DA]_n and Cyclo[n]thiophenes C[n]T were studied with STM. Different patterns and nanostructures for different molecule-symmetries and diameters (1-5 nm) of the cycles were found.

These nanostructured surfaces will be studied with an AFM in tapping mode. We want to investigate if these self-assembly-structures will form some overstructures on a larger lengthscale.

O 14.49 Mon 18:00 P2

Observation of Distinct Topographic/Electronic Features in Cobalt Porphyrin Layers on Silver (111) — ●K. COMANICI, H. MARBACH, F. MAIER, F. BUCHNER, K. FLECHTNER, T. LUKASCZYK, J. M. GOTTFRIED, and H.-P. STEINRÜCK — Lehrstuhl für Pysikalische Chemie II, Universität Erlangen-Nürnberg, Egerlandstraße 3, D-91058 Erlangen

Metalloporphyrins are of special interest due to their functionality in technological processes and biological molecules like chlorophyll and hemoglobin. The properties of metalloporphyrins can be modified e.g. by changing a central metal atom and different ligands. Keeping or reversibly changing the oxidation state of the involved central metal atom is crucial for the functionality of the porphyrin in natural and technological processes. The approach of this work is to prepare and investigate monolayers of different porphyrins under ultra clean conditions in an ultra high vacuum (UHV) environment. We studied different metalloporphyrins on a silver (111) surface by means of scanning tunneling microscopy (STM) and ultraviolet photoelectron spectroscopy (UPS). Ordered porphyrin layers imaged with sub-molecular resolution were found. A particular interesting feature was observed for two different cobalt porphyrins. A fraction of these Co porphyrins appear as "pits" in the STM image. These pits tend to vanish at lower bias voltages. One possible explanation for these features is to interpret them as different oxidation states of the central cobalt atoms.

O 14.50 Mon 18:00 P2

Azobenzene containing ligands for photoresponsive self-assembled monolayers on gold — ●M. TROJTA¹, B. KROHN¹, T. WEIDNER¹, M. MEIER², F. BRETTHAUER², D. ENDERS³, U. SIEMELING², and F. TRÄGER¹ — ¹Institut für Physik, Universität Kassel, Kassel — ²Institut für Chemie, Universität Kassel, Kassel — ³Kirchhoff Institut für Physik, Universität Heidelberg, Heidelberg

The new azobenzene-derivatized 1,2-dithiolanes (**1**) (a five membered ring with two sulfur and three carbon atoms) was synthesised and used for the preparation of self-assembled monolayers (SAM) on gold. Azobenzene derivatives can be switched between their "cis" and "trans" isomers by irradiation with light and represent the most widely studied building blocks for photoresponsive SAMs. However, in SAMs based on thiols and disulfides on gold, the chromophores are densely packed and show little free volume to allow photoisomerisation. The binding unit of **1** with its two attachment points and increased size should lead to considerable void space between the individual "azo" units which protrude from the surface. Photoswitching was confirmed by IR-spectroscopy. The results were compared to azobenzene containing disulfides (**2**), which showed no evidence for photoresponsive behaviour. In addition, the kinetics of film formation of **1** and **2** have been compared by *in situ* optical second harmonic generation. The adsorption of **1** is best described by first order Langmuir kinetics at an adsorption rate of $2.2 \cdot 10^{-4} \text{ s}^{-1}$. For **2** the data reveal second order Langmuir kinetics at a rate of $9.0 \cdot 10^{-3} \text{ s}^{-1}$. Film thickness of $(11 \pm 1) \text{ \AA}$ for **1** and $(12 \pm 1) \text{ \AA}$ for **2** were obtained from spectroscopic ellipsometry in accord with monolayer formation.

O 14.51 Mon 18:00 P2

Structure and morphology of organic films of PTCDI-C8 on silicon dioxide — ●TOBIAS KRAUSS¹, ESTHER BARENA^{1,2}, and HELMUT DOSCH^{1,2} — ¹Max-Planck-Institut für Metallforschung, Heisenbergstrasse 3, 70569 Stuttgart, Germany — ²Institut für Theoretische und Angewandte Physik, Universität Stuttgart, 70550 Stuttgart, Germany

Since it has been proved that the charge transport within semiconductor organic films is strongly dependent on their morphology and structural order, their controlled ordered growth is a primary task to optimize the organic film electrical and optical properties. Here we focus on thin films of an n-type organic semiconductor, PTCDI-C8 (N,N*-dioctyl-3,4,9,10-perylene tetracarboxylic diimide), deposited on SiO₂/Si by organic molecular beam epitaxy (OMBE) in ultra-high vacuum (UHV). We show that PTCDI-C8 forms extraordinary well-ordered films of standing molecules. By combining x-ray diffraction studies and Atomic Force Microscopy (AFM) we present results on the structure (perpendicular and parallel to the film surface) and morphology as a function of the substrate temperature.

O 14.52 Mon 18:00 P2

Electrochemical and Thermal Stability of Self-Assembled Mercaptohexanol Monolayers on Gold Surfaces — ●CHRISTINE HAUTMANN¹, KENJI ARINAGA^{1,2}, ERIKA PRINGSHEIM¹, MARC TORNOW¹, SHOZO FUJITA², NAOKI YOKOYAMA², ULRICH RANT¹, and GERHARD ABSTREITER¹ — ¹Walter Schottky Institut, Technische Universität München, Garching, Germany — ²Fujitsu Laboratories, Atsugi, Japan

Self assembled monolayers of mercaptoalkanol are widely used to functionalize solid substrates in aqueous environments. Recently, they have

gained great importance as an essential element in advanced DNA layer architectures on gold surfaces. In a two-step adsorption process, mercaptohexanol (MCH) is used to backfill exposed surface areas after oligonucleotide assembly. By forming a dense sub-layer MCH prevents non-specific DNA-Au interactions, thus improving the functionality of DNA molecules on the surface. Although this procedure has been adopted by numerous groups, little is known about the durability of mercaptohexanol SAM when exposed to various environmental conditions.

In this contribution, we elucidate the electrochemical as well as thermal stability of MCH-layers in aqueous solutions. Using electrochemical blocking experiments and impedance spectroscopy, we probe the stability of the layers for varying electrochemical substrate potentials. In addition, we study the durability of the layers when repeatedly performing temperature cycles up to 85°C. Understanding the behavior of MCH-SAMs under these conditions is essential with respect to the electrical manipulation of DNA on Au surfaces and DNA-sensing in particular.

O 14.53 Mon 18:00 P2

VUV-IR ellipsometry for structural characterisation of anisotropic films — ●K. HINRICH¹, S. D. SILAGHI², C. COBET^{1,3}, N. ESSER¹, and D.R.T. ZAHN² — ¹ISAS - Institute for Analytical Sciences, Department Berlin, Albert-Einstein-Str. 9, 12489 Berlin, Germany — ²Chemnitz University of Technology, Semiconductor Physics, 09107 Chemnitz, Germany — ³TU Berlin, Institute of Solid State Physics, Hardenbergstr. 36, 10623 Berlin, Germany

Thin films of bio-molecules and smart materials are of increasing interest in the field of nanotechnology and the design of bio-sensors or new types of electronic and optoelectronic devices. Further advancement in these fields requires detailed understanding of structural properties of such thin films and interfaces. This contribution presents the high potential of ellipsometry for the investigation of composition and molecular structure in thin anisotropic bio-films using the VUV - IR spectroscopic ellipsometry [1,2]. Infrared and VUV optical properties of thin films are correlated to vibrational and electronic excitations. Therefore the corresponding spectra are well suited for structural analysis, while the application of VIS ellipsometry for this purpose is often limited by the similarity of refractive indices for many organic materials. In particular for the investigated films of four different DNA bases the dielectric functions were determined and interpreted with respect to the average orientation of molecules. [1] K. Hinrichs, M. Gensch, N. Esser, Appl. Spectrosc. 59 (2005) 272(A)-282(A). [2] K. Hinrichs, S. D. Silaghi, C. Cobet, N. Esser and D. R. T. Zahn, phys. stat. sol. b 242 (2005) 2681.

O 14.54 Mon 18:00 P2

Influence of the film morphology on the diffusion of Ag and Au into thin films of the organic semiconductor diindenoperylene — ●MICHAEL SCHARNBERG¹, KLAUS RÄTZKE¹, RAINER ADELUNG¹, FRANZ FAUPEL¹, STEPHAN MEYER², and JENS PFLAUM² — ¹Christian Albrechts Universität Kiel — ²3. Physikalisches Institut, Universität Stuttgart

The application of organic-based field effect transistors (OFETs) for large scale low-cost electronic devices has lead to intense research. Diindenoperylene (DIP) thin films on SiO₂ are a prominent system due to their high structural out-of-plane order. While bottom contact OFET structures can be realized easily, preparation of top contacts might cause diffusion of metal atoms (typically Au) deep into the organic film, thereby changing the injection properties at the interface. Recently, we could establish a very sensitive radiotracer technique to measure even tiny concentrations of atoms [1]. The results show cluster formation on the surface and a low concentration of noble metal atoms dispersed throughout the film indicating that most of the metal atoms are immobilized near the surface due to agglomeration. The results for noble metal atoms in DIP films will be presented here. The structural influence, namely the crystallinity and mosaicity of the organic layer on the metal diffusion will be discussed as it is a fundamental question also for other organic electronic devices like organic solar cells or OLEDs. Furthermore, the results obtained for Ag and Au will be compared. [1] Scharnberg et al., App.Phys.Lett. 86, 024104 (2005)

O 14.55 Mon 18:00 P2

STM Investigation of Oligopyridine Nanostructures Based on Weak Hydrogen Bonds — ●CHRISTOPH MEIER, KATHARINA LANDFESTER, and ULRICH ZIENER — Organische Chemie III, Makromolekulare Chemie und Organische Materialien, Universität Ulm, Albert-Einstein-Allee 11, D-89081 Ulm, Germany, ulrich.ziener@uni-ulm.de

A series of oligopyridine compounds was investigated by scanning tunnelling microscopy (STM) considering their self-assembly at the HOPG/liquid interface. They are all constitutional isomers, exhibiting the same overall molecular shape. A systematic change in the position of the nitrogen atoms in the terminal pyridine units causes different monolayer structures. The results show that the 2D nanostructures of the oligopyridines are dominated by weak intermolecular hydrogen bonds. The packing pattern can be generalised based on a geometrical model which is determined by the relative orientations of the directional H-bonding interactions.

The observed monolayers exhibit further functional subunits and highly ordered voids which can be used as potential binding sites for several guest units. These results can be used for the development of a new concept of 2D crystal engineering based on weak C-H*N hydrogen bonds as subtle directional forces which opens a new pool of building blocks in surface nano patterning.

O 14.56 Mon 18:00 P2

2D oligopyridine networks on HOPG - solid/gas versus solid/liquid interface — ●K. TONIGOLD¹, A. BREITRUCK¹, CH. MEIER², U. ZIENER², H.E. HOSTER¹, K. LANDFESTER², and R.J. BEHM¹ — ¹Department of Surface Chemistry and Catalysis, University of Ulm, D-89069 Ulm — ²Department of Macromolecular Chemistry and Organic Materials, University of Ulm, D-89069

Ordered 2D structures formed by oligopyridine compounds on HOPG have been studied by STM i) after vapor deposition of the molecules in UHV and ii) at the solid liquid interface in the presence of an organic solvent with the molecules dissolved in it. For both interfaces we find highly ordered networks stabilized by hydrogen bonds. In UHV, the structure geometry mainly depends on the coverage, which is easily varied via duration and rate of the deposition. At the solid-liquid interface, the structure is more easily varied via the choice of the utilized organic solvent. Similarities and differences between the structures at both interfaces are discussed, including the actual influence of the organic solvent on the structures and their formation.

O 14.57 Mon 18:00 P2

Ab-initio calculation of STM images of Si(111)-(2x1) and of PTCDA:Ag(111) — ●MICHAEL ROHLFING¹, J. K. GARLEFF², A. KRAFT³, S. K. M. JÖNSSON¹, F. S. TAUTZ¹, R. TEMIROV¹, R. G. ULBRICH², and M. WENDEROTH² — ¹International University Bremen, School of Engineering and Science, Bremen, Germany — ²4. Physikalisches Institut, Universität Göttingen, Germany — ³Institut für Mess- und Regelungstechnik, Universität Hannover, Germany

We discuss the calculation of STM images on the basis of ab-initio electronic-structure theory, employing the approach of Tersoff and Hamann. One of the key ingredients is the careful evaluation of electronic wave functions up to 10 Angstrom outside the surface. To this end, we calculate each wave function close to the surface, take its two-dimensional Fourier transform, and extrapolate each Fourier component to the height of the tip, allowing to evaluate the LDOS and resulting tunneling current at the tip position. In the case of the Si(111)-(2x1) surface the two dangling-bond surface bands lead to high-contrast STM features with characteristic spatial shifts between both bands, as we also observe in experiment [1]. In the case of a monolayer of PTCDA on Ag(111), high-resolution images are obtained in theory and experiment, as well, allowing for an accurate determination of adsorption sites and for a systematic comparison between theory and experiment regarding trends with varying tip height and voltage.

[1] J. K. Garleff, M. Wenderoth, K. Sauthoff, R. G. Ulbrich, and M. Rohlfing, Phys. Rev. B 70, 245424 (2004).

O 14.58 Mon 18:00 P2

Surface State on Ultrathin fcc γ -Mn(111) Films on Au(111) — ●YURY DEDKOV¹, ELENA VOLOSHINA², MIKHAIL FONIN³, ULRICH RUEDIGER³, and GERNOT GUENTHERODT⁴ — ¹Institut für Festkörperphysik, Technische Universität Dresden, 01062 Dresden, Germany — ²Max-Planck-Institut für Physik komplexer Systeme, Nöthnitzer Str. 38, 01187 Dresden, Germany — ³Fachbereich Physik, Universität Konstanz, 78457 Konstanz, Germany — ⁴II. Physikalisches Institut, RWTH Aachen, 52056 Aachen, Germany

Crystallographic as well as electronic structure of thin Mn films on Au(111) surface has been investigated by means of scanning tunneling microscopy (STM) and angle-resolved photoelectron spectroscopy (ARPES) at room temperature. A structural phase transition from the fcc γ -Mn to the cubic α -Mn in thin Mn layers on Au(111) is accompanied by the changes in the electronic structure of thin Mn films as observed by ARPES. For the 1 ML of α -Mn on the Au(111) surface a peak at 0.8 eV of binding energy is observed in photoemission spectra, which disappears for Mn films thicker than 3 ML. Using *ab initio* band structure calculations this state at 0.8 eV is identified as a $\bar{\Gamma}$ -centered $3d_{z^2}$ -like surface state.

O 14.59 Mon 18:00 P2

Growth and electronic structure of thin NiO(111) films — ●ALEXANDER GOTTBERG¹, EUGEN WESCHKE¹, ALEXANDER HELMKE¹, ENRICO SCHIERLE¹, KRISHNAKUMAR S. R. MENON², and GÜNTER KAINDL¹ — ¹Institut für Experimentalphysik, Freie Universität Berlin, Arnimallee 14, 14195 Berlin, Germany — ²Surface Physics Division, Saha Institute of Nuclear Physics, 1/AF, BidhanNagar, Kolkata 700 064, India

The polar (111) surfaces of the rocksalt structure are matter of experimental and theoretical interest. They are difficult to prepare and exhibit surface reconstructions. For these reasons, little is known experimentally about the NiO(111) surface, in particular about its electronic structure. We have prepared NiO(111) thin films by Ni evaporation in oxygen atmosphere on Ag(111) thin-film substrates grown on W(110). The growth and structural properties were studied by hard x-ray scattering in situ, indicating layer-by-layer growth up to a film thickness of about 8 layers. Hexagonal LEED patterns show a (1x1) surface structure. The valence electronic structure of the NiO(111) films was studied by angle-resolved photoemission with synchrotron radiation, revealing pronounced dispersion of d-derived states. Surprisingly, we find high density of states at the Fermi energy for the present films, in spite of the fact that NiO is known to be an insulator.

O 14.60 Mon 18:00 P2

Electronic structure of pristine and Rb adsorbed VSe₂ — ●MICHAEL HELLE¹, MATTHIAS FRANK¹, MARTIN MARCZYNSKI¹, KAI ROSSNAGEL¹, LUTZ KIPP¹, ANTON TADICH², PETAR STOJANOV², ERIC HUWALD², NATHANIEL JANKE-GILMAN², JOHN RILEY², and ROBERT LECKEY² — ¹Institut für Experimentelle und Angewandte Physik, Universität Kiel, D-24098, Germany — ²Physics Department, La Trobe University, Melbourne, Australia

An interesting and useful property of layered transition metal dichalcogenides is their ability to intercalate electron donating atoms between the layers. This can be exploited for storing alkali ions, e.g. like in battery cells as well as for the tailoring of the host electronic structure. The aim of this work was to find out about electronic effects such as charge transfer and reduced band dispersions perpendicular to the layers induced by the deposition of alkali atoms, Rb in particular, on the surface of the layered charge density wave compound VSe₂. The electronic and geometric structures of VSe₂ have been investigated in detail prior and after evaporation of Rb at room temperature by angle-resolved photoemission spectroscopy (ARPES) and low energy electron diffraction (LEED). The ARPES data have been collected at BESSY II using a 2nd generation toroidal spectrometer developed by La Trobe University, Melbourne, Australia with an energy resolution of $\Delta E < 0.2$ eV and an angle resolution of $\Delta\theta < 0.5^\circ$.

This work is supported by DFG Forschergruppe FOR 353.

O 14.61 Mon 18:00 P2

One-Dimensional Electronic Structure of Gd chains on Si(111) — ●K.M. DÖBRICH¹, J.L. MCCHESEY², E. ROTENBERG², G. KAINDL¹, F.J. HIMPSEL³, and K. STARKE¹ — ¹Fachbereich Physik, Freie Universität Berlin — ²Advanced Light Source, Lawrence Berkeley National Laboratory, U.S.A. — ³Department of Physics, University of Wisconsin Madison, U.S.A.

Confining the propagation of electrons to one dimension leads to dramatically different band structures compared to those found in bulk crystals. Decorating a surface with a sub-monolayer amount of material is a natural approach for creating 1D structures. For some cases, e.g. Au on Si(111), the formation of atomic chains was reported. Recently, Gd was observed to induce a chain-like 5×2 reconstruction of the Si(111) surface [1], similar to Au. In contrast to the non-magnetic systems investigated before, Gd provides a large magnetic moment of $7\mu_B$ per atom. One-dimensional Gd-induced bands were observed by angle-resolved photoemission spectroscopy (ARPES) in the Si bandgap [2].

In the present work, Si(111) 5×2 Gd was studied by ARPES using synchrotron radiation at beamline 7.0.1 of the Advanced Light Source. We have investigated a wide range of k-space which allows us to distinguish between features of the electronic structure of Si(111) 5×2 Gd, Si(111) $\sqrt{3} \times \sqrt{3}$ -R30-Gd and Si(111) 7×7 .

[1] A. Kirakosian *et al.*, *Surf. Sci.* **498**, L109 (2002).

[2] T. Okuda *et al.*, *J. Electron Spectrosc. Relat. Phenom.* **137-140**, 125 (2004).

O 14.62 Mon 18:00 P2

Surface and quantum well states in Ag mono- and multilayers on Au(111): A high-resolution line-width study by ARPES — ●FRANK FORSTER, EUGEN GERGERT, AZZEDINE BENDOUNAN, and FRIEDRICH REINERT — Experimentelle Physik II, Universität Würzburg, Am Hubland 97074 Würzburg, Germany

Due to their strong localization on the (111) surfaces of noble metals Shockley states are a powerful tool for the study of different adsorption processes on these systems. Furthermore they are suitable model systems for the investigation of many-body interactions like electron-electron, electron-phonon and electron-impurity scattering by angular resolved photoelectron spectroscopy (ARPES) ($\Delta E = 3$ meV, $\Delta\theta = 0.3^\circ$). We present data on mono- and multilayers of Ag on Au(111). The ordered layer-by-layer growth allows a systematic study on the thickness dependence of the Ag layer on the surface electronic structure.

While the band mass of the spin-orbit split Au surface state increases with increasing Ag coverage, the binding energy and the Rashba term shift gradually to lower values. Additionally the line-width of the surface state becomes smaller although the density of defects on the surfaces increases. A further coverage of Ag generates new states in the bulk band gap of Au(111) with very narrow line-width. These quantum well states are confined in the Ag layer and show — like surface states — a quasi two-dimensional character with parabolic dispersion but a much smaller sensitivity on surface contamination.

O 14.63 Mon 18:00 P2

The Kondo-resonance in photoemission spectra on Ce and Yb thin-film systems — ●ANDREAS NUBER, MARKUS KLEIN, AZZEDINE BENDOUNAN, FRANK FORSTER, and FRIEDRICH REINERT — Universität Würzburg, Am Hubland, D-97074 Würzburg, Germany

The physical properties of Kondo systems are determined by interaction between localized 4f states and conduction electrons which leads to a characteristic spectral resonance at the Fermi-level. This so called Kondo-resonance has been investigated thoroughly in the last two decades by various techniques, in particular on lanthanide systems [1]. The basis for a consistent understanding of these properties can be studied directly by angle resolved photoelectron spectroscopy (ARUPS). This requires highly-ordered single-crystalline surfaces that have to be prepared in situ by appropriate methods. For bulk single crystals this preparation can be rather troublesome. In order to get rid of these problems we have prepared thin film systems containing the rare-earth elements Yb and Ce by in situ evaporation. Our ARUPS results (res. ~ 3 meV) show that these thin films and surface alloys have a long range order and can be used for a systematic study of band dispersions, crystal field effects and Kondo properties. We discuss the spectroscopic results in the framework of the Single Impurity Anderson model (SIAM) and compare the results with already existing data from bulk single crystals, with special respect to surface effects.

[1] Handbook on the Physics and Chemistry of Rare Earths, edited by K.A. Gschneidner, Jr., L. Eyring and S. Hüfner, North-Holland, Amsterdam - New York - Oxford, 1982-2002

O 14.64 Mon 18:00 P2

Energy dispersion of 4f-derived emissions in photoelectron spectra of the heavy-fermion compound YbIr_2Si_2 — ●S. DANZENBÄCHER¹, YU. KUCHERENKO², C. LAUBSCHAT¹, D.V. VYALIKH¹, Z. HOSSAIN³, CH. GEIBEL³, N. MANNELLA⁴, X.J. ZHOU⁴, W. YANG⁴, Z.-X. SHEN⁴, and S.L. MOLODTSOV¹ — ¹Institut für Festkörperphysik, Technische Universität Dresden, D-01062 Dresden, Germany — ²Institute of Metal Physics, National Academy of Sciences of Ukraine, UA-03142 Kiev, Ukraine — ³Max Planck Institut für Chemische Physik fester Stoffe, Nöthnitzer Str. 40, D-01187 Dresden, Germany — ⁴Stanford Synchrotron Radiation Laboratory and Department of Applied Physics, Stanford University, Stanford, California 94305, USA

In the present work we report on an angle-resolved PE study of the heavy-fermion system YbIr_2Si_2 . Our experiments reveal YbIr_2Si_2 to be mixed-valent with a mean valency of 2.9 at a temperature of 15 K. At the outermost surface layer, Yb is found to be divalent with a 4f BE of about 0.5 eV. A parabolic band with hole-like dispersion around the $\bar{\Gamma}$ point is observed, that crosses the almost dispersion-free Yb 4f¹³ surface signal in the Brillouin zone. Around the intersection points the f emission splits into two dispersive components separated from each other by about 0.2 eV. In the region of the $\bar{\Gamma}$ point also the 4f¹³ bulk emission at E_F reveals a similar \mathbf{k} dependent splitting related to the interaction with parabolic bands of electron-like dispersion that cross E_F close to the $\bar{\Gamma}$ point. The dispersion of the interacting 4f¹³ states is explained in terms of a simplified periodic Anderson model by a \mathbf{k} dependence of the electron hopping matrix element.

O 14.65 Mon 18:00 P2

ARUPS and XPS studies of phenylazobenzoic acid on the layered material HfS_2 — ●MEIKE QUITZAU, CLAAS THEDE, BRIDGET MURPHY, JAROSLAW IWICKI, KAI ROSSNAGEL, and LUTZ KIPP — Institut für Experimentelle und Angewandte Physik, Universität Kiel, D-24098 Kiel

The photoisomerisation process is very interesting in particular for molecular switches and image storing devices. Phenylazobenzoic acid $\text{C}_{13}\text{H}_{10}\text{N}_2\text{O}_2$, a derivative of azobenzene, changes under irradiation of light of 365 nm from the *trans* to the *cis* conformation. This photoisomerisation process is reversible at a wavelength of 438 nm. In this study phenylazobenzoic acid was evaporated onto a HfS_2 substrate under UHV conditions and electronic structure changes were measured by X-ray and angle resolved photoemission spectroscopy using synchrotron radiation delivered by the BW3 and HONORMI beamlines at HASYLAB. The XPS measurements confirm the adsorption of phenylazobenzoic acid on HfS_2 . Furthermore, the observed core level shifts give information about a possible photoisomerisation of the phenylazobenzoic acid on HfS_2 . Changes in valence band maximum and band structure after evaporation with phenylazobenzoic acid were observed.

This work is supported by the DFG Forschergruppe FOR 353.

O 14.66 Mon 18:00 P2

Photoemission Studies of Liquid Water and Aqueous Acid and Base Solutions — ●BERND WINTER¹, MANFRED FAUBEL², INGOLF V. HERTEL¹, CHRISTIAN PETTENKOFER³, STEPHEN E. BRADFORTH⁴, and PAVEL JUNGWIRTH⁵ — ¹Max-Born-Institut, Berlin — ²MPI für Dynamik und Selbstorganisation, Göttingen — ³Hahn-Meitner-Institut, Berlin — ⁴University of Southern California, Los Angeles — ⁵Academy of Sciences, Prague

The electronic structure of liquid aqueous solutions is probed in a water jet by photoemission (PE) spectroscopy employing 100-1200 eV photons. The O1s PE spectra of liquid water exhibit minor differences for surface vs bulk water. Also in solute water, measured in aqueous alkali halide solutions, the O1s shift is no larger than 0.2 eV. The Auger spectrum of liquid water is nearly identical with previous reports for water clusters (Oehrwall et al., JCP 123, 054310, 2005). Strong well-resolved spectator Auger shifts, on the order of 3 eV, for resonant excitation, would appear to correlate with different H₂O local structures. From valence PE studies of aqueous NaOH and HCl solutions the spectral signature of the lowest IP of OH⁻ at 9.2 eV and of the second lowest IP of H₃O⁺ at 20 eV are obtained. Both values agree with our ab initio and molecular dynamics calculations; the observed IP of hydronium is strongly supportive for an Eigen rather than a Zundel-like core.

O 14.67 Mon 18:00 P2

Electronic structure of pentacene crystals — ●JAROSLAW IWICKI, BRIDGET MURPHY, MEIKE QUITZAU, KAI ROSSNAGEL, and LUTZ KIPP — Institut für Experimentelle und Angewandte Physik, Universität Kiel, D-24098, Germany

Organic semiconductors, such as pentacene, are promising candidates for several applications, including electronic devices. In order to develop an understanding for the transport mechanism and conduction properties in pentacene, it is necessary to know the band structure of the material. The pentacene crystals were prepared by physical vapor growth according to Ref.[1]. An angle-resolved photoemission spectroscopy (ARPES) investigation of the electronic structure of pentacene crystals was carried out using the ASPHERE spectrometer at beamline W3.2 at HASYLAB. ARPES data will be presented and discussed.

[1] R.A Laudise, Ch. Kloc, P.G. Simpkins, T. Siegrist, J. Cryst. Growth **187**, 449 (1998).

Work supported by the DFG Forschergruppe FOR 353.

O 14.68 Mon 18:00 P2

Angle Resolved Photoemission Spectroscopy at VUV-FEL — ●MARTIN MARCZYNSKI, MATTHIAS KALLAENE, TIM RIEDEL, SOENKE HARM, KAI ROSSNAGEL, and LUTZ KIPP — Institut für Experimentelle und Angewandte Physik, Universität Kiel, D-24098, Germany

Free Electron Lasers (FELs) are new kinds of light sources that can generate very brilliant ultrashort and coherent photon pulses. Employing 38 eV FEL radiation delivered by the VUV-FEL beamline PG2 at HASYLAB we performed angle resolved photoemission spectroscopy (ARPES) measurements on layered crystals. Electronic structure and space charge effects were investigated as a function of FEL pulse intensity. ARPES spectra were taken on a single shot basis using a hemispherical analyzer with a multichannel detector capable of detecting energy and angle of the photoelectrons in parallel.

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O 14.69 Mon 18:00 P2

Innershell absorption spectroscopy of amino acids at all relevant absorption edges — ●YAN ZUBAVICHUS^{1,2}, ANDREY SHAPORENKO¹, MICHAEL GRUNZE¹, and MICHAEL ZHARNIKOV¹ — ¹Angewandte Physikalische Chemie, Universität Heidelberg, INF 253, 69120, Heidelberg — ²Institute of Organoelement Compounds, Russian Academy of Sciences, 28 Vavilov st., 119991 Moscow, Russia

Application of X-ray absorption spectroscopy to bioorganic objects opens new possibilities for study of biologically-relevant processes at molecular level. However, such studies are difficult for various reasons, including the complexity of the molecular composition and radiation sensitivity of the target objects, so that the simplest of these objects, such as e.g. proteinogenic amino acids, which are building blocks of biological macromolecules, should be studied at first. Keeping this goal in mind, we acquired the C, N, and O K-edge near-edge X-ray absorption fine structure (NEXAFS) spectra of the 22 most common proteinogenic alpha-amino acids in the zwitter-ionic form. The spectra were collected from solvent-free polycrystalline powder films of the amino acids in the partial electron yield mode. Spectral features common to all amino acids, as well as distinctive fingerprints of specific subgroups of these compounds were identified and analyzed in detail. The obtained spectral library is an important step to establish such a powerful technique as NEXAFS spectroscopy to study complex systems of biological significance. This work was supported by BMBF (05 KS4VHA/4 and 05 KS4WWA/6) and the Russian Foundation for Basic Research (05-03-32871a).

O 14.70 Mon 18:00 P2

Slow electron backscattering spectroscopy as a technique for studies of electronic energy structure of semiconductors — ●L.A. KIZMAN¹, T.YU. POPIK¹, V.M. FEYER², O.B. SHPENIK¹, and YU.V. POPIK³ — ¹Institute of Electron Physics, Ukr. Nat. Acad. Sci., Uzhhorod, Ukraine — ²CNR-IMIP, Area della Ricerca di Roma 1, CP10, I-00016 Monterotondo Scalo, Italy — ³Uzhhorod National University, Uzhhorod, Ukraine

Using the technique of slow (0-5 eV) monoenergetic (~30 meV) electron backscattering spectroscopy, the processes of excitation of surface and bulk electron states of Si, Ge, and GaAs surfaces of various modifications. The effect of treatment, crystal orientation and chemical purity of the surface on the processes of elastic and inelastic scattering of slow monoenergetic electrons is revealed. The energy dependences of the intensity

of the scattered low-energy electrons and characteristic loss spectra at various incident electron energies are studied for the semiconductors under investigation. The slow electron elastic and inelastic backscattering spectra are shown to be very sensitive to the surface condition and their fine structure results from the excitation of surface and bulk electron states.

O 14.71 Mon 18:00 P2

Surface States of Stretched Ag(111) Surfaces — ●ROLF ÖTTKING and JUERGEN A. SCHAEFER — Institut für Physik und Zentrum für Mikro- und Nanotechnologien, Technische Universität Ilmenau Postfach 100565, 98684 Ilmenau

We present first-principles- (DFT-) calculations for the electronic states of stretched Ag(111)- surfaces using projector-augmented waves (PAW-) pseudopotentials and a plane wave basis set. Starting from the energy-minimalised bulk configuration of the stretched crystal, we derive the relaxation of the first 3 silver layers of a 7-layer slab of stretched Ag(111). Electronic state calculations yield the projected surface band structure in $\Gamma \bar{X} \bar{M} \bar{\Gamma}$ - direction. We analyse the changes in the projected DOS and identify the shift of the surface electronic states of Ag(111).

O 14.72 Mon 18:00 P2

Self-interaction-corrected pseudopotentials for SiC, MgO and LiF. — ●B. BAUMEIER, P. KRÜGER, and J. POLLMANN — Institut für Festkörpertheorie, Universität Münster, Wilhelm-Klemm-Str. 10, 48149 Münster

Calculations of the electronic properties of solids, as resulting from density functional theory (DFT) within local density approximation (LDA) show typical shortcomings, most noticeably the systematic underestimate of the band gap in semiconductors and insulators. These problems are partially attributed to an unphysical self-interaction inherent in the common DFT-LDA.

One approach to overcome these shortcomings is the construction of nonlocal, norm-conserving pseudopotentials which incorporate self-interaction corrections (SIC), based on calculations for the respective constituent atoms. These atomic pseudopotentials are transferred to the bulk system by adequate modifications. We have studied the applicability of such SIC-pseudopotentials to the bulk crystals of cubic (3C) and hexagonal (2H, 4H, 6H) polytypes of SiC, as well as the ionic crystals MgO and LiF. Our results show significant improvements over standard LDA results and are in much better agreement with experimental data and also – where available – with the results of considerably more elaborate quasiparticle calculations.

O 14.73 Mon 18:00 P2

Diffusion of interstitial carbon atom in graphite studied by Van der Waals-corrected density functional theory — ●YUCHEN MA^{1,2}, A.S. FOSTER², A.V. KRASHENINNIKOV², and R.M. NIEMINEN² — ¹School of Engineering and Science, International University Bremen, P.O. Box 750 561, D-28725 Bremen, Germany — ²Laboratory of Physics, Helsinki University of Technology, P.O. Box 1100, Helsinki 02015, Finland

Present first-principle methods based on density functional theory (DFT) fail to describe the VdW interaction in graphite correctly. An empirical long-range dispersion term is incorporated into the DFT-based VASP code within the GGA in order to study the diffusion of interstitial carbon atom in graphite.

On a graphene sheet, the ground state of carbon adatom has been calculated to form a bridge-like structure by forming two bonds with two atoms in the graphene. By VASP code, a metastable state is found for the adatom. In this metastable state, the adatom pushes one atom in the graphitic network out of the graphene plane and these two atoms form a symmetric structure with respect to the graphene plane.

Calculations by both the VASP code and the VdW-corrected VASP code show that in AB-stacking graphite single interstitial carbon atom prefers to form four bonds with adjacent two graphene layers, i.e. two bonds with each layer. The diffusion along the c-axis is through the metastable state discussed above and the diffusion energy along this path is about 1.0 eV. Our calculations show that the diffusion of single interstitial in graphite is isotropic.

O 14.74 Mon 18:00 P2

Theoretical and experimental approaches to the characterization of reflective nano-focusing photon sieves — ●DIRK RAHN, JAN BARTUSSEK, CHRISTIAN HAMANN, JENS BUCK, MATTHIAS KALLÄNE, SÖNKE HARM, KAI ROSSNAGEL, and LUTZ KIPP — Institut für Experimentelle und Angewandte Physik, Universität Kiel, D-24098, Germany

For many applications, such as nonospectroscopy at modern light sources, it is necessary to focus synchrotron radiation to spot sizes in the sub-micrometer range and, at the same time, achieve a separation of zero and first order light. Reflecting optics, in particular reflecting photon sieves, fulfil these requirements. In this work an analytical model [1-2] has been extended to describe the intensity distribution in the focal plane for reflective geometry. This opens up the possibility to calculate the intensity distribution for a large section of the focal plane and a volume around the focus. A variety of different effects have been simulated, such as chromatic aberration and off-axes source positions, providing a better understanding for reflective optics. A comparison of simulated and measured focus properties will be presented and discussed. [1] Qing Cao, J. Jahns, J. Opt. Soc. Am. A, 19, 1005 (2002) [2] Qing Cao, J. Jahns, J. Opt. Soc. Am. A, 20, 2387 (2003).

O 14.75 Mon 18:00 P2

Investigation of polymer structures with a 2-photon photoelectron emission microscope (2P-PEEM) — ●CHRISTOPH SENFT, JENS SCHÜTTE, LILIENKAMP GERHARD, and DAUM WINFRIED — Institut für Physik und Physikalische Technologien, TU Clausthal, Leibnizstrasse 4, D-38678 Clausthal-Zellerfeld

Our photoelectron emission microscope (PEEM) has been combined with a femtosecond Ti:sapphire laser system for surface imaging using 2-photon photoemission (2PPE). A home-built frequency conversion system provides 100 fs pulses at the second, third and fourth harmonic wavelength of the laser. Energy-filtered images of the surface are obtained with an electrostatic double-90° energy filter. Recently, *hot spots* have been reported in a 2P-PEEM study of silver particles on silicon and assigned to plasmon excitations in the particles [1]. We have observed similarly enhanced 2P-PEEM intensities from polystyrene particles on platinum. A marked increase of 2PPE intensity at small wavelengths of excitation can be explained by HOMO-LUMO transitions in the polymer particles. We did not find indications for Mie-resonances in the particle-surface system. We will also discuss the behavior of dielectrics in a PEEM such as energy shifts and charging under femtosecond laser illumination.

[1]: O. Schmidt et al., Appl. Phys. B74 (2002) 223

O 14.76 Mon 18:00 P2

Non-linear Photoemission Electron Microscopy on silver islands by use of frequency doubled fs-laser pulses — ●JAWAD SLIEH, ULF KLEINEBERG, and ULRICH HEINZMANN — Molecular and Surface Physics, University of Bielefeld, Germany

Multiphoton photoemission from nanosized silver islands evaporated on silicon wafer substrates has been studied using of a Photoemission Electron Microscope (PEEM) coupled to a frequencydoubled Ti:Sa system. The fs-laser pulses generated by the Ti:Sa oscillator (77 MHz repetition rate) exhibit a pulse duration of 30-50 fs, a pulse energy of 3nJ and a center photon energy of 3.1 eV. This photon energy is lower than the work function of silver (4.6 eV) and thus no linear photoemission takes place. Furthermore, linear photoemission from the same samples has been investigated by illumination with light from a mercury discharge source (4.9 eV). The experimental results are compared and discussed in terms of the shape and size dependence of the multiphoton photoemission process.

O 14.77 Mon 18:00 P2

SMART: The first operating spectro-microscope with aberration correction — ●FLORIAN C. MAIER¹, THOMAS SCHMIDT¹, HELDER MARCHETTO², ULRICH GROH¹, PIERRE L. LÉVESQUE², TOMÁŠ SKÁLA², RAINER FINK³, HANS-JOACHIM FREUND², EBERHARD UMBACH¹, and THE SMART-COLLABORATION^{1,2,3,4,5,6,7} — ¹Univ. Würzburg — ²Fritz-Haber-Institut, Berlin — ³Univ. Erlangen-Nürnberg — ⁴Technische Univ. Clausthal — ⁵Technische Univ. Darmstadt — ⁶Carl Zeiss, Oberkochen — ⁷BESSY GmbH, Berlin

The lateral resolution in photoelectron emission microscopy (PEEM) is basically limited by aberrations, which can only be overcome by suitable correction techniques. The SMART (Spectro-Microscope with

Aberration-correction for Resolution and Transmission enhancement) is worldwide the first operating electron microscope which uses an electrostatic tetrode mirror combined with a highly symmetric magnetic beam-splitter to compensate simultaneously for both, the chromatic and spherical aberrations. SMART aims at a lateral resolution below 2 nm with an energy resolution of at least 100 meV and is therefore the most ambitious project in the field of spectroscopic microscopy. In addition to the high lateral resolution a gain in transmission of up to two orders of magnitude is obtained. The instrument excels in a variety of contrast mechanisms (photo-emitted and reflected electrons) and in different operation modes (microscopy, spectroscopy and diffraction) and therefore enables a comprehensive surface characterization using various methods quasi-simultaneously. Project funded by BMBF under contract no. 05 KS4WWB/4

O 14.78 Mon 18:00 P2

Positron annihilation induced Auger electron spectroscopy at Au-layers on Cu and Si — ●JAKOB MAYER¹, CHRISTOPH HUGENSCHMIDT^{1,2}, and KLAUS SCHRECKENBACH^{1,2} — ¹Technische Universität München, Physikdepartment E21, James-Franck-Str., 85748 Garching — ²Technische Universität München, ZWE FRM-II, Lichtenbergstr. 1, 85748 Garching

At the new positron source NEPOMUC at the FRM-II in Munich a low-energy (15eV) positron beam with an intensity of 10^7 - 10^8 moderated positrons per second is available. This enables positron annihilation induced Auger electron spectroscopy (PAES) within a short measurement time (few hours/spectrum). Up to now qualitative PAES measurements of Au on Cu have been performed to show the feasibility of this technique.

At present, Au covered single crystals of Cu and Si are prepared in order to determine the sensitivity of this technique quantitatively. For this purpose, the thickness of the Au layer is even chosen in the submonolayer range (0.1 ML-10 ML). For the analysis of the spectra besides the layer thickness of the adsorbed material its positron affinity (A_+) as well as the A_+ of the substrates has to be taken into account. Therefore the systems Au/Si and Au/Cu were chosen, since the A_+ of Si ($A_{+,Si} = -6.95$) is similar to the A_+ of Au ($A_{+,Au} = -6.30$), whereas in the latter system the A_+ of the Cu substrate is much larger ($A_{+,Cu} = -4.57$) than $A_{+,Au}$. The results of the measurements are always compared with conventional AES.

O 14.79 Mon 18:00 P2

Single-Shot Infrared Ellipsometry with a Free Electron Laser and its potential applications — ●MICHAEL GENSCH¹, JONGSEOK LEE², KARSTEN HINRICHS¹, NORBERT ESSER¹, WOLFGANG SEIDEL³, ARNULF RÖSELER¹, and ULLRICH SCHADE² — ¹ISAS - Institute for Analytical Sciences, Department Berlin, Albert-Einstein-Str. 9, 12489 Berlin, Germany — ²Berliner Elektronenspeicherring-Gesellschaft für Synchrotronstrahlung mbH, Albert-Einstein-Str. 15, 12489 Berlin, Germany — ³Research Center Rossendorf, Institute of Nuclear and Hadron Physics, Bautzner Landstraße 128, 01328 Dresden, Germany

In this contribution, a novel division of amplitude polarimeter (DOAP) approach for single-shot infrared ellipsometry with a free electron laser source is presented. The set-up enables the simultaneous determination of the ellipsometric parameters by determining two ratios of intensities so that variations of the pulse power essentially do not affect the measurement. The present set-up utilizes electrical lock-in technique to the macro pulse structure of the FEL. In a first beam time awarded in autumn 2005, we determined successfully the optical response of thin polymeric films on silicon. Thus, we establish the proof-of-principle and the precision of the instrument. The high brilliance of the FEL combined with the DOAP principle gives unique opportunities for e.g. micro-focus, imaging or pump-probe ellipsometry as well as mapping ellipsometry of ultra thin films.