

SURFACE PHYSICS

OBERFLÄCHENPHYSIK (O)

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OVERVIEW OF INVITED TALKS AND SESSIONS

(lecture rooms TRE Phys, PHY C213, WIL A317, WIL B321, WIL C207, HSZ 02)

Invited Talks

O 1.1	Mon	09:30	(TRE Phys)	Structure defines the nanoworld: Thin films, surfaces and nano-particles , <u>Christian Kumpf</u>
O 2.1	Mon	10:15	(TRE Phys)	Ab initio description of electronic excitations at surfaces , <u>Olivia Pulci</u>
O 8.1	Mon	14:00	(TRE Phys)	Electronic properties of SiC surfaces and interfaces - fundamental and technological aspects , <u>Th. Seyller</u>
O 15.1	Tue	09:30	(TRE Phys)	Control of coherent electron motion and adsorbate diffusion at surfaces by femtosecond laser excitation , <u>Jens Güdde</u>
O 16.1	Tue	10:15	(TRE Phys)	Ab initio Ice Growth at Metal Surfaces , <u>Angelos Michaelides</u>
O 22.1	Tue	14:00	(TRE Phys)	Understanding Scanning Tunneling Microscopy Experiments on Transition-Metal Structures , <u>Stefan Heinze</u>
O 23.1	Tue	14:45	(TRE Phys)	Organic molecule adsorption on solid surfaces: Chemical bonding, mutual polarisation and dispersion interaction* , <u>Wolf Gero Schmidt</u>
O 30.1	Thu	09:30	(TRE Phys)	Electronic control of molecular dynamics inside a single molecule; towards molecular nano-machines , <u>Gérald Dujardin</u> , <u>Geneviève Comtet</u> , <u>Mathieu Lastapis</u> , <u>Marta Martin</u> , <u>Damien Riedel</u>
O 31.1	Thu	10:15	(TRE Phys)	Scanning Tunneling Microscopy of Adsorbates on Insulating Films: From the Imaging of Individual Molecular Orbitals to the Manipulation of the Charge State , <u>Jascha Repp</u>
O 37.1	Thu	14:00	(TRE Phys)	Fuel Cells linking Catalysis and Electrochemistry. A challenge to Surface Science , <u>Jens R. Rostrup-Nielsen</u> , <u>N. Christiansen</u>
O 45.1	Fri	10:15	(TRE Phys)	Surface electron dynamics on the atomic scale , <u>Alexander Föhlisch</u>

Sessions

O 1	Invited talk Kumpf	Mon 09:30–10:15	TRE Phys	O 1.1–1.1
O 2	Invited talk Pulci	Mon 10:15–11:00	TRE Phys	O 2.1–2.1
O 3	Adsorption I	Mon 11:15–12:45	TRE Phys	O 3.1–3.6
O 4	Nanostructures I	Mon 11:15–13:00	PHY C213	O 4.1–4.7
O 5	Electronic structure I	Mon 11:15–13:00	WIL A317	O 5.1–5.7
O 6	Scanning probe techniques I	Mon 11:15–13:00	WIL B321	O 6.1–6.7
O 7	Surface reactions I	Mon 11:15–13:00	WIL C207	O 7.1–7.7
O 8	Invited talk Seyller	Mon 14:00–14:45	TRE Phys	O 8.1–8.1
O 9	Organic films I	Mon 15:00–17:45	TRE Phys	O 9.1–9.11
O 10	Semiconductor surfaces and interfaces	Mon 15:00–17:45	PHY C213	O 10.1–10.11
O 11	Epitaxy and growth I	Mon 15:00–17:30	WIL A317	O 11.1–11.10
O 12	Methods	Mon 15:00–17:15	WIL B321	O 12.1–12.9

O 13	Solid-liquid interfaces	Mon 15:00–17:45	WIL C207	O 13.1–13.11
O 14	Poster session I (Adsorption, Epitaxy and growth, Phase transitions, Surface reactions, Organic films, Electronic structure, Methods) (sponsored by Omicron Nanotechnology GmbH)	Mon 18:00–21:00	P2	O 14.1–14.79
O 15	Invited talk Gdde	Tue 09:30–10:15	TRE Phys	O 15.1–15.1
O 16	Invited talk Michaelides	Tue 10:15–11:00	TRE Phys	O 16.1–16.1
O 17	Adsorption II	Tue 11:15–13:00	TRE Phys	O 17.1–17.7
O 18	Nanostructures II	Tue 11:15–13:00	PHY C213	O 18.1–18.7
O 19	Electronic structure II	Tue 11:15–13:00	WIL A317	O 19.1–19.7
O 20	Epitaxy and growth II	Tue 11:15–13:00	WIL B321	O 20.1–20.7
O 21	Phase transitions	Tue 11:15–13:00	WIL C207	O 21.1–21.7
O 22	Invited talk Heinze (Gaede-Preis)	Tue 14:00–14:45	TRE Phys	O 22.1–22.1
O 23	Invited talk Schmidt	Tue 14:45–15:30	TRE Phys	O 23.1–23.1
O 24	Adsorption III	Tue 15:45–18:30	TRE Phys	O 24.1–24.11
O 25	Organic films II	Tue 15:45–18:30	PHY C213	O 25.1–25.11
O 26	Particles and clusters I	Tue 15:45–18:30	WIL A317	O 26.1–26.11
O 27	Scanning probe techniques II	Tue 15:45–18:45	WIL B321	O 27.1–27.12
O 28	Surface reactions II	Tue 15:45–18:30	WIL C207	O 28.1–28.11
O 29	Poster session II (Nanostructures, Magnetism, Particles and clusters, Scanning probe techniques, Time-resolved spectroscopy, Structure and dynamics, Semiconductor surfaces and interfaces, Oxides and insulators, Solid-liquid interfaces)	Wed 14:30–17:30	P2	O 29.1–29.84
O 30	Invited talk Dujardin	Thu 09:30–10:15	TRE Phys	O 30.1–30.1
O 31	Invited talk Repp	Thu 10:15–11:00	TRE Phys	O 31.1–31.1
O 32	Adsorption IV	Thu 11:15–13:00	TRE Phys	O 32.1–32.7
O 33	Scanning probe techniques III	Thu 11:15–13:00	PHY C213	O 33.1–33.7
O 34	Particles and clusters II	Thu 11:15–13:00	WIL A317	O 34.1–34.7
O 35	Organic films III	Thu 11:15–13:00	WIL B321	O 35.1–35.7
O 36	Structure and dynamics	Thu 11:15–13:00	WIL C207	O 36.1–36.7
O 37	Invited talk Rostrup-Nielsen	Thu 14:00–14:45	TRE Phys	O 37.1–37.1
O 38	Adsorption V	Thu 15:00–18:00	TRE Phys	O 38.1–38.12
O 39	Nanostructures III	Thu 15:00–18:00	PHY C213	O 39.1–39.12
O 40	Oxides and insulators	Thu 15:00–18:00	WIL A317	O 40.1–40.12
O 41	Electronic structure III	Thu 15:00–17:30	WIL B321	O 41.1–41.10
O 42	Symposium Electron transfer processes II	Thu 15:00–17:30	WIL C207	O 42.1–42.5
O 43	Time-resolved spectroscopy I	Thu 17:30–18:30	WIL C207	O 43.1–43.4
O 44	Postdeadline session	Thu 20:00–21:00	HSZ 02	O 44.1–44.1
O 45	Invited talk Fhlisch	Fri 10:15–11:00	TRE Phys	O 45.1–45.1
O 46	Adsorption VI	Fri 11:15–13:00	TRE Phys	O 46.1–46.7
O 47	Organic films IV	Fri 11:15–13:00	PHY C213	O 47.1–47.7
O 48	Nanostructures IV	Fri 11:15–13:00	WIL A317	O 48.1–48.7
O 49	Electronic structure IV	Fri 11:15–13:00	WIL B321	O 49.1–49.7
O 50	Time-resolved spectroscopy II	Fri 11:15–13:00	WIL C207	O 50.1–50.7

Annual General Meeting of the Section Surface Physics

Thu 19:30–20:00 HSZ 02

Preliminary agenda:

- Report of speaker
- Election of section speaker and vice speaker
- Other things

Postdeadline session O44

Thursday, 20:00-21:00, Lecture hall HSZ 02, 21:00-24:00 Restaurant of Leibniz-Institut IWF (Helmholtzstrasse)

Deadline for invitation is February 15, 2006

The session is sponsored by SPECS GmbH together with BESTEC GmbH, VTS CREATEC GmbH, and SURFACE CONCEPT.

JOINT SESSIONS WITH OTHER SECTIONS**Symposium SYET Ultrafast electron transfer processes at surfaces**

Thursday 10:00-13:00, HSZ 04

Together with sections MA, MM

Sessions

– Invited, Keynote, Contributed Talks and Posters –

O 1 Invited talk Kumpf

Time: Monday 09:30–10:15

Room: TRE Phys

Invited Talk

O 1.1 Mon 09:30 TRE Phys

Structure defines the nanoworld: Thin films, surfaces and nanoparticles — ●CHRISTIAN KUMPF — Exp. Physik II, Univ. Würzburg

Nano-scaled systems like ultra-thin films, surfaces and nanoparticles dominate several fields of modern physics. In many cases it is possible to deliberately tune and hence design the properties of these systems. A detailed knowledge about their geometric structure is essential since this represents the key for a fundamental understanding of the optical, electronic or magnetic properties. In this contribution several examples of structural investigations of unconventional systems are presented, which are based on results obtained from modern diffraction techniques:

Thin films of magnetic half-metallic materials epitaxially grown on semiconductor surfaces are discussed as candidates for spin injection.

The degree of spin polarization depends strongly on the quality of the interfaces and layers. These properties are investigated for pseudomorphically strained layers of the half-Heusler compound NiMnSb.

The second example is the adsorption of large organic molecules on metal surfaces. The molecules were believed to be only weakly bonded, however, recently an increasing number of evidences for strong chemisorption was found. We report on x-ray standing waves (XSW) and LEED-IV measurements on NTCDA and Sn-phthalocyanine on Ag(111).

Finally we report on a new approach for the structural analysis of very small (< 5nm) nanoparticles based on synchrotron radiation diffraction data. In contrast to conventional methods our approach enables the investigation of detailed structural parameters like size-distributions, shape, relaxation, stacking faults and other lattice imperfections.

O 2 Invited talk Pulci

Time: Monday 10:15–11:00

Room: TRE Phys

Invited Talk

O 2.1 Mon 10:15 TRE Phys

Ab initio description of electronic excitations at surfaces — ●OLIVIA PULCI — ETSF, CNR-INFM, Dept. of Physics University of Rome Tor Vergata, Rome, ITALY

Structural, electronic and optical properties of complex systems are nowadays accessible thanks to the impressive development of theoretical approaches and computer power.

Nanostructures, surfaces and even biological systems can now be stud-

ied within ab-initio methods fully including exchange and correlation effects.

We will review the Many-Body Perturbation Theory based on the Green's function formalism, and present examples of GW and excitonic calculations for systems ranging from nanocrystals to liquid water.

Applications to the study of the band structure, electron affinity and optical properties of diamond, silicon, and germanium surfaces will be discussed in details.

O 3 Adsorption I

Time: Monday 11:15–12:45

Room: TRE Phys

O 3.1 Mon 11:15 TRE Phys

Ligand Effects Observed For The CO Adsorption At CoPt-Alloys — ●DANIELA FENSKE, DIRK HOOGESTRAAT, DENIS GRESHNYK, STEFANIE NEUENDORF, HOLGER BORCHERT, WAI-LEUNG YIM, THORSTEN KLÜNER, and KATHARINA AL-SHAMERY — Carl v.Ossietzky University Oldenburg, Faculty V, Institute of Pure and Applied Chemistry, Germany

The use of bimetallic compounds instead of monometallic catalysts can strongly enhance the efficiency of heterogeneous catalysts which may be attributed either to structural and/or to ligand effects. Results on the influence of the adsorption of CO at CoPt-alloys will be reported as a function of surface composition. The alloys were obtained by evaporating a thin film of Co-atoms onto a Pt(111) crystal under UHV-conditions and subsequent annealing to various temperatures. The final composition of the surface itself could be tuned because Pt tends to segregate at the surface as a function of temperature. The exact surface composition of the different alloys was investigated by XPS. FT-IRAS as well as TPD measurements exhibited that CO-adsorption strongly depends on the actual surface composition which is mainly attributed to strong ligand effects (either preferential adsorption at Pt- (Pt rich surfaces) or Co-sites (Co rich surfaces)). Within TPD desorption peaks are lower than for pure platinum but larger than for pure cobalt sites. Supplementary data on a Co₃Pt(111) single crystal will be presented. Theoretical calculations (DFT) reveal the dependence between surface composition, the composition of the second and third layer and changing IR-frequencies and desorption temperatures.

O 3.2 Mon 11:30 TRE Phys

Changes in CO adsorption behavior on stepped platinum surfaces induced by preadsorbed silver — ●BARBARA TRÄNKENSCHUH, REGINE STREBER, JOHANNES SCHÖCK, CHRISTIAN PAPP, REINHARD DENECKE, and HANS-PETER STEINRÜCK — Lehrstuhl für Physikalische Chemie II, Universität Erlangen-Nürnberg, Egerlandstr. 3, 91058 Erlangen

The influence of preadsorbed silver on the adsorption of CO on stepped platinum surfaces was studied using a combination of high-resolution X-ray photoelectron spectroscopy (XPS) and a supersonic molecular beam set-up. Gambardella et al. [1] have shown that on stepped Pt surfaces silver grows via an 1D row-by-row growth mode for small coverages (< 0.5 ML), starting at the step edges. In our study we deposited different amounts of silver onto Pt(355)=[5(111)x(111)] and Pt(644)=[5(111)x(100)] at 300 K and monitored the growth behavior by XPS in the Ag 3d and Pt 4f binding energy region. Thereafter, CO was dosed at low temperatures and simultaneously C 1s spectra were measured to determine the time-dependent occupation of the different adsorption sites, which can be distinguished by high-resolution XPS. For Ag coverages up to one monatomic row at the step edges, mainly the occupation of the CO step adsorption sites is changed. For higher Ag coverages, also changes in the CO adsorption behavior on the terraces were observed, due to the decreasing free Pt terrace width. Supported by the DFG (STE 620/4-3).

[1] P. Gambardella et al., Physical Review B 61 (2000) 2254.

O 3.3 Mon 11:45 TRE Phys

The influence of steps on the activated adsorption of methane on platinum: a molecular beam / high-resolution XPS study. — •CHRISTIAN PAPP, BARBARA TRÄNKENSCHUH, REGINE STREBER, THOMAS FUHRMANN, REINHARD DENECKE, and HANS-PETER STEINRÜCK — Lehrstuhl für Physikalische Chemie II, Universität Erlangen-Nürnberg, Egerlandstr. 3, 91058 Erlangen.

We investigated the activated adsorption of methane on Pt(644) and Pt(355) to examine the influence of steps on the sticking coefficient and, thus, on the reactivity of these surfaces. Both samples have (111) terraces and differ only in the step orientation: Pt(644) has (100) steps and Pt(355) has (111) steps. To overcome the barrier for methane dissociation at UHV conditions, we used a supersonic molecular beam set-up. From measurements on Pt(111)[1], methyl (CH_3) has been identified as the product of the dissociative adsorption. By using high resolution in-situ XP spectroscopy we are able to distinguish between methyl adsorbed at step and terrace sites. The adsorption processes were analysed separately, leading to relative sticking coefficients for step and terrace adsorbed molecules, with a different kinetic energy dependence. Additionally, we investigated the thermal evolution of the adsorbed species to study the influence of the steps on the dehydrogenation process. A comparison to corresponding results for flat Pt(111)[2] will be presented. Supported by the DFG (STE 620/4-3).

[1] Fuhrmann et al., Chem. Phys. Lett. 390 (2004) 208.

[2] Fuhrmann et al., New J. Phys. 7 (2005) 107.

O 3.4 Mon 12:00 TRE Phys

Buckled iodine layers on Pt(100): evidence of a charge density wave? — •BJÖRN BRAUNSCHWEIG and WINFRIED DAUM — Institut für Physik und Physikalische Technologien, TU Clausthal, Leibnizstrasse 4, D-38678 Clausthal-Zellerfeld

The atomic structure of well-defined iodine-covered Pt(100) surfaces was examined by scanning tunnelling microscopy (STM) in air and electrolyte. At high iodine coverage the well-known ($\sqrt{2} \times 5\sqrt{2}$)R45°-I adlattice on an unreconstructed Pt(100) substrate is observed. The adlayer consists of iodine rows which predominantly run along the [010] direction and form a characteristic double-row structure. Our STM images of the I-Pt(100) surface obtained in air show that the surface is covered with two distinctly different ($\sqrt{2} \times 5\sqrt{2}$)R45°-I phases: one phase with weak buckling of the double-rows parallel to the steps along the [010] direction, and a second phase of strongly buckled iodine double-rows perpendicular to the steps. The buckling of both domains strongly depends on the tunneling resistance and is reversible. No buckling is observed in a 0.1M HClO_4 electrolyte for a wide range of tunneling conditions, in accordance with previous work. We suggest that the iodine adsorbate induces a periodic lattice distortion (Peierls distortion) of the substrate yielding a charge density wave. The distortion of the charge density may be lifted or enhanced by the strong electric field of the electric double layer of the Pt/electrolyte interface and by the tip-induced field at the Pt/air interface, respectively.

O 4 Nanostructures I

Time: Monday 11:15–13:00

O 4.1 Mon 11:15 PHY C213

Self-Organized Titanium Oxide Nanotube-Layers: Formation and Applications — •JAN MACAK and PATRIK SCHMUKI — University of Erlangen Nuremberg, Dept. of Materials Science, LKO, Martensstr. 7, 91058 Erlangen, Germany

The presentation shows approaches to achieve electrochemical fabrication of self-organized high aspect ratio titanium oxide nanotubes. Key to obtain highly defined tubes is an optimized and controlled anodization of Ti in fluoride containing solutions. In general, the morphology of the tubular layers is affected strongly by the electrochemical parameters such as solution pH and anodization voltage. By optimizing the local electrochemical conditions within the tubes layers consisting of highly ordered TiO_2 nanotubes with a length of several micrometers can be grown on Ti surfaces. The diameters that can be obtained range from 20 nm to 200 nm * typical wall thicknesses are in the range of 10-20 nm. Except for the formation of the tubes also (potential) applications will be discussed. Titanium oxide is a highly functional material that has numerous interesting properties, for example, in solar energy conversion, catalysis of decomposition of organic compounds (self-cleaning), wettability and

O 3.5 Mon 12:15 TRE Phys

Adsorption modes of ethene on Pt(111) and $\text{Cu}_3\text{Pt}(111)$ from vibrational spectroscopy and DFT calculations — •CONRAD BECKER, JAN HAUBRICH, THOMAS PELSTER, and KLAUS WANDEL — Institut für Physikalische und Theoretische Chemie der Universität Bonn, Wegelerstr. 12, 53115 Bonn

The adsorption of ethene on Pt(111) and $\text{Cu}_3\text{Pt}(111)$ at 100K has been investigated experimentally using high resolution electron energy loss spectroscopy (HREELS) and temperature programmed desorption (TPD). The spectra suggest two significantly different adsorption modes, which can be characterized as a bridged di- σ -mode on Pt(111) and a more weakly bound atop mode on $\text{Cu}_3\text{Pt}(111)$. Using the Vienna ab initio simulation package (VASP) we have computed the bonding geometries and energies as well as the vibrational spectra of the di- σ -mode and the atop mode. As expected the di- σ -mode is the strongest bonding mode on Pt(111). When the molecule is, however, forced to an atop position - a situation that corresponds to the bonding on the $\text{Cu}_3\text{Pt}(111)$ surface - the most favourable configuration is a metalla cycle, which is characterized by two σ -bonds on a single Pt atom. Furthermore, the adsorption energy of the metalla cycle is significantly smaller than that of the di- σ -mode, which reflects the findings of the TPD experiments. Based on DFT calculations a complete assignment of the modes in the HREELS spectra is performed.

O 3.6 Mon 12:30 TRE Phys

Investigations on segregation in modern hydrogen storage alloys — •MARK SCHÜLKE¹, JANOS GIBER², GABOR KISS², MARTIN LAMMERS³, KARL-HEINZ MÜLLER^{1,3}, and HUBERT PAULUS³ — ¹University of Applied Sciences of South Westphalia, Luebecker Ring 2, 59494 Soest, Germany — ²Technical University of Budapest, Institute of physics, Chair of atom physics, H-1111 Budapest, Budafoki ut 8, Hungary — ³Institute for Technology and Knowledge Transfer (TWS), Luebecker Ring 2, 59494 Soest, Germany

Before the first use hydrogen storage alloys have to be activated by means of several heating cycles combined with hydrogen flushing. According to former publications, the key mechanism to the understanding of the activation process is surface segregation induced by selective oxidation. [1] But it is also known from previous experiments with model systems that the thermodynamic segregation of alloy components and of oxygen solved in the bulk influences the hydrogen absorption as well.

Samples of the AB_2 Laves phase alloy $\text{Ti}_{0.95}\text{Zr}_{0.05}\text{Mn}_{1.53}\text{V}_{0.47}\text{Fe}_{0.08}\text{Al}_{0.02}$ with an oxygen content of ca. 0.9 at% (from manufacturing) were tempered for different periods of time (30 s, 1 min, 1 h, 5 h) at 100°C and 200°C and analyzed by means of different surface analysis methods (SNMS, XPS, AES, depth profiles) afterwards. In addition to oxygen, Mn and Fe are enriched in a surface layer with a thickness of about 20 nm.

In future investigations the influence of defined surface conditions on the hydrogen absorption shall be examined.

[1] L. Schlappbach in: Hydrogen in Intermetallic Compounds II, Topics in Applied Physics, vol. 67, ed. L. Schlappbach, Springer, 1992.

Room: PHY C213

biocompatibility. Therefore this simple approach to produce this highly defined nanoscopic form of TiO_2 bears a high potential for technological exploitation.

O 4.2 Mon 11:30 PHY C213

Metallic Multilayer TiSi_2 Nanocontacts — •SVEND VAGT¹, JAN RÖNSPIES¹, TAMMO BLOCK¹, VOLKMAR ZIELASER², and HERBERT PFNÜR¹ — ¹Institut für Festkörperphysik, Universität Hannover — ²Institut für Angewandte und Physikalische Chemie, Universität Bremen

For electrical investigations of nanosized structures, macroscopic contacts pads have to fulfill several prerequisites like low resistivity, chemical purity and inertness, a defect free substrate, and well defined boundaries. By MBE in an UHV-chamber, we produced a stack of alternating Si, Ti, and Si layers on a structured Si sample. After transport through air, an annealing step up to 750°C in UHV forms the highly conducting C54 crystal structure. The Si capping layer efficiently protects the underlying Ti layer against oxidation. Only low temperature annealing is then required afterwards for cleaning and oxide removal. Generation of a deep trench at the boundary of TiSi_2 and Si at the surface was avoided by a

Si starting layer. Lateral diffusion of Ti into silicon, as shown by [1] for simple thin Ti pads on Si, is vital for the understanding of the contacting of nanostructures to the contactpads. We will compare our results of SAM, STM, and STS measurements of the pad boundaries of the multilayer silicide pads with [1], and discuss the requirements for contacting a one-dimensional electrically conducting system, and show as an example the contacting of Ag and Pb nanowires.

[1] Palermo et. al., Appl. Phys. Lett., Vol. 81, No.19, 2002

O 4.3 Mon 11:45 PHY C213

Atomic structure and electronic properties of self-assembled dysprosium-silicide nanowires on Si(001) — ●MARTINA WANKE¹, CHRISTIAN PREINESBERGER¹, SYLVIA HAGEDORN¹, GERD PRUSKIL¹, MARIO DÄHNE¹, DENIS VYALIKH², FRIEDRICH SCHILLER², SERGEIJ MOLODTSOV², and CLEMENS LAUBSCHAT² — ¹Institut für Festkörperphysik, Technische Universität Berlin, D-10623 Berlin — ²Institut für Festkörperphysik, Technische Universität Dresden, D-01219 Dresden

We report on high-resolution scanning tunneling microscopy of the self assembly of dysprosium-silicide nanowires on planar and vicinal Si(001) surfaces. These nanowires have widths of 15 to 100 Å and lengths exceeding several 1000 Å. They are found to grow in two domains with different nanowire directions on different substrate terraces, which is related to the geometry of the dangling bonds at the Si(001)2x1 surface. This two-domain growth can be suppressed when the nanowires are prepared on vicinal Si(001) substrates with an angle of 4° in [110] direction.

Two types of such nanowires are formed depending on the preparation conditions. Using high-resolution scanning tunneling microscopy, the atomic structure of both nanowire types is derived. It is shown that anisotropic strain in combination with the Si(001) surface anisotropy is the driving force for nanowire formation.

Angle-resolved photoelectron spectroscopy on vicinal substrates shows an anisotropic metallicity of the nanowires. Thus these nanowires are an interesting model system for one-dimensional metallicity. This project was supported by DFG, project number DA 408/11.

O 4.4 Mon 12:00 PHY C213

Direct Growth of Mesoscopic Copper Wires by Electrodeposition — ●SHENG ZHONG^{1,2}, THOMAS KOCH^{1,2}, HARALD ROESNER², HORST HAHN², EBERHARD NOLD³, TORSTEN SCHERER², MU WANG⁴, STEFAN WALHEIM², and THOMAS SCHIMMEL^{1,2} — ¹Institute of Applied Physics, University Karlsruhe, D-76128 Karlsruhe, Germany — ²Institute of Nanotechnology (INT), Forschungszentrum Karlsruhe, D-76021 Karlsruhe, Germany — ³Institute for Materials Research I (IMF I), Forschungszentrum Karlsruhe, D-76021 Karlsruhe, Germany — ⁴National Laboratory of Solid-State Microstructures, Nanjing University, Nanjing 21009, China

One-dimensional metallic nanowires have attracted considerable attention in recent years because of their potential use as interconnects in future generations of nanometer-scale electronics. For example, in the field of interconnects in electronics especially copper plays an important role. There are few methods to fabricate nanowires that are long, aligned, free standing and metallic. One of the most successful approaches to prepare metallic nanowires is the deposition of metal guided by appropriate templates. In this paper, a new method is demonstrated to self-assemble long, straight, free-standing and thin copper wires consisting of well-orientated single crystalline domains. The wires are directly reduced from copper sulfate solution in the presence of a direct current electric field without templates, surfactants and additives. We present a detailed study of the structure of these thin copper wires with a diameter down to 120 nm by SEM, FIB, TEM and SAMS.

O 4.5 Mon 12:15 PHY C213

Formation of a contacted nanobridge without micropatterning — ●S. WILLE¹, S. WU¹, F. H. GOJNY², M. H. G. WICHMANN², B. FIEDLER², K. SCHULTE², and R. ADELUNG¹ — ¹Lehrstuhl für Materialverbunde, Technische Fakultät der CAU Kiel, Kaiserstr. 2, 24143 Kiel, Germany — ²Kunststoffe und Verbundwerkstoffe, Technische Universität Hamburg-Harburg (TUHH), Denickestr. 15, 21073 Hamburg, Germany

There are many applications for carbon nanotubes in research nowadays. In our approach we use double wall carbon nanotubes (DWCNTs) as a substrate. Starting with an epoxy-DWCNT composite, there are only a few steps to get a nanobridge structure, suitable for, e.g. a H_2 -sensor. As first step, μm -scale channels were fabricated by etching the composite. These cracks were found to be bridged by the DWCNTs. The bridges themselves can be used as a substrate of a metal-nanostructure (e.g. Au, Pd). By evaporating under a small angle, we make use of the shadowing of the crack walls. This avoids a shortcut and covers simultaneously the channels bridged by the DWCNTs with metal. The obtained metal tubes that form around the carbon nanotubes determine the conductivity of the ensemble. The details of the formation process will be discussed as well as possible applications.

O 4.6 Mon 12:30 PHY C213

Direct Observation of Individual Defects on Carbon Nanotubes by Dynamic Force Microscopy — ●MAKOTO ASHINO and ROLAND WIESENDANGER — Institute of Applied Physics and Microstructure Research Center, University of Hamburg, Jungiusstr. 11, D-20355 Hamburg

Single-walled carbon nanotubes (SWNTs) have attracted much attention due to their unusual mechanical and unique electronic properties, which can provide great opportunity for fabricating nanoscale devices. Actual implementation of the SWNT devices demands a thorough understanding of the structural and electronic properties not only of perfect SWNTs but also of defective SWNTs because some kinds of defects are naturally included and can cause drastic changes of their properties. Recently, we have successfully achieved atomic resolution for imaging SWNTs by dynamic force microscopy (DFM) in ultrahigh vacuum and at low temperature [1]. The DFM, operated by the frequency modulation technique in non-contact regime, has enabled "true" atomic resolution for imaging non-periodic features and point defects. Here, we present atomic resolution imaging of individual defects in the SWNTs. As in the case of Ref. 1, we observed the SWNTs on a graphite substrate under feedback control to maintain a constant frequency shift of the cantilever oscillation with a constant amplitude operation. The images obtained suggest the existence of localized defects. Through detailed analysis of the image contrasts, we will topologically characterize those defects.

[1] M. Ashino, *et al.*, Phys. Rev. Lett. **93**, 136101 (2004).

O 4.7 Mon 12:45 PHY C213

Innovative Quantum Devices based on C₆₀ -Nanodots — ●OLIVER S. SENFTLEBEN, TANJA STIMPEL-LINDNER, HERMANN BAUMGÄRTNER, and IGNAZ EISELE — Institut für Physik EIT9.1, Universität der Bundeswehr München, 85577 Neubiberg

Thermal evaporation of pure C₆₀ molecules is very suitable for the fabrication of new quantum devices. Observation of quantum effects like Coulomb-Blockade or coherent tunnelling can only be observed at room temperature if capacities are in the range of sub-atto-farad regime to exceed thermal noise. Hence the feasibility of extremely thin oxides as well as the behaviour of C₆₀ under high temperatures (400-850°C) and oxygen atmosphere is of very high importance. Experiments have been performed in a UHV chamber to avoid any surface contamination during process and to allow in-situ process control with AES, LEED, STM and STS. Thermal oxidation of Si has been studied under several pressures (10⁻⁵ to 10⁻³ mbar) and temperatures (RT to 850°C). The experiments have shown that oxide-growth is possible up to a thickness of 2 nm. C₆₀ films of different coverage have then been studied under these environmental conditions. C₆₀ on pure Si shows no chemical reaction with oxygen up to 800°C and a pressure of 10⁻⁴ mbar. This has been verified by STM and AES. The behaviour of C₆₀ on SiO₂ during annealing has been observed under UHV conditions and oxygen pressures up to 10⁻⁴ mbar. First experiments indicate a weaker binding of C₆₀ to the SiO₂ than to the Si(100)-2x1 surface and therefore a higher desorption rate at elevated temperatures. Finally first STS results of C₆₀ on UHV grown oxides are presented.

O 5 Electronic structure I

Time: Monday 11:15–13:00

Room: WIL A317

O 5.1 Mon 11:15 WIL A317

Probing of bulk band edges by STM: An ab initio analysis — ●ALEXEY DICK and JÖRG NEUGEBAUER — Max-Planck-Institut für Eisenforschung, Düsseldorf, Germany

Scanning tunneling microscopy (STM) is an extensively used surface-sensitive tool that allows to address an ever extending range of surface phenomena. Recently it became possible to study electron dynamics by analyzing electron standing wave patterns created in the vicinity of surface imperfections. In the past these studies had been mainly restricted to surface states since bulk states have been assumed to decay too fast in the vacuum region accessed by STM.

To analyze whether STM can be extended to access bulk properties such as the dispersion of the projected bulk band edge (BBE), we have performed a theoretical STM study on various noble metal (110) surfaces. A repeated slab geometry and density functional theory based on a plane-wave pseudopotential approach have been employed to accurately describe surface properties.

A careful analysis of our results explains well recent experimental studies on silver (110) surfaces [1]. It shows that probing of the BBE is possible due to coupling of the bulk and surface states and an enhancement of the bulk state density at the edge of the projected bulk bands. Such an enhancement occurs due to the bulk band-folding in the direction perpendicular to a surface. Since the underlying effect is general, our results can be used to understand the resolution of the BBE on other metallic surfaces.

[1] J.I. Pascual *et al.*, submitted to Phys. Rev. Lett.

O 5.2 Mon 11:30 WIL A317

Stark-Effect in STM induced Light Emission — ●GERMAR HOFFMANN¹, PETER JOHANSSON², and RICHARD BERNDT³ — ¹Institut für Angewandte Physik und Zentrum für Mikrostrukturforschung, Universität Hamburg, 20355 Hamburg, Germany — ²Department of Natural Sciences, University of Örebro, Sweden — ³IEAP, Christian-Albrechts-Universität zu Kiel, 24098 Kiel

The tunnelling current in a scanning tunnelling microscope gives rise to the emission of photons. Owing to the small lateral dimension of the tunnelling current filament high lateral resolution can be achieved. The effect can be used for optical spectroscopy of nanoscale objects such as individual molecules. In STM induced light emission of Na layers on Cu(111) photon emission spectra reflect quantum well transitions. The energy of these transitions can be varied by the electric field of the tip, akin to a Stark effect. We will present experimental observations and numerical calculations for clean substrates, a number of Na coverages and various quantum well states. The results will be discussed in relation to recent observations of STM-induced molecular fluorescence.

O 5.3 Mon 11:45 WIL A317

Electronic structure of the 6H-SiC(11 $\bar{2}$ 0) non-polar surface — ●MARCO BERTELLI¹, JAN HOMOTH¹, MARTIN WENDEROTH¹, RAINER G. ULBRICH¹, ANGELA RIZZI¹, M. CLELIA RIGHI², and ALESSANDRA CATELLANI³ — ¹IV. Physikalisches Institut, Georg-August Universität Göttingen, Germany — ²CNR-INFM National Center on nanoStructures and bioSystems at Surfaces (S³) and Dipartimento di Fisica, Università di Modena e Reggio Emilia, Modena, Italy — ³CNR-IMEM, Parco Area delle Scienze, Parma, Italy and S³

We studied the 6H-SiC(11 $\bar{2}$ 0) surface reconstruction by means of combined cross-section scanning tunneling microscopy and ab-initio simulations. The n-doped Si-terminated 6H-SiC(0001) substrates were cleaved in ultra high vacuum and measured in-situ by STM at room temperature. The experimental results show an unreconstructed surface. The surface unit cell resembles the stacking sequence of the 6H polytype. The most prominent feature in the occupied state images within the cell is a depression at the inversion point.

In agreement with the experimental observation, the theoretical calculations predict a relaxed surface, but no reconstruction. Correspondingly bond lengths and angles change along the stacking sequence only for the outermost layer, with Si atoms moving inwards of ca. 0.22 Å. C atoms positions are almost unchanged, but for a depression of 0.07 Å at inversion. In general, the up and down arrangement of C and Si atoms is responsible for the observed features in STM images: filled states appear to be concentrated on the carbon atoms and the empty states on the Si atoms.

O 5.4 Mon 12:00 WIL A317

Neutral phosphorus atoms in Si(111)-2×1 stabilize local buckling of π -bonded chains — ●J. K. GARLEFF¹, M. WENDEROTH¹, R. G. ULBRICH¹, C. SÜRGER², H. V. LÖHNEYSSEN^{2,3}, and M. ROHLFING⁴ — ¹IV. Physikalisches Institut der Universität Göttingen, Friedrich-Hund-Platz. 1, 37077 Göttingen, Germany — ²Physikalisches Institut and DFG Center for Functional Nanostructures (CFN), Universität Karlsruhe, 76128 Karlsruhe, Germany — ³Forschungszentrum Karlsruhe, Institut für Festkörperphysik, 76021 Karlsruhe, Germany — ⁴School of Engineering and Science, International University Bremen, P. O. Box 750561, 28725 Bremen, Germany

Substitutional phosphorus (P) atoms in the Si(111)-2×1 surface have been studied with scanning tunneling microscopy at 8 Kelvin. The unexpected *neutral* charge state of embedded P atoms at low temperature has been established by experimental observation: (i) Peak positions in the differential conductance at the P atom and on the clean Si surface coincide. (ii) The P-induced contrast pattern is restricted to a single or double π -bonded chain. (iii) Atomic corrugation significantly changes around charged defects, but remains unaffected at P atoms. The absence of extra charge at substitutional P atoms in Si(111)-2×1 proves that its electronic properties are dominated by the surface states. The surface band gap of clean Si(111)-2×1 itself strongly decreases to higher temperature. This points on weaker buckling of the π -bonded chains at increased temperature. We explain the spectroscopic contrast of P atoms at room temperature [1] by a locally stabilized buckling of the π -chains.

[1] T. Trappmann *et al.*, Europhys. Lett. **38**, 177 (1997)

O 5.5 Mon 12:15 WIL A317

Visualization of the Molecular Jahn-Teller effect in an insulating K4C60 Monolayer — ●ANDRE WACHOWIAK^{1,2}, R. YAMACHIKA², K. H. KHOO², Y. WANG², M. GROBIS², D.-H. LEE², STEVEN G. LOUIE², and M. F. CROMMIE² — ¹Institute of Applied Physics, University Hamburg, 20355 Hamburg, Germany — ²Department of Physics, University of California at Berkeley, Berkeley, CA, USA

Unlike atoms in an elemental solid, the building blocks of a molecular solid are more susceptible to tuning. C60 based bulk solids can be tuned between metallic, insulating and superconducting states by changing the charge state and/or local environment of the constituent molecules. This flexibility arises through a sensible interplay between intramolecular Coulomb interaction, electron-phonon coupling, and local charging on an energy scale comparable to the narrow electronic bandwidth. By low temperature scanning tunneling microscopy we have examined how molecular electronic structure is strongly influenced due to charge doping and local electron-phonon interaction in extended monolayer films. In particular, the Jahn-Teller effect, a charge-induced mechanical deformation of molecular structure, is directly visualized at the single molecule level in an insulating K4C60 monolayer[1]. [1] A. Wachowiak *et al.* Science 310 (2005) 468

O 5.6 Mon 12:30 WIL A317

Scanning Tunneling Microscopy (STM) and Spectroscopy (STS) Investigation of Ultra-thin Epitaxial Nobel Metal Films on Sapphire — ●CHRISTOF DIETRICH, BERNDT KOSLOWSKI, GERD KÄSTLE, HANS-GERD BOYEN, and PAUL ZIEMANN — Abteilung Festkörperphysik, Universität Ulm, D-89069 Ulm

Ultra-thin epitaxial Au(111) and Ag(111) films have been prepared on (0001)-oriented sapphire with a niobium buffer layer. Despite their thickness of just 2nm, the noble metal films are electrically conductive and, according to XRD, exhibit excellent epitaxial properties as well as outstanding smoothness over macroscopic scales [1,2]. Room temperature STM measurements revealed highly ordered smooth surfaces with large terraces and mono-atomic steps. STS measurements on these samples reproducibly showed prominent signatures which can be nicely explained by quantum well states due to the confinement of the electrons perpendicular to the film. Additionally, a thickness-dependent shift of the onset of the Shockley-like surface state was observed in the I(V) spectra possibly indicating a thickness dependent strain in the films.

[1] Growth of thin, smooth, epitaxial (111) oriented Gold films on c-cut Sapphire; G.Kästle, H.-G. Boyen, B. Koslowski, A. Plettl, F. Weigl and P. Ziemann, Surf. Sci. 498, 168 (2002). [2] Size-Effect of the resistivity of thin epitaxial Gold Films, G. Kästle, H.-G. Boyen, A. Schröder, P. Ziemann, Phys. Rev. B 70, 165414 (2004).

O 5.7 Mon 12:45 WIL A317

STM study of subsurface impurities in noble metals — ●A. WEISMANN, M. WENDEROTH, N. QUAAS, and R. G. ULBRICH — Universität Göttingen, IV. Physikalisches

Isolated subsurface Co-atoms embedded in noble metals (Cu, Ag) were prepared under UHV-conditions by codeposition of host metal and impurity compound from two e-beam evaporators. Surface charge density oscillations in the vicinity of these impurities were investigated by low temperature Scanning Tunneling Microscopy and Spectroscopy at 8K. While isotropic surface-state Friedel-oscillations around surface impurities were studied extensively in the past decade, bulk charge density

oscillations have not been reported in this context. Here we show that interesting effects arise from the anisotropy of the host metals bandstructure. Most prominent is the effect of electron focussing: the out-scattered wave is not a spherical wave as in the isotropic case but shows a preferential propagation in certain directions. This shapes the observed LDOS-pattern decisively. In this study we concentrate on the energy dependency of these bulk state interference patterns. We quantitatively compare the observed STM and STS data to calculations. For this we used the electrons retarded Greensfunction of the host material to describe the propagation process and calculated the surface LDOS by considering interference processes between an incoming and a scattered wave.

O 6 Scanning probe techniques I

Time: Monday 11:15–13:00

Room: WIL B321

O 6.1 Mon 11:15 WIL B321

Scanning optical nearfield investigation of thin metal films — ●MAXIMILIAN ASSIG, KAI HODECK, and MARIO DÄHNE — Institut für Festkörperphysik, Technischen Universität Berlin, D-10623 Berlin

We present a setup to investigate the optical nearfield of thin film samples such as metal films with subwavelength spatial resolution. Simultaneously observing the topography and the luminescence of the sample we are able to correlate structural and optical properties. When illuminating the sample from reverse in total reflection geometry, we are able to probe the near field of the sample either by collection through an etched fiber tip or by scattering with a gold tip. In the latter case, the scattered light is collected in the far field, using distance modulation to detect selectively the scattered nearfield-signal of the sample. We present first results on the nearfield properties of a thin gold film containing nanometer scale holes with two different diameters.

O 6.2 Mon 11:30 WIL B321

Scattering scanning near-field optical microscopy on anisotropic dielectrics using a free electron laser light source — ●SUSANNE SCHNEIDER¹, J. SEIDEL¹, S. GRAFSTRÖM¹, C. LOPPACHER¹, M. CEBULA¹, L. M. ENG¹, S. WINNERL², D. STEHR², and M. HELM² — ¹Institute of Applied Photophysics, University of Technology Dresden, D-01062 Dresden — ²Forschungszentrum Rossendorf, D-01328 Dresden

Scattering scanning near-field optical microscopy (s-SNOM) is based on the interaction between an optically scattering nano-particle (AFM tip) and a dielectric sample. The size of the scatterer defines the optical resolution of the microscope, which is on the order of a few nanometers. On that scale, the optically anisotropic properties of most samples have to be taken into account [1].

To examine the influence of optical anisotropy on the scattering signal, we excite a ferroelectric sample close to its phonon resonance in the mid infrared regime. As the precisely tunable light source at infrared wavelengths we used a free electron laser (FEL). We have measured the near-field signal at several wavelengths while scanning the sample, as well as the tip-sample distance dependence of the scattered light signal for the 1st, 2nd, and 3rd harmonic signal. The anisotropy is revealed for different sample orientations. Not only are we presenting the first tunable IR near-field measurements on ferroelectric lithium niobate and barium titanate single crystals, but furthermore are our measurements in excellent accordance with recent calculations of optical anisotropy in such systems [1].

[1] S. Schneider, et al., Phys. Rev. B 71, 115418 (2005)

O 6.3 Mon 11:45 WIL B321

Optical versus mechanical contrast mechanism in dynamic apertureless SNOM — ●RALF VOGELGESANG, ALPAN BEK, RUBEN ESTEBAN, and KLAUS KERN — Max Planck Institut für Festkörperforschung

In dynamic mode apertureless or scattering-type scanning near-field optical microscopy (SNOM) an oscillating scanning probe tip excites optical interactions at a surface. Ideally, the local optical information can be extracted by lock-in amplification at a higher harmonic of the oscillation frequency. This signal, however, is easily contaminated by mechanical crosstalk.

We have developed a quantitative model to specify the proper conditions [1]. We show that the contrast mechanism is in general a combination of both spatially nonlinear optical interaction and temporally

anharmonic mechanical tip motion. Our algebraic analysis provides a systematic framework to identify and control the relative influence of the competing contrast origins.

[1] A. Bek, R. Vogelgesang, and K. Kern, Appl. Phys. Lett., 87, 163115 (2005)

O 6.4 Mon 12:00 WIL B321

Plasmon propagation through a border between different layered systems observed by SNOM — ●ANDREAS ENGLISCH, STEFAN GRIESING, and UWE HARTMANN — Institute of Experimental Physics, University of Saarbrücken, P.O. Box 151150, D-66401 Saarbrücken, Germany

Quasi-twodimensional optics with plasmons involving refraction and reflection can be realized by different approaches. One possibility is to use elements consisting of a structured thin dielectric layer deposited on the plasmon-supporting surface. The resulting individual layers are the metal film with and without dielectric coating. The electromagnetic eigen modes are characterized by an effective refractive index which determines the propagation parallel to the plane of the layers (x-y plane). The behavior of plasmons or other modes incident to a border between two different multilayers is not known in detail. SNOM measurements are presented which show the intensity distribution at the border between different layered systems: Due to the different decay length perpendicular to the x-y plane within both subsystems a near-field is formed at the border which extends across an area of several tens of microns. Although the intensity is confined to the x-y plane it cannot be modelled just by the interference of plasmons or other eigen modes of the given layered structure. In order to explain the observed intensity pattern an approach is introduced which is based on three-dimensional diffraction theory. Under particular conditions the border causes strong electromagnetic losses. The origin of these intrinsic or radiative losses is discussed in particular.

O 6.5 Mon 12:15 WIL B321

Nonlinear nano-optics: tip-enhanced spectroscopy based on optical frequency conversion at a metal tip — ●MATTHIAS DANCKWERTS, MICHAEL BEVERSLUIS, and LUKAS NOVOTNY — Institute of Optics, University of Rochester, Rochester NY 14627 (USA)

At a sharp gold tip illuminated with pulsed laser light at 800 nm, the interaction of the electromagnetic field with the metal leads to the generation of frequency-doubled light as well as a supercontinuum arising from 2-photon excited interband transitions. In the case of multi-wavelength illumination, mixing signals such as DFG and SFG and higher-order processes like 4-wave mixing are observed. Due to the local field enhancement, the source of this radiation is highly confined to within nanometers at the apex of the tip, hence the tip is acting as a nanometric light source.

This offers a range of nanoscopic optical spectroscopies, where the tip acts as a source, not as a scatterer of light emitted from an object. The measured light is spectrally well-separated from the excitation, allowing for essentially background-free detection. For an application, we show optical extinction measurements with a lateral resolution of 30 nm. Further, experiments utilizing the continuum radiation from the tip for elastic scattering measurements at nanostructures such as carbon nanotubes are discussed.

O 6.6 Mon 12:30 WIL B321

Video-rate Scanning Probe Microscopes: solving the problem of resonances induced by the non-linear piezo material. — ●G.J.C. VAN BAARLE^{1,2}, W.M. VAN SPENGEN¹, W.A. VAN LOO¹, R. SCHAKEL¹, L. CRAMA¹, J.W.M. FENKEN¹, M.J. ROST^{1,2}, and T.H. OOSTERKAMP¹ — ¹Kamerlingh Onnes Laboratory, Leiden University, P.O. box 9504, 2300 RA Leiden, The Netherlands — ²Leiden Probe Microscopy BV, P.O. box 9504, 2300 RA Leiden, The Netherlands

For a wide variety of surface and interface phenomena in both fundamental and applied contexts, it is becoming increasingly important to visualize them with atomic or molecular resolution combined with high speeds. We report on the recent progress we made in the development of fast scanning probe techniques, and demonstrate that the current bottleneck for fast imaging is given by the mechanical properties of the scanner rather than the control electronics. This has been confirmed by testing several home-built and commercial instruments. In order to optimize the scanners for high speeds, we take into account the influences of piezo non-linearity. We present experimental results showing the existence of both non-linear super- and subharmonic resonances. In addition, we also consider the strength of the non-linear effects as a function of piezo geometry. Preliminary results indicate that the above problems can be circumvented by actuating the piezo scanner with the well-known, but in the context of SPM technology not commonly used, 'charge control' technique instead of the more standard method of 'voltage control'.

O 6.7 Mon 12:45 WIL B321

Using the Constant-Excitation Mode as a Spectroscopy Tool in Ambient Conditions — ●JAN-ERIK SCHMUTZ, MARCUS SCHÄFER, and HENDRIK HÖLSCHER — Center for Nanotechnology (CeNTech) and Physics Institute, University of Münster

Dynamic modes are often used in scanning force microscopy in order to improve the resolution compared to conventional contact mode. In air and liquids the so-called "tapping mode" is often applied where the cantilever is oscillated with a fixed frequency near the sample surface. In vacuum, however, the so-called frequency modulation mode (FM mode) - based on a self-driven cantilever - has several advantages. Nonetheless, this technique is not limited to vacuum conditions as shown for ambient conditions and liquids. Recently, we demonstrated that the closely related constant excitation mode (CE mode) [1] allows dynamic force spectroscopy in ambient conditions [2,3]. This technique delivers not only high resolution pictures but also information about material properties like adhesion and elasticity. In difference to the tapping mode it enables the continuous measurement of the tip-sample interaction potential. Here we present an extension of this approach towards a 3D technique. By mapping systematically the frequency shift on top a single DNA strand, we created an iso-potential map of the sample potential [4]. We discuss advantages compared to conventional techniques.

[1] H. Ueyama, Y. Sugawara, S. Morita, *Appl. Phys. A* 66, S295 (1998). [2] H. Hölscher, B. Gotsmann, A. Schirmeisen, *Phys. Rev. B* 68, 153401 (2003). [3] H. Hölscher, B. Anczykowski, *Surf. Sci.* 579,21 (2005). [4] J.-E. Schmutz, M.M. Schäfer, H. Hölscher (submitted).

O 7 Surface reactions I

Time: Monday 11:15–13:00

Room: WIL C207

O 7.1 Mon 11:15 WIL C207

Comparison of chemically and photo induced electronic excitations on gold surfaces — ●BEATE MILDNER, PETER THISSEN, ECKART HASSELBRINK, and DETLEF DIESING — Institut für Physikalische Chemie, Universität Duisburg Essen

Within an adiabatic picture exothermic surface reactions dissipate their excess energy into adsorbate and substrate vibrations. Deviations from this behavior are manifested in internal electronic excitation of the reaction products or in electronic excitations of the metal. The latter ones can be detected by the emission of electrons from the surface. However, this is only possible, when the energy of the electrons is larger than the work function of the metal. Electronic excitations with smaller energies can be detected as internal currents in tunnel or Schottky devices, whose barriers are smaller than the metals work function. We use Ta-TaOx-Au tunnel junctions as detectors for electronic excitations. In the course of the recombination reaction of atomic hydrogen on the gold surface chemically induced tunnel currents are observed. The band structure of the tunnel devices can be modified by the application of a bias voltage between the Ta and Au layers allowing an energy selective detection of the chemically excited charge carriers. This experiment is compared with the energy selective detection of photo induced tunnel currents. We used laser diodes with $h\nu = 1.95, 1.53, 1.37, 1.27$ eV. The spectrum of the chemically induced excitations agrees best with that observed for a photo excitation with $h\nu = 1.27$ eV, a value which is close to the exothermicity of the Langmuir-Hinshelwood reaction between two adsorbed hydrogen atoms of approx. 1.4 eV.

O 7.2 Mon 11:30 WIL C207

Description and analysis of non-adiabatic effects in surface processes using a mixed quantum-classical framework. — ●CHRISTIAN CARBOGNO and AXEL GROSS — Abteilung Theoretische Chemie, Universität Ulm, Albert-Einstein-Allee 11, 89069 Ulm

Impressive improvements in treating excited states have been achieved during the last decade and now allow a numerical calculation of *ab initio* potential energy surfaces for many systems. Nevertheless, to perform dynamical simulations on these surfaces still represents a considerable challenge: A full quantum treatment of both electrons and nuclei is computationally not feasible at the moment for complex, realistic systems. We have used a mixed quantum-classical approach [1] in order to describe the dynamics of electronically non-adiabatic processes at surfaces [2]. The computational efficiency of this method allows a high-dimensional treatment of these processes by including many nuclear degrees of freedom and/or electronic states. We have studied the influence of several phys-

ical and numerical parameters (e.g. number of electronic states) on the non-adiabatic reaction dynamics and compared the results with the experiment and full quantum simulations, in particular for charge-transfer processes in molecule-surface scattering and for laser-induced desorption from surfaces [2].

[1] J. C. Tully, *J. Chem. Phys.* **93**, 1061 (1990)

[2] C. Bach *et al.*, *Israel J. Chem.* **45**, 45 (2005)

O 7.3 Mon 11:45 WIL C207

Non-adiabatic spin-transfer and electronic friction during chemisorption simulated with TDDFT — ●ECKHARD PEHLKE and MICHAEL LINDENBLATT — Institut für Theoretische Physik und Astrophysik, Christian-Albrechts-Universität Kiel, 24098 Kiel

When atoms interact with a surface, part of their chemisorption energy is transferred into electron-hole pair excitations. This can result in the emission of exoelectrons, or chemicurrents over Schottky barriers as observed by Nienhaus *et al.* [1]. We simulate such non-adiabatic processes using time-dependent spin-density functional theory together with Ehrenfest dynamics for the motion of the nuclei. Results for the chemisorption of H-atoms on the Al(111) surface will be presented. Upon approach of the surface, the local spin polarization of the hydrogen atom is transferred to the substrate electrons. For an incoming H-atom with thermal energies, the energy dissipated into electron-hole pairs amounts to order of 0.1 eV for the initial part of the trajectory up to the first reflection of the H atom at the surface potential. The variation of the local spin polarization at the H-atom is compared to the Newns-Anderson model by Mizielinski *et al.* [2].

[1] H. Nienhaus, *Surf. Sci. Rep.* **45**, 1 (2002).

[2] M.S. Mizielinski, D.M. Bird, M. Persson, S. Holloway, *J. Chem. Phys.* **122**, 084710 (2005).

O 7.4 Mon 12:00 WIL C207

Influence of the isotope effect on chemicurrent detection — ●DAVID KRIX, RAMONA NÜNTHEL, and HERMANN NIENHAUS — Experimental Physics, University of Duisburg-Essen, 47048 Duisburg, Germany

Hot charge carriers created in the exothermic reaction of atomic hydrogen and atomic deuterium with silver have been detected with the use of thin film Ag/p-Si(111) Schottky diodes. In thin film diodes excited holes can penetrate the metal film. If the holes are sufficiently energetic they can surpass the Schottky barrier and can be detected as a so called chemicurrent. The intensity of the chemicurrent is influenced by the transport process in the device. An exponential attenuation depending on the film

thickness is observed. The experimental data show an isotope effect in the absolute intensity and attenuation length for deuterium vs. hydrogen. Chemicurrents as much as three times larger have been observed while exposing the devices to hydrogen than is the case with deuterium. The attenuation length of hot holes is found to be larger for hydrogen than for the deuterium case. The results are in agreement with theoretical predictions of electronic excitations by chemical reactions within the electronic friction model.

O 7.5 Mon 12:15 WIL C207

Copper Dissolution Reaction (CDR) in the Presence of a Binary 2D-Compound: CuI on Cu(100) — •MINH HAI NGUYEN THI, PETER BROEKMANN, and KLAUS WANDEL — Institut für Physikalische und Theoretische Chemie, Universität Bonn, Wegelerstr. 12, D-53115 Bonn

The anodic copper dissolution reaction (CDR), has been studied by means of Cyclic Voltammetry (CV) and in-situ scanning tunnelling microscopy (STM) at the electrochemical solid/liquid interface. Exposing the Cu(100) electrode surface to an acidic and iodide containing electrolyte (5 mM H₂SO₄, 1 mM KI) leads to the formation of an electro-compressible/decompressible c(px 2)-I adsorbate layer at potentials close to the onset of the CDR. At these positive potentials mobile CuI species originating mainly from step-edges cause the local exceeding of the CuI solubility product, thereby giving rise to the nucleation and growth of a laterally well ordered 2D-CuI film. As this process occurs at potentials well below the potential regime of the 3D-CuI bulk formation we refer to it as under potential formation (UPF) of a binary compound. The formed 2D-CuI film exhibits symmetry properties and nearest neighbour distances that are similar to the (111) lattice of the crystalline bulk CuI phase (zinc blende type). Surprisingly, the 2D-CuI film on Cu(100) does not act as a passivation layer against the copper dissolution which proceeds via an inverse step flow mechanism.

O 7.6 Mon 12:30 WIL C207

Mass transport with pulses in an excitable surface reaction: Rh(110)/K/NO + H₂ — •HONG LIU¹, LING ZHOU², SEBASTIAN GÜNTHER³, and RONALD IMBIHL¹ — ¹Institute for Physical Chemistry, Hannover University, Callinstr. 3-3a, D-30167 Hannover, Germany — ²Division of Engineering and Applied Sciences, Harvard University, Pierce Hall, 29 Oxford St., Cambridge, MA 02138, USA — ³LMU München, Department Chemie, Butenandstr.11 E, 81377 München, Germany

O 8 Invited talk Seyller

Time: Monday 14:00–14:45

Room: TRE Phys

Invited Talk

O 8.1 Mon 14:00 TRE Phys

Electronic properties of SiC surfaces and interfaces - fundamental and technological aspects — •TH. SEYLLER — Lehrstuhl für Technische Physik, Universität Erlangen-Nürnberg, Erwin-Rommel-Straße 1, 91058 Erlangen, Germany

The wide band gap semiconductor silicon carbide (SiC) is the first choice material for power electronic devices operating at high voltages, high temperatures, and high switching frequencies. Due to their importance for crystal growth, processing, and device fabrication, the electronic properties of SiC surfaces and interfaces to other materials such as metals and dielectrics are of particular interest from both, fundamental as well as technological point of view. The first part of the presenta-

tion deals with the electronic properties of unreconstructed SiC surfaces. Unreconstructed, H-terminated SiC surfaces which are passivated in a chemical as well as an electronic sense are obtained in a thermal hydrogenation process. Using these surfaces as a starting point it is possible to prepare unreconstructed (1×1) surfaces with one dangling bond per unit cell. These surfaces show indications for strong electron correlation effects. The second part of the presentation is concerned with the electronic properties of interfaces to SiC. It is demonstrated that deposition of Al₂O₃ on H-terminated SiC(0001) leads to interfaces which are lower in defects than the thermally grown SiO₂/SiC interface. Finally, we will focus on the band alignment of graphite on SiC and discuss consequences of the observed Schottky barriers for the formation of rectifying and ohmic contacts on SiC.

O 9 Organic films I

Time: Monday 15:00–17:45

Room: TRE Phys

O 9.1 Mon 15:00 TRE Phys

STM and LEED studies of α -sexithiophene on Au(111) — •MARIO KIEL, KLAUS DUNCKER, CHRISTIAN HAGENDORF, and WOLF WIDDRA — Martin-Luther-Universität Halle-Wittenberg, FB Physik, D-06120 Halle(Saale)

The growth of α -sexithiophene (6T) on the close-packed Au(111) surface has been studied by scanning tunneling microscopy (STM) and low energy electron diffraction (LEED). The evaporation of the 6T molecules from a home-built Knudsen cell and measurements have been performed at a base pressure of 1×10^{-10} mbar. STM images reveal rows of equiv-

O 7.7 Mon 12:45 WIL C207

Two-dimensional polymeric network formed via a surface reaction — •CARSTEN BUSSE^{1,2}, SIGRID WEIGELT¹, KURT V. GOTHELF³, CHRISTIAN BOMBIS¹, THOMAS STRUNSKUS², CHRISTOF WÖLL², FLEMMING BESENBACHER¹, and TROLLE R. LINDEROTH¹ — ¹Department of Physics and Astronomy, and iNANO, University of Aarhus, DK-8000 Aarhus C, Denmark — ²Lehrstuhl für Physikalische Chemie I, Ruhr-Universität Bochum, D-44780 Bochum, Germany — ³Department of Chemistry, and iNANO, University of Aarhus, DK-8000 Aarhus C, Denmark

Molecular assemblies on surfaces are often held together via weak forces (van-der-Waals interaction, hydrogen bonding). In order to form more stable, covalently bond structures, we explored chemical reactions between adsorbed molecules. A tri-aldehyde with a large, conjugated backbone was deposited under UHV-conditions in submonolayer coverage on Au(111). The resulting 2D-islands were exposed to a background pressure of a reactive di-amine. After annealing to 450 K, STM reveals the formation of a network structure that consists of large (molecular mass up to 6 kDa) polymer-like macromolecules. We were able to study the connectivity and the varying local binding patterns with sub-molecular resolution. The structure of the macromolecules leads to the conclusion that a chemical reaction between the aldehyde and the amine takes place. Increasing the initial tri-aldehyde coverage leads to a dense, monolayer-high polymer film covering the whole surface. Changing the structure of the educts leads to very similar reactions. We obtained additional information on this process by XPS and NEXAFS.

alent 6T molecules with one molecule per unit cell. The rows are rotated by 9° with respect to the [112] direction and span large Au(111) terraces (~100 nm). Six symmetry-equivalent domains are possible, however step-induced structures with the molecular axis along the step edges are strongly favored. This can be also seen by higher spot intensities in LEED, visible due to a small crystal miscut. On the terrace, the herring bone (22×√3) reconstruction of the clean Au(111) surface is stretched by about 15% upon 6T monolayer adsorption. This is interpreted as adsorbate-induced strain in the first Au(111) layer.

O 9.2 Mon 15:15 TRE Phys

Comparison of gas- and condensed phase NEXAFS spectra of large organic molecules — ●FLORIAN HOLCH¹, DOMINIQUE HÜBNER¹, ACHIM SCHÖLL¹, RAINER FINK², and EBERHARD UMBACH¹ — ¹Universität Würzburg, Experimentelle Physik II — ²Universität Erlangen, Physikalische Chemie II

The interaction between most large organic molecules in the solid state is commonly believed to be solely due to electrostatic and van-der-Waals forces. An analysis of these intermolecular effects requires a comparison of high-quality spectroscopic data of gaseous and condensed organic molecules. In this work we present high-resolution NEXAFS spectra of 1,4,5,8-naphthalene-tetracarboxylic acid dianhydride (NTCDA) and acenaphthenequinone (ANQ) in the gas phase and solid state. For the gas phase experiments a new experimental set-up has been used that allows the measurement of substances with high sublimation temperatures. A detailed Franck-Condon analysis of the *vibronic* fine structure of the NTCDA spectra at the C K-edge yields consistent results for both phases. In contrast, pronounced differences in the *electronic* features between gas phase and condensate can be demonstrated. This corroborates the results for ANQ that also suggest an involvement of the π^* -orbitals of the aromatic core in the intermolecular interaction. Our findings thus indicate that intermolecular forces can be much stronger than commonly believed and may even cause the formation of intermolecular bonds. The project is financed by the BMBF under contract 05KS4WWC/2

O 9.3 Mon 15:30 TRE Phys

Long-range order and polymerisation of sexithiophene on Ag(100) surfaces – a STM study — ●KLAUS DUNCKER, SEBASTIAN WEDEKIND, CHRISTIAN HAGENDORF, and WOLF WIDDRA — Martin-Luther-Universität Halle-Wittenberg, 06120 Halle, Fb Physik

High-temperature scanning tunneling microscopy (STM) is used to study the morphology of the first few monolayers of α -sexithiophene (6T) on Ag(100) surfaces at room and elevated temperatures. The 6T molecules have been evaporated from a homebuilt Knudsen cell at a base pressure of the UHV chamber of 1×10^{-10} mbar.

Several molecular superstructures coexist in different domains within the monolayer. They can be divided into two groups with either one or two molecules in the unit cell. Common to all, the flat-lying 6T molecules are oriented with their long axis parallel to [011] and [0 $\bar{1}$ 1] crystallographic directions of the Ag-substrate. As the predominant superstructure with two molecules in the unit cell we find a (9/0)(2/5) structure with a pair of chirally equivalent, parallel molecules in the unit cell. Additionally, a herring bone-like structure is found with two non-linear molecules in the unit cell forming rows in highly-ordered domains. STM images with submolecular resolution reveal flat molecules which have undergone a cis-trans isomerization exclusively between the 4th and 5th thiophene ring and which align in rows of left- and right-handed molecules.

Whereas earlier studies indicate molecular dissociation of the first monolayer during thermal desorption, we have identified by STM polymerization to long chains and polythiophene networks after annealing to about 440 K and multilayer desorption.

O 9.4 Mon 15:45 TRE Phys

Novel Tripod Ligands for Prickly Self-Assembled Monolayers — ●TOBIAS WEIDNER¹, ANDREAS KRÄMER², MICHAEL ZHARNIKOV³, ANDREY SHAPORENKO³, DOMINIK ENDERS⁴, ULRICH SIEMELING², and FRANK TRÄGER¹ — ¹Institut für Physik, Universität Kassel, Kassel — ²Institut für Chemie, Universität Kassel, Kassel — ³Angewandte Physikalische Chemie, Universität Heidelberg, Heidelberg — ⁴Kirchhoff Institut für Physik, Universität Heidelberg, Heidelberg

Self-assembled monolayers (SAMs) consisting of laterally separated and non-interacting functional units are of great current interest in sensor- and molecular electronics applications. We used the new ligands PhSi(CH₂SMe)₃ (**1**) and Ph-*p*-C₆H₄-Si(CH₂SMe)₃ (**2**) to prepare such SAMs on gold. In **1** and **2** the rigid rod type units Ph and Ph-*p*-C₆H₄, respectively, are connected to the central Si atom at the vertex of the tripod binding unit that can be anchored on the surface with three instead of a single binding site via thioether head groups. In particular, owing to the relative size of the binding unit, the SAMs are expected to exhibit considerable void space between individual Ph and Ph-*p*-C₆H₄ units which protrude from the surface.

Film formation was investigated *in situ* by optical second harmonic generation and ellipsometry, revealing a two-step process. SAMs of **2** were further investigated by *ex situ* methods, *viz.* high-resolution XPS (HRXPS), IR-spectroscopy, and STM. The most important results are as

follows: HRXPS showed three different binding states of sulfur. Dense packing of the tripod anchor groups on the surface has been verified with a substantially lower density of the biphenyl pricks.

O 9.5 Mon 16:00 TRE Phys

Molecule-molecule vs. molecule-substrate interactions in 2D oligopyridine networks — ●H.E. HOSTER¹, M. ROOS¹, CH. MEIER², A. BREITRUCK¹, B. PLUHAR¹, M. SEYFRIED¹, K. TONIGOLD¹, and R.J. BEHM¹ — ¹Abt. Oberflächenchemie und Katalyse, Universität Ulm, 89069 Ulm — ²Abt. Organische Chemie III, Universität Ulm, 89069 Ulm

Oligopyridines vapor deposited onto single crystalline surfaces form highly ordered 2D networks with a geometry mainly determined by the coverage. We have analysed such networks on HOPG, Au(111), and Ag(111)-like adlayers on Ru(0001). Variations of the substrate in some cases alter details within the structures such as intermolecular distances or aspect ratios of unit cells, while in other instances certain molecular arrangements are only found on one type of surface. We assume the local constellations of the molecules and as a consequence also the unit cells of the resulting superstructures to be dominated by intermolecular interactions via hydrogen bonds. On the other hand, both the 2D networks and the planar single molecules appear to prefer certain lateral alignments with respect to the substrate, as obvious in closer analyses of domain orientations and STM-images showing molecular adlayers with the Au(111) herringbone reconstruction shining through. This points towards a significant contribution of the adlayer/substrate interface to the overall energy, which causes an adaptation of the respective 2D-layer to the respective substrate up to a repetitive occupation of equivalent adsorption sites, *i.e.*, a commensurate or at least quasi-epitaxial layer.

O 9.6 Mon 16:15 TRE Phys

Two step adsorption of phenyl-functionalized tripod ligands on gold — ●TOBIAS WEIDNER¹, ANDREAS KRÄMER², TIGRAN VARTANYAN³, ULRICH SIEMELING², and FRANK TRÄGER¹ — ¹Institut für Physik, Universität Kassel, Kassel — ²Institut für Chemie, Universität Kassel, Kassel — ³Vavilov State Optical Institute, St Petersburg, Russia

Further progress in organic monolayer preparation depends on the thorough understanding of thin film formation processes. In this contribution *in situ* optical second harmonic generation (SHG) measurements have been employed to study the adsorption kinetics of the new tripod thioether ligands PhSi(CH₂SMe)₃ and Ph-*p*-C₆H₄-Si(CH₂SMe)₃ on gold substrate from solution. Previous characterization by *in situ* ellipsometry and a number of *ex situ* methods, *viz.* high-resolution XPS, FTIR-RAS, and STM indicated dense packing of the tripod anchor groups on the surface with a substantially lower density of the biphenyl moieties. To characterize the adsorbate-substrate interaction quantitatively a new method based on SHG measurements at different temperatures was developed. The rate of adsorption was found to decrease from $2.4 \cdot 10^{-3} \text{ s}^{-1}$ to $3.4 \cdot 10^{-4} \text{ s}^{-1}$ when the solution temperature was raised from 2.5 to 49 degrees centigrade (at constant concentration). This contra intuitive behavior is explained by a two-step adsorption model assuming that stable chemical bonds are formed subsequent to a weakly bound precursor state. The theoretical description of such a model allows us to obtain an estimate of the enthalpy of the physisorbed state, a parameter difficult or impossible to determine by other techniques.

O 9.7 Mon 16:30 TRE Phys

Coverage dependent structure of 2D networks formed by oligopyridines on Ag(111)/Ru(0001) Bonds — ●ACHIM BREITRUCK¹, MATTHIAS ROOS¹, CHRISTOPH MEIER², ULRICH ZIENER², MONA SEYFRIED¹, HARRY E. HOSTER¹, and ROLF J. BEHM¹ — ¹Department Surface Chemistry and Catalysis, University of Ulm, 89069 Ulm — ²Department Macromolecular Chemistry and Organic Materials, University of Ulm, 89081 Ulm

Oligopyridines form highly ordered 2D networks on a number of single crystal surfaces [1]. They are of interest both for the physical background of their structure formation itself and for their possible utilization as self assembling templates for nanostructuring. In the present study, layers of increasing coverage have been vapor deposited in UHV onto Ag(111)-like adlayers on Ru(0001). STM analyses reveal at least 5 different highly ordered structures, with a geometry depending on the coverage and, in some cases, the temperature during and after deposition. The coverage dependence is an immediate consequence of the geometry of the utilized oligopyridines, which at higher packing densities forces the molecules into local constellations with less network stabilizing hydrogen bonds

per molecule. This also involves a coverage dependent adsorption energy, which allows to safely transform one structure into another by partial desorption of the adlayer.

[1] U. Ziener, J.-M. Lehn, A. Morran, M. Möller, Chem. Eur. J., 2002, 8(4), 951-957

O 9.8 Mon 16:45 TRE Phys

High thermal stability of electron cross-linked aromatic self-assembled monolayers — ●MOHAMED EL-DESAWY, ANDREY TURCHANIN, and ARMIN GÖLZHÄUSER — Physik Supramolekularer Systeme, Universität Bielefeld, Universitätsstr. 25, 33615 Bielefeld

We report on the thermal stability of e-beam cross-linked biphenylthiol (BPT) self-assembled monolayers (SAMs) on gold surfaces. The monolayers were formed from solution and cross-linked by low-energy electrons (50-200 eV). The SAMs were then thermally annealed in ultra high vacuum. Long annealing times and slow heating rates were employed to follow temperature induced changes at conditions close to thermal equilibrium. After each heating step, the films were analyzed by X-ray photoelectron spectroscopy (XPS). For non cross-linked BPT, at $\sim 420\text{K}$ the carbon coverage abruptly decreases to $\sim 20\%$, which is accompanied by a breaking of C-S bonds. In cross-linked BPT, despite a C-S bond cleavage in the same temperature range, the carbon matrix shows only gradual changes with increasing temperature. Even at $\sim 1000\text{K}$, the SAM coverage has only decreased to $\sim 80\%$. Hence, cross-linked SAMs show a much higher thermal stability than non cross-linked ones. This is of importance for technological applications of SAM coatings.

O 9.9 Mon 17:00 TRE Phys

On the Origin of a Phase Transition in clean Porphyrin Films on a Silver (111) Surface — ●H. MARBACH, K. COMANICI, F. BUCHNER, F. MAIER, and H.-P. STEINRÜCK — Lehrstuhl für Physikalische Chemie II, Universität Erlangen-Nürnberg, Egerlandstraße 3, D-91056 Erlangen

Organic molecules play a prominent role for the development of new materials and molecular devices. An important group of such molecules are porphyrins. Their versatility and distinct chemical and electronic properties make them promising candidates for tailored catalytic processes and as building blocks for nanoscaled electronic devices. The properties of porphyrins can be modified e.g. by introducing or changing a central metal atom and different ligands. We studied different porphyrins on a silver (111) surface by means of scanning tunneling microscopy (STM) in ultra high vacuum (UHV). The preparation of the porphyrin layers was done in UHV via sublimation techniques. Different ordered phases and spatiotemporal behaviors were observed for different central metal atoms and porphyrin ligands. In particular for a specific Cobalt porphyrin (Co-TTBPP) two different phases (square and hexagonal) were observed. In a time series of STM images the transition from the hexagonal to the square phase was studied. Based on these observa-

tions and the comparison with the ordered square structures of similar porphyrins the underlying mechanism is interpreted as an activated process.

O 9.10 Mon 17:15 TRE Phys

Electroless metal deposition on the surface of aromatic self-assembled monolayers — ●CHRISTOPH T. NOTTBOHM, ANDREY TURCHANIN, and ARMIN GÖLZHÄUSER — Physik Supramolekularer Systeme, Universität Bielefeld, Universitätsstr. 25, 33615 Bielefeld

We investigated the palladium-catalysed electroless deposition (ELD) of copper on amino-terminated, cross-linked biphenyl self-assembled monolayers (SAMs). Cross-linking as well as the generation of surface amino groups is achieved by irradiation with low-energy electrons. The cross-linked SAM acts as a diffusion barrier, suppressing the catalyst-free ELD of copper on the gold substrate. Immobilization of a catalyst on the surface of the SAM is achieved by the reduction of Pd(II) ions that are coordinated to the surface amino groups. This was verified by angle resolved X-ray photoelectron spectroscopy (APXPS). Using a stencil mask to locally generate surface amino groups, it was shown by atomic force microscopy that copper is only deposited in irradiated areas. This indicates that copper deposition occurs only at the catalytic site.

O 9.11 Mon 17:30 TRE Phys

Temperature effect in branching of photochemical reactions — ●ZHARNIKOV MICHAEL¹, ANDREY SHAPORENKO¹, ANDREA BAUMER², DIETRICH MENZEL³, and PETER FEULNER³ — ¹Angewandte Physikalische Chemie, Universität Heidelberg, Im Neuenheimer Feld 253, D-69120 Heidelberg — ²Walter Schottky Institut, Am Coulombwall 3, D-85748 Garching — ³Physikdepartment E20, Technische Universität München, D-85747 Garching

Radiation-induced damage represents a severe constraint for the characterization of organic and biological materials by advanced electron or x-ray spectroscopy and microscopy. A possibility to reduce damage is cooling of the samples down to cryogenic temperatures. The protective effect of cooling is commonly related to hindrance of mass transport in the object, whereas the basic irradiation-induced bond cleavage is believed to be unaffected. To prove this hypothesis we studied radiation damage of self-assembled monolayers, which are prototypes of thin organic layers and highly organized biological systems. We demonstrate that the effect of cooling is twofold. It freezes the structure, but by decreasing the mobility of fragments it also changes the branching of various photochemical reactions, thereby strongly modifying the cross sections as well as the products of irradiation induced processes. Two limiting cases could be identified. Reactions involving transport of single atoms and small fragments proceed nearly independent of temperature. Reactions requiring transport of heavy fragments are, however, efficiently quenched by cooling. We speculate that bonds can recombine if the fragments are forced to stay in place due to their reduced mobility at low temperatures.

O 10 Semiconductor surfaces and interfaces

Time: Monday 15:00-17:45

Room: PHY C213

O 10.1 Mon 15:00 PHY C213

Investigation of geometrical properties of NiMnSb-Half-Heusler thin films by X-ray reflectivity measurements. — ●ANDREAS STAHL, CHRISTIAN KUMPF, and EBERHARD UMBACH — Experimentelle Physik II, Universität Würzburg

The Half-Heusler alloy NiMnSb is an important material which may be utilized for the fabrication of spintronic devices due to its unusual half-metallic properties. It can be grown in high crystalline quality on InGaAs/InP substrates, however, as for all heteroepitaxial systems mechanical stress is an important factor which influences crystalline quality, film growth, and magnetic properties. One example is a magnetic anisotropy which depends on the thickness of the Half-Heusler layer [1].

We present a series of x-ray reflectivity measurements on MBE-grown NiMnSb thin films from 10nm to 200nm thickness. Some of the samples were capped with an amorphous Au/Ti layer in order to avoid oxidation in air. The reflectivity scans were performed at the six-circle-diffractometer at BW2, HASYLAB, Hamburg. We discuss important parameters like the layer thicknesses, the roughnesses of the interfaces and the electron densities of the Half-Heusler layers [2].

[1] A. Koveshnikov et al.: J. Appl. Phys. \textbf{97}, 073906 (2005).

[2] A. Stahl et al.: to be published.

O 10.2 Mon 15:15 PHY C213

Morphology of ultrathin manganese silicide films on Si(001) and Si(111) substrates — ●MAHBUBE HORTAMANI, PETER KRATZER, and MATTHIAS SCHEFFLER — Fritz-Haber Institut, Faraday weg 4-6, 14195 Berlin, Germany

Recently, the field of spintronics has attracted much attention since it provides knowledge for a novel type of electronic devices that use the electron's spin, in addition to its charge, for processing and storage of data. Ferromagnetic metal/semiconductor interfaces hold great promise for fabrication of such devices. Covering Si with a layer of Mn intermetallic compounds is one possibility to produce such interfaces. We investigate the stability of Mn_xSi_y films on Si for various stoichiometries and atomic structures of the films, using density functional theory with the GGA-PBE functional and the FP-APW+lo method. We find that for ultrathin film growth on the Si substrate, the manganese-silicon multilayers with 1:1 stoichiometry (MnSi) are more stable than a pure Mn film or other silicide compounds. The formation of the B20 structure on the Si(111) substrate is found to be thermodynamically more stable than films of other structures. While the B20 structure is not compatible with the Si(001), we suggest a closely lattice-matched B2 structure to form on this surface. By simulating the proposed B2 structure on both (001) and

(111) surfaces, we find that the film formation on Si(111) is energetically favorable. However, the films on Si(001) are metastable compared to formation of MnSi islands, and hence Volmer-Weber growth is expected. In all MnSi films on Si(111) the Mn atoms in the interface and surface layer have sizable magnetic moments.

O 10.3 Mon 15:30 PHY C213

In/Si(111): Chain structure and metal-insulator transition — ●ANDREY STEKOLNIKOV, JÜRGEN FURTHMÜLLER, and FRIEDHELM BECHSTEDT — Friedrich-Schiller-Universität Jena, Institut für Festkörpertheorie und -optik, Max-Wien-Platz 1, D-07743 Jena

Atomic geometry and electronic structure of quasi-one-dimensional (1D) In/Si(111) systems with 4×1 , 4×2 , and 8×2 translational symmetries are studied by means of *ab-initio* calculations. While the 4×1 structure shows metallic behavior, the 4×2 (8×2) reconstruction leads to a pure semiconducting phase. For 4×2 (8×2) reduction of the total energy and formation of the energy gap are related to an additional bonding within the double In zig-zag chains. Simulated STM images show a good agreement with experimental ones. The geometry of In chains is very sensitive to all possible interactions. Several local minima may occur on the total-energy surface. The description of In-In and In-Si bonds plays an important role. The influence of the exchange and correlation within density functional theory calculations as well as In *d*-electrons is discussed in detail.

O 10.4 Mon 15:45 PHY C213

Optical properties of the Si(113) 3×2 ADI surface — ●KATALIN GAAL-NAGY — Dipartimento di Fisica, Università degli Studi di Milano, Via Celoria 16, 20133 Milano (Italy)

We have investigated the optical properties of the 3×2 ADI reconstruction which is the most stable structure of the (113) surface of silicon. The calculations have been done within the plane-wave pseudopotential approach to the density-functional theory as implemented in ABINIT [1] and TOSCA [2]. Besides, also a semi-empirical tight-binding approach has been used. In a first step, tests on the atomic geometry, the slab thickness, and the electronic structure have been performed. The optical properties have been derived using the matrix elements of the momentum operator through the calculation of the *x* and *y* contribution to the imaginary part of the polarizability, from which the RAS (reflectance anisotropy spectra) can be obtained. With a layer-by-layer analysis the surface contributions have been disentangled from the ones of the bulk-part of the slab. Finally, we compare our results with available theoretical and experimental data.

[1] <http://www.abinit.org>

[2] <http://users.unimi.it/etsf/tosca.html>

O 10.5 Mon 16:00 PHY C213

Investigation of the System Hafnium/Silicon(100) by means of XPS and X-ray Photoelectron Diffraction (XPD) — ●C. FLUECHTER^{1,2}, D. WEIER^{1,2}, S. DREINER¹, M. SCHÜRMANN¹, U. BERGES^{1,2}, M.F. CARAZZOLNE³, A. DE SIERVO^{3,4}, R. LANDERS^{3,4}, G.G. KLEIMAN⁴, C. WESTPHAL^{1,2}, and E. HENSCHER¹ — ¹Experimentelle Physik 1 - Universität Dortmund, Otto-Hahn-Str.4, D 44221 Dortmund, Germany — ²DELTA - Universität Dortmund, Maria-Göppert-Meier-Str. 2, D 44227 Dortmund, Germany — ³Laboratório Nacional de Luz Sincrotron, C.P. 6192, 13084-971 Campinas, SP, Brazil — ⁴Instituto de Física - Universidade Estadual de Campinas, C.P. 6165, 13083-970 Campinas, SP, Brazil

The ongoing miniaturization of transistor devices in the semiconductor industry calls for a new gate dielectric, replacing silicon oxide (SiO₂) that has been used for decades. One of the candidates, i.e. hafnium oxide (HfO₂), is investigated in this work by studying ultrathin films of the pre system HfSi/Si(100) via XPS, LEED and Photoelectron Diffraction with a magnesium x-ray source. Several heating curves are presented showing that, unlike for thick layers, no phase transitions of the ordered HfSi films can be observed. Also, an island formation of the annealed film is indicated. Simulations of the structure of the system are shown and compared to experimental diffraction patterns. We propose a possible interface structure for Hf/Si(100) to bulk Si. Finally, possibilities for oxidizing and transforming the prepared HfSi into HfO₂ are introduced.

O 10.6 Mon 16:15 PHY C213

Photothermal patterning of H-terminated silicon substrates: Writing nanostructures with a micron-sized laser beam — ●RAFAEL BAUTISTA, THORSTEN BALGAR, STEFFEN FRANZKA, NILS HARTMANN, and ECKART HASSELBRINK — Universität Duisburg-Essen, Fachbereich Chemie, Universitätsstr. 5, 45141 Essen

A focused beam of an argon ion laser at a wavelength of 514 nm is used for rapid large-area patterning of H-terminated Si(100) substrates under ambient conditions [1]. The technique allows for the preparation of well-confined, ultrathin oxide structures with a lateral dimension significantly below the diffraction limited laser spot diameter of the optical setup. In particular, at a focal spot diameter of about 2.5 μm oxide lines with a width from several microns down to 300 nm are prepared. At even smaller spot diameters structures with a lateral dimension below 200 nm are reached. The patterning experiments under ambient conditions are complemented by investigations in an ultrahigh vacuum environment. A simple thermokinetic analysis of the data allows to estimate effective kinetic parameters of the patterning process and reproduce the experimentally observed functional dependence of the line width on the incident laser power and the writing speed. The underlying highly super-linear dependence of the overall patterning process on the laser intensity is traced back to the interplay between the laser-induced transient local temperature rise and the thermally activated hydrogen desorption.

[1] T. Balgar, S. Franzka, N. Hartmann, E. Hasselbrink, Langmuir 20 (2004) 3525.

O 10.7 Mon 16:30 PHY C213

Photothermally induced dehydroxylation on surface-oxidized silicon substrates: A simple means for the fabrication of submicron-structured hydrophilic/hydrophobic templates — ●NILS HARTMANN, THORSTEN BALGAR, STEFFEN FRANZKA, and ECKART HASSELBRINK — Universität Duisburg-Essen, Fachbereich Chemie, Universitätsstr. 5, 45141 Essen

Patterns with alternating hydrophilic and hydrophobic domains are widely used to control and study processes at surfaces in many fields of material science. We recently reported a laser-assisted procedure for the fabrication of hydrophobic patterns on hydrophilic, surface-oxidized silicon substrates [1]. Local irradiation with a highly focused laser beam at a wavelength of 514 nm results in photothermal dehydroxylation and converts the affected surface areas from hydrophilic to hydrophobic. The patterns are stable for weeks or longer, even if the samples are stored at ambient conditions. Contrary to ordinary avenues to hydrophilic/hydrophobic patterns no coating is required. This makes the procedure extremely simple and robust. Routine patterning can be carried out over large areas at fast writing speeds under ambient conditions. At a focal spot diameter of about 2.5 μm , hydrophobic lines with a width down to 0.4 μm are prepared. The laterally varying hydrophilicity provides an opportunity to further functionalize the surface. In particular, as shown here, the patterned substrates represent suitable templates for the directed self-assembly of organic monolayers.

[1] T. Balgar, S. Franzka, E. Hasselbrink, N. Hartmann, Appl. Phys. A, in press.

O 10.8 Mon 16:45 PHY C213

Sum-frequency generation study of hydrogen diffusion on vicinal Si(100) surfaces induced by resonant IR laser excitation — ●XU HAN, KRISTIAN LASS, and ECKART HASSELBRINK — Fachbereich Chemie, Physikalische Chemie, Universität Duisburg-Essen, Universitätsstr. 5, D-45141 Essen

We report first measurements of a new way (non-thermal, non-electronic excitation) of inducing adatom diffusion. Under selective resonant excitation by tunable IR laser pulses, hydrogen diffusion between step sites or from step edges onto terraces of a vicinal Si(100) surface has been demonstrated. The state of the adsorbate has been monitored by means of IR-visible sum-frequency generation spectroscopy (using ps laser pulses). Hydrogen preferentially binds to the step edges on a Si(100) surface with D_B or S_B steps. For saturation coverage the stretch vibration of step-bonded monohydrides has been found at 2087 cm⁻¹, with a small blue shift at lower coverages. Hydrogen diffusion from D_B or S_B step edges to other weakly bonded sites at steps can be enhanced by resonant IR laser excitation at temperatures well below the threshold for thermally activated surface diffusion of hydrogen. Alternatively, hydrogen can also diffuse onto terraces, where the frequencies of isolated monohydride, monohydride with neighboring dihydride, and dihydride are 2100, 2104 and 2107 cm⁻¹, respectively, with a small red shift at lower coverages.

O 10.9 Mon 17:00 PHY C213

MOMBE growth of ZnO on SiC - a photoemission study — ●STEFAN ANDRES¹, CHRISTIAN PETTENKOFER¹, and THOMAS SEYLLER² — ¹Hahn-Meitner-Institut, Glienicke Str. 100, D-14109 Berlin, Germany — ²Institut of Technical Physics, University of Erlangen, Erwin-Rommel-Str. 1, D-91058 Erlangen, Germany

Zinc oxide (ZnO) is a semiconductor with a direct band gap of 3.3eV and therefore an interesting candidate for future applications in the area of opto-electronics in the UV regime or transparent electronics.

We report on the growth of thin ZnO films on 6H-SiC(0001) substrates. The films were grown using Metal Organic Molecular Beam Epitaxy (MOMBE). Changes in surface morphology and electronic structure during film growth were investigated by low energy electron diffraction (LEED) and photoelectron spectroscopy (PES), respectively. The qualitative LEED images show that highly oriented ZnO(0001) films are formed. However, faceting of the surface is observed during the initial stages of ZnO growth and also beyond the monolayer coverage. A careful quantitative and qualitative examination of the SiC and ZnO core and valence band levels reveals the growth mode to be of the Frank v.d. Merwe type. Furthermore, we will comment on the the band alignment of the SiC/ZnO interface.

O 10.10 Mon 17:15 PHY C213

RF-sputtered indium-tin-oxynitride films investigated by photoelectron spectroscopy — ●MARCEL HIMMERLICH¹, MARIA KOUFAKI², MANOLIS SIFAKIS², STEFAN KRISCHOK¹, ELIAS APERATHITIS², and JUERGEN A. SCHAEFER¹ — ¹Institut für Physik und Zentrum für Mikro- und Nanotechnologien, TU Ilmenau, P.O. Box 100565, 98684 Ilmenau, Germany — ²Microelectronics Research Group, IESL, Foundation for Research & Technology-HELLAS, P.O. Box 1527, 71110 Heraklion, Crete, Greece

Indium-tin-oxide (ITO) and indium-tin-oxynitride (ITON) thin films have been fabricated by rf-sputtering in Ar or N₂ plasma, respectively. The deposition was performed on pre-cleaned Si using an ITO target (80% In₂O₃ + 20% SnO₂). During the growth procedure the gas flow was controlled to maintain a total pressure of 5×10⁻³ Torr in the cham-

ber. The dependence of the surface chemical composition and the electronic properties on the rf power were examined using photoelectron spectroscopy (XPS, UPS). Changes upon annealing were investigated by rapid thermal annealing in N₂ atmosphere as well as by in vacuo heating combined with a monitoring of the gas desorption using a quadrupole mass spectrometer. The observed differences in the carrier concentration are well correlated with the existence or absence of an oxygen reduced phase in the films, as can be seen by a high binding energy feature in the O1s, Sn3d and In3d core levels. A complex incorporation of nitrogen into the ITON films was found which reveals itself in the existence of 5 different N1s states. Annealing above 550°C resulted in a release of nitrogen combined with the formation of the oxygen reduced phase.

O 10.11 Mon 17:30 PHY C213

XPS and XPD studies on the system Hafnium(oxide) on Si(100) using soft x-rays — ●D. WEIER^{1,2}, C. FLÜCHTER^{1,2}, S. DREINER¹, M. SCHÜRMAN¹, U. BERGES^{1,2}, M.F. CARAZZOLNE³, A. PANCOTTI³, R. LANDERS^{3,4}, G.G. KLEIMAN⁴, C. WESTPHAL^{1,2}, and E. HENSCHERL¹ — ¹Experimentelle Physik 1 - Universität Dortmund, Otto-Hahn-Str.4, D 44221 Dortmund, Germany — ²DELTA - Universität Dortmund, Maria-Göppert-Meier-Str. 2, D 44227 Dortmund, Germany — ³Laboratório Nacional de Luz Sincrotron, C.P. 6192, 13084-971 Campinas, SP, Brazil — ⁴Instituto de Física - Universidade Estadual de Campinas, C.P. 6165, 13083-970 Campinas, SP, Brazil

Continuous down-scaling of the silicon based MOSFETs results in gate lengths of less than 100 nm. Scaling down the gate dielectric to less than 15 Å is not possible using SiO₂ because of an increasing leakage current. Presently, there are many high-k candidates discussed as a substitution for SiO₂ as the gate dielectric. One of the most promising candidates is HfO₂. In this work ultrathin films of HfSi on Si(100) were studied by XPD to investigate possible interface structures between Silicon and Hafnium. It will be shown that a modified C49 structure is found for HfSi by a comparison of experimental with simulated diffraction patterns. Further on, experimental XPS and XPD results for the systems HfO/Si(100) are shown.

O 11 Epitaxy and growth I

Time: Monday 15:00–17:30

Room: WIL A317

O 11.1 Mon 15:00 WIL A317

Steering induced growth anisotropy as a probe for long range interaction — ●HERBERT WORMEESTER, FRITS RABBERING, TEUN WARNAAR, and BENE POELSEMA — University of Twente, Enschede, The Netherlands

Grazing incidence homo-epitaxy of 0.5 ML on Cu(001) leads to anisotropic structures as determined with high-resolution LEED. This is the result of attractive forces between the surface and the incoming particle. The trajectory of an incoming particle changes so dramatically that a large deposition flux enhancement on protruding structures results [1]. Trajectory calculations based on an attractive Lennard-Jones potential were combined with a kMC simulation that treats the surface diffusion processes in order to investigate the evolution of the observed anisotropy. Modifications of this potential at short range distances only slightly influence the anisotropy, while modifications at long range has a significant influence on the anisotropy as observed during sub-monolayer growth. This enables to probe the long range interaction. The experimental feasibility of the detailed probing will be discussed. [1] S. van Dijken, L.C. Jorritsma and B. Poelsema, Phys. Rev. Lett. 82 4038 (1999)

O 11.2 Mon 15:15 WIL A317

Pulsed Laser Deposition of Fe on Cu Single Crystal Surfaces - Investigations by STM and Time-of-Flight Spectroscopy — ●GEORG RAUCHBAUER¹, ANDREAS BUCHSBAUM¹, HANNES SCHIECHL¹, WERNER RUPP¹, MICHAEL SCHMID¹, PETER VARGA¹, and ALBERT BIEDERMANN² — ¹Institut für Allgemeine Physik, Technische Universität Wien — ²Institut für Materialphysik, Universität Wien

In order to understand the influence of growth conditions on structure, morphology and properties we investigated ultrathin pulsed laser deposited Fe films on Cu. The main analysis technique employed was

scanning tunneling microscopy (STM), allowing us to determine the structure of the surfaces. For measuring the energy distribution of the ablated species, a time-of-flight (TOF) spectrometer, applicable for ions as well as for neutrals, has been constructed. At low coverage, low laser fluence leads to bilayer island growth while higher laser fluences result in layer-by-layer growth. We observed intermixing of Fe and Cu in the films which is caused by implantation of Fe with high kinetic energy. With increasing laser fluence, an increasing number of Fe atoms is implanted. The TOF spectra show hyperthermal energies of the neutrals, high degrees of ionization up to several dozen percent and kinetic ion energies of 50 to 150 eV, depending on the laser fluence. The ion energies can be related to the different growth modes observed.

O 11.3 Mon 15:30 WIL A317

Initial growth of Cu islands on Cu(100) by pulsed laser deposition — ●ANDREAS DOBLER and THOMAS FAUSTER — Lehrstuhl für Festkörperphysik, Universität Erlangen, Staudtstr. 7, D-91058 Erlangen

We investigated the initial growth of Cu islands on a Cu(100) surface for coverages below 0.3 monolayers with scanning tunneling microscopy. According to nucleation theory, the island density increases with the deposition flux F proportional to $F^{1/2}$. For thermal deposition at room temperature the critical nucleus i is about three atoms. Although the instantaneous flux of pulsed laser deposition is about 10⁴ times higher than in the case of thermal deposition, the island density is of the same order of magnitude for both deposition methods. When the flux is increased due to higher laser intensity, the number of islands decreases which cannot be explained by nucleation theory.

O 11.4 Mon 15:45 WIL A317

Al-Enriched Surface Phases on NiAl(100) — ●ROLAND SCHURR, ANDREAS KLEIN, LUTZ HAMMER, and KLAUS HEINZ — Lehrstuhl für Festkörperphysik, Universität Erlangen-Nürnberg, Staudtstr. 7, D-91058 Erlangen

The thermal evolution of Al-films evaporated on the cold NiAl(100) surface was studied by means of LEED, STM and AES. Deposition of several monolayers of Al at 100 K on clean NiAl(100) leads to rather flat but poorly ordered epitaxial films with (111) orientation. With annealing at about 500 K reordering occurs within the films leading to both pseudomorphic (100) grains and epitaxially aligned (111) oriented grains of pure Al as identified by comparison with single crystal LEED intensity spectra. With increasing temperature Al dissolves into the bulk leading to a sequence of different Al-rich surface phases of NiAl(100). At first a $(\sqrt{5} \times \sqrt{5})R26.6^\circ$ phase at about 600 K appears, followed by a 1D-incommensurate superstructure at about 750 K. This can be tentatively ascribed to a transition state towards the then following structure, an Al-rich $c(\sqrt{2} \times 3\sqrt{2})R45^\circ$ phase ($=$ "(3 \times 3)diag"), which develops at 800 K. Further annealing eventually produces a (1 \times 1) structure which corresponds to the (100) surface of stoichiometric NiAl. At even higher temperatures (>1150 K) Al starts to desorb from the surface leading to another "(3 \times 3)diag" phase of the Ni-enriched surface known since earlier [1]. LEED intensity spectra taken from both "(3 \times 3)diag" phases differ completely proving the existence of two distinct phases with the same periodicity. [1] D.R. Mullins and S.H. Overbury, Surf. Sci. 199 (1988) 141

O 11.5 Mon 16:00 WIL A317

Growth and structure of ultrathin Ni-films on Ir(100)-(1 \times 1) — ●W. MEYER¹, B. GÜMLER¹, A. KLEIN¹, A. SCHMIDT¹, L. HAMMER¹, S. MÜLLER¹, K. HEINZ¹, and J. REDINGER² — ¹Festkörperphysik, Universität Erlangen-Nürnberg, Staudtstr. 7, D-91058 Erlangen — ²Center for Computational Material Science, Vienna University of Technology, Gumpendorferstr. 1A, A-1060 Vienna

We report on the growth and atomic structure of epitaxial Ni-films on the metastable (1 \times 1)-phase of Ir(100) in the coverage regime 1 - 4 ML using STM, quantitative LEED and first principle calculations. The lateral misfit for Ni on the Ir(100) substrate is +8.8% so that layer-by-layer growth should not be expected. The STM studies reveal flat growth of the first Ni-layer whilst the second film layer does not close completely but third layer islands start to grow. It comes as a surprise that the films return to an almost ideal layer-by-layer growth for the 3 and 4 ML coverages. Quantitative LEED was applied to determine the atomic structure of the surfaces. The Ni-films are heavily tetragonally distorted with an average contraction of 12.3% of the inner film layers and 14.4% for the top layer spacing relative to the Ni bulk value. The experimental observation can be understood in combination with the DFT calculations: The surface formation enthalpy for the 2 ML film is less favourable than a combination of 1 ML and 3 ML islands. For higher film thickness surface roughening does not yield a sizable energy gain. Hence, only formation of a 2 ML film is energetically hindered. The relaxed film structure calculated by DFT agrees well with the LEED results apart from the top layer spacing for which DFT predicts an enhanced contraction.

O 11.6 Mon 16:15 WIL A317

Large Film Stress of Fe, Co, and Ni monolayers on Ir(100) — ●Z. TIAN, C.S. TIAN, D. SANDER, and J. KIRSCHNER — Max-Planck-Institut für Mikrostrukturphysik,

The mechanical stress of ferromagnetic monolayers(ML), which are deposited on different surface reconstructions of Ir(100) (1 \times 1, 5 \times 1-Hexagonal, 5 \times 1-H) is measured with an optical bending beam technique during growth. Both Co and Ni show a large positive film stress of 17 and 15 GPa, respectively, during the initial stage of the growth(1-2ML). This stress corresponds to the calculated value based on continuum elasticity with a misfit strain of 8.8% for fcc-Co and 9.1% for Ni. The same magnitude of stress is measured irrespective of the surface reconstruction. A kink in the stress vs. coverage curve at 2 ML can be tentatively ascribed to the end of pseudomorphic growth. Ongoing deposition leads to a lower film stress, which relaxes to less than 2 GPa as the thickness increases above 10ML. The growth of Fe leads to a compressive film stress of -10 GPa in the thickness range 2-12 ML. This stress magnitude corresponds to the epitaxial misfit induced stress, if we take the lattice constant of bcc-Fe as a reference. We conclude that pseudomorphic growth of Fe ends around 12 ML. The results are discussed in view of film structure and morphology as obtained by in-situ LEED and MEED measurements and previous STM work[1]. Lattice strain is often the decisive factor which determines the magnetic anisotropy of ferromagnetic monolayers (ML). [1] L. Hammer, W. Meier, A. Schmidt and K. Heinz: Phys. Rev. B **67**, 125422 (2003).

O 11.7 Mon 16:30 WIL A317

Two new phases of CO monolayers on Ag(100) — ●HANS-CHRISTOPH PLOIGT, FRANÇOIS PATTHEY, MARINA PIVETTA, and WOLF-DIETER SCHNEIDER — Ecole Polytechnique Fédérale de Lausanne, Institut de Physique des Nanostructures, CH-1015 Lausanne, Switzerland

We used low-temperature scanning tunneling microscopy to characterise the growth mode of CO monolayers on a cold Ag(100) substrate. CO was dosed at substrate temperatures between 150 K and 250 K. The CO was adsorbed on the substrate and formed two new phases in the sub-monolayer regime which coexist in the studied temperature range. One is a slightly disordered hexagonal phase without translational symmetry. The average intermolecular distance is 440 ± 20 pm. The other one has a rectangular lattice unit cell with the dimensions $a = 1.62 \pm 0.12$ pm and $b = 0.83 \pm 0.06$ pm. For a substrate temperature above 250 K, CO desorption was observed.

O 11.8 Mon 16:45 WIL A317

A LEEM study of structure, morphology and composition of ultrathin Ag/films on Pt(111) — ●ESTHER VAN VROONHOVEN and BENE POELSEMA — Solid State Physics; MESA+ Institute for Nanotechnology; University of Twente; P.O.Box 217; AE 7500 Enschede; The Netherlands

The growth of ultra-thin silver films on Pt(111) at 750 K has been studied in real time and - space using Low Energy Electron Microscopy, LEEM. Our results demonstrate that the system is considerably more complex than appreciated so far. The LEEM/LEED results reveal a highly mobile film-substrate system. In the sub-monolayer regime they exhibit an intriguing sequence of surface confined alloying up till $\theta(\text{Ag}) = 0.5$ ML and de-alloying (both consistent with existing literature), phase separation, partial strain relieve at $\theta(\text{Ag}) \sim 0.8$ ML, reentrant alloying and accompanying build-up of strain as indicated by return of the monolayer film to the pseudomorphic state. During growth of the second layer more Pt is dissolved into the Ag-bilayer until the strain is finally relieved by the formation of wide trenches along <11-2> azimuth directions, in line with <1-10> being the soft direction under compressive strain. The full de-alloying and approach towards the bulk immiscibility of silver and platinum is reached only in third monolayer, accompanied by remarkable rearrangements at the interface.

O 11.9 Mon 17:00 WIL A317

Growth of different adatom systems on a Moiré superstructure induced by Pt deposition on WSe₂ — ●DENYS MAKAROV, ROGER PALLESCH, GÜNTER SCHATZ, and MANFRED ALBRECHT — University of Konstanz, Department of Physics, D-78457 Konstanz, Germany

The morphology and structure of Pt deposited on a WSe₂(0001) van der Waals surface was investigated by reflection high energy electron diffraction (RHEED) and compared to scanning tunneling microscopy (STM) and spectroscopy (STS). The growth of Pt at 450 °C is characterized by an initial three-dimensional growth of (111)-orientated nanostructures followed by coalescence of the nanostructures. After a Pt thickness of about 3 nm a clear (4 \times 4) superstructure appears, which is a result of strong Se diffusion towards the growth surface, forming most likely a PtSe₂ alloy on the top surface. Due to the lattice mismatch between the Pt(111) layers and the PtSe₂ top layer a Moiré pattern is created. The investigation of the Pt growth on WSe₂ at different deposition temperatures shows that the Moiré structure is established at about 300 °C. With the presence of the Moiré pattern the surface potential becomes a 2D periodical function of the local density of states near the Fermi level. Thus, the extrema of the local density of states can act as "pinning" sites for adatom nucleation. This approach for nanostructuring employing a self-organized Moiré pattern in the WSe₂/Pt system was attempted by the deposition of different adatom systems including metals (Co, Cr) and organic molecules (C₆₀).

O 11.10 Mon 17:15 WIL A317

Metastable and Stable Structures of In on W(110) — ●MARTIN GABL¹, MAREK TRZCIŃSKI², NORBERT MEMMEL¹, ANTONI BUKALUK², and ERMINALD BERTEL¹ — ¹Institute of Physical Chemistry, University of Innsbruck, A-6020 Innsbruck, Austria — ²Institute of Mathematics and Physics, University of Technology and Agriculture, Pl-85796 Bydgoszcz, Poland

The growth of indium on W(110) at submonolayer coverages was studied by low energy electron diffraction (LEED) and scanning tunnelling microscopy (STM). At room temperature with increasing coverage three

indium-induced overlayer structures - (3x1), (1x4) and (1x5) - are observed. The (3x1) structure corresponds to an overlayer with 1 atom/unit cell of the In-overlayer and an ideal coverage of 0.33 ML. The (1x4) structure is essentially interpreted as a Moire-pattern between the W(110) substrate and a slightly distorted In(111) layer in Nishiyama-Wassermann orientation. The atom density in the (1x4) overlayer matches that of a close-packed In(111) layer within 2%. The (1x5) structure is interpreted as a compressed monolayer, where the areal density of In exceeds that of

an In(111) monolayer by 8%. Upon annealing or aging at room temperature the In atoms of the (3x1) structure agglomerate into islands with the high-coverage (1x4) structure. Hence the (3x1) structure - although being ordered - is only metastable. This transition can also be induced by exposure to oxygen. Obviously oxygen first adsorbs onto the free W(110) surface and compresses In atoms into densely-packed islands of (1x4) periodicity rather than oxidizing the indium adlayer.

O 12 Methods

Time: Monday 15:00–17:15

Room: WIL B321

O 12.1 Mon 15:00 WIL B321

Near-field effects in heat transfer under UHV conditions — •ULI F.-WISCHNATH, ACHIM KITTEL, and ANDREAS KNÜBEL — Uni Oldenburg, Fak. V, C. v. Ossietzky Str., 26111 Oldenburg

The heat transfer between a sample and a probe in an STM based SThM (Scanning Thermal Microscope) is dominated by near field radiation when approaching to small separations under UHV conditions. The nature of this evanescent part of the radiation is subject to ongoing discussions, especially the dependencies on temperature difference and distance.

We have measured the heat transfer between a gold-platin thermoelement as probe and different samples. The classical theory of fluctuating charge carriers predicts a strong increase when approaching the sample. This can be observed for separations ranging from roughly 100 nm down to the order of one nanometer. For even smaller separations a nearly constant value is found showing the breakdown of the classical theory.

We were able to trace the increase of the heat transfer above the far field value up to separations of about 100 nm due to a new production process of the thermoelement. The more filigree new probe has its sensitive area about 100 times closer to the very end of the tip and has a ten times greater thermal resistance. This results in an increase in sensitivity by a factor of 15 compared to the ones used previously.

O 12.2 Mon 15:15 WIL B321

Characterization of a time-of-flight spectrometer using photoemission with higher harmonic radiation — •ANDREA MELZER, ALVARO WULFF, JINXIONG WANG, and THOMAS FAUSTER — Lehrstuhl für Festkörperphysik, Universität Erlangen-Nürnberg, Staudtstr. 7, D-91058 Erlangen

By focussing laser pulses with 1.4 mJ energy, 30 fs pulse length and 779 nm wavelength from a multipass amplifier at a repetition rate of 1 kHz into argon photon energies up to 52 eV are generated. A grating monochromator with two interchangeable toroidal gratings (250 and 950 lines/mm) is used to select individual harmonics. A time-of-flight spectrometer for electrons is designed with a large detection angle of 34°. A fast detection electronics is used with a time-resolution of 200 picoseconds to obtain an energy resolution in the meV range. A Cu(111) surface was used to characterize the time-of-flight spectrometer and the results are compared to data obtained on the same surface with a hemispherical energy analyzer.

O 12.3 Mon 15:30 WIL B321

Improvement of temporal resolution on Ultrafast Electron Diffraction (UED) experiments — •MATTHIAS WIELENS, ANJA HANISCH, BORIS KRENZER, and MICHAEL HORN-VON HOEGEN — Universität Duisburg-Essen, Institut für Experimentelle Physik, Lotharstrasse 1, 47057 Duisburg

For Ultrafast Electron Diffraction experiments studying transient phenomena at surfaces and in bulks upon laser excitation a high temporal resolution is essential. In our surface sensitive Reflection High Energy Electron Diffraction setup the resolution is limited by the so called "velocity mismatch" between the velocity of light and the much lower velocity of high energy electrons. Due to their grazing incidence the electron pulse needs a few 10 ps to travel across the sample. The excitation by the fs laser pulses at normal incidence with the pulse front parallel to the surface, however, occurs instantaneously. Thus, temporal overlap is not given. In consequence, this leads to an averaging of the observation of transient phenomena during the time the electron pulse probes the sample.

A solution to this problem is to tilt the pulse front of the laser pulses with respect to the propagation direction at such an angle that ensures

temporal overlap between the pulse fronts of the two beams. For 10 keV electrons with a grazing angle of incidence of 5° this requires a tilt angle of almost 80°!

We present an experimental setup that facilitates such a large tilt angles and will demonstrate the improvement in temporal resolution of our ultrafast electron diffraction setup.

O 12.4 Mon 15:45 WIL B321

How the solid state matrix affects the chemical shift of core-level binding energies: A novel method to take the induction effect into account — •KUNYUAN GAO, THOMAS SEYLLER, and LOTHAR LEY — Institut für Physik der Kondensierten Materie, Lehrstuhl für Technische Physik, Universität Erlangen-Nürnberg, Erwin-Rommel-Str. 1, D-91058 Erlangen, Germany

Small binding energy variations of core levels, i.e., chemical shifts provide useful information about the chemical environment of the atom under investigation. With the widespread use of synchrotron radiation as excitation source for photoelectron spectroscopy a vastly improved spectral resolution compared to conventional laboratory sources allows the unambiguous identification of components with chemical shifts less than a tenth of an eV. As a consequence, the interpretation of the chemical shift in complex systems such as mixed oxides requires to take charge transfer beyond the first coordination shell into account. A novel scheme is presented that allows to include these so-called induction effects in estimates of chemical shifts based on the electronegativities of the constituent elements. The method is a judicious extension of Sanderson's original approach [1] towards network structures. At each point of departure from Sanderson, the method is tested successfully against the rigorous Sanderson formalism. For three crucial examples of relevance in semiconductor technology, our new method yields predictions in excellent agreement with experiment. [1] R.T. Sanderson, Chemical Bonds and Bond Energy, Academic Press, London, 1971, p.17.

O 12.5 Mon 16:00 WIL B321

Van der Waals Interaction: A Universal Semiempirical Supplement to DFT Tested for Various Systems — •FRANK ORTMANN¹, WOLF G. SCHMIDT², and FRIEDHELM BECHSTEDT¹ — ¹Institut für Festkörpertheorie und -optik, Friedrich-Schiller-Universität, Max-Wien-Platz 1, 07743 Jena, Germany — ²Universität Paderborn, Fakultät für Naturwissenschaften, Theoretische Physik, Warburger Str. 100, 33100 Paderborn, Germany

Theoretical investigations of surface adsorbed molecules are generally carried out using Density Functional Theory within the Local Density Approximation (LDA) or the Generalized Gradient Approximation (GGA). One driving force for the adsorption process of molecules are van der Waals interactions (see [1] and [2]). Unfortunately LDA and GGA are incapable of accounting for long-range correlations for inhomogeneous systems by construction.

We supplement the DFT with a semiempirical long-range correlation term based on the London formula [3] for van der Waals interaction to cure this lack. Here we examine the transferability of the present approach to different structures and to investigate the universality with respect to the atom species under consideration.

[1] F. Ortmann and W. G. Schmidt and F. Bechstedt, Phys. Rev. Lett. **95**, 186101 (2005)

[2] M. Preuss and W. G. Schmidt and F. Bechstedt, Phys. Rev. Lett. **94**, 236102 (2005)

[3] F. London, Z. Phys. Chem. **Abt. B11**, 222 (1930)

O 12.6 Mon 16:15 WIL B321

Efficiency of numerical atom-centered basis functions in all-electron electronic-structure theory: the absolute-convergence limit — •VOLKER BLUM, JÖRG BEHLER, RALF GEHRKE, KARSTEN REUTER, and MATTHIAS SCHEFFLER — Fritz-Haber-Institut, Faradayweg 4-6, D-14195 Berlin, Germany

The most fundamental choice in practical electronic structure calculations is the underlying basis set. For structures with large empty regions (surfaces, clusters, molecules), numeric atom-centered orbitals (NAO's) are attractive [1,2]. However, the question of basis set convergence is often skirted by relying on fixed basis set libraries and error cancellation; a straightforward route to establish the basis set limit does not exist.

We here investigate the routine feasibility of meV-level *absolute* convergence in all-electron total-energy calculations with NAO basis sets (confined atomic, ionic, or hydrogen-like), using as examples small molecules and clusters (N₂, Cu₂, Cu₄, Cu₁₀). (i) We show how to establish a systematic (over-)converged NAO basis set limit. (ii) To construct minimal-sized converged basis sets, we pick individual functions one by one from large candidate function pools, using non-selfconsistent superposition potentials for maximum efficiency. ~50 basis functions per atom are needed for meV-level convergence in each case. (iii) We find that converged basis sets are transferable to self-consistent potentials, and from one structure to another. The total energy errors from underconverged basis sets depend systematically on the interatomic distance.

[1] B. Delley, J. Chem. Phys. **92**, 508 (1990).

[2] J.M. Soler *et al.*, J. Phys.: Condens. Matter **14**, 2745 (2002)

O 12.7 Mon 16:30 WIL B321

The influence of sample properties and finite resolution on the results of surface-XPCS measurements — •ROBERT FENDT¹, CHRISTIAN GUTT², AYMERIC ROBERT³, ANDERS MADSEN³, and METIN TOLAN¹ — ¹Exp. Physik 1a, Univ. Dortmund — ²HASYLAB, Hamburg — ³ESRF, Grenoble, France

Surface-sensitive XPCS is a powerful technique for in-situ measurements on a fluctuating surface. However, recent experimental results clearly show that assuming the Fraunhofer limit (which holds in the case of PCS) is an over-simplification in the case of XPCS, yielding the need for a new theoretical treatment [1, 2]. In the case of low-viscosity liquids, which is considered here, one expects an oscillating behaviour (due to capillary waves) of the correlation function, i. e. for a homodyne setup, $G_{\text{hom}}(\vec{q}, \tau) = 1 + C \cos^2(\omega(\vec{q})\tau) \exp(-2\Gamma(\vec{q})\tau)$ with the contrast $0 < C \leq 1$. However, under special circumstances, a "heterodyne" function $G_{\text{het}}(\vec{q}, \tau) = 1 + C \cos(\omega(\vec{q})\tau) \exp(-\Gamma(\vec{q})\tau)$ is observed [3, 4]. This behaviour can be understood as a resolution effect, i. e., a finite experimental resolution $dq > 0$ enables the specular reflection from the surface to function as a static reference signal [2]. Surprisingly, recent experiments [3] suggest a possible dependence of dq on the sample material. This would essentially mean that the usual separation of specular and off-specular scattering might not be valid in the case of SXPCS.

[1] M. Sprung *et al.*: ESRF 2004, unpub.

[2] T. Gadheri: PHD thesis, to be publ.

[3] R. Fendt *et al.*: ESRF 2005, unpub.

[4] C. Gutt *et al.*: PRL 91, 076104 (2003)

O 12.8 Mon 16:45 WIL B321

An Energy Dispersive beamline for NEXAFS and other CFS/CIS studies — •D. R. BATCHELOR¹, TH. SCHMIDT¹, R. FOLLATH², CH. JUNG², R. FINK³, M. KNUPFER⁴, A. SCHÖLL¹, and E. UMBACH¹ — ¹Exp.Physik II, Univ. Würzburg — ²BESSY GmbH — ³Phys. Chem. II, Univ. Erlangen — ⁴IFW Dresden

Energy dispersive NEXAFS is a quite well known technique in the Hard X-Ray region. It is however not so well known in the Soft X-Ray region [1]. By combining the energy dispersion of a monochromator and the imaging properties of a hemispherical electron analyser the simultaneous detection of electron distribution curves as a function of photon energy is possible. The dispersion of the monochromator is projected on to the sample and subsequently imaged in the non dispersive plane of the analyser. Such an instrument is able to fully exploit the small spot size of state-of-art synchrotron monochromators and modern electron energy analysers with 2D imaging detectors. The parallel detection enables a large parameter space to be efficiently sampled such that, e.g., high energy resolution can be combined with short time scales in the ms range. We present the design for an upgrade of an existing beamline and a pilot experiment utilising the low angular divergence of a PGM which is operated at low C_{ff} values. The advantages and need for such an experimental setup will be illustrated using traditional CFS/CIS data of organic thin films.

Funded by BMBF under contract no. 05KS4WWC/2

[1] K. Amemiya, H. Kondoh, T. Yokoyama, T. Ohta, Journal of Electron Spectroscopy and Related Phenomena **124** (2002) 151 – 164

O 12.9 Mon 17:00 WIL B321

New potentialities at the ESRF surface diffraction beamline ID03 — •N.M. JEUTTER, I. POPA, D. WERMELLE, H. ISERN-HERREA, E. PAISER, L. PETIT, T. DUFRANE, and R. FELICI — ESRF, 6 Rue Jules Horowitz, 38000 Grenoble, France

The ESRF surface diffraction beamline ID03 has been devoted to structural and dynamical studies of surfaces and interfaces since 1993. Structural and dynamical studies like epitaxial growth, surface kinetics and phase transitions resulted in many publications. The hutch 1 diffractometer can host small UHV, catalysis and electrochemistry cells. In the hutch 2 the diffractometer coupled with a large UHV chamber, allows the studying of the structures and the kinetics of adsorbates or homostructures. A refurbishment program is currently underway. An upgrade of the monochromator takes place in order use the full brightness of the undulator source, and to allow for an easier control on the selected used beam energy. The optics of the beamline will be improved in order to achieve a focussing at the sample of the order of few squared microns. The modernisation of the experimental hutch 2 will allow users to install their own UHV systems and will simplify the changing of the samples on the provided chamber. Aim of this contribution is to show to the surface science community the status of the ID03 refurbishment plan and the new opportunities provided by the upgraded instrumentation.

O 13 Solid-liquid interfaces

Time: Monday 15:00–17:45

Room: WIL C207

O 13.1 Mon 15:00 WIL C207

The corrosion behaviour of surface- and heat-treated magnesium alloy WE43 in Simulated Body Fluid — •PETRA GUNDE, PETER J. UGGOWITZER, and JÖRG F. LÖFFLER — Laboratory of Metal Physics and Technology, ETH Zurich, Switzerland

Due to similar mechanical properties between magnesium and the human bone and due to the biocompatibility and non-toxicity of magnesium, it might be considered as an absorbable implant. In the present work, the corrosion behaviour of the magnesium alloy WE43 in simulated body fluid (SBF) was investigated. The corrosion rate of the samples was worked out using two methods; the conventional weight-loss method and the hydrogen evolution method where magnesium-loss is calculated based on the amount of evolved hydrogen. Different surface and heat treatments were applied to WE43 samples and their influence on the corrosion behaviour was characterised by immersion in SBF, X-ray diffraction and impedance spectroscopy. All methods indicate that the corrosion resistance is significantly increased by these surface treatments.

The outstanding corrosion resistance of such treated WE43 samples is assumed to result in a relatively thick and less crack-afflicted protective oxide layer. In conclusion, surface treatments as performed in this work, significantly influence the degradation behaviour of WE43 specimens.

O 13.2 Mon 15:15 WIL C207

Excess non-specific Coulomb ion adsorption at the metal electrode/electrolyte solution interface — •ALEXANDER M. GABOVICH, YURI I. REZNIKOV, and ALEXANDER I. VOITENKO — Institute of Physics, prospekt Nauki 46, 03028, Kiev, Ukraine

Excess ion adsorption G induced by the polarization image forces in the system of a metal electrode/symmetric electrolyte solution separated by an insulating interlayer have been calculated. The adopted theoretical scheme involves the Coulomb Green's function in a three-layer system with sharp interfaces and specular reflection at them. The influence of the spatial dispersion of the dielectric permittivities $E(k)$ in all the three media on the image force energy $W(x)$ and the adsorption G has been an-

alyzed (k is a transferred wave-vector). A comparison with the classical model, where $E = \text{const}$, has been carried out. It has been shown that both the Debye-Hückel ion screening and the spatial dispersion of the solvent contribution to the overall dielectric function of the electrolyte solution lead to the qualitative difference with the results for the classical model. In particular, in a wide range of ion concentrations n a thin interlayer $L = 10$ Angstroms effectively screens out the attractive influence of the metallic electrode, so that the net Coulomb adsorption becomes repulsive. The approach and the results obtained qualitatively describe two physically different situations. Specifically, the introduced interlayer corresponds either to the dense near-electrode (inner) electrolyte layer or to the intentionally deposited control coating of arbitrary thickness.

O 13.3 Mon 15:30 WIL C207

Modeling electrocatalysis – electro-oxidation of Pt(111) — •TIMO JACOB and MATTHIAS SCHEFFLER — Fritz-Haber Institut der MPG, Faradayweg 4-6, 14195 Berlin, Germany

Electrochemical reactions (such as in fuel cells) usually occur under conditions of finite temperature, pressure, and electrode potential, implying a very involved situation, possibly leading to novel surface materials. Especially the presence of an electrode potential, which results in the formation of an electric double-layer, affects the composition and structure of the electrode/electrolyte-interface.

Towards a more realistic treatment of electrocatalysis we developed an appropriate theory in which the electrode of the interface is assumed to be in contact with a *bulk-electrode* reservoir (at chemical potential μ_{el}) while the electrolyte is in contact with a *bulk-electrolyte* reservoir. Although we are in the process of simulating the entire electric-double layer self-consistently, the present approach already allows us to estimate the limits of the expected effects.

As a first application we studied the electro-oxidation of Pt(111) by calculating the $p/T/\phi$ -phase diagram. The obtained behavior, that positive electrode potentials stabilize higher oxygen coverages, is in qualitative agreement with cyclic-voltammetry experiments.

O 13.4 Mon 15:45 WIL C207

ATR-IR spectroscopic measurements of cooperative effects during CO electro-oxidation on Pt film electrodes — •JOHANNES BOLTEN¹, ANTOINE BONNEFONT², SAURADIP MALKHANDI¹, and KATHARINA KRISCHER¹ — ¹Physik Department E19, Technische Universität München, James Franck Str. 1, 85748 Garching — ²Université Louis Pasteur, 4 rue Blaise Pascal, 67070 Strasbourg Cedex, France

Attenuated total reflection infrared (ATR-IR) spectroscopy allows the in-situ observation of surface coverages under reaction conditions. When combined with a flow cell, adsorbate coverages under stationary conditions can be monitored. Employing ATR-IR spectroscopy in a flow-cell, we present studies on nonlinear phenomena during CO electro-oxidation on Pt film electrodes. In particular, we investigate the dynamics in the bistable and oscillatory regime of this reaction. The studies allow us to draw conclusions on the physico-chemical mechanism of the oscillations. Moreover, simultaneous measurements of CO and anion coverages make it possible to analyze the adsorption dynamics in the presence of both species, allowing to detect cooperative effects.

O 13.5 Mon 16:00 WIL C207

Ensemble size effects in the electrochemical properties of PtRu/Ru(0001) and PdRu/Ru(0001) surface alloys — •H.E. HOSTER, A. BERGBREITER, E. FILONENKO, and R.J. BEHM — Abt. Oberflächenchemie und Katalyse, Universität Ulm, 89069 Ulm

Atomically smooth PtRu and PdRu surface alloys can be prepared in UHV by vapor deposition of Pt or Pd on Ru(0001), respectively, followed by heating to 1000-1350 K. This leads to an incorporation of Pt (Pd) mainly into the outermost layer, which then contains fractions of Pt (Pd) immediately determined by the amount deposited initially. The lateral atomic distribution in the 2D alloys, however, is significantly different in PdRu compared to PtRu. As in bulk alloys, Pt and Ru are well miscible also in two dimensions, coming along with a nearly random atomic distribution. Pd and Ru, on the other hand, are bulk immiscible and also show a clear tendency towards phase separation on a low nm-scale in the studied surface alloys. Atomic distribution and surface density of distinct adsorption ensembles are derived from STM images and quantitatively related to certain features in electrochemical adsorption and reaction data, which provides insights into the ensemble size requirements of typical adsorbates and reactants.

O 13.6 Mon 16:15 WIL C207

Potential dependence of the step line tension on vicinal gold surfaces — •GUILLERMO BELTRAMO, MARGRET GIESEN, and HARALD IBACH — Institut für Schichten und Grenzflächen, ISG4, Forschungszentrum Jülich, Jülich 52425, Germany

The step line tension β per atom plays a crucial role in the electrochemical deposition and dissolution of metals, and in particular, in the creation of nanostructures and their dynamical properties. Recently (1,2) we demonstrated how step energies can be measured in electrolyte by island studies. Now, we introduce a new method to analyze steps energies on metal electrodes.

We present Electrochemical Impedance Spectroscopy studies (EIS) of stepped Au(100) electrodes in electrolyte. Following the model proposed by Schmickler and Ibach (3) one can determine the step line tension, and from the shift of the potential of zero charge (pzc) the dipole moment of the step. Here we will present results obtained in weakly adsorbing electrolytes (sulfuric and perchloric acid). The results will be discussed.

(1) Farad. Disc. 121 (2002) 27.

(2) J. Electroanal. Chem. 524-525 (2002) 194.

(3) Physical Rev. Lett. 91 (2003) 016106.

O 13.7 Mon 16:30 WIL C207

Electrochemistry of Two Dimensional Copper Sulphide Films on Au(111) Studied by in situ STM and Cyclic Voltammetry — •DANIEL FRIEBEL, CHRISTIAN SCHLAUP, and KLAUS WANDEL — Institut für Physikalische und Theoretische Chemie, Wegelerstr. 12, D-53115 Bonn, Germany

For the electrochemical preparation of ultrathin copper sulphide films on Au(111), Cu underpotential deposition from 1 mM CuSO₄ + 0.1 M H₂SO₄ is followed by two consecutive electrolyte exchanges for (i) *acid blank* solution (0.1 M H₂SO₄) and (ii) *reactive* solution (0.5 mM Na₂S + 0.1 M NaOH). We can stabilize the first up layer ($\theta_{Cu} = 2/3$) with its well-known ($\sqrt{3} \times \sqrt{3}$)R30° structure in the acid blank solution for over 2 hours. In the reactive solution, we observe islands of two ordered Cu_xS phases: a rectangular and, at higher potentials, an incommensurate hexagonal phase. Cu-free, S-covered Au(111) regions are identified by their characteristic ($\sqrt{3} \times \sqrt{3}$)R30° structure. At strongly anodic potentials, Cu_xS is irreversibly dissolved. The latter process cannot be directly observed with STM because HS⁻(aq) is oxidized to S₈(ads) multilayers. Therefore, we have extended our investigations by a third electrolyte exchange, subsequent to Cu_xS formation, for *alkaline blank* solution (0.1 M NaOH), to get further insights into the Cu_xS electrooxidation. Obviously, anodic Cu dissolution in alkaline solutions is enhanced by complexation of Cu(II) with bi- or polysulphides.

O 13.8 Mon 16:45 WIL C207

Exploring the diamond/aqueous electrolyte interface — •JOSE ANTONIO GARRIDO, STEFAN NOWY, ANDREAS HÄRTL, JORGE HERNANDO, and MARTIN STUTZMANN — Walter Schottky Institut, Technische Universität München, Am Coulombwall 3, 85748 Garching

The diamond surface is a unique platform for the investigation of the charged solid/liquid interfaces. Both carbon-hydrogen (C-H) and carbon-oxygen (C-O) surface groups are stable in aqueous solutions, and show a completely different behavior in terms of wetting by water and the resulting charge state. Furthermore, under certain conditions a highly conductive p-type channel is induced at the surface of H-terminated undoped diamond films, which can be used for charge sensing applications. In this contribution, we report on the electrochemical characterization of modified C-H and C-O diamond surfaces in contact with aqueous electrolytes. For this purpose, we have investigated surface conductive single crystalline films as well as boron-doped metal-like polycrystalline and nitrogen-containing ultrananocrystalline diamond films. Using impedance spectroscopy we study the influence of different surface terminations on the interfacial capacitance. Surface charging processes have been investigated as a function of electrolyte pH. The effect of screening and/or specific adsorption of electrolyte ions will be discussed. This work has direct implications for an understanding of the pH and ion sensitivity of diamond surfaces, as well as the physisorption of charged biomolecules on these surfaces.

O 13.9 Mon 17:00 WIL C207

In-plane structure of liquid 8CB layers confined between mica sheets — ●HARALD REICHERT¹, THOMAS BECKER², HELMUT RATHGEN³, and FRIEDER MUGELE³ — ¹MPI for Metal Research, 70569 Stuttgart — ²Universität Ulm, 89081 Ulm — ³University of Twente, 7500 AE Enschede, NL

The ongoing miniaturization of both microelectromechanical and microfluidic devices creates an increasing interest in transport properties of liquids near solid-liquid interfaces and in confinement. For simple liquids confined between atomically smooth solid substrates, it has been shown that the molecules arrange into layers parallel to the surfaces. The question whether the structure of thin confined liquid layers changes from a liquid-like structure (for thicker layers) to a more solid-like structure (monolayer regime) is highly controversial. Direct measurements of the in-plane structure of thin confined liquid layers have not been performed up to now.

We have developed a new x-ray diffraction setup which allows us to study the in-plane structure of liquid layers as a function of temperature. We present the first results of time and temperature dependent measurements of the in-plane structure of liquid crystal 8CB confined between two mica sheets.

O 13.10 Mon 17:15 WIL C207

Probing interfaces of particle suspensions using vibrational sum frequency scattering — ●SYLVIE ROKE — Max-Planck Institute for Metals Research, Heisenbergstr. 3, Stuttgart, Germany

Many important chemical, physical and biological phenomena occur at interfaces of particles in suspension. Most of the tools presently available to study these interfaces use invasive techniques or model systems. Ideally, one would want a non-invasive technique that allows to study interface structure and dynamics with molecular specificity.

We have for the first time used the nonlinear optical technique vibrational sum frequency generation to study the interfaces of sub-micron particles in suspension. As a model system we use a suspension of silica particles covered with alkane (C18) chains [1]. We obtain information about the molecular structure (molecular order and orientation) as well

as particle morphology, by analyzing both the spectra as well as the angle dependent scattered intensity. Finally, we show that the interfacial order and structure is strongly influenced by the solvent [3].

[1] S. Roke, W. G. Roeterdink, J. E. G. J. Wijnhoven, A. V. Petukhov, A. W. Kleyn and M. Bonn, Phys. Rev. Lett., 91, 258302 (2003)

[2] S. Roke, M. Bonn, A. V. Petukhov, Phys. Rev. B, 70, 115106 (2004)

[3] S. Roke, J. Buitenhuis, J. C. van Miltenburg, M. Bonn and A van Blaaderen, J. Phys. Condens. Matter, 17, S3469 (2005)

O 13.11 Mon 17:30 WIL C207

Benzene diffusion measurements using neutron and helium spin-echo — ●PETER FOUQUET¹, HOLLY HEDGELAND², ANDREW P. JARDINE², GIL ALEXANDROWICZ², WILLIAM ALLISON², and JOHN ELLIS² — ¹Institut Laue-Langevin, BP 156, F-38042 Grenoble Cedex, France — ²Cavendish Laboratory, Madingley Road, Cambridge CB3 0HE, UK

The accurate description of surface-molecule interaction potentials is crucial for a correct description of molecule dynamics in systems with a large fraction of molecules close to a surface, such as zeolithes, mesoporous confinements and real catalysts. Here we present a new approach using two techniques that will allow to extract the surface contribution to the dynamics of molecules in confinements by measuring bulk diffusion (neutron spin-echo, NSE) and surface diffusion (helium spin-echo, HeSE) on the same system on identical length scales. NSE is an established technique for the analysis of dynamics in the ps to 100 ns time window at molecular length scales in bulk samples. Recently, surface sensitivity could be introduced by translating the NSE principle to helium atom scattering [1].

In a prototype experiment we could show the complementarity of NSE and HeSE by studying benzene diffusion on graphite(0001) surfaces. We characterized the specific response by the two techniques in respect of signal, diffusion mechanism and possible excitation of phonons. The measured diffusion mechanisms and constants agree well between the two techniques and also with recent MD calculations.

[1] A.P. Jardine et al., Science 304 (2004) 1790.

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"/{a}tsverlag 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, ERMINALD 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 reconstruction 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) D_{5h} and D_{5d} 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, Kyiv-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 TaS_2 — ●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 TaS_2 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 Jülich GmbH, 52425 Jülich — 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 meV/Å at RT

and 0.02 meV/Å 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 SiO_2 .

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 $T_c=78$ K 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. Teegenkamp 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)-(2×1), 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)-(2×1) 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 3×3 surface prepared by Si deposition and subsequent annealing and a ($\sqrt{3} \times \sqrt{3}$) R30° 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 3×3 surface three new stable reconstructions 2 $\sqrt{3}$ ×2 $\sqrt{3}$ R30°, 3×3 and 5×5 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° surface the evolution of the core level spectra after Au deposition and annealing was found to be distinctly different compared to the Si-rich 3×3 surface. Only one stable reconstruction, a 3×3 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(4×2) but not on SiC(001)-(3×2)? 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(4×2) surface while it hardly interacts with SiC(001)-(3×2) 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(4×2) 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 3×2 surface, on the contrary, H₂ 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)-(3×2) — ●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)-(3×2) 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)-(3×2) 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. Sorptionisothermes of C₃H₇OH 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 HENTSCH¹, 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° 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 C₂H₂. 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 Epitaxial Rutile TiO₂(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. TiO₂ 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(2x2) 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 $1.15 \times 10^{18} / \text{m}^2$ (= 0.56 CO molecules per TiO₂(011)-(2x1) 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 $C_{60}/Au(111)$ 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 $C_{60}/Au(111)$ 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.

Quadrupol 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 ÜMBACH¹ — 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-tetracarboxylicacid 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/Holzminde/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-perylenetetra-carboxylic acid-dianhydride (PTCDA) induces a surface rearrangement by step bunching and subsequent faceting. 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-diine) like C[3T-DA]_n, Cyclo(quinquethiophen-diine), 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 BARRENA^{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 mercaptoalkanols 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. HINRICHS¹, 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 \cdots 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. MCCHESENEY², 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 YbIr₂Si₂ — ●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 YbIr₂Si₂. Our experiments reveal YbIr₂Si₂ 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 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 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 HfS₂ — ●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 C₁₃H₁₀N₂O₂, 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 HfS₂ 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 HfS₂. Furthermore, the observed core level shifts give information about a possible photoisomerisation of the phenylazobenzoic acid on HfS₂. 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.

This work is supported by *Innovationsfond des Landes Schleswig-Holstein*.

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 $\Gamma X' M \bar{\Gamma}$ - 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, LILLENKAMP 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 HUGEN-SCHMIDT^{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 10⁷-10⁸ 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 sub-monolayer 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 GENSCHE¹, 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.

O 15 Invited talk GÜDDE

Time: Tuesday 09:30–10:15

Room: TRE Phys

Invited Talk

O 15.1 Tue 09:30 TRE Phys

Control of coherent electron motion and adsorbate diffusion at surfaces by femtosecond laser excitation — ●JENS GÜDDE — Fachbereich Physik und Zentrum für Materialwissenschaften, Philipps-Universität, D-35032 Marburg

Diffusion of adsorbates is usually a thermally activated process. The corresponding rate can be influenced only by varying the substrate temperature, which may also induce unwanted competitive surface reactions. In particular for metal surfaces, however, the diffusive motion of adsorbates is strongly coupled to electron-hole pair excitations within the substrate, which makes it possible to induce diffusion also by optical excitation of metal electrons. I will show for atomic oxygen on vicinal Pt(111) that femtosecond-pulse laser excitation is capable of inducing

lateral motion of oxygen atoms even at low substrate temperatures. By applying a sequence of two laser pulses, the diffusion rate can be controlled by varying their time-delay. In this way it is possible to study the coupling between electronic excitation and diffusive motion in the time domain.

While the diffusive adsorbate motion is excited by an incoherent distribution of electrons, the primary laser excitation is coherent and allows a more sophisticated control of motion at surfaces. In the second part of my talk I will show for a copper surface how a multiphoton excitation scheme can be used to induce coherent electron motion at surfaces, i.e. a coherent DC current, the direction of which can be controlled by the relative phase of the excitation pulses. The current is detected with high sensitivity by time-resolved photoemission.

O 16 Invited talk Michaelides

Time: Tuesday 10:15–11:00

Room: TRE Phys

Invited Talk

O 16.1 Tue 10:15 TRE Phys

Ab initio Ice Growth at Metal Surfaces — ●ANGELOS MICHAELIDES — Fritz-Haber-Institut der Max-Planck-Gesellschaft, Faradayweg 4-6, D-14195 Berlin, Germany

Few physical processes are as ubiquitous or feature more prominently in our daily lives than the nucleation of water into ice. Typically this process is aided by a so-called ice nucleating agent; a microscopic substrate that in essence catalyses the nucleation process. Remarkably little is known, however, about these seemingly simple "catalytic" processes, particularly at the all-important atomic and molecular level.

Here we present the results of density-functional theory simulations for ice nucleation on model (metal) substrates, which aim to put our understanding of catalysed ice nucleation on a much firmer footing. A particular focus will be placed on how the competing influences of substrate reactivity and water cluster-substrate epitaxial mismatch conspire to yield a rich variety of (novel) ice-like structures. Moreover, the key molecular clusters that are accessed en route to ice crystal growth will be presented and how these differ from gas phase water clusters discussed.

This work has been performed in collaboration with Matthias Scheffler

O 17 Adsorption II

Time: Tuesday 11:15–13:00

Room: TRE Phys

O 17.1 Tue 11:15 TRE Phys

FORMATION OF ULTRATHIN CdS-FILMS ON Cu(111) - AN IN-SITU STM and EX-SITU SXPS STUDY — ●SASCHA HÜMANN¹, PETER BROEKMANN¹, RALF HUNGER², THOMAS MAYER², WOLFRAM JAEGERMANN², and KLAUS WANDEL¹ — ¹Institut für Physikalische und Theoretische Chemie der Universität Bonn, Wegelerstr. 12, 53115 Bonn — ²Institut für Materialwissenschaft, Technische Universität Darmstadt, Petersenstr. 23, 64287 Darmstadt

Electrochemical Atomic Layer Epitaxy is a useful method to grow thin layers of semiconductor compounds at solid/liquid interfaces. In this contribution we present combined ECSTM and synchrotron x-ray photoelectron spectroscopy (SXPS) data dealing with the epitaxial growth of ultrathin CdS-films on a Cu(111) electrode surface. We observed that the atomic structure and the morphology of the resulting CdS film strongly depend on the first layer adsorbed on the copper substrate. The first preparation route of the CdS-films started with a $(\sqrt{7} \times \sqrt{7})R19.1^\circ$ sulfide adlayer on the Cu(111) surface. This root 7 phase could be maintained upon emersion and successfully transferred into the UHV. We observed corresponding LEED images and SXPS data supporting the results of the ECSTM studies. Cd deposition on the root 7 sulfide phase at a potential of -375 mV vs. RHE results in the formation of a CdS-phase revealing a complex dislocation network. After transfer to UHV the composition and chemical nature of the film constituents was analysed. A different CdS phase was obtained when sulfide anions were adsorbed on the Cd precovered copper surface. The corresponding LEED pattern shows a $(\sqrt{3} \times \sqrt{3})R30$ unit cell.

O 17.2 Tue 11:30 TRE Phys

Correlation of Structure and Femtosecond Electron Dynamics during Crystallization of Amorphous D₂O/Cu(111) — ●JULIA STÄHLER¹, MICHAEL MEHLHORN², UWE BOVENSIEPEN¹, KARINA MORGENSTERN², and MARTIN WOLF¹ — ¹Freie Universität Berlin, Fachbereich Physik, Arnimalle 14, 14195 Berlin, Germany — ²Universität Hannover, Institut für Festkörperphysik, Appelstraße 2, 30167 Hannover, Germany

The structure, i.e. molecular arrangement, of an adsorbate layer strongly influences the electron transfer dynamics across the interface since it determines bond strengths and periodicity of the lattice and therefore localized and delocalized states in the adlayer. Using two techniques, low-temperature scanning tunneling microscopy (STM) and time-resolved two-photon photoelectron (2PPE) spectroscopy, we investigate the correlation of the structure and electron dynamics in ultrathin D₂O layers on Cu(111). We find that crystallization of initially porous amorphous ice clusters, which are adsorbed at $T < 90$ K, occurs via three metastable phases. The latter are prepared by annealing to 118 K, 131 K, and 145 K. The stable, crystallized phase is reached by heating to 149 K. These different stages of crystallization are characterized by clear changes in the time-dependent photoelectron spectra. We observe that localization probability and lifetime of the solvated electrons, which are highly sensitive to changes in their local molecular surrounding, strongly depend on the ice structure. Additionally the dependence of image potential states on the ordering in the D₂O layer will be discussed.

O 17.3 Tue 11:45 TRE Phys

Energy resolved quadrupole alignment of H₂ desorbing from Cu(100) — ●CARSTEN THEWES, MARCO RUTKOWSKI, and HELMUT ZACHARIAS — Physikalisches Institut, Westfälische Wilhelms-Universität, 48149 Münster

Measurements of the energy dependent quadrupole alignment for associative desorption of H₂ from Cu(100) were performed. The analysis includes different rotational states in the vibrational ground state $v''=0$ and the first vibrationally excited state $v''=1$. State selective detection of the desorbing molecules is realised by the (VUV+UV)-REMPI techniques. For the excitation step in the $B^1\Sigma_g^+ \leftarrow X^1\Sigma_u^+$ Lyman bands of H₂ photon energies around 110 nm are used. In $v=0$ the angular momenta $J=1,2,3,4,5$ and 8 while in $v''=1$ measurements for $J''=2,3,4$ could be detected. The acquired energy dependent alignment factor $A_0^{(2)}$ shows a preferentially positive value between 0,2 and 0,4, thus helicopter motion of the desorbing molecules is observed. $A_0^{(2)}$ increases at low kinetic energies close to the respective translational barrier of the two states, i.e. around 300 meV and 200 meV for $v''=0$ and 1, respectively. For

higher energies (1100 meV for $v=0$, 800 meV for $v=1$) a decrease of the quadrupole alignment is observed, as expected. Based on theoretical calculations of the quadrupole alignment [1] possible reaction mechanisms will be discussed.

[1] M.F. Somers, D.A. McCormack, G.J. Kroes, R.A. Olsen, E.J. Baerends and R.C. Mowrey; *J. Chem. Phys.*, 117, 6673 (2002)

O 17.4 Tue 12:00 TRE Phys

Adsorption and C 1s NEXAFS Spectra of Three Phenylpropenes on Cu(111) — ●C. KOLCZEWSKI¹, F. J. WILLIAMS², R. L. CROPLEY², R. M. LAMBERT², and KLAUS HERMANN¹ — ¹Fritz-Haber-Institut der MPG, Faradayweg 4-6, 14195 Berlin, Germany — ²Department of Chemistry, University of Cambridge, Cambridge CB2 1 EW, UK

In this study we present equilibrium geometries of trans-methylstyrene, α -methylstyrene and allylbenzene adsorbed on Cu(111) obtained from density functional theory (DFT) calculations using $\text{Cu}_{73}\text{-C}_9\text{H}_{10}$ clusters. All molecules are found to adsorb with their phenyl ring lying flat on the surface. However, the position of the side chain varies: allylbenzene adsorbs with its propenyl chain pointing away from the surface whereas for trans-methylstyrene and α -methylstyrene the side chains are closer to the surface but differ in their relative arrangement of C=C bonds and allylic hydrogens. These results can explain the different epoxidation rates measured for the three molecules by simple geometric arguments. The calculated geometries are also used to evaluate theoretical angle resolved C 1s NEXAFS spectra which can be compared with experimental spectra and yield excellent agreement. This confirms the adsorption geometries obtained in the present study and underlines the geometric interpretation of the epoxidation behavior of the phenylpropenes.

O 17.5 Tue 12:15 TRE Phys

LT-STM study of electronic and vibronic properties of single C_{60} on Cu(111) and Ag(100). — ●ANNA STRÓZECKA, JOSEF MYSLIVEČEK, and BERT VOIGTLÄNDER — Institut für Schichten und Grenzflächen (ISG3), Forschungszentrum Jülich, D-52425 Jülich

A low temperature scanning tunneling microscope (LT-STM), due to its high stability, allows addressing single molecules on the surfaces. Density of States (DOS) spectrum of C_{60} on Cu(111), measured by STS (Scanning Tunneling Spectroscopy) technique, shows features corresponding to molecular orbitals of a free molecule. The shifting and splitting of the peaks indicate charge transfer from the substrate to the fullerene cage. Peaks in the IETS vibrational spectrum (Inelastic Electron Tunneling Spectroscopy) can be assigned to the vibrational modes of C_{60} . Two different intramolecular modes are observed: $H_g(\omega_2)$ and $H_g(\omega_5)$.

The lateral manipulation was used to precisely control the position of C_{60} on Ag(100). The plot of the tip height during the manipulation shows that the buckyballs are pulled along the surface.

O 17.6 Tue 12:30 TRE Phys

Vibrations of ethylene on smooth and roughened single crystal copper surfaces — ●MARTIN BINDER, OLAF SKIBBE, and AN-NEMARIE PUCCI — Kirchhoff-Institut für Physik, Universität Heidelberg, INF 227, 69120 Heidelberg

The adsorption of ethylene on cold evaporated and annealed copper surfaces and on copper single crystal surfaces has been investigated with Raman spectroscopy and infrared reflection absorption spectroscopy in the past [1]. In order to clarify some remaining questions concerning the assignment of the spectral features to the adsorption sites, we performed high resolution electron energy loss spectroscopy (HREELS) on smooth and slightly roughened single crystal surfaces. Roughening was achieved by utilising ion bombardment without adjacent annealing and evaporating small amounts of copper at low temperatures, respectively.

[1] C. Siemes, A. Bruckbauer, A. Goussev, A. Otto, M. Sinther, and A. Pucci. *J. Raman Spectrosc.* 32 (2001), 231-239 and references therein

O 17.7 Tue 12:45 TRE Phys

Velocity distributions of NO desorbed from $\text{C}_{60}/\text{Cu}(111)$ by UV laser excitation — ●DANIEL GRIMMER, TIM HÖGER, and HELMUT ZACHARIAS — Westfälische-Wilhelms Universität, Physikalisches Institut, Wilhelm-Klemm-Str. 10, 48149 Münster

NO laser desorption experiments have been performed using C_{60} grown on a poly-Cu crystal. A bimodal distribution of the kinetic energy results in a fast and a slow channel. The fast channel peaks at a velocity of $v=1000$ m/s for low rotational states and increases to 1300 m/s for high rotational states. The slow channel's velocity can be fitted by a Maxwellian flux distribution of $T_{kin}=110$ K showing deviations at slow velocities (*Surf. Sci.*, submitted).

For C_{60} epitaxially grown on Cu(111) similar results with respect to the kinetic energies and rotational population are obtained. A slightly higher vibrational population is detected.

In these experiments the velocity was inferred from the arrival time in a pump-probe arrangement. The transformation of the delay into a velocity distribution then yields very slow molecules, too slow to be explained by thermal desorption since the kinetic temperature is clearly much below the surface temperature. Diffusion processes or long-lived excited states could cause such a delayed desorption.

Here we present new velocity distributions of NO desorbed from $\text{C}_{60}/\text{Cu}(111)$ directly measured by a field-free flight time tube.

This work has been supported by the Deutsche Forschungsgemeinschaft via the Schwerpunktprogramm SPP1093 under project number Za110/21.

O 18 Nanostructures II

Time: Tuesday 11:15–13:00

Room: PHY C213

O 18.1 Tue 11:15 PHY C213

Surface Plasmon Polariton Excitation on Tuneable Nanostructured Surfaces — ●DOMINIC ZERULLA¹, STEPHANIE REHWALD^{1,2}, BRIAN ASHALL¹, GILLIAN DOYLE¹, MICHELLE GALVIN¹, MICHAEL BERNDT^{1,2}, and KLAUS SCHIERBAUM² — ¹UCD Dublin, School of Physics, Dublin 4, Ireland — ²Heinrich-Heine-University Düsseldorf, Materialwissenschaft, 40225 Düsseldorf, Germany

Surface Plasmon Polaritons (SPPs) allow for extremely surface sensitive spectroscopic methods like Surface Plasmon Resonance (SPR) or Surface Enhanced Raman Scattering (SERS) which, play a fast-growing role in the Life Sciences.

The conditions for their excitation by photons are quite restrictive. On smooth metal surfaces a Kretschmann or Otto-type attenuated total reflection (ATR) setup is needed to generate an SPP. Using periodically nano- or mesostructured surfaces liberates from the ATR-restrictions, but a rigid nanostructure only allows for the excitation of SPPs for a single, fixed wavelength at a given angle of incidence. In order to gain more flexibility, e.g. in the light of tuneable laser sources, we are the first to design tuneable nanostructured surface on which a plasmon excitation is possible over a broad wavelength region. The nanostructures consist of a polymer base upon which the periodic structure is generated. Subsequently, the system is coated with a suitable metal (e.g. silver, gold,

or aluminium) but is still tuneable with respect to changes in the excitation wavelength. The effect is proved by showing the full, experimentally derived dispersion relation of the SPP in comparison to theoretical predictions.

O 18.2 Tue 11:30 PHY C213

Electron confinement in nm-size vacancy islands — ●GUILLEMIN RODARAY¹, HAIFENG DING^{1,2}, DIRK SANDER¹, and JÜRGEN KIRSCHNER¹ — ¹Max-Planck-Institut für Mikrostrukturphysik, Weinberg 2, D-06120 Halle — ²Department of Physics, Nanjing University, Nanjing, China

We have studied the electron confinement in hexagonal vacancy islands on Cu(111) by low temperature scanning tunneling microscopy (STM). Hexagonal vacancy islands on Cu(111) are formed upon deposition of sub-monolayer amounts of Co at 320 K [1]. The vacancy islands are one atomic layer deep (0.2 nm), and are surrounded by straight step edges, which form hexagons with sizes in the nm range. Surface state electrons of Cu(111) are scattered at the vacancy hole edge. This gives rise to characteristic electron standing wave patterns inside the vacancy hole and on the terraces surrounding the hole. These electron standing waves are imaged and analyzed by scanning tunneling spectroscopy (STS) at 7 K. The dispersion relation of the confined electrons is derived for differ-

ent vacancy hole diameters ranging from 5–15 nm and compared to those measured at straight terrace step edges. The origin of the standing wave pattern in the hole is discussed in view of the quantum corral model [2].
 [1] J. de la Figuera, J. E. Prieto, C. Ocal, R. Miranda, Phys. Rev. B **47**(1993)13043; M. Klaua, H. Höche, H. Jenniches, J. Barthel, J. Kirschner, Surf. Sci. **381**(1993)106.
 [2] H. C. Manoharan, C. P. Lutz, D. M. Eigler, Nature **403** (2000) 512; V.S. Stepanyuk, L. Niebergall, W. Hergert, P. Bruno, Phys. Rev. Lett. **94**(2005)187201.

O 18.3 Tue 11:45 PHY C213

Controllable molecular Ag contacts on Si(100) and Si(111) via electromigration — ●GERNOT GARDINOWSKI, JEDRZEJ SCHMEIDEL, CHRISTOPH TEGENKAMP, and HERBERT PFNÜR — Institut für Festkörperphysik, Universität Hannover, Appelstrasse 2, 30167 Hannover, Germany

In order to characterize single molecules and nanostructures electrically, contacts with a well-defined geometry and size are essential. We present a electromigration method, that leads to thin vertical and small lateral contacts of high yield, which are particularly interesting for STM/AFM investigations. In a first step, we are using electron beam lithography on a two-resist combination (PMMA/LOR3B) on Si(100) and Si(111). We demonstrate, that it is possible to create nanobridges due to underetching. The latter can be used for a three dimensional stairs-like growth by evaporating of Ag at different angles. Film-thicknesses down to ≈ 4 nm and lateral dimensions below 100 nm has been realised so far. This is important for heat dissipation during the planar breakjunction process and also for thin contacts for further investigations via STM/AFM. Contactpads have been tested by SEM/AFM/AES. In a second step, we are using a computer-based controlled electromigration method at ≈ 80 K. First measurements indicates gaps around 1 nm, which has been characterized electrically.

O 18.4 Tue 12:00 PHY C213

In-situ Monitoring of Particle Plasmon Excitation in Ag-nanostructures — ●LIVIU I. CHELARU, DAGMAR THIEN, MICHAEL HORN-VON HOEGEN, and FRANK MEYER ZU HERINGDORF — Institut für Experimentelle Physik, Universität Duisburg-Essen, Duisburg, Germany

Although the Mie-Plasmon in Ag islands and particles is well known, it is still a challenge to analyze the plasmonic behaviour of single Ag particles and nanowires on surfaces. Photoemission Microscopy offers a way to directly observe particle plasmons by means of two photon photoemission. Here, the plasmon as an intermediate state completely dominates the photoemission signal; a first photon is used to excite a particle plasmon before a second photon triggers the plasmon-assisted photoemission. We will show, that the particle plasmon evolves during growth of Ag islands and wires on 4 degree vicinal Si(001) and demonstrate that depending on the size of the particle only distinct plasmon modes can be excited. The strong nonlinear nature of the two-photon photoemission process allows to image the fringe field pattern around the particle on the surface and to directly correlate the particle plasmon excitation with the lateral dimensions of the particle.

O 18.5 Tue 12:15 PHY C213

Surface plasmon on sputtered Ag(110) measured by reflectance difference spectroscopy — ●L.D. SUN, J.M. FLORES-CAMACHO, M. HOHAGE, and P. ZEPPENFELD — Institut of Experimental Physics, Johannes Kepler University Linz, Altenberger str. 69, A4040 Linz, Austria

The surface plasmon resonance on sputtered Ag(110) has been investigated by Reflectance Difference Spectroscopy (RDS). The Ag(110) clean surface was exposed to Ar ion bombardment and its effects on the optical anisotropic response were monitored by means of RDS. The spectra exhibit a pronounced peak around the established surface plasmon resonance at about 3.66 eV. We believe that this feature is induced by the well known rippled pattern formed by the Ar ion sputtering on the clean Ag(110)[1], whose periodicity along the [001] direction allows for the coupling of the dispersion relations of surface plasmon and light in an excitation grating mode. The effects of annealing at room temperature and sputtering with other ions (Ne, He) will be discussed as well.

[1] S. Rusponi, C. Boragno and U. Valbusa, Phys. Rev. Lett. **78**, 2795 (1997).

O 18.6 Tue 12:30 PHY C213

Excitation of surface plasmon polaritons at surface grooves in bulk metals and thin film metal waveguides — ●J. RENGER¹, S. GRAFSTRÖM¹, J. SEIDEL¹, P. OLK¹, L.-M. ENG¹, C. AKHMADALIEV², L. BISCHOFF², B. SCHMIDT², D. TAVERNA³, and J.-C. WEEBER³ — ¹Institute for Applied Photophysics, University of Technology Dresden, D-01062 Dresden, Germany — ²Forschungszentrum Rossendorf, Institute of Ion Beam Physics and Materials Research, D-01314 Dresden, Germany — ³Laboratoire de Physique de l'Université de Bourgogne, UMR CNRS 5027, F-21078 Dijon, France

We explore different approaches to excite surface plasmon polaritons (SPPs), aiming at strong enhancement and localization of the electromagnetic field. The SPP is excited by focussing laser light onto a small single groove or a grating having a finite number of periods. Such grooves cancel the requirement of momentum conservation, and makes the excitation of surface waves possible. The metallic structures were fabricated by high resolution focused ion beam milling (25 keV Ga⁺, IMSA-Orsay Physics FIB) into photolithographic pre-patterned 60 nm thick aluminium thin-film metallic waveguides. Our multiple multipole calculations show a characteristic dependence on both the width and the depth of the grooves, as well as a strong impact of the angle of incident laser light. Hence, this allows the selective excitation of SPP modes propagating at the air/metal or metal/glass interface. Experimental observation of SPPs was performed using scanning near-field optical microscopy with uncoated etched fiber probes. These results confirm the excitation of SPP modes at grooves.

O 18.7 Tue 12:45 PHY C213

Nanostructuring of NiMnSb(110): influences on surface magnetic properties — ●CHRISTIAN EICKHOFF^{1,2}, HRISTO KOLEV¹, GEORGI RANGELOV¹, LIFENG CHI¹, and MARKUS DONATH¹ — ¹Physikalisches Institut, Westfälische Wilhelms-Universität Münster, Wilhelm-Klemm-Str. 10, 48149 Münster, Germany — ²now at: Max-Born-Institut, Max-Born-Str. 2a, 12489 Berlin, Germany

The magnetic and electronic properties, crystal structure and surface morphology at the (110) surface of the ferromagnetic half-Heusler alloy NiMnSb have been investigated by means of magneto-optical Kerr effect, appearance potential spectroscopy, low-energy electron diffraction and atomic-force microscopy.

A standard sputter-anneal preparation procedure leads to a stoichiometric surface which is predicted to show a high spin polarisation at the Fermi level. We observed, in contrast, a reduced surface magnetic signal. Atomic-force microscopy reveals a nanostructuring of the NiMnSb surface which proceeds with the number of preparations. The changed morphology of the NiMnSb surface is made responsible for the observed reduced surface magnetization [1].

[1] H. Kolev, G. Rangelov, J. Braun, and M. Donath: *Reduced surface magnetization of NiMnSb(001)*, Phys. Rev. B **72**, 104415 (2005)

O 19 Electronic structure II

Time: Tuesday 11:15–13:00

Room: WIL A317

O 19.1 Tue 11:15 WIL A317

Surface state lifetimes from scanning tunnelling spectroscopy: A theoretical analysis — ●MICHAEL BECKER¹, SIMON CRAMPIN², and RICHARD BERNDT¹ — ¹Institut für Experimentelle und Angewandte Physik, Christian-Albrechts-Universität zu Kiel, 24098 Kiel, Germany — ²Department of Physics, University of Bath, Bath BA2 7AY, United Kingdom

Recently the discrepancy between image state lifetimes measured by means of the scanning tunneling microscope (STM) and two-photon-photoemission spectroscopy was lifted [1]. The electric field applied in STM was shown to cause an increase in both the efficiency of the image state decay channels as well as their number. In the light of this work, we theoretically investigate the impact of the STM induced electric field on the inelastic electron-electron damping rate of the electron- and hole-like

excitations in the Shockley surface state band at Ag(111). Our calculations within the GW approximation of many-body theory are based upon the approach developed by Chulkov and coworkers [2]. The results indicate that under typical tunnelling conditions the STM does not significantly alter the surface state wavefunction and so previous STM derived Shockley state lifetimes need not be corrected.

[1] S. Crampin, Phys. Rev. Lett. **95**, 046801 (2005)

[2] E. V. Chulkov, I. Sarria, V. M. Silkin, J. M. Pitarke, and P. M. Echenique, Phys. Rev. Lett. **80**, 4947 (1998)

O 19.2 Tue 11:30 WIL A317

Image-Potential States of Reconstructed Au(100) — ●M. ALEXANDER SCHNEIDER, GERO WITTICH, LUCIA VITALI, and KLAUS KERN — Max-Planck-Institute for Solid State Research, 70569 Stuttgart, Germany

Electrons in image-potential states form an exemplary two-dimensional electron gas at the surface of many metals. As the major weight of the electron wavefunctions is found in the vacuum region they are attractive for studying the mechanisms limiting electron lifetimes which are larger than that of other electronic states in metal systems.

However, despite the low overlap with the surface region of a crystal, defects at surfaces modify the electronic states considerably. This is demonstrated in a low-temperature Scanning Tunneling Spectroscopy (STS) study of the image-potential states of reconstructed Au(100) (5x27). The interaction with the reconstruction introduces band-gaps in the dispersion of the image-potential states and causes a spatial anisotropy of the image potential states. STS allows to study the behavior of the electrons at defects like dislocations or step edges. We will discuss to what extent the (scattering) surface potential can be reconstructed from STS measurements.

O 19.3 Tue 11:45 WIL A317

Structure of the Adatom Electron Band of the Si(111)-7x7 Surface — ●JOSEF MYSLIVEČEK¹, ANNA STRÓZECKA¹, JAN ŠTEFFL², PAVEL SOBOTÍK², IVAN OŠTÁDAL², and BERT VOIGTLÄNDER¹ — ¹Institut für Schichten und Grenzflächen (ISG 3) and cni – Center of Nanoelectronic Systems for Information Technology, Forschungszentrum Jülich, 52425 Jülich, Germany — ²Charles University, Faculty of Mathematics and Physics, Department of Electronics and Vacuum Physics, V Holešovičkách 2, 180 00 Praha 8, Czech Republic

Using a low temperature scanning tunnelling spectroscopy we map the wave functions of the electrons in the adatom band of the Si(111)-7x7 surface in real space. We observe the splitting of the adatom electron states to “ring” (corner adatom) and “dimer” (center adatom) structures in agreement with recent theory and determine the relative energies of these structures. A high resolution of our measurement is a tradeoff for the loss of absolute energy scale due to transport limitations in tunnelling spectroscopy of semiconductors at low temperatures.

O 19.4 Tue 12:00 WIL A317

Unoccupied surface state on Pt(111) revealed by scanning tunneling spectroscopy — ●JENS WIEBE¹, FOCKO MEIER¹, KATSUSHI HASHIMOTO¹, GUSTAV BIHLMAYER², STEFAN BLÜGEL², PAOLO FERRIANI¹, STEFAN HEINZE¹, and ROLAND WIESENDANGER¹ — ¹Institute of Applied Physics, Hamburg University, D-20355 Hamburg, Germany — ²Institut für Festkörperforschung, Forschungszentrum Jülich, D-52425 Jülich, Germany

Surface states are known to play a crucial role in chemistry, magnetism and for the growth properties of surfaces of noble metals and late fcc transition-metals (Ni, Pd, Pt). For noble-metal (111) surfaces it is well known that a partly occupied surface state resides far inside the projected bulk *sp*-band gap. The situation is more complex for the transition-metals. Ni(111) has a partly occupied surface state, while the corresponding surface state on Pd(111) is unoccupied and far above the Fermi energy E_F . For Pt(111) the situation was controversial so far.

We measured the dispersion of an unoccupied surface state on Pt(111) by imaging scattering states at point defects and step edges using scanning tunneling spectroscopy. By comparison to first-principles electronic structure calculations the state is assigned to an *sp*-derived surface band at the lower edge of the projected bulk band-gap. In $dI/dV(V)$ -curves, the onset of the surface-state band appears as a rather broad feature. Its shape results from two spin-orbit split branches with nearly linear

dispersion, one of them merging into bulk states at higher energies. We found no indications for a surface state below E_F . [1]

[1] J. Wiebe, *et al.*, Phys. Rev. B **72**, 193406 (2005)

O 19.5 Tue 12:15 WIL A317

STS study of Fe monomers and multimers on InAs(110) surfaces — ●TOMOHIRO MATSUI, CHRISTIAN MEYER, LILLI SACHAROW, and ROLAND WIESENDANGER — Institute of Applied Physics, University of Hamburg

The local density of states on and around single Fe atoms (monomers) and Fe multimers (dimers, trimers and tetramers both perpendicular and parallel to the As rows of the substrate) on n-InAs(110) surfaces were studied by scanning tunneling spectroscopy at $T \sim 6$ K.

Different states are observed for a monomer as peaks in the tunneling spectrum: The most prominent peak is spatially localized mainly on the Fe atom, while the other states are spread to the As or In atoms next to the Fe. Their shapes are strongly anisotropic reflecting the asymmetry of the substrate lattice. The peak structure changes by manipulating the atom laterally suggesting different bonding configurations of the Fe to the substrate.

On multimers, the main peak related to the Fe is found at lower energies. The peak shifts in energy from one side to the other side of the multimer. However, this behavior is observed only for the perpendicular case presumably because of the asymmetry of the substrate lattice. For the parallel tetramers, on the other hand, three symmetric states are observed. The first is extended over the whole tetramer, while the others are localized on the end or the middle atoms of the tetramer.

O 19.6 Tue 12:30 WIL A317

Image states on ferromagnetic surfaces explored by tunneling spectroscopy — ●ANDRE KUBETZKA, MATTHIAS BODE, and ROLAND WIESENDANGER — Institute of Applied Physics, University of Hamburg, Jungiusstr. 11, 20355 Hamburg, Germany

Above metal surfaces a series of hydrogenlike states can exist in the potential well created by the attractive image potential and the surface projected bulk band gap, which hinders a decay into the crystal, with energies between the Fermi and the vacuum level. These so-called image or image-potential states have been investigated in the past by inverse photoemission (IPE) and tunneling spectroscopy [1].

In ferromagnets the band gap is spin dependent which results in a small spin-splitting of these states. The first experimental investigation with spin-resolved IPE determined a value of 18 meV for Ni(111) [2]. We will present first results for image states on Fe(110), employing low temperature spin-polarized scanning tunneling spectroscopy.

[1] G. Binnig *et al.*, Phys. Rev. Lett. **55**, 991 (1985)

[2] F. Passek and M. Donath, Phys. Rev. Lett. **69**, 1101 (1992)

O 19.7 Tue 12:45 WIL A317

Organic small bandgap semiconductors: Electronic properties of quaterrylene derivatives on Au(111) — ●ROBERT FRANKE, CHRISTIAN WAGNER, SEBASTIAN FRANKE, and TORSTEN FRITZ — Institut für Angewandte Photophysik, George-Bähr-Straße 1, 01069 Dresden

The understanding of the electronic properties of organic thin films is of large interest for their application in novel devices. As the electronic properties of perylene derivatives [1] and other medium-sized planar aromatic molecules [2] have already been studied intensively, we have now investigated larger organic molecules, namely quaterrylene (QT) and quaterrylenebisdicarboximide (QTCDI) on Au(111) in UHV. This class of materials is especially interesting due to their long-wavelength absorption in the NIR.

Ultrathin films of QTCDI and QT were investigated by Tunnelling Spectroscopy. In case of QTCDI we found a HOMO-LUMO gap of about 2.2 eV. This result is in good agreement with our optical measurements of QTCDI on mica where the optical gap is found to be 1.8 eV, indicating an exciton binding energy of about 0.4 eV. For thin QT films we obtained an electronic bandgap of 2.5 eV, which fits nicely to the fact that the smaller QT-molecule is expected to have a larger gap than the larger QTCDI molecule.

[1] M. Toerker, T. Fritz, H. Proehl, R. Gutierrez, F. Großmann, and R. Schmidt PRB **65** (2002) 245422 [2] H. Proehl, M. Toerker, F. Sellam, T. Fritz, and K.Leo PRB **63** (2001) 205409

O 20 Epitaxy and growth II

Time: Tuesday 11:15–13:00

Room: WIL B321

O 20.1 Tue 11:15 WIL B321

In-situ diffraction studies of homoepitaxial electrochemical growth on Au(100) — ●KLAUS KRUG, JOCHIM STETTNER, and OLAF M. MAGNUSSEN — Institut für Experimentelle und Angewandte Physik, Christian-Albrechts-Universität, 24098 Kiel

The surface structure and growth behaviour of Au(100) electrodes during electrodeposition in HAuCl_4 -containing HCl solution has been studied in-situ by high-energy surface x-ray diffraction in transmission geometry. Using a "hanging meniscus" cell structural data can be obtained parallel to electrochemical measurements. To distinguish the effects of the interface structure on the deposition process from effects caused by different deposition rates, measurements were performed under diffusion limited deposition conditions. By time-dependent measurements of the x-ray intensity at selected positions along specular and non-specular crystal truncation rods a complex potential-dependent growth behavior was found: With decreasing potential transitions from step-flow deposition to layer-by-layer growth, manifested by layering oscillations in the x-ray intensity, then to 3D growth, and finally back to layer-by-layer growth were observed. The latter occurred parallel to the formation of the "hex" reconstruction on the Au(100) surface. This growth behavior can be explained by the effect of Cl adsorbates and the Au surface structure on the mobility of Au adatoms.

O 20.2 Tue 11:30 WIL B321

surface Debye Temperatur of thin Bi(111) on Si(001) — ●RABIH KHANAFER, ANDREAS JANZEN, BORIS KRENZER, GIRIRAJ JNAWALI, HICHEM HATTAB, and MICHAEL HORN-VON HÖGEN — Universität-Duisburg-Essen, Institut für experimentelle Physik, 47057 Duisburg

Experiments with time resolved electron diffraction at surfaces require materials with a low surface Debye temperature to ensure high sensitivity for transient surface temperature changes upon excitation by ultrashort laser pulses. In order to study the heat dissipation in thin films from monolayer thickness up to bulk properties additionally require high quality heteroepitaxial growth. Bismuth films on Si(001) act as ideal model system for such investigations.

Bismuth with a bulk Debye temperature of 119 K shows a surface Debye temperature of only 48 K [1]. Deposition of Bismuth at room temperature on Si(001) results in the formation of continuous, smooth and well oriented Bi(111) films even for a thickness as low as 3 nm. The surface Debye temperature has been determined by LEED, SPA-LEED and RHEED as function of film thickness and electron energy. Between 80 and 100 eV a decrease of the surface Debye temperature from 46 K to 33 K is observed followed by an increase to 48 K at 190 eV. This behaviour agrees well with the maximum of surface sensitivity around 100 eV.

The use of these films in a ultrafast electron diffraction experiment will be presented.

[1] R. M. Goofman, G. A. Somorjai, J. Chem. Phys. **52**, 6325 (1970)

O 20.3 Tue 11:45 WIL B321

Epitaxial growth of Bi(111) on Si(001) studied by SPA-LEED: Morphology and Lattice Accommodation — ●GIRIRAJ JNAWALI, HICHEM HATTAB, BORIS KRENZER, and MICHAEL HORN VON HOEGEN — Universität Duisburg-Essen, Fachbereich Physik, Lotharstr. 1, 47057 Duisburg

Deposition of Bismuth at 150 K results in the formation of epitaxial films. The LEED pattern shows diffuse spots reflecting a hexagonal orientation in two Bi(111) domains rotated by 90°. With increasing coverage only a ring of intensity remains, reflecting rotational disorder. The ring disappears after annealing to 200 K. Annealing to 350 K reduces surface roughness and very flat surfaces are obtained with sharp LEED spots. Further annealing to 470 K leads to dewetting of the film which can be observed from LEED pattern. The surface morphology is studied by Spot Profile Analysing Low Energy Electron Diffraction during deposition and annealing. The lattice constant $a_{0,\text{Bi}(111)} = 4,54 \text{ \AA}$ of Bi(111) matches perfectly by a factor of 11:13 with the lattice constant $a_{0,\text{Si}(001)} = 3,84 \text{ \AA}$ of the Si(001) surface in one direction. In the perpendicular direction the row distance $a_{0,\text{Bi}(111)} \sin 60^\circ = 3,94 \text{ \AA}$ of the Bi(111) film almost matches the Si(001) lattice constant. For the films thicker than 2 nm the remaining lattice mismatch of 2.5 % is relieved by a disordered array of interfacial dislocations which is observed by spot

splitting in the LEED pattern. From the distance between the satellite spots we conclude an almost strain relieved growth of the Bi(111)-film on the Si(001) surface.

O 20.4 Tue 12:00 WIL B321

Epitaxial growth of thin Fe-films on GaAs(110) at 80K — ●L. WINKING, M. WENDEROTH, J. HOMOTH, and R. G. ULBRICH — Universität Göttingen, IV. Physikalisches Institut

The best conditions for the epitaxial growth of Fe on GaAs(001) or GaAs(110) were reported to be at substrate temperatures of about 175°C [1]. Nevertheless the highest spin injection efficiencies were reported for films grown at 10-15°C, due to the reduced intermixing at the Fe/GaAs heterointerface [2]. At lower substrate temperatures Fe films showed an increasing number of defects towards a nanoclustered film.

We present a combined LEED and STM study of thin Fe films that were deposited at 80K on in-situ cleaved GaAs(110). The film thickness ranges from a sub-monolayer coverage up to several monolayers. After annealing to RT Fe films of more than 3 ML thickness show the well known LEED pattern of Fe(110) and demonstrate the good epitaxial quality of the film. STM topographies of these annealed films show clear evidence for a 2D layer-by-layer growth, in contrast to the well known 3D cluster growth of thin Fe films deposited at RT or above. Our study demonstrates that low temperature deposition of Fe on GaAs leads to thin epitaxial films of good quality. Due to the low substrate temperature the described preparation scheme may be a key technique to suppress intermixing at the Fe/GaAs heterointerface.

This work was supported by the SFB 602 TP A7.

[1] P. M. Thibado et al., PRB 53, R10481 (1996)

[2] A. T. Hanbicki et al., APL 80, 1240 (2002)

O 20.5 Tue 12:15 WIL B321

Influence of strain on the dynamics of III – V semiconductor surfaces — ●HANNES GUHL and FRANK GROSSE — Halbleitertheorie, Institut für Physik an der Humboldt-Universität Newtonstr. 15, 12489 Berlin

Thermodynamic equilibrium and growth kinetics of the InAs(001) surface under static homogeneous or inhomogeneous strain is investigated by kinetic Monte Carlo simulations. Its input, a strain dependent cluster expansion for the In and As interaction energies, is solely determined by ab initio density functional theory calculations. The surface interactions can be simplified under anneal conditions and mapped onto a multi-state Potts model with generalized interactions. The As-interaction along the As-dimer rows changes from attractive (compressive strain) to repulsive (tensile strain). Furthermore, the overall increased binding of As-dimers on compressed surfaces leads to slower As-dynamics and an increased density. The main step in the island nucleation is the formation of In pairs on the As-dimers rows [1]. Their increased binding energy under tensile strain leads to an increased island density in the initial stages of growth.

[1] F. Grosse, W. Barvosa-Carter, J. Zinck, M. Wheeler, M.F. Gyure, Phys. Rev. Lett. 89, 116102 (2002).

O 20.6 Tue 12:30 WIL B321

Kinetic roughening during polymer film growth: Monte-Carlo simulations and experiments — ●CHRISTIAN VREE¹, JOHANNA RÖDER², HANS-ULRICH KREBS², and S. G. MAYR¹ — ¹I. Physikalisches Institut, Universität Göttingen — ²Institut für Materialphysik, Universität Göttingen, Friedrich-Hund-Platz 1, 37077 Göttingen, Germany

Surface evolution during polymer thin film deposition is investigated with the help of Monte-Carlo simulations and compared with experiments. Vapor deposition of chainlike model polymers onto a substrate is simulated where the polymer chains are implemented as linear chains of inseparably bonded particles which subsequently relax via a reptation type of dynamics after deposition. We investigate the impact of processing parameters on kinetic roughening, and find a crossover from single particle behavior to continuous growth behavior in early growth stages which has been observed in former experiments as well. The continuous growth behavior is characterized by a growth exponent $\beta = 0.20 \pm 0.02$ and a roughness exponent $\alpha = 0.38 \pm 0.02$ for most preparation conditions. In the high thickness regime a strong roughening and concurrent structural change of morphologies is observed. On the experimental side

polycarbonate films are prepared with pulsed laser deposition and characterized with scanning force microscopy. We find a growth exponent $\beta = 0.23 \pm 0.04$ and a roughness exponent $\alpha = 0.68 \pm 0.04$. We acknowledge the SFB 602, TP B3 for financial support.

O 20.7 Tue 12:45 WIL B321

Optical in situ monitoring of deoxidation of III-V-semiconductors in MOVPE — ●A. OESTEREICH¹, C. KASPARI¹, M. PRISTOVSEK¹, and W. RICHTER² — ¹Technische Universität Berlin, Institut für Festkörperphysik, Hardenbergstr. 36, 10623 Berlin — ²Università degli Studi di Roma "Tor Vergata", Via della Ricerca Scientifica 1, 00133 Roma, Italy

O 21 Phase transitions

Time: Tuesday 11:15–13:00

Room: WIL C207

O 21.1 Tue 11:15 WIL C207

Inplane order observed at the liquid surface of eutectic AuSi above bulk melting temperature — ●REINHARD STREITEL¹, VENKAT BALAGURUSAMY¹, PETER PERSHAN¹, OLEG SHPYRKO², and ALEXEI GRIGORIEV³ — ¹Harvard University, Cambridge, MA — ²Center for Nanoscale Materials, Argonne National Lab, IL — ³University of Wisconsin-Madison, WI

The liquid surface of eutectic AuSi shows inplane order above bulk melting temperature ($T=361^\circ$ Celsius). Similar behaviour was not observed in any other binary alloy to date. In comparison to other Au based alloys AuSi shows anomalous, enhanced specular X-ray reflectivity ($q_z = 1.0 - 2.5 \text{ \AA}$) indicating a pronounced surface layering. GID measurements at different temperatures show reversible structural changes at the surface about 12° Celsius above bulk melting temperature. For low temperatures (above T_{melt} and below $T_{melt} + 12^\circ$ Celsius) GID measurements indicate a powder like 2D inplane structure of the eutectic surface. At higher temperatures (380° Celsius) GID measurements indicate a structural change. At $T=430^\circ$ Celsius no stable phase is present. The inplane correlation length estimated from the FWHM for the low temperature phase is about $200nm$.

O 21.2 Tue 11:30 WIL C207

Submonolayer coverage of long chain alkanes at SiO₂/air interfaces: Molecular mobility, phase transition, and structure formation — ●RALF KÖHLER and HANS RIEGLER — MPI für Kolloid- und Grenzflächenforschung, Abt. Grenzflächen, 14424 Potsdam, Germany

The ordering behavior of submonolayers of long chain alkanes at SiO₂/air interfaces is a surprisingly complex phenomenon. Below the surface melting point two-dimensional nucleation and structure formation occurs. The observed fractal crystallites (1,2) can be related to a process analogous to diffusion-limited aggregation (3). One can distinguish three growth scenarios depending on the initial thickness of the liquid alkane film, i.e., due to different supply conditions to the growth front. The system also shows a reversible (equilibrium)-coexistence of solid domains and remaining fluid film in between. The melting temperature of the two-dimensional domains depends on the total amount of alkane at the surface and follows the liquid-drop model for melting of low-dimensional systems (4) if one introduces a critical length, i.e., a critical film thickness, into this model. On-line optical microscopy observations are presented and analyzed. 1) A.Holzwarth et al., Europhys.Lett. 52, 653 (2000) 2) H.Schollmeyer et al., Langmuir 19, 5042 (2003) 3) L.Knüfing et al., Langmuir 21, 992 (2005) 4) K.K.Nanda et al., PRA 66, 013208 (2002)

O 21.3 Tue 11:45 WIL C207

Thermal switching due to a surface phase transition. — ●JUSTIN WELLS, JESPER KALLEHAUGE, and PHILIP HOFMANN — Institute for Storage Ring Facilities and iNano center, University of Aarhus, Denmark.

Temperature induced surface phase transitions such as charge density waves (CDWs) have recently been studied extensively because of the interesting basic physics of these quasi two dimensional systems. Although changes in surface electronic structure due to such phase transitions have been well studied, a direct influence on the physical properties appears not to have been measured.

We report on the surface conductivity of Si(111)+Ag($\sqrt{3} \times \sqrt{3}$) as it undergoes a surface phase transition. A temperature dependent switch-

ing of the surface conductivity between $\approx 10^{-6} \Omega^{-1}$ and $10^{-3} \Omega^{-1}$ can be seen. The transition temperature is around 200 K, but small changes in the surface preparation can shift the transition temperature by at least 20 K

Such a strong conductivity change due to a surface phase transition has applications as an ultimately small thermal switch, with a switching temperature that can be controlled by the surface preparation.

The measurements of surface conductivity have been made under UHV conditions in our newly developed micro 4 point probe. As a demonstration of the instrument, Si(111) 7×7 has also been studied, and the surface and bulk conductivities are clearly distinguishable. This is confirmed by observing the effect of changing the bulk properties (by changing the doping) and changing the surface properties (by the adsorption of silver).

O 21.4 Tue 12:00 WIL C207

Unusual reversible disorder-order transition in Br/Pt(110) below 100 K — ●ENRICO DONÀ and ERMINGALD BERTEL — Institut für Physikalische Chemie, Innrain 52a, Innsbruck Austria

The temperature dependence of Bromine overstructures on Pt(110) has been investigated by variable-temperature scanning tunneling microscopy (VT-STM). Surprisingly, for the c(2x2) structure formed at a coverage of 0.5 monolayers (ML) at room temperature it was found that the long-range order disappears upon lowering the temperature. Strongly anisotropic domains elongated along the [1-10] directions are formed, which exhibit local (2x1) or c(2x2) symmetry. In addition, areas with a local (3x1) geometry are also observed. While it is known from DFT calculations that the (2x1) phase is energetically slightly favoured with respect to the c(2x2) phase, the (3x1) phase is believed to be distinctly higher in energy [1]. The present data seem to indicate that the three phases are almost degenerate at $T \sim 50$ K, whereas at room temperature the c(2x2) phase is stabilised. Possible mechanisms for this phenomenon are entropic stabilisation or an incipient Peierls transition into an incommensurate phase.

[1] J. Redinger, R. Zucca, private communication

O 21.5 Tue 12:15 WIL C207

A Low-Energy Electron Diffraction Study of Phase Transitions in Br/Pt(110) — ●SIMON PENNER, THOMAS LÖRNING, and ERMINGALD BERTEL — Institut für Physikalische Chemie, Innrain 52a, A-6020 Innsbruck, Austria

Peak shape analysis of low-energy electron diffraction spots recorded as a function of temperature are used to analyse phase transitions in c(2x2) and (3x1) Bromine overstructures on Pt(110). A well-defined one-dimensional order-disorder transition at 370 K in the c(2x2) structure indicates the existence of long-range interactions within the adsorbate layer consistent with a quasi-1D electronic structure. Lowering the temperature to ~ 100 K leads to an unexpected decrease in the long-range order consistent with observations by variable-temperature STM. It is shown that the decay of the long-range order cannot be attributed to contamination but seems to be related to fluctuations which involve the substrate atoms as well. Similar experiments carried out for various Br coverages 0.5 monolayers (ML) $< \Theta < 0.67$ ML also point to the possibility that the substrate plays an essential role in driving the phase transitions. A possible explanation in terms of a Peierls mechanism is discussed.

O 21.6 Tue 12:30 WIL C207

Dynamics of electrons in a Mott insulator — ●LUCA PERFETTI — Freie Universität Berlin, Arnimallee 14, D-14195 Berlin

We monitor the photoelectrons emitted by a Mott insulator after the absorption of an intense laser pulse. This experiment allows to visualize directly the ultrafast melting of the insulating phase and the coherent excitation of a coupled phonon mode. The Mott phase is fully restored after 1 ps but a coherently excited phonon induces electronic oscillations lasting longer than 20 ps. As a consequence, the effects of electron-electron and electron-phonon interactions can be clearly disentangled.

O 21.7 Tue 12:45 WIL C207

Interface melting of ice at deeply buried ice-silicondioxide interfaces investigated with high energy x-ray reflectivity —

●SEBASTIAN SCHOEDER^{1,2}, SIMON ENGEMANN¹, HARALD REICHERT¹, HELMUT DOSCH¹, JÖRG BILGRAM³, and VEIJO HONKIMÄKI² — ¹Max-Planck-Institut für Metallforschung, Heisenbergstraße 3, D-70569 Stuttgart — ²ESRF, 6 rue Jules Horowitz, F-38000 Grenoble — ³ETH Zürich, Schafmattstr. 16, CH-8093 Zürich

Ice interfaces play a key role in many technological and environmental phenomena. Yet the properties of the ice interface are poorly understood, especially at conditions close to the melting point. It is well established that surface melting occurs at the free ice surface. However only very few and contradictory measurements exist for the melting of ice at buried interfaces. We have investigated the temperature dependence of the structure of ice in contact with silicondioxide by x-ray reflectivity measurements exploiting a high energy x-ray beam from a 3rd generation synchrotron source. The high penetration length of this radiation allows us to investigate interface phenomena through macroscopic amounts of material. We show that interface melting can be observed at the ice - silicondioxide interface for both crystalline and amorphous substrates and give values for the thickness of the quasi-liquid layer.

O 22 Invited talk Heinze (Gaede-Preis)

Time: Tuesday 14:00–14:45

Room: TRE Phys

Prize Talk

O 22.1 Tue 14:00 TRE Phys

Understanding Scanning Tunneling Microscopy Experiments on Transition-Metal Structures — ●STEFAN HEINZE — Institut für Angewandte Physik, Universität Hamburg, Jungiusstrasse 11, 20355 Hamburg

Scanning tunneling microscopy (STM) is one of the most important techniques to characterize nanostructures on surfaces with a resolution down to the atomic scale. However, the interpretation of such measurements is not trivial, especially on the atomic scale, due to contributions to the tunneling current from various sources such as structural, electronic, chemical, and magnetic properties. Successful interpretation approaches, e.g. the Tersoff-Hamann model, rely on an accurate description of the electronic structure of the sample. Hence, the combination with modern

density functional theory (DFT) calculations has proven a powerful tool for the understanding of STM experiments.

Here, the theory of STM is applied to structures on transition-metal surfaces and a transparent method is introduced to correlate bandstructure features with STM measurements. With this approach surprising effects such as bias-dependent corrugation reversal, imaging of buried nanostructures, and even the detection of small spectroscopic signals due to spin-orbit coupling can be explained based on the electronic structure. Further, the theory of spin-polarized STM (SP-STM) is presented and the potential of SP-STM to unravel complex, e.g. non-collinear, magnetic structures on the atomic scale is demonstrated. A particular striking example is the verification of a two-dimensional antiferromagnetic structure in a monolayer of Fe, the prototypical ferromagnet, on W(001).

O 23 Invited talk Schmidt

Time: Tuesday 14:45–15:30

Room: TRE Phys

Invited Talk

O 23.1 Tue 14:45 TRE Phys

Organic molecule adsorption on solid surfaces: Chemical bonding, mutual polarisation and dispersion interaction* — ●WOLF GERO SCHMIDT — Theoretische Physik, Universität Paderborn, Pohlweg 55, 33098 Paderborn

Many new and exciting electronic devices are based on the organic functionalisation of semiconductor surfaces. Weak interactions of molecules with template substrates, on the other hand, allow for studying molecular self-organisation at the fundamental level.

Here I discuss some of the most relevant bonding scenarios for the adsorption of organic molecules on solid surfaces from the perspective of first-principles calculations. Covalent bonds formed with semiconductor surfaces significantly modify the structural and electronic properties of

both the adsorbed molecules and the substrate [1,2]. In many instances of organic molecule adsorption on metals, mutual polarisation leads to substantial charge transfer and re-hybridisation, despite small adsorption energies [3]. Subtle effects related to the lowering of the kinetic energy of the valence electrons as well as dispersion forces, finally, govern the interaction between the organic molecules and chemically inert substrates such as graphite [4].

*in collaboration with F. Bechstedt, F. Fuchs, K. Seino, M. Preuss (Jena) and A. Hermann (Auckland).

- [1] K Seino, WG Schmidt, F Bechstedt, PRB 69, 245309 (2004).
- [2] A Hermann, WG Schmidt, F Bechstedt, JPCB 109, 7928 (2005).
- [3] M Preuss, WG Schmidt, F Bechstedt, PRL 94, 236102 (2005).
- [4] F Ortman, WG Schmidt, F Bechstedt, PRL 95,186101 (2005).

O 24 Adsorption III

Time: Tuesday 15:45–18:30

Room: TRE Phys

O 24.1 Tue 15:45 TRE Phys

Adsorption of Molecular Oxygen on Metal Surfaces — ●CHRISTIAN MOSCH and AXEL GROSS — University of Ulm, Albert-Einstein-Allee 11, D-89069 Ulm

The dissociation barrier of O₂ on the aluminum (111) surface has been of large interest in the past years since the theoretical description within density functional theory (DFT) using the generalized gradient approximation (GGA) failed to reproduce the barrier that is found in experiments. Recently a dynamical description of this process assuming that the oxygen molecule does not adiabatically switch to a singlet state near the surface but stays in its gas phase triplet state has provided an explanation for this problem [1].

We investigate the problem from another point of view. We systematically study the adsorption process of O₂ on Al (111) in detail using both a planewave based slab approach within the GGA approximation as well as a gaussian based cluster method going beyond the local DFT approximations, thus elucidating the dependence of the theoretical results on the treatment of the electronic correlation. In addition, we will also address the adsorption of O₂ on Pt/Ru overlayer structures.

- [1] J. Behler, B. Delley, S. Lorenz, K. Reuter, and M. Scheffler, Dissociation of O₂ at Al(111): The role of spin selection rules. Phys. Rev. Lett. **94**, 036104 (2005)

O 24.2 Tue 16:00 TRE Phys

The ordering behavior of oxygen at Pd(100) studied with a first-principles lattice-gas Hamiltonian approach — ●YONGSHENG ZHANG, JUTTA ROGAL, and KARSTEN REUTER — Fritz-Haber-Institut, Faradayweg 4-6, D-14195 Berlin, Germany

We study the mesoscopic ordering behavior of oxygen on Pd(100) from first-principles by parametrizing a lattice-gas Hamiltonian (LGH) with density-functional theory data. Using this LGH we carry out mesoscopic Monte Carlo simulations in order to obtain the surface phase diagram for sub-monolayer coverages or as a function of the oxygen pressure. The calculated lateral interactions between oxygen atoms adsorbed in fourfold hollow sites are dominated by a first-nearest neighbor repulsion. Together with a smaller second nearest-neighbor repulsion and a third nearest-neighbor attraction, this stabilizes both experimentally known ordered structures, namely a $p(2 \times 2)$ and a $c(2 \times 2)$ phase. The critical temperatures for the order-disorder transition are found to be in good agreement with experimental values from low-energy electron diffraction measurements [1]. The population of bridge sites at higher coverages is critically discussed.

[1] S.-L. Chang and P.A. Thiel, J. Chem. Phys. **88**, 2071 (1988).

O 24.3 Tue 16:15 TRE Phys

A first-principles statistical mechanics investigation of the stability of a thin surface oxide in reactive environments — ●JUTTA ROGAL, KARSTEN REUTER, and MATTHIAS SCHEFFLER — Fritz-Haber-Institut, Faradayweg 4-6, D-14195 Berlin, Germany

Sufficiently oxygen-rich environmental conditions lead to the formation of oxides at metal surfaces. This could for example happen under the oxygen-rich conditions of high-pressure oxidation catalysis, and oxide films forming in the reactive environment could then actuate the catalytic behavior that is traditionally ascribed to the pristine transition metal substrate. At more noble metals with their rather unstable bulk oxides, the focus is here primarily on the relevance of so-called "surface oxides", i.e. nanometer thin oxide films.

Using the CO oxidation over Pd(100) as example, we investigate the composition and stability of this model catalyst in the reactive environment with a first-principles statistical mechanics approach. In a first step we consider the surface in *constrained* thermodynamic equilibrium with an O₂ and CO gas phase. Under ambient gas phase conditions representative of technological CO oxidation catalysis the known $(\sqrt{5} \times \sqrt{5})R2^\circ$ surface oxide structure on Pd(100) is then indeed the most stable structure. In a second refined step we explicitly consider the effect of the reaction kinetics on the stability of this surface oxide through first-principles kinetic Monte Carlo simulations. Our simulations indicate that the stability of this surface oxide depends intricately on the ratio of reactant partial pressures in the environment.

O 24.4 Tue 16:30 TRE Phys

High-Pressure Oxidation of Pd(111) Single Crystal Surface: In-situ X-ray Diffraction studies — ●NIKOLAI KASPER, A. STIERLE, P. NOLTE, and H. DOSCH — Max - Planck-Institut für Metallforschung, Heisenbergstr. 3, D 70569 Stuttgart, Germany

The interaction of molecular oxygen with a Pd(111) single crystal surface has been studied in a wide temperature and pressure range (30 - 800 °C and 10⁻¹⁰ mbar - 1 bar, respectively). The stability regions of the surface oxide Pd₅O₄ and the bulk PdO have been obtained. Independent on the oxygen partial pressure, only chemisorbed oxygen layers form below 300 °C. The Pd₅O₄ surface oxide exhibits rather narrow stability (p , T) region - it can be formed only at temperatures $300^\circ \leq T \leq 650^\circ \text{C}$. Increasing pressure induces the transformation of the surface oxide into the PdO bulk oxide. The formation of unstable Pd₅O₄ structure has been observed during the decomposition of bulk oxide. The chemisorbed oxygen layers transform directly into the bulk PdO at the temperatures above 650 °C. From comparison of the stability diagram with the results of DFT-calculations one can easily see the effect of kinetic hindrance in formation of both surface and bulk oxides at low temperatures ($300^\circ \leq T < 450^\circ \text{C}$), similar to the case of Pd(100) oxidation [1]. The crystal structure of Pd₅O₄ obtained from crystal truncation rod measurements agrees with the literature data [2].

Financial support of this work is acknowledged from the European Union under contract no. NMP3-CT-2003-505670 (NANO2).

[1] E. Lundgren *et al.*, Phys. Rev. Lett., **88**, 246103 (2002)

[2] E. Lundgren *et al.*, Phys. Rev. Lett., **92**, 046101 (2004)

O 24.5 Tue 16:45 TRE Phys

Origin of anomalous surface lattice expansion in Pd(001) — ●HOLGER L. MEYERHEIM¹, S. H. KIM¹, J. H. SEO², J.-S. KIM³, J. BARTHEL¹, and J. KIRSCHNER¹ — ¹MPI f. Mikrostrukturphysik, 06120 Halle — ²Dept. of Ophthalmic Optics, Chodang Univ. (Korea) — ³Dept. of Physics, Sook-Myung Women's Univ. (Korea)

We present a systematic study of the hydrogen induced anomalous expansion of the top layer spacing, $d_{\{12\}}$, using low-energy electron diffraction and surface x-ray scattering. After exposure of 6 Langmuirs of hydrogen at 150 K sample temperature, the hydrogen atoms occupy the surface hollow sites and a lattice expansion of $\Delta d_{\{12\}} = +4.7\%$ is determined in agreement with theoretical predictions (5.2%). Heating the sample above the hydrogen desorption temperature ($T_{\{D\}} \approx 340^\circ \text{K}$), leads to an almost complete relaxation of $d_{\{12\}}$ to the bulk value of 1.945 Å. Similarly, no expansion is observed for clean Pd(001) prepared by rapid cooling after thermal treatment to remove hydrogen. Hydrogen re-adsorption from the residual gas atmosphere and possibly hydrogen agglomeration in the near surface region leads to an expansion of $d_{\{12\}}$ in the 2-3% range as observed in previous experiments. On the basis of our results, surface magnetism as a mechanism to trigger lattice expansion in Pd(001) needs not to be invoked.

O 24.6 Tue 17:00 TRE Phys

Hydrogen adsorption dynamics on clean and precovered Pd(100) surfaces from first principles — ●AXEL GROSS — Department of Theoretical Chemistry, University of Ulm, 89069 Ulm/Germany

Ab initio molecular dynamics simulations based on density functional theory (DFT) calculations have been performed to study the adsorption of H₂ on clean and hydrogen-covered Pd(100) surfaces. In the simulations, the surface atoms have been treated dynamically thus allowing a realistic description of the energy transfer from the impinging molecules to the substrate. On the clean surface, the sticking probability is hardly influenced by the recoil of the metal substrate atoms because of the large mass mismatch. However, if the H₂ molecules impinge on a hydrogen-covered surfaces with coverages $\Theta_{\text{H}} \leq 0.5$, the recoil of the preadsorbed hydrogen atoms causes a significant enhancement of the sticking probability. This leads to a H₂ sticking probability which is much larger than what one would expect from a simple site-blocking picture. For higher coverages, the repulsive interaction between the hydrogen atoms has to be taken into account which partially counterbalances the promoting effect of the recoil.

O 24.7 Tue 17:15 TRE Phys

SFG and TDS studies of CO adsorption on Pd nanoparticles supported by Nb₂O₅ and Fe₃O₄ thin films — ●FRANK HÖBEL, ATULA BANDARA, GÜNTHER RUPPRECHTER, and HANS-JOACHIM FREUND — Fritz-Haber-Institut der Max-Planck-Gesellschaft, Faradayweg 4-6, 14195 Berlin, Germany

CO adsorption on Nb₂O₅- and Fe₃O₄-supported Pd nanoparticles was studied by sum frequency generation (SFG) vibrational spectroscopy from ultrahigh vacuum (UHV) to 100 mbar, and by thermal desorption spectroscopy (TDS) under UHV. Differences between the Pd-Nb₂O₅/Cu₃Au(100) and Pd-Fe₃O₄/Pt(111) model catalysts will be discussed. Heating the Pd-Nb₂O₅ system to 300 K resulted in an irreversible decrease in CO chemisorption associated with a phase shift in the SFG spectra. This indicates a modification of the electronic structure of the particles and a formation of mixed Pd-NbO_x sites. Pd-Fe₃O₄ model catalyst, on the other hand, were rather stable up to ~600 K. For 10 nm Pd particles no pronounced changes were observed by SFG and TDS spectra, both methods revealing well-ordered particle facets. However, smaller Pd particles (~6 nm) showed different CO bands in SFG, pointing to rougher surfaces, and also phase changes occurred during annealing. Possible surface modifications during annealing (TDS) will be discussed

O 24.8 Tue 17:30 TRE Phys

STM/STS investigations of Cu-phthalocyanine molecules on Al₂O₃/Ni₃Al(111) — ●A. KRUPSKI^{1,2}, M. MOORS¹, S. DEGEN¹, M. KRALJ¹, C. BECKER¹, and K. WANDEL¹ — ¹Institute of Physical and Theoretical Chemistry, University of Bonn, Germany. — ²Institute of Experimental Physics, University of Wrocław, Poland.

LT-STM and STS have been used to investigate the growth of Cu-phthalocyanine (C₃₂H₁₆N₈Cu) molecules on an ultrathin Al₂O₃ oxide

film grown on the $Ni_3Al(111)$ surface [1] as a function of coverage and annealing temperature. For sub- and monolayer coverage and a deposition temperature of 140 K two different planar molecular adsorption configurations rotated by 30° with respect to each other were observed with sub molecular resolution in the STM images. For θ_{CuPc} about 1 ML, before completion of the first layer, the growth of a second layer was already observed. The measured distance of 0.35 nm between 1st and 2nd layer corresponds to the distance between layers in the a modification of crystalline CuPc. By the use of STS the lowest unoccupied molecular orbital (LUMO) of the adsorbed CuPc molecules has been identified at an energy of 1.2 eV. The lateral distribution of the electronic states of the CuPc has been analysed and mapped by STS. The $C_{32}H_{16}N_8Cu$ molecules grown at 140 are thermal stable up to 350 K against shape changes upon prolonged annealing to temperatures up to 350 K. A template effect of the underlying oxide film on the CuPc growth, as has been observed for metals like Pd [2], has not been found.

[1] S. Degen et al., Surf. Sci. Lett. 576 (2005) L57.

[2] S. Degen et al., Faraday Discuss. 125 (2003) 343.

O 24.9 Tue 17:45 TRE Phys

Self-Organization of Au Atoms on a polar FeO film — ●EMILE D. L. RIENKS, NIKLAS NILIUS, HANS-PETER RUST, and HANS-JOACHIM FREUND — Fritz-Haber-Institut der Max-Planck-Gesellschaft, Faradayweg 4-6, 14195 Berlin

On polar oxide surfaces, the large surface dipole can have a significant effect on the adsorption characteristics. We have explored this effect using a mono-layer thick film of FeO grown on Pt(111). In this system a surface dipole is built up between the positive Fe and the negative O layers. A lattice mismatch between the FeO film and the Pt substrate gives rise to a Moiré pattern, in which Fe atoms alternately occupy on-top, fcc and hcp positions on the Pt lattice. Modulations of the surface dipole have been observed within the Moiré unit cell that can be traced back to the structural inhomogeneity of the film. Single Au atoms, deposited at 10 K, preferentially bind to the region of the Moiré cell with the largest surface dipole. This indicates a significant role of electrostatic interaction in the binding. In addition, the Au atoms display a remarkably small tendency to form clusters upon increasing the coverage. Instead,

a hexagonal network of single atoms with a lattice constant of 2.5 nm is formed. Electrostatic repulsion between polarized or partially charged Au atoms can account for this phenomenon.

O 24.10 Tue 18:00 TRE Phys

Organic Molecule Intercalation in TaS_2 — ●SUJIT KUMAR DORA and OLAF MAGNUSSEN — Institut für Experimentelle und Angewandte Physik, Christian-Albrecht-Universität, Germany, Leibnizstr. 19, 24118 Kiel

Transition metal dichalcogenides are ideal host materials for the intercalation of organic molecules, resulting in large change of structural and electronic properties. In this study the atomic-scale mechanisms of the electrochemical intercalation/deintercalation of pyridine and octylamine (both 0.01 M solution pH 3) in $1T - TaS_2$ was investigated by in-situ electrochemical STM and cyclic voltammetry. Intercalation starts at potentials negative of $-0.45 V$ vs SCE. The STM observations show characteristic structural changes in the surface morphology during this process indicating an important role of surface defects, such as holes and steps. In particular, the formation of holes, step flow etching and the formation of small islands of submonolayer height were observed.

O 24.11 Tue 18:15 TRE Phys

Rb adsorption and intercalation on TaS_2 — ●PATRICK SCHMIDT, JÖRG KRÖGER, and RICHARD BERNDT — Institut für Experimentelle und Angewandte Physik, Universität Kiel, D-24098 Kiel, Germany

We report results of scanning tunnelling microscopy at room temperature (RT) and low temperature (LT, 9 K) of TaS_2 exposed to Rb. All samples are prepared by evaporating several monolayers of Rb at RT. STM topographs at RT show a $\sim 1 \text{ \AA}$ deformation of the first layer of TaS_2 on a $\sim 1000 \text{ \AA}$ lateral scale indicating Rb intercalation. Additionally the step height of TaS_2 -Rb is increased by 3 \AA compared to pristine TaS_2 . This value corresponds to the ionic radius of Rb. Finally, the hexagonal $\sqrt{13} \times \sqrt{13}$ charge density wave of TaS_2 changes to a rectangular phase. After evaporating ~ 4 monolayer (ML) of Rb we observe at LT Rb adatoms residing at maxima of the charge density wave. For higher exposure (~ 9 ML) the pattern changes to unordered arrangement of maxima with a typical nearest neighbour distance of 11 \AA .

O 25 Organic films II

Time: Tuesday 15:45–18:30

Room: PHY C213

O 25.1 Tue 15:45 PHY C213

Electronic Effects in the Adsorption Structure of Organic Molecules: STM and STS of Phthalocyanines and Naphthalocyanines on Graphite — ●THIRUVANCHERIL G. GOPAKUMAR and MICHAEL HIETSCHOLD — Chemnitz University of Technology, Institute of Physics, Solid Surfaces Analysis Group, D-09107 Chemnitz, Germany.

The adsorption structure and electronic properties of various metal phthalocyanines and naphthalocyanines organized on graphite surface have been investigated using STM and STS. PdPc and PtPc show similar type of adsorption structure (quadratic lattice) although the central metal atoms are different, however PtPc (300°) adlayer shows almost three times thermal stability compared to PdPc ($80-90^\circ$). Naphthalocyanine shows a distorted quadratic superstructure, the difference is expected in this case due to the long arms of the molecule (additional benzene ring) compared to phthalocyanine. The metal (Sn) naphthalocyanine shows quite interesting superstructure (hexagonal) compared to all other molecules studied may be due to the geometry (non-planar) arises due to the large Sn^{2+} ionic radii. These differences in the adsorption structures give insight in to how internal electrical properties of molecules affect the adsorption structure. Moreover we demonstrate the tip-sample distance dependant tunneling spectroscopy of these molecules which gives quantitative information about the electronic properties especially the transport at the molecule-substrate interface in the adlayer.

O 25.2 Tue 16:00 PHY C213

Combined investigation of the disordered phases of PTCDA on $Ag(111)$ with STM and STS — ●RUSLAN TEMIROV, SERGUEY SOUBATCH, and STEFAN TAUTZ — International University Bremen, Bremen, Germany

Adsorption of large organic molecules is a topic of increasing importance. Among other materials PTCDA has got a lot of attention as a model system for studying complex absorption phenomena. Due

to the unique properties of its chemisorptive bond PTCDA demonstrates a commensurate monolayer growth on $Ag(111)$. Such ordered PTCDA/ $Ag(111)$ interface has been characterized recently on atomic scale using STM, STS and NXSW techniques [1],[2]. In our contribution we present a study of the disordered PTCDA overlayers grown on $Ag(111)$ at 100K. We studied the structure and the thermal stability of the layer employing Low Temperature STM. Electronic properties of the interface have been characterized by STS on a single molecular scale. STM induced single molecular manipulation combined with the STS measurements have been used for the tracking of the changes of interface electronic structure during the transition of the disordered film into the ordered one. These data are further used for the identification of the nature of the disordered PTCDA phases on $Ag(111)$.

[1] A. Hauschild et al. Phys. Rev. Lett. 94, 0360106 (2005)

[2] A. Kraft et al. submitted

O 25.3 Tue 16:15 PHY C213

Self-assembled monolayers of molecular switches - azobenzene carrying alkanethiols on gold — ●R. SCHMIDT¹, W. FREYER¹, T. GIESSEL¹, K. HERRMANN¹, H. PRIMA GARCIA¹, R. WEBER¹, and M. WEINELT^{1,2} — ¹Max Born-Institute, Berlin, Germany — ²Freie Universität Berlin, Germany

Alkanethiols form self-assembled monolayers (SAMs), e.g., bound to gold films via the sulphur headgroup and are thus promising candidates for molecular devices. For this purpose the thiols need to be functionalized by an appropriate endgroup. We chose azobenzene a cis-trans-conformation switch. Adsorption measurements prove that in solution azobenzene attached to decanethiols switches reversibly upon irradiation at 360 nm and 450 nm.

By NEXAFS-spectroscopy (U41 at BESSY II) we investigated both the azobenzene-decanethiol adsorption geometry and its subsequent change upon irradiation. The layers are well ordered at 90 K, but less ordered

at 300 K. Switching seems to be seldom reproducible. However, the temperature dependence of both the adsorption geometry and the switching process makes conceivable a fundamental change of the isomerization energetics at the surface. Autoionization after resonant excitation (N1s, C1s to π^*) reveals strong Resonant-Raman-Auger contributions. Thus charge transfer between azobenzene switch and Au substrate is substantially slowed down by the thiol spacer.

O 25.4 Tue 16:30 PHY C213

Intermolecular, interface, and dipole-dipole interactions in organic thin films — ●ACHIM SCHÖLL¹, SELAMI YILMAZ¹, CHRISTOPH STADLER¹, SATOSHI KERA², and EBERHARD UMBACH¹ — ¹Exp. Phys. II, Univ. Würzburg, Germany — ²Faculty of Engineering, Chiba Univ., Japan

The interactions at metal-organic interfaces are of crucial importance for electronic devices, since they influence the layer morphology and the charge carrier transport through the interface due to the formation of interface dipoles and band offsets. We present a high-resolution PES and NEXAFS study on the adsorption behaviour and interface interaction of ordered thin films of the molecules titanium- (TiO-Pc) and vanadyl-phthalocyanine (VO-Pc), which offer the possibility to tune the work function change of metal surfaces due to their high static dipole moments. Strong changes in the XPS and NEXAFS data of TiO-Pc consistently show the chemisorptive bonding of the first layer. In addition, UPS and work function measurements clearly indicate a parallel orientation of the molecular dipoles which increases the work function by ~0.1 eV in comparison to non-polar adsorbates. A further increase of the coverage leads to the formation of a second layer with anti-parallel dipoles and reduced work function. The careful analysis of the high-resolution XPS and NEXAFS data shows no significant covalent contribution to the intermolecular interaction. However, the desorption temperature of the second layer is increased by more than 150 K in respect to the multilayer, which is attributed to dipole-dipole interaction. This project is financed by the BMBF under contract 05KS4WWC/2.

O 25.5 Tue 16:45 PHY C213

Metal Electrodes to the Molecular World: Evidence for Size-dependent Interactions — ●H.-G. BOYEN¹, P. ZIEMANN¹, U. WIEDWALD¹, V. IVANOVA², M. MANOLOVA², D.M. KOLB², S. SAKONG³, A. GROSS³, A. ROMANYUK⁴, M. BÜTTNER⁴, and P. OELHAFEN⁴ — ¹Abteilung Festkörperphysik, Universität Ulm, D-89069 Ulm — ²Abteilung Elektrochemie, Universität Ulm, D-89069 Ulm — ³Abteilung Theoretische Chemie, Universität Ulm, D-89069 Ulm — ⁴Institut für Physik, Universität Basel, Klingelbergstr. 82, CH-4056 Basel

Organic molecules generally need to be attached to metal electrodes via chemical bonds in order to take advantage of their electrical properties for molecular electronics applications. These chemical bonds, on the other hand, might have strong impact on the electronic properties of the metal leads themselves at the metal/molecule interface.

Here we report experiments aiming to unravel the electronic structure of the metal at the metal/molecule interface representing the early stage of electrode formation. For this purpose, strictly 2-dimensional Pd islands of different size are prepared on top of 4-mercaptopyridine (4MP) Self-Assembled Monolayers (SAMs) by means of a novel electro-chemical approach. Electron spectroscopy together with density functional theory reveal strong interactions between the organic molecules and the metal atoms forming the electrical contact resulting in a drastically reduced density of states at the Fermi level for a nearly closed Pd monolayer and even non-metallic properties in case of nanometer-sized islands.

O 25.6 Tue 17:00 PHY C213

Optimizing the charge carrier injection from Au electrodes in organic electronic devices — ●STEPHAN RENTENBERGER¹, ANTJE VOLLMER², EGBERT ZOJER¹, and NORBERT KOCH³ — ¹Institute of Solid State Physics, Graz University of Technology, Petersgasse 16, A-8010 Graz, Austria — ²Berliner Elektronenspeicherring-Gesellschaft für Synchrotronstrahlung mbH, Albert-Einstein-Str. 15, D-12489 Berlin, Germany — ³Humboldt-Universität zu Berlin, Institut f. Physik, Newtonstrasse 15, D-12489 Berlin, Germany

The performance of organic-based devices (e.g. light emitting diodes, transistors) is governed by two key factors: charge carrier transport within the active organic material and injection of charge carriers from the electrodes into the organic layer. We demonstrate that the work function of Au electrodes can be increased by exposure to UV/ozone.

Consequently, the hole injection barriers (HIBs) between such Au electrodes and organic materials were lowered by as much as 1.4 eV compared to untreated Au electrodes. HIBs were measured using photoelectron spectroscopy. The lowering of HIBs was observed for a wide variety of organic materials [N,N'-diphenyl-N,N'-bis(1-naphthyl)-1,1'-biphenyl-4,4'-diamine, sexiphenyl, sexithiophene, poly-(3-hexylthiophene), and poly-fluorene], which indicates the universal applicability of our Au electrode modification method.

O 25.7 Tue 17:15 PHY C213

Molecular Lifetime Contrast in Thin Pentacene Layers — ●F.-J. MEYER ZU HERINGDORF, D. THIEN, P. KURY, L.I. CHELARU, and M. HORN-VON HOEGEN — Institut für Experimentelle Physik, Universität Duisburg-Essen, Lotharstrasse 1, 47057 Duisburg

Whenever excited electrons are required to tailor specific properties of a thin film, the decay of the initial excitation over time defines an intrinsic limit for the performance. To determine the lifetime of such an electronic excitation in a heterogeneous layer requires a combination of microscopic and spectroscopic methodologies. We used an ultrahigh vacuum spectroscopic photoemission microscope (SPE-PEEM) together with a fs Ti:Sapphire laser to study the decay of electronic excitations in thin films of the aromatic molecule pentacene. This molecule, deposited on a Si surface, initially forms a wetting layer of flat-lying molecules, while subsequent layers stand upright and develop a typical dendritic shape. The change in morphology is reflected in the decay channels for the electronic excitation: while we determine a time constant of less than 200fs for the wetting layer, the lifetime in the dendritic islands is more than twice as high as the wetting layer. Mapping of the lifetime reveals that the morphology of the layer is in fact different for islands of different heights.

O 25.8 Tue 17:30 PHY C213

Determination of the transport gap by UPS and IPES — ●STEFAN KRAUSE, DETLEF EICH, BENEDETTA CASU, and EBERHARD UMBACH — Experimentelle Physik II, Universität Würzburg

The transport gap in semiconductors is defined as the minimum energy needed to produce a separated electron and hole. In a conventional semiconductor such as Si or GaAs this gap can be determined by means of optical absorption taking into account that the optical gap is only slightly smaller than the transport gap because of the small exciton binding energy (few meV). Organic materials are in general believed to have very weak intermolecular interaction leading to a localized charge and hence to a large exciton energy. Thus transport and optical gap may differ by several 100 meV. Then, other methods like UPS and IPES are needed to measure the position of the highest occupied and lowest unoccupied molecular orbital directly. We did such measurements for the organic molecules PTCDA, Alq3 and Cu-Pc and compared the results to those obtained from GaAs, Si, HgTe, and CdTe. In both groups of materials, the peak-to-peak distances of the leading peaks in UPS and IPES are much larger (1-3 eV) than the optical gap, i.e. also much larger than the known or expected exciton energies. The agreement is much better if one uses the peak onsets in all cases. However, then the exciton energies in organic materials are surprisingly small. The origin of the failure of the peak-to-peak approach and the implications of the findings will be discussed.

O 25.9 Tue 17:45 PHY C213

A Metal Surface as a Complex Ligand: Adsorption of Co(II)-Porphyrins on Ag(111) — ●T. LUKASCZYK, K. FLECHTNER, K. COMANICI, H. MARBACH, F. MAIER, J. M. GOTTFRIED, and H.-P. STEINRÜCK — Universität Erlangen-Nürnberg, Lehrstuhl für Physikalische Chemie II, Egerlandstr. 3, D-91058 Erlangen, Germany

Metalloporphyrins control the decisive steps in various natural and technological processes that often involve the reversible attachment of a molecular ligand on the central metal ion. In order to study this key step on a model compound in a solvent-free environment, we investigated ordered monolayers of Tetraphenylporphyrin-Co(II) and Tetrakis-(3,5-di-tert-butylphenyl)porphyrin-Co(II) on Ag(111). First, we focused on the interaction of the Co- d_{z^2} orbital with the Ag surface, because the coordination of an additional ligand is most likely mediated by this orbital. We made use of the different "heights" of the molecules to vary the distance between the Co atom and the Ag substrate. The monolayers were studied with XPS, UPS, and LEED. In the Co 2p_{3/2} photoemission signal, a peak appears at 778.3 eV that is absent at multilayer coverages and that probably reflects the interaction of the Co ion with the Ag substrate.

Complementary evidence for this interaction is provided by a new signal close to E_F in the monolayer UP spectrum. The UP signal position varies with the Co-Ag distance, as expected from MO theory. This work was supported by the DFG through SFB 583.

O 25.10 Tue 18:00 PHY C213

Electronic structure of thin organic films on metal surfaces studied by UV- and resonant photoemission — ●AZZEDINE BENDOUNAN, FRANK FORSTER, ACHIM SCHÖLL, JOHANNES ZIROFF, EBERHARD UMBACH, and FRIEDRICH REINERT — Experimentelle Physik II, Universität Würzburg, am Hubland, 97074 Würzburg, Germany

We present high-resolution photoemission data on the valence band structure of organic thin films on noble metal surfaces, in particular on the epitaxial systems PTCDA/Ag(111) and NTCDA/Ag(111). The valence band of one monolayer PTCDA on Ag(111) is characterized by two spectral features located close to the Fermi energy. Both features are associated to the formation of a strong chemical bond between the substrate and the molecule. The binding energy of these features show an immediate dependence on the PTCDA film thickness. The NTCDA molecule is less strongly bonded to the Ag(111) substrate, but also for this system the formation of hybrid orbitals can be observed in the photoemission spectra. The observed HOMO structure shifts slightly as the NTCDA coverage increases. Moreover, by combination of NEXAFS and resonant photoemission data, we identify the NTCDA and Ag contributions to the various peaks in the photoemission spectrum. In addition, an information is obtained about the coherent and incoherent processes

occurring after excitation by analysis of the evolution of the Auger and photoemission features in the resonant photoemission spectra.

O 25.11 Tue 18:15 PHY C213

In-situ electrical investigations of the growth of dihexyl-oligothiophenes in organic field effect transistors — ●TORSTEN BALSTER, TOBIAS MUCK, ARNE HOPPE, JÖRG SEEKAMP, and VEIT WAGNER — International University Bremen, Bremen, Germany

Optimized contact properties are essential for applications of thin film organic field effect transistors (OFET) enabling higher current level and switching frequencies. We have grown thin films of dihexyl-oligothiophene with 4 to 7 thiophene rings (DHnT) on Ti/Au bottom contact transistor templates in ultrahigh vacuum, because the energetic difference between the HOMO and the Fermi energy of the Au contact is varied by the number of chromophores in oligothiophenes. The channel width of the transistors ranges from 100 down to 5 μm . The in-situ electrically characterized samples of these thiophene derivatives demonstrates oscillatory behaviour of the charge carrier mobilities during growth indicating layer-by-layer mode. The onset of the current could be found in excess of 2/3 of a monolayer, whereas saturation after more than 2 monolayers is observed. Furthermore, higher mobilities (up to 10^{-1}Vs/cm^2 for DH7T) could be found for increasing number of thiophene rings at optimized growth temperatures (190°C) of the sample. The voltage drops at the source and drain electrode are independently determined by means of 4-point measurements using additional, screened electrodes within the organic channel showing a major drop up to 1 V for DH6T at the source electrode.

O 26 Particles and clusters I

Time: Tuesday 15:45–18:30

Room: WIL A317

O 26.1 Tue 15:45 WIL A317

Growth and in-situ oxidation of Rhodium nanoparticles on $\alpha - \text{Al}_2\text{O}_3(0001)$ — ●PHILIPP NOLTE, A. STIERLE, N. KASPER, C. ELLINGER, N.Y. JIN-PHILIPP, G. RICHTER, and H. DOSCH — Max-Planck-Institute for Metals Research, Heisenbergstraße 3, 70569 Stuttgart

To understand the catalytic activity of 4d transition metal nanoparticles, it is important to study their oxidation behaviour. In general, due to their reduced dimensions and their interaction with the support, the oxidation will differ from the corresponding single crystal surfaces, for example in the ability to form surface oxide layers. We studied the growth and oxidation of Rh particles on the $\alpha - \text{Al}_2\text{O}_3(0001)$ surface.

Rh-nanoparticles on $\alpha - \text{Al}_2\text{O}_3(0001)$ can be grown by electron beam evaporation in UHV. As we deduce from x-ray diffraction, the particles grow (111)-oriented and epitaxially. The surface lattice can nearly be described by a $R(\sqrt{3} \times \sqrt{3})30^\circ$ -orientation on the substrate, but with a lattice mismatch of 2%. For an effective material deposition of 2 nm, the formation of flat particles with the shape of truncated hexagonal pyramids could be observed by transmission electron microscopy.

In an in-situ x-ray diffraction experiment at the MPI-MF beamline at ANKA, we studied changes of Crystal Truncation Rods of the Sapphire surface after evaporation of Rh to obtain information about the metal-support interface. The formation of Rh_2O_3 could be observed in an atmosphere of molecular oxygen with $p = 3 \cdot 10^{-2}$ mbar and a substrate Temperature $T_S = 400^\circ \text{C}$.

O 26.2 Tue 16:00 WIL A317

Deviations in exp. and calc. sputtering yields of Cu, Ag, and Au with keV noble gas ions — ●WOLFGANG ECKSTEIN¹ and RAINER BEHRISCH² — ¹IPP, 85748 Garching, MPI — ²IPP, 85748 Garching, MPI

The sputtering yields of metals have been calculated for noble gas ions at different incident energies with the program TRIM.SP. The results in dependence on the incident energy have been approximated with an algebraic formula. In the plots representing the energy dependence of the sputtering yield, the sputtering yields which have been measured by different authors are introduced. For most solids the measured yields scatter within a factor of two around the calculated curves. However, for the noble metals Cu, Ag, and Au the measured yields are systematically about a factor of two higher than the calculated values. Possible reasons for this discrepancy are that the surface binding energy is lower than the heat of sublimation taken in the TRIM.SP calculations. This may be caused by surface roughening during ion bombardment. Surface

atoms may be moved to places with a lower binding energy. Due to the roughening also atom clusters may be released, which is not included in TRIM.SP program. Another reason could be deviations in the interaction potential used as input in the calculations.

O 26.3 Tue 16:15 WIL A317

Growth of supported gold nanoparticles: the influence of substrate material, temperature, and laser irradiation — ●N. BORG, D. BLÁZQUEZ-SÁNCHEZ, C. HENDRICH, H. OUACHA, F. HUBENTHAL, and F. TRÄGER — Institut für Physik and Center for Interdisciplinary Nanostructure Science and Technology - CINSaT, Universität Kassel, Heinrich-Plett-Straße 40, D-34132 Kassel

In order to tailor the optical properties of metal nanoparticles (NPs) for different applications, a variety of parameters must be considered and can be changed. Here, the substrate material as well as its temperature during growth has been varied systematically to clarify the influence of these parameters. Gold nanoparticles (AuNPs) with radii ranging from 0.5 to 12 nm were prepared under ultrahigh vacuum conditions by deposition of gold atoms on quartz, sapphire and titanium dioxide substrates followed by Volmer-Weber-growth. As a consequence of this self-organised assembly we obtained NP ensembles with a broad size and shape distribution where the shape is strongly correlated to the size of the NP. We measured the influence of the substrate material, and the temperature on the shape of the particles. In addition, the method of laser assisted growth has been applied to further tailor the NPs. This technique was developed in our group and takes advantage of the optical properties of metal NPs to overcome the correlation between the shape and the size, the objective being to produce NPs with desired, well-defined shapes and variable sizes. Depending on the wavelength and the fluence of the laser light we can stabilise the mean axial ratio of the AuNPs at values ranging from 0.19 to 0.98 independent of size.

O 26.4 Tue 16:30 WIL A317

Oxidation of mass-selected Au_n clusters ($n=2-9$) on SiO_2/Si — ●RAINER DIETSCHKE, DONG CHAN LIM, MORITZ BUBEK, YOUNG DOK KIM, and GERD GANTEFÖR — Fachbereich Physik, Universität Konstanz, 78464 Konstanz

Mass-selected Au cluster anions consisting of less than 9 atoms were deposited on etched Si wafer surfaces covered with native oxide layers. Oxidation and reduction of the Au clusters were studied using X-ray Photoelectron Spectroscopy (XPS). For $n=2,4,6,8$ exposures of the clusters to atomic oxygen environments result in the appearance of additional peaks at the Au 4f level, which are characteristic for the Au-oxide formation.

For the odd numbered clusters, the Au-oxide formation is much less pronounced. In particular, it can be observed that there is no characteristic feature of the Au-oxide formation for Au₇. This result suggests that each additional atom can drastically change chemical properties of the deposited clusters consisting of the less than 9 atoms. Moreover, the even-odd pattern indicate that chemistry of the clusters correlates with electronic structures rather than with specific adsorption/reaction sites.

O 26.5 Tue 16:45 WIL A317

Dynamic final state effect for the photoemission of gold clusters on graphite: comparison with scanning-tunneling spectroscopy — ●HEINZ HÖVEL and INGO BARKE — Universität Dortmund, Experimentelle Physik I, 44221 Dortmund, Germany

We present an experimental study for the electronic properties of metal clusters on surfaces. For the specific case of the confined Shockley surface state on the top (111) facets of gold clusters on graphite [1] we were able to detect the quantized electronic structure with two independent experimental techniques, scanning tunneling spectroscopy (STS) and ultraviolet photoelectron spectroscopy (UPS). Here we present new UPS data and their analysis which shows a quantitative agreement if we compare the density of states, extracted from the STS spectra by averaging over the cluster size distribution, with the UPS spectra using a deconvolution to compensate the dynamic final state effect [2] which leads to a systematic asymmetric broadening of all valance band UPS features [3].

[1] I. Barke, H. Hövel, Phys. Rev. Lett. **90**, 166801 (2003).

[2] H. Hövel, B. Grimm, M. Pollmann, B. Reihl, Phys. Rev. Lett. **81**, 4608 (1998).

[3] H. Hövel, I. Barke, Prog. Surf. Sci., submitted for publication.

O 26.6 Tue 17:00 WIL A317

Electronic and geometric structures of Au nanostructures on HOPG studied using XPS and STM — ●IGNACIO LOPEZ, DONG CHAN LIM, RAINER DIETSCHKE, and YOUNG DOK KIM — Department of Physics, Universität Konstanz. D-78457, Germany

Au nanostructures grown on mildly sputtered Highly Ordered Pyrolytic Graphite (HOPG) surfaces were studied using Scanning Tunneling Microscopy (STM) and X-ray Photoelectron Spectroscopy (XPS), and the results were compared with those of Ag on the same substrate. By varying defect densities of HOPG and Au coverages, one can create Au nanoparticles with various sizes. At high Au coverages, it is observed that Au structures significantly deviate from the ideal truncated octahedral structure: the existence of many steps between different Au planes can be observed, most likely due to high activation barriers for the Au atoms on the topmost plane of the Au structures jumping over the step edges down to the next plane. This result implies that the particle growth at room temperature is strongly limited by kinetic factors. Using XPS, much less positive core level shifts of the Au 4f level with decreasing particle size was found, compared to the core level shifts of the Ag 3d level in the similar particle size range on HOPG. Together with our results of the Auger analysis of the Ag data, we suggest that the metal/substrate charge transfer is an important factor to determine the core level shifts of the metal nanoparticles on HOPG, i.e. Ag is (partially) positively charged, whereas Au negatively on HOPG. It is demonstrated that XPS can be a useful tool to study metal-support interactions, which can play an important role for e.g. heterogeneous catalysis.

O 26.7 Tue 17:15 WIL A317

Spectroscopic properties of molecules in small gold-nanoparticle aggregates — ●M. RINGLER, S. FUNK, M. BOROWSKI, T. SOLLER, A. SUSHI, G. RASCHKE, T. A. KLAR, and J. FELDMANN — Photonics and Optoelectronics Group, Physics Department and CeNS, Ludwig-Maximilians-Universität München, Germany

Plasmonic properties of metallic nanostructures alter the spectroscopic properties of their nano-environment. Understanding and controlling this phenomenon is of utmost interest both from a fundamental point of view and with regard to sensing applications. Fluorophores attached to single gold-nanoparticles are quenched by energy transfer [1] and radiative rate suppression [2], on nano-structured metal films, enhanced fluorescence is observed [3]. We will discuss the intermediate regime of small aggregates of a few nanoparticles. We will present experimental results of their joint influence on the properties of attached or enclosed molecules.

[1] Dulkeith et al., Phys. Rev. Lett. **89**, 203002 (2002)

[2] Dulkeith, Ringler et al., Nano Lett. **5**, 585 (2005)

[3] Lakowicz, Anal. Biochem. **337**, 171 (2005)

O 26.8 Tue 17:30 WIL A317

Dynamics of gold nanoparticles on the surface of thin polymer films — ●SIMONE STREIT¹, HENNING STERNEMANN¹, CHRISTIAN GUTT², VIRGINIE CHAMARD³, AYMERIC ROBERT⁴, and METIN TOLAN¹ — ¹Exp. Physik I, Universität Dortmund, 44221 Dortmund, Germany — ²DESY (HASYLAB), Notkestr. 85, 22607 Hamburg, Germany — ³LTPCM, 1130 rue de la piscine, 38402 St Martin d'Hères, France — ⁴ESRF, BP 220, 38043 Grenoble Cedex, France

Surface x-ray photon correlation spectroscopy (XPCS) is used to measure the dynamic structure factor $S(q, \tau)$ of nanometer sized gold particles moving on the surface of thin polymer films. Above the glass transition of the polymer the dynamic structure factor is found to follow the peculiar form $S(q, \tau) \sim \exp[-(t/\tau)^\alpha]$. For the exponent a value $\alpha = 1.5$ is observed, representing a faster than exponential decay of the correlation function. A dispersion relation from $q = 0.01$ to 0.06 \AA^{-1} is obtained, corresponding to lengthscales of several hundred Å. The relaxation time τ scales as q^{-1} in contrast to the q^{-2} behavior of simple Brownian diffusive motion. This type of correlation function corresponds to a power law distribution of particle velocities which has also been observed e.g. in aging bulk soft matter systems. The special form of the dynamic structure factor characterizes the hyperdiffusive motion of the gold nanoparticles.

O 26.9 Tue 17:45 WIL A317

Negative differential resistance and nonclassical capacitive behavior in networks of metal clusters — ●HUIJING ZHANG, DIRK MAUTES, and UWE HARTMANN — Institute of Experimental Physics, University of Saarbrücken, P. O. Box 151150, D-66041 Saarbrücken

Monolayers of small metal clusters of type Au₅₅[P(C₆H₅)₃]₁₂Cl₆ were investigated with a low-temperature ultrahigh vacuum scanning tunneling microscope. Apart from the usual charge-quantization phenomena, such as Coulomb blockade and staircase, negative differential resistance was observed by performing measurements at distinct locations on the cluster layers. The latter phenomenon can be understood from a "gate" effect caused by neighboring clusters and involving a nonclassical behavior of the capacitances generated by the nanoscale metal particles.

O 26.10 Tue 18:00 WIL A317

Measurement of the size of embedded metal clusters by mass spectrometry, transmission electron microscopy and small angle X-ray scattering — ●C. HENDRICH¹, L. FAVRE¹, D. N. IEVLEV¹, A. N. DOBRYNIN¹, P. LIEVENS¹, K. TEMST¹, W. BRAS², U. HÖRMANN³, E. PISCOPIELLO³, and G. VAN TENDELOO³ — ¹Laboratorium voor Vaste-Stoffysica en Magnetisme, K.U.Leuven, Leuven, Belgium — ²DUBBLE@ESRF, Netherlands Organisation for Scientific Research (NWO), Grenoble, France — ³Elektronenmicroscopie voor Materiaalonderzoek, Universiteit Antwerpen, Antwerp, Belgium

We investigated ensembles of nanometer sized Au, Co, Er and FePt clusters which were embedded in MgO grown simultaneously on mica substrates. The particles were produced by a laser vaporization source and characterized by time-of-flight mass spectrometry before embedding them into the matrix. The size distribution of the clusters before sample preparation was compared to that obtained by transmission electron microscopy after preparation. These well characterized samples were used for investigations by small angle X-ray scattering (SAXS). By using the Guinier analysis to evaluate the scattering data we could extract the average radii of the embedded clusters. We found a good agreement of this data with the cluster sizes obtained from the mass spectra and with the dimensions determined from the transmission electron micrographs. Furthermore, we also investigated samples which were produced at an elevated substrate temperature and found an increased average cluster radius in the SAXS measurements which we attribute to diffusion and coalescence emerging at higher sample temperatures.

O 26.11 Tue 18:15 WIL A317

Tailoring the dimensions of colloidal gold nanoparticles by laser irradiation — ●F. VOGEL, C. HENDRICH, F. HUBENTHAL, and F. TRÄGER — Instiut für Physik and Center for Interdisciplinary Nanos-structure Science and Technology - CINSaT, Universität Kassel, Heinrich-Plett-Straße 40, D-34132 Kassel

Colloidal gold nanoparticles (AuNPs) are used in many different fields and, especially for industrial applications, are often needed in large quantities. However, a substantial drawback of most production methods is that the prepared AuNPs exhibit broad size and shape distributions. In this contribution, we present our recent experiments with the objec-

tive of tailoring the size of AuNPs in solution with laser light in order to overcome the drawback mentioned above. In our experiments colloidal AuNPs were prepared by wet chemical reduction of HAuCl_4 . Post-synthesis irradiation with laser light permits tailoring of the dimensions of the nanoparticles by diffusion of surface atoms and, especially at high fluences, removal of atoms. Thus, it is possible to eliminate all particles of undesired sizes and shapes by choosing appropriate photon energies and light intensities.

First experiments on colloidal AuNPs with a mean radius of $\langle r \rangle = (7.5 \pm 1.5)$ nm show a pronounced reduction of the HWHM (half width at half maximum) of the surface plasmon resonance (SPR) from 0.37 eV to 0.21 eV and an increased absorption at higher photon energies by the modified AuNPs. The increase and shift of the SPR to higher photon energies can be attributed to a narrowed shape distribution. Consequences of the laser treatment for the size distribution are under examination.

O 27 Scanning probe techniques II

Time: Tuesday 15:45–18:45

Room: WIL B321

O 27.1 Tue 15:45 WIL B321

Towards the analysis of force interactions of atomically defined tip-sample contacts — •DANIEL BRAUN¹, THOMAS KÖNIG¹, JENS FALTER², ANDRÉ SCHIRMEISEN^{1,3}, HENDRIK HÖLSCHER³, MARCUS LIEBMANN⁴, UDO D. SCHWARZ², and HARALD FUCHS^{1,3} — ¹Institute of Physics, University of Münster, Münster, Germany — ²Department of Mechanical Engineering, Yale University, New Haven, CT, USA — ³Center for Nanotechnology (CeNTech), University of Münster, Münster, Germany — ⁴II. Institute of Physics B, RWTH Aachen, Aachen, Germany

In recent years, the atomic force microscope (AFM) has been established as a tool for the imaging of surfaces with atomic resolution. However, a reliable interpretation of the observed atomic-scale contrast is often difficult since the exact structural configuration of the tip apex is generally unknown. A determination of the position of the last atoms of the tip is possible using field ion microscopy (FIM). We have built an AFM for operation at low temperatures and under ultra high vacuum (UHV) conditions based on a design that has previously been published [1]. However, significant changes in the design were necessary as the original design uses silicon cantilevers as force sensors, which are not suited for FIM. Therefore, we implemented a tuning fork as force sensor [2], allowing us to choose an appropriate tip material such as tungsten while maintaining atomic-scale resolution capabilities in AFM mode. First experimental results with both microscopy methods will be presented.

[1] W. Allers et al., Rev. Sci. Instrum. 69, 221 (1998)

[2] F. J. Giessibl, Appl. Phys. Lett. 76 1470 (2000)

O 27.2 Tue 16:00 WIL B321

Quantitative analysis of ferroelectric domain imaging with piezoresponse force microscopy* — •TOBIAS JUNGK, ÁKOS HOFFMANN, and ELISABETH SOERGEL — Institute of Physics, University of Bonn, Wegelerstraße 8, 53115 Bonn, Germany

The contrast mechanism for ferroelectric domain imaging via piezoresponse force microscopy (PFM) is investigated. A novel analysis of PFM measurements is presented which takes into account the background frequency spectrum caused by the experimental setup. Thereby all generally required features of PFM imaging with respect to phasing, amplitude, and frequency dependence are satisfied. This allows, for the first time, a quantitative analysis of the domain contrast which is in good agreement with the expected values for the piezoelectric deformation of the sample. Consequences of the inherent experimental background on the amplitude of the domain contrast (enhancement, nulling, inversion) as well as on the shape and the location of the domain boundaries are discussed.

*Financial support of the DFG (FOR 557) and of the Deutsche Telekom AG is gratefully acknowledged.

O 27.3 Tue 16:15 WIL B321

Measurement and simulation of grain boundaries in thin film solar cell absorbers — •CASPAR LEENDERTZ, FERDINAND STREICHER, TOBIAS EISENBARTH, SUSANNE SIEBENTRITT, SASCHA SADEWASSER, and MARTHA CH. LUX-STEINER — Hahn-Meitner-Institut, Glienicke Str. 100, 14109 Berlin

Kelvin probe force microscopy (KPFM) uses electrostatic forces for the spatially resolved measurement of surface potentials. Using KPFM we studied the potential barrier at grain boundaries of CuGaSe_2 semiconductor thin films for solar cell applications. The long range electrostatic interaction complicates quantitative data interpretation. Therefore, we developed 3D simulations using finite element methods to estimate the spatial variation of the measured surface potentials as a function of the barrier height and doping concentration. We find that the deviation between measured and true barrier height strongly depends on the sample

doping, i.e. the measured barrier height increases from 55% to 70% of the true barrier height when the doping drops from $5 \times 10^{16} \text{cm}^{-3}$ to $3 \times 10^{15} \text{cm}^{-3}$.

O 27.4 Tue 16:30 WIL B321

High resolution nc-AFM investigation of the adsorption of PTCDA on ultrathin KBr films — •CHRISTIAN LOPPACHER¹, U. ZERWECK¹, L.M. ENG¹, S. GEMMING^{2,3}, G. SEIFERT², C. OLBRICH³, K. MORAWETZ³, and M. SCHREIBER³ — ¹Institute of Applied Photophysics, University of Technology Dresden, D 01062 Dresden — ²Institute of Physical Chemistry and Electrochemistry, TU Dresden, D-01062 Dresden, Germany — ³Institute of Physics, TU Chemnitz, D-09107 Chemnitz, Germany

Ordered growth of 3,4,9,10-perylene-tetracarboxylic-dianhydride (PTCDA) on Ag(111) partially covered by one or two monolayers KBr was investigated by noncontact AFM with molecular resolution. Different adsorption patterns are found on the pure substrate, the one covered by a single monolayer, and the one covered by two monolayers KBr. Simulations with an extended Ising-type model reproduce these experimental patterns very well [1]. The adsorbate-adsorbate and the adsorbate-substrate interaction parameters obtained from the simulation are discussed in respect to the interactions at the Ag(111)–KBr interface.

[1] K. Morawetz, C. Olbrich, S. Gemming et al., Phys. Rev. Lett., (submitted)

O 27.5 Tue 16:45 WIL B321

Investigation of dissipative interaction between probe and ligand-stabilized clusters by NC-AFM — •GEORGETA RADU and UWE HARTMANN — Institute of Experimental Physics, Saarland University, P.O. Box 151150, D-66041 Saarbrücken, Germany

In recent years, noncontact atomic force microscopy (NC-AFM) became a powerful tool for imaging at high resolution as well as for probing specific surface properties. A major advantage of NC-AFM is the ability to distinguish between conservative and dissipative interactions. In order to investigate the dissipative interaction between the AFM probe and individual clusters, thin films of ligand-stabilized Au_{55} clusters on an Au(111) substrate have been prepared. The NC-AFM images show locally ordered Au_{55} monolayer islands with single cluster resolution. Dissipative interactions can be investigated by NC-AFM by measuring the damping of the cantilever oscillation as a function of the probe-sample distance. Damping-versus-distance measurements were performed on individual clusters as well as on the bare substrate. A distance dependence corresponding to the electric-field mediated Joule-dissipation [1] was found for the energy dissipated above individual clusters as well as on the bare substrate. No additional energy dissipation due to the mechanical deformation of the ligand shell under the action of the oscillating tip was observed. This is in agreement with the theoretical calculations by Couturier et al. [2].

[1] W. Denk and D. Pohl, Appl. Phys. Lett. 59, 2171 (1991)

[2] G. Couturier et al., J. Phys. D: Appl. Phys. 34, 1266 (2001)

O 27.6 Tue 17:00 WIL B321

Site-Specific Dynamic Force Spectroscopy on NaCl — •ANDRÉ SCHIRMEISEN, DOMENIQUE WEINER, and HARALD FUCHS — Institute of Physics and CeNTech, University of Münster, Wilhelm-Klemm-Str.10, 48149 Münster, Germany

Dynamic force microscopy under ultrahigh vacuum conditions is an established tool to obtain atomically resolved images of flat surfaces. Recent advances in the technique as well as the interpretation of the un-

derlying physical mechanisms has led to the method of dynamic force spectroscopy, which enabled researchers to determine the forces acting between tip and sample. We have measured the frequency shift and the damping curves using non-contact atomic force spectroscopy of an atomically resolved NaCl surface in ultrahigh vacuum at room temperature. Unfortunately, room temperature measurements usually suffer from considerable temperature drift effects, thus making reliable site-specific force spectroscopy a difficult task. Combining fast data acquisition with a site-averaging technique we obtained reproducible spectroscopy curves. From these spectroscopy curves we calculate the force and the energy dissipation and find that both channels depend strongly on the specific lattice sites. Furthermore, we have investigated the influence of atomic surface defects on the spectroscopy curves.

O 27.7 Tue 17:15 WIL B321

Theoretical Analysis of Q -controlled Dynamic Force Microscopy in Ambient Conditions — •DANIEL EBELING^{1,2}, HENDRIK HÖLSCHER^{1,2}, HARALD FUCHS^{1,2}, and UDO D. SCHWARZ³ — ¹Center for Nanotechnology (CeNTech), Münster — ²Physics Institute, University of Münster — ³Department of Mechanical Engineering, Yale University, New Haven, USA

The so-called Q -control method allows the active modification of the effective cantilever damping in dynamic force microscopy (DFM) by increasing or decreasing the Q -value of the cantilever [1]. This feature can be used in different ways to improve the imaging capabilities of DFM in air. Even though the Q -control method has been frequently applied in numerous experimental studies in recent years [2, 3] and the necessary driving electronics is commercially available, it is striking that an in-depth analytic description that would allow a rigorous theoretical explanation of the various features of Q -controlled dynamic force microscopy (QC-DFM) is still missing. Here, we present an analysis of QC-DFM based on the analytical solution of the equation of motion and on numerical simulations considering a model tip-sample interaction force in both cases. Explicit formulas allowing for the calculation of all relevant parameters like gain, phase, and amplitude are given. The detailed analysis of these formulas explains the observed imaging characteristics of QC-DFM.

[1] B. Anczykowski et al., Appl. Phys. A 66, S885 (1998)

[2] J. Tamayo et al., APL 77, 582 (2000)

[3] A. Grant et al., Ultramicroscopy 97, 2919 (2003)

O 27.8 Tue 17:30 WIL B321

Hydrogen-altered Gd(0001) surfaces investigated by dynamic force microscopy — •RENE SCHMIDT, ALEXANDER SCHWARZ, and ROLAND WIESENDANGER — Institute of Applied Physics, University of Hamburg, Jungiusstr. 11, D-20355 Hamburg

Adsorbates from residual gases alter the electronic and magnetic properties of rare earth metals. Here, the chemisorption process of hydrogen on Gd(0001) islands epitaxially grown on W(110) is investigated by means of dynamic force microscopy in UHV. Frequency shift vs. bias curves show a potential difference of 0.6 V between clean and H-covered regions on Gd(0001) islands. This originates from a charge transfer between hydrogen and gadolinium, leading to a bias voltage dependent contrast in DFM images, i.e., H-covered gadolinium surface areas appear depressed for negative or elevated for positive bias voltages, respectively. These results are discussed with respect to photoemission and STM studies, which indicate, that adsorbed hydrogen locally destroys the surface state with d_{z^2} -like orbital symmetry and induces a decreasing differential conductivity near the Fermi level at low bias voltages.

O 27.9 Tue 17:45 WIL B321

Detection of electrical forces with a capacitive cantilever device — •A.-D. MÜLLER¹, F. MÜLLER¹, A. KÄPPEL², and M. HIETSCHOLD² — ¹Anfatec Instruments AG, Melanchthonstr.28, 08606 Oelsnitz, Europe. — ²TU Chemnitz, Solid Surfaces Analysis Group, 09107 Chemnitz, Europe.

The detection of electrical forces in dynamic mode AFM allows to observe contact potential differences between tip and sample as well as carrier concentration variations. For this, additional voltages are applied to the tip, while the additional electrical signals are evaluated with lock-in amplifiers. In order to observe locally generated potentials in its surrounding surface region, multiple tip cantilevers can be utilized.

This work investigates the applicability of multiple tip cantilever devices for electrical force microscopy. In contrast to conventional AFM, the tips in this devices are independently movable in vertical direction

and the tip sample forces are sensed by displacement current detection [1]. Imaging of electrical properties with this devices is shown at the example of dopant patterns on n-silicon. In order to improve the understanding of the image contrast, the results are compared with numerical simulations of the electrical force interaction in dependence on applied voltage magnitudes.

[1] A.-D. Müller, F. Müller, M. Hietschold, Th. Gessner, Curr. Appl. Phys. 5, 629 (2005).

O 27.10 Tue 18:00 WIL B321

Temperature dependence of point-contact friction on silicon — •LARS JANSEN^{1,2}, ANDRÉ SCHIRMEISEN^{1,2}, HENDRIK HÖLSCHER^{1,2}, and HARALD FUCHS^{1,2} — ¹Institute of Physics, University of Muenster, Wilhelm-Klemm-Str. 10, 48149 Muenster — ²CeNTech, Center for Nanotechnology, Gievenbecker Weg 11, 48149 Muenster

Due to the rising importance of the tribological properties of silicon in industrial applications like micro-electro mechanical systems (MEMS), the friction between two silicon bodies is of high interest. In order to investigate the tribological properties, we have measured the frictional forces between a Si-tip and a Si(111)-surface at different sample temperatures in the range of 30 K to 300 K by cooling the sample with a flow cryostat, using liquid nitrogen and liquid helium. The measurements are performed with a commercial Atomic Force Microscope under ultra high vacuum conditions. The temperature dependence of the friction coefficient, given by the ratio of friction to load, shows a large variation by a factor of 3-9 within the investigated temperature range with a maximum around 100 K. Furthermore, we found a drastic change in the velocity dependence of the friction. Above 150 K the friction is virtually independent of the velocity in the range from 200 nm/s to 20.000 nm/s, while below 150 K the friction is proportional to logarithm of the velocity. These findings are of great interest for the design and functionality of MEMS devices.

O 27.11 Tue 18:15 WIL B321

Relating structure and friction: Energy dissipation during the lateral manipulation of antimony nanoparticles — •MARKUS HEYDE¹, CLAUDIA RITTER², KLAUS RADEMANN², and UDO D. SCHWARZ³ — ¹Fritz-Haber-Institute of the Max-Planck-Society, Faradayweg 4-6, D-14195 Berlin, Germany — ²Institute of Chemistry, Humboldt University Berlin, Brook-Taylor-Str. 2, 12489 Berlin, Germany — ³Department of Mechanical Engineering, Yale University, P.O. Box 208284, New Haven, CT 06520-8284, USA

Despite its daily-life importance, the fundamentals of friction are still insufficiently understood. In particular, the interplay between friction, "true" contact area, and crystalline structure at the interface is an issue of current debate. Recently, a new technique had been introduced that allows determining the threshold energy dissipated during the lateral displacement of small nanoparticles on suitable substrates as a function of the particle-substrate contact area [1]. Here, we present results of an extensive study of antimony nanoparticles 1000 nm² to 100000 nm² in size moved in air on graphite substrates. Complementary studies by electron microscopy reveal the internal structure of the islands, showing a transition from amorphous to crystalline of the island's cores at about 10000-15000 nm² size, while the surface layers are composed of amorphous antimony oxide in all cases. However, despite the similarities of the amorphous surface layer, islands with crystalline core show significantly higher energy dissipation during motion than the ones with amorphous core. Possible reasons for this effect are discussed.

[1] Ritter et al., Phys. Rev. B 71, 085405 (2005).

O 27.12 Tue 18:30 WIL B321

Influence of wettability on microtribological properties of microsystems — •WOLFRAM HILD¹, YONGHE LIU¹, MICHAEL SCHUCH¹, MATTHIAS SCHERGE², and JUERGEN A. SCHAEFER¹ — ¹Institut für Physik und Zentrum für Mikro- und Nanotechnologien, TU Ilmenau, P.O. Box 100565, 98684 Ilmenau, Germany — ²IAVF Antriebstechnik AG, Im Schlebert 32, 76187 Karlsruhe

The capillary force formed by water at smooth hydrophilic surfaces plays a crucial role in the performance and reliability of microelectromechanical systems. Capillary forces may lead to malfunctions. The negative influence of water can be excluded by various techniques, e.g. by using hydrophobic Self Assembled Monolayers (SAMs). We report the influence of wettability on the microtribological properties of Si. A microtribometer with a force resolution of 100 nN was employed to study the tribological properties of hydrophilic and hydrophobic microcontacts

in air and immersed in water. The wettability of silicon surfaces was changed by etching with piranha solution (contact angle [CA] immeasurably small) and by SAMs (CA 110°). Micro friction was measured as a

function of external load and sliding velocity in both environments. The influence of wettability on friction and adhesion is discussed.

O 28 Surface reactions II

Time: Tuesday 15:45–18:30

Room: WIL C207

O 28.1 Tue 15:45 WIL C207

CO-Oxidation measurements on Au/TiO₂ model catalysts — ●S. KIELBASSA¹, J. BANSMANN¹, F. WEIGL², H.G. BOYEN², P. ZIEMANN², and R.J. BEHM¹ — ¹Dept. of Surface Chemistry and Catalysis, University of Ulm — ²Dept. of Solid State Physics, University of Ulm

Model catalysts with tuneable particle size and distance parameters on flat surfaces open new opportunities for studying the influence of particle sizes and separations on the catalytic activity. However, the overall small active surface, approximately 1:500th of 1mg of a comparable powder catalyst, results in a very low total product conversion which is difficult to detect, especially in higher pressure regimes (1atm). Our model catalysts consist of Au particles with defined particle sizes (1-5nm) and separations (30-100nm) prepared by a micellar approach on flat TiO₂(110) single crystal surfaces. For the catalytic measurements, we use a novel design of a reactor with a very small volume (0.003ml) and constant gas-flow (0.0005ml) to detect the oxidation of CO. The reactor is situated in the load-lock of a UHV-chamber, which gives us the opportunity to characterize the samples in-situ with AFM and XPS without moving them through air. Results of the influence of particle sizes and separations on the activity are discussed.

O 28.2 Tue 16:00 WIL C207

Adsorption and Oxidation of CO on Au/TiO₂ model catalysts — ●THOMAS DIEMANT¹, ZHONG ZHAO¹, JOACHIM BANSMANN¹, HUBERT RAUSCHER², and R. J. BEHM¹ — ¹Abt. Oberflächenchemie und Katalyse, Universität Ulm, D-89069 Ulm — ²Institute for Health and Consumer Protection, European Commission, Joint Research Centre, I-21020 Ispra

Metal oxide supported gold catalysts have attracted considerable attention in the last years because of their surprising activity in a number of reactions such as the low temperature CO oxidation. We have studied the interaction of both pure CO and reactive CO/O₂ gas mixtures with planar Au/TiO₂ model catalysts at gas pressures up to 100 mbar and the activity of the model systems for CO oxidation in simultaneous kinetic and in-situ IR measurements (PM-IRAS). The possible evolution of additional surface species (carbonates, formates), which has been observed on real catalysts under similar conditions, was monitored. The results of this work will be compared with results from real catalysts, consequences for the reaction mechanism will be discussed.

O 28.3 Tue 16:15 WIL C207

Analysis of the compensation effect observed in first-principles kinetic Monte Carlo simulations of heterogeneous catalysis — ●HAKIM MESKINE, KARSTEN REUTER, and MATTHIAS SCHEFFLER — Fritz-Haber-Institut, Faradayweg 4-6, D-14195 Berlin, Germany

First-principles kinetic Monte Carlo (kMC) simulations for heterogeneous catalysis provide quantitative microscopic insight into the steady-state catalytic activity, fully accounting for the correlations, fluctuations and spatial distributions of the chemicals at the catalyst surface [1]. Density-functional theory is employed to accurately obtain the energetics of the manifold of relevant processes, while a correct statistical mechanics treatment of their interplay is taken care of by the kMC algorithm. In the application of this approach to the CO oxidation at a RuO₂(110) model catalyst, we compute the composition and structure of the surface in reactive environments ranging from ultra-high vacuum to technologically relevant conditions with pressures of the order of atmospheres and elevated temperatures. The catalytic activity is narrowly peaked in environments, where the surface kinetics builds a disordered and dynamic adsorbate composition at the surface. Our analysis shows that the strong process interplay makes this resulting optimum mix at the catalyst surface highly adaptive.

[1] K. Reuter, D. Frenkel, and M. Scheffler, Phys. Rev. Lett. **93**, 116105 (2004).

O 28.4 Tue 16:30 WIL C207

Hot electron mediated associative desorption of hydrogen from Ru(001): insights from theory and experiment — ●STEFFEN WAGNER¹, CHRISTIAN FRISCHKORN¹, MARTIN WOLF¹, MATS PERSSON², and ALAN C. LUNTZ³ — ¹Freie Universität Berlin — ²Chalmers University of Technology, Göteborg — ³Dansk Fysik Institut Odense

Hot electron mediated associative desorption of hydrogen from a hydrogen covered Ru(001) surface was investigated both experimentally and theoretically. The hot electron distribution created by femtosecond-laser irradiation was proven to mediate H₂ desorption [1]. The desorbing hydrogen molecules were investigated regarding isotope effects, fluence dependence and energy transfer to the different molecular degrees of freedom [1, 2]. For the latter, different energy content in the different degrees of freedom was found. Those experimental findings are compared with the outcome of two-dimensional trajectory calculation, which take into account the electron mediated activation of the adsorbate via electronic friction. The friction coefficients are obtained from DFT calculations. This concept has been proven to be successful for the consideration of non-adiabatic effects in activated associative desorption and vibrational damping of adsorbed molecules [3,4]. Thus, we are able to give a microscopic description of the experimental observations.

[1] Denzler et al, Phys. Rev. Lett. 91, 226102 (2003) [2] Wagner et al, Phys. Rev. B 72, 205404 (2005); [3] Luntz, Persson, J.Chem. Phys. 123, 074704 (2005) [4] Persson, Hellsing, Phys. Rev. Lett. 49, 662 (1982)

O 28.5 Tue 16:45 WIL C207

Ammonia oxidation on Pt single crystal surfaces in an intermediary pressure range up to 1 mbar — ●YINGFENG ZENG¹, SEBASTIAN GÜNTHER², LING ZHOU³, and RONALD IMBIHL¹ — ¹Institute for Physical Chemistry, Hannover University, Callinstr. 3-3a, D-30167 Hannover, Germany — ²LMU München, Department Chemie, Butenandstr. 11 E, D-81377 München, Germany — ³Division of Engineering and Applied Sciences, Harvard University, Pierce Hall, 29 Oxford St., Cambridge, MA 02138, USA

The kinetics of ammonia oxidation on Pt(443), Pt(533) and Pt(100), have been investigated under stationary reaction condition in the 10⁻⁴ to 10⁻² mbar range with low-energy electron diffraction (LEED), ellipsometry and rate measurement. Rate hysteresis in T-cycling occurs associated with structural modification of the Pt substrate is verified by LEED measurements with Pt(533) and Pt(443). Surprisingly, the occurrence of a hysteresis depends on the total pressure. For Pt(533) and Pt(443) we found a hysteresis at 10⁻³ mbar, but no hysteresis at P ≥ 10⁻² mbar, on Pt(443) hysteresis vanishes at P ≤ 10⁻⁴ mbar. On Pt(100) we found under all conditions a very broad hysteresis due to the phase transition of substrate from (1 × 1) to hex. The origin of the P-dependent hysteresis on Pt(443) and Pt(533) is discussed in terms of reversible and irreversible structural changes of the Pt surfaces.

O 28.6 Tue 17:00 WIL C207

Methanol steam reforming on Zn/Pd(111) — ●REINHARD DENECHE, ERCAN ÜNVEREN, ARMIN REINDL, HEIKO WUSTMANN, and HANS-PETER STEINRÜCK — Lehrstuhl für Physikalische Chemie II, Universität Erlangen-Nürnberg, Egerlandstr. 3, 91058 Erlangen

Hydrogen as energy source for mobile applications can be obtained by steam reforming of methanol over Pd/ZnO catalysts. On other supported Pd catalysts, the addition of Zn increases the selectivity and the rate of hydrogen formation [1].

In order to prepare the active PdZn alloy, 3 or 6 ML Zn are deposited on Pd(111) at 300 K and alloyed at 500 to 600 K. The adsorption of methanol and consequently the reaction with water at different temperatures are investigated in-situ in a pressure range from ultra-high-vacuum up to 0.3 mbar by "high-pressure" X-ray photoelectron spectroscopy [2]. For methanol adsorption, CH_xO (x=0-3) and CH₃OH species are found on the catalyst surface. In contrast to Pd(111), nearly no dissociation to CH_x was observed, suggesting different reaction pathways. Coadsorption of methanol and water leads to reduced intensity of the CH_xO (x=0-3)

species, signalling a reaction process. Gas phase analysis complements these results. Supported by DFG (SPP 1091).

[1] N. Iwasa et al., *J. Chem. Eng. Japan* 37 (2004) 286

[2] J. Pantförder et al., *Rev. Sci. Instrum.* 76 (2005) 014102

O 28.7 Tue 17:15 WIL C207

Adsorption and Reaction of Methanol on Partially Oxidized Pd Model Catalysts — ●BJÖRN BRANDT¹, TOBIAS SCHALOW¹, SWETLANA SCHAUERMANN¹, JÖRG LIBUDA², and HANS-JOACHIM FREUND¹ — ¹Fritz-Haber-Institut der Max-Planck-Gesellschaft, Department of Chemical Physics, Faradayweg 4-6, 14195 Berlin, Germany — ²Friedrich-Alexander-Universität Erlangen-Nürnberg, Lehrstuhl für Physikalische Chemie II, Egerlandstrasse 3, 91058 Erlangen, Germany

The chemical state of metal nanoparticles under oxidizing reaction conditions and its influence on the reactivity is a subject of enduring discussion for many catalytic systems. On transition metal surfaces, a variety of different oxygen species has been reported, whose role in reaction kinetics is poorly understood. In this study we present first results on the interaction of methanol with well-defined Pd/Fe₃O₄ model catalysts, applying molecular beam methods combined with TR-IRAS. Previously, we have shown that oxidation of iron oxide supported Pd particles above 500 K results in the formation of Pd oxides, located primarily at the particle/support interface. We probe the reactivity of partially oxidized and pristine metallic Pd nanoparticles for methanol decomposition and oxidation. On the pristine Fe₃O₄ support, the formation of stable methoxy species was observed up to 350 K. On Pd particles, methanol decomposition undergoes two competing reaction pathways, resulting in formation of CO and carbonaceous species. The influence of Pd particle oxidation on the two decomposition pathways was studied by transient and steady-state experiments, combined with TR-IRAS.

O 28.8 Tue 17:30 WIL C207

Formation and Activity of Partially Oxidized Pd Nanoparticles — ●TOBIAS SCHALOW¹, BJÖRN BRANDT¹, MATHIAS LAURIN¹, SEBASTIEN GUIMOND¹, HELMUT KUHLENBECK¹, DAVID E. STARR¹, SHAMIL K. SHAIKHUTDINOV¹, SWETLANA SCHAUERMANN¹, JÖRG LIBUDA², and HANS-JOACHIM FREUND¹ — ¹Fritz-Haber-Institut der Max-Planck-Gesellschaft, Department of Chemical Physics, Faradayweg 4-6, 14195 Berlin, Germany — ²Friedrich-Alexander-Universität Erlangen-Nürnberg, Lehrstuhl für Physikalische Chemie II, Egerlandstrasse 3, 91058 Erlangen, Germany

The formation and reactivity of different oxygen species formed on iron-oxide supported Pd nanoparticles are studied by combining well-defined model catalysts, molecular beam experiments and various surface science techniques. It is shown that at temperatures above 500 K, large amounts of oxygen can be stored in form of a thin Pd oxide layer at the particle support interface, which can be reversibly accumulated and depleted. The formation of this interface oxide layer, however, shows a strong particle size dependence: While for small particles the oxygen storage capacity is limited by the amount of metal available, for large particles strong kinetic hindrances and a limited amount of accessible interface sites inhibit the oxygen storage process. Consequently, a pronounced maximum in oxygen storage capacity is found for particles of about 7 nm in diameter. Furthermore it is demonstrated how the formation and reduction of this interface oxide layer affects the activity of the catalyst towards CO oxidation under reaction conditions.

O 28.9 Tue 17:45 WIL C207

On the oxidation and reduction of Co nanoparticles on thin aluminum oxide films — ●TOBIAS NOWITZKI¹, THOMAS RISSE², VOLKMAR ZIELASEK¹, and MARCUS BÄUMER¹ — ¹Institut für Angewandte und Physikalische Chemie, Universität Bremen, Leobener Str. NW II, 28359 Bremen — ²Abteilung Chemische Physik, Fritz-Haber-Institut der Max-Planck-Gesellschaft, Faradayweg 4-6, 14195 Berlin

Cobalt is used as a catalyst for the hydration of carbon monoxide, the so called Fischer-Tropsch process. As a model catalyst for this reaction, Co nanoparticles on thin aluminum oxide films have been studied in ultrahigh vacuum (UHV) with respect to their oxidation and reduction behaviour. The Co particles were prepared in UHV by physical vapor deposition on a thin aluminum oxide film grown on a NiAl(110) single crystal. X-ray photoelectron (XP) and thermal desorption (TD) spectroscopy data show that Co particles are entirely oxidized at room temperature. After heating to temperatures > 500 K, XPS shows mostly metallic Co, indicating reduction, while TDS shows a mixture of metallic and oxidic components, revealing the existence of a thin surface oxide. Our results indicate that the surface oxide formation depends on particle size. We also find that carbon monoxide can dissociate on metallic particles, which is interesting for the Fischer-Tropsch reaction. In the XP spectra, the oxidic component of the Al 2p substrate signal is increased after heating in presence of the Co particles. Obviously, the aluminum oxide film gets thicker during this procedure, enhancing its thermal stability.

O 28.10 Tue 18:00 WIL C207

EPOXIDATION OF ETHYLENE ON SILVER STUDIED BY HIGH-PRESSURE STM — ●R. REICHEL, M. RÖSSLER, S. GÜNTHER, and J. WINTTERLIN — Ludwig-Maximilians-Universität, Department Chemie, 81377 München, Germany

Using an improved high pressure scanning tunneling microscope (STM) we have investigated the epoxidation of ethylene on silver surfaces. The setup consists of a high-pressure cell (up to 1 bar) housing the STM that is attached to an ultra-high vacuum chamber and to a gas analysis system containing a mass spectrometer. In the STM cell catalytic reactions can be performed under pressure and temperature conditions close to those of industrial catalytic processes, both in batch and flow mode. In the UHV chamber single crystal surfaces are prepared under clean surface-science conditions, and standard surface science techniques are used for post-reaction analysis of the sample surface. It has been achieved to detect a reaction to give ethylene oxide at pressures of approximately 1 mbar and at temperatures around 500 K. Atomic resolution was obtained on an Ag(111) surface under epoxidation conditions. Several different surface structures were observed, suggesting that more than one species of oxygen is involved in this reaction.

O 28.11 Tue 18:15 WIL C207

SCANNING TUNNELING MICROSCOPY INVESTIGATIONS OF THE STRUCTURAL BASIS FOR CATALYST DEACTIVATION — ●S. MARCHINI, S. GÜNTHER, and J. WINTTERLIN — Ludwig-Maximilians-Universität, Department Chemie, 81377 München, Germany

Deactivation and poisoning is an essential phenomenon in industrial catalysis. A poison can influence both the activity and the selectivity of the catalyst chemically, by modifying the electronic properties of the surface, or physically, by altering the geometry or blocking the active sites of the catalyst. We here present a scanning tunneling microscopy investigation of the formation of a graphitic layer on the Ru(0001) surface. Prolonged annealing of the sample causes carbon segregation from the bulk of the crystal and the formation of a superstructure whose coverage increases up to saturation upon increasing the heating temperature to 1400K. LEED measurements show that the structure is incommensurate (~12.5x12.5) and rotationally aligned to the surface. STM images exhibit a Moiré pattern with a periodicity of 28Å and whose structure could be atomically resolved. The system exhibits an interesting spectroscopic behavior: images taken with different tunneling voltages show strong changes in the way the structure appears, revealing the presence of a composite surface electronic structure.

O 29 Poster session II (Nanostructures, Magnetism, Particles and clusters, Scanning probe techniques, Time-resolved spectroscopy, Structure and dynamics, Semiconductor surfaces and interfaces, Oxides and insulators, Solid-liquid interfaces)

Time: Wednesday 14:30–17:30

Room: P2

O 29.1 Wed 14:30 P2

Non-paraxial Talbot effect at arrays of microspheres and microstructures — ●MANUEL GONÇALVES, ANDRÉ SIEGEL, ALEXANDER GIGLER, and OTHMAR MARTI — Department of Exp. Physics, University of Ulm, D-89069 Ulm, Germany

The Talbot effect, known in optics since the middle of the 19th century was observed in atom optics in 1995. Since then, an increasing attention has been drawn to this effect in both classical and atom optics. One of the reasons for that is the connection between the Talbot effect and the optical coherence. However, most of the theoretical analysis has been based on the paraxial approximation of optical rays. In some cases this approach is inadequate.

We have measured the Talbot effect for two-dimensional arrays of microspheres, on flat surfaces, and for microstructured surfaces using colloidal crystals as templates. These structures can focus strongly plane waves generating very sharp light sources. We show that if the size of light sources is of the order of the wavelength, or even smaller, the conventional paraxial approach to calculate the Talbot length z_T fails.

We have developed a theoretical model based on the scalar diffraction theory to calculate the field in the Fresnel region, without using the paraxial approximation. The results obtained are in good agreement with the experimental measurements. By contrary, the simulations based on the Fresnel diffraction were not observed experimentally.

O 29.2 Wed 14:30 P2

Ultraflat Ternary Nanopatterns Fabricated via Colloidal Lithography — ●MICHAEL HIMMELHAUS, OLIVER WORSFOLD, CONOR WHITEHOUSE, and JONATHAN WRIGHT — Bionanotechnology Research Project, R&D Division, Fujirebio, Inc., 51 Komiya-cho, Hachioji-shi, Tokyo 192-0031, Japan

Colloidal lithography on mica has been combined with subsequent thermal evaporation, sputtering, and template-stripping processes to produce ultraflat ternary nanopatterns of large lateral extension. As confirmed by atomic/friction force microscopy (AFM/FFM) the patterns provide a new type of model surface particularly useful for applications that demand proper distinction between surface chemistry and topography. By right choice of materials for fabrication of the inorganic pattern, the resulting features can be selectively functionalized with self-assembled monolayers, thereby altering surface properties of the addressed regions only. We found that the size of the circular patches, which can be fabricated by our method, is reduced to 60% of the nominal diameter of the colloidal particles used to produce the colloidal mask. Accordingly, the minimum size of circular features that can be fabricated by colloidal lithography is significantly reduced.

O 29.3 Wed 14:30 P2

Electronic properties of the Si(557)-Au surface investigated by STM and STS — ●M. SAUTER¹, R. HOFFMANN¹, C. SÜRGER¹, and H. v. LÖHNEISEN^{1,2} — ¹Physikalisches Institut und DFG Center for Functional Nanostructures (CFN), Universität Karlsruhe, D-76128 Karlsruhe — ²Forschungszentrum Karlsruhe, Institut für Festkörperphysik, D-76021 Karlsruhe

The Si(557)-Au surface is investigated by scanning tunneling microscopy (STM) and spectroscopy (STS) at different temperatures. Previous photoemission data were interpreted in terms of a one-dimensional metallic band at room temperature [1]. However, at $T = 260$ K the photoemission intensity near the Fermi energy vanishes. This has been attributed either to a Peierls transition [1] or to a shift of the Fermi energy [2]. At room temperature our STM images confirm the chainlike structure due to adatoms adjacent to a diffuse row attributed to the step edge. At $T = 77$ K images of unoccupied electronic states show a splitting of the step-edge structure but no doubling of periodicity in contradiction with the interpretation of a Peierls transition. In addition, we present high-resolution images that reveal a substructure at the location of the Au-Si bonds. Current-distance measurements have been performed in order to investigate the k -dependence of the tunneling spectra.

[1] J. R. Ahn *et al.*, Phys. Rev. Lett. **91**, 196403 (2003).

[2] D. Sánchez-Portal *et al.*, Phys. Rev. Lett. **93**, 146803 (2004).

O 29.4 Wed 14:30 P2

Preparation und characterization of molecular Ag nano contacts via electromigration — ●JEDRZEJ SCHMEIDEL, GERNOT GARDIŃSKI, CHRISTOPH TEGENKAMP, and HERBERT PFNÜR — Institut für Festkörperphysik, Universität Hannover, Abteilung Oberflächen, Appelstrasse 2, 30167 Hannover, Germany

In order to obtain electrical characteristics from molecules and nanostructures, atomically well-defined and stable contacts are of high importance, which can be manufactured reproducibly, e.g. under UHV conditions to minimize further contamination.

We create nanogaps using an electromigration technique. For heat dissipation different geometries have been fabricated by using e-beam lithography on mono(PMMA)- and bi-layer(PMMA/LOR3B) photo-resist systems. The latter is used to create nano-bridges due to underetching. In a following step Ag is evaporated on H-terminated Si(100) or Si(111) surfaces at different angles, thus forming flat Ag films in between thicker Ag contacts, which are around 50nm high and laterally separated by 200nm. The evaporation is done at 80K, i.e. continuous Ag films are obtained already for 10ML in the central part. The widths of the initial structure is around 30nm. The chemistry and the structure on the mesoscopic scale is controlled by AES, SEM and AFM. In a final step, after bonding the structures, computer-controlled electromigration is performed using a high precision current source. For excluding thermal mobility and reducing the breakdown speed, the sample has been cooled down to LN₂ temperature. As revealed from I-V characteristics, gaps of around 1nm are formed.

O 29.5 Wed 14:30 P2

Preparation of metal nanodroplets and solidification under zero-g conditions — ●ANJA HABENICHT, PAUL LEIDERER, and JOHANNES BONEBERG — Universität Konstanz, Fachbereich Physik, LS Leiderer, 78457 Konstanz

Flat metal nanostructures on inert substrates (e.g. glass) are illuminated by single intensive laser pulses with fluences above the melting threshold. The liquid structures produced in this way are far from their equilibrium shape and a dewetting process sets in. On a timescale of a few nanoseconds the liquid contracts toward a sphere. During this contraction the center of mass moves upward, which can lead to detachment of droplets from the surface due to inertia. The velocity of the detaching nanodroplets is measured with a light barrier technique and compared with the velocity deduced from simple estimations for the dewetting process [1].

Further we show impact experiments where the droplets are landed on another substrate. The particles cool down during the flight due to thermal radiation. They solidify either during flight or when impacting on the substrate. By catching at different distances, the landing temperature and thus, if still liquid, the time on the substrate while liquid can be varied. Snapshots of different stages of droplet impact are shown.

[1] A. Habenicht, M. Olapinski, F. Burmeister, P. Leiderer, J. Boneberg. Science 309 (2005) 2043

O 29.6 Wed 14:30 P2

Double layers from polycyclic aromatic hydrocarbons as studied by STM and STS — ●MIN AI¹, FRANK JÄCKEL¹, JI SHAN WU², KLAUS MÜLLEN², and JÜRGEN P. RABE¹ — ¹Humboldt University Berlin, Department of Physics, Newtonstr. 15, 12489 Berlin — ²Max-Planck-Institut für Polymerforschung, Ackermannweg 10, 55128 Mainz

We present the investigation of functionalized hexa-perihexabenzocoronenes (HBC) by scanning tunneling microscopy (STM) and spectroscopy (STS) at the liquid-solid interface. For star-shaped HBC derivatives different mono- and double layer structures were observed depending on the solvent that can be incorporated [1]. For composites of electron rich HBC derivatives (donors) with electron acceptors different architectures were observed, some of which can be solved with atomic precision using as additional information the spectroscopic data obtained from STS [2]. The potential for prototypical single-molecule electronic devices is discussed.

[1] Jäckel, F.; Ai, M.; Wu, J.; Müllen, K.; Rabe, J.P. *J. Am. Chem. Soc.* 2005, 127, 14580. [2] Jäckel, F.; Watson, M.D.; Müllen, K.; Rabe, J.P. submitted.

O 29.7 Wed 14:30 P2

Lithographic Fabrication of Clean Nanostructures by Means of Electron-Beam Induced Deposition (EBID) — ●M. SCHIRMER, T. LUKASCZYK, H. MARBACH, and H.-P. STEINRÜCK — Universität Erlangen-Nürnberg, Lehrstuhl für Physikalische Chemie II, Egerlandstraße 3, D-91058 Erlangen, Germany

EBID is the electron induced decomposition of chemical compounds and the resulting deposition of the non-volatile fragments. By utilizing a sharp spot of electrons well defined deposit structures in the nanometer range can be achieved in a controlled manner. A common difficulty is the contamination of the deposits due to e.g. residual gases. To avoid this problem an ultra high vacuum chamber is utilized. The integrated UHV electron column creates an electron-beam approximately 2 nm in diameter. This instrument in combination with a lithographic package enables the controlled fabrication of clean nanostructures via EBID. For the characterization of the obtained structures the following probe techniques are housed in the same UHV chamber: scanning tunnelling microscopy, scanning Auger electron microscopy and scanning electron microscopy. To generate pure carbon structures the hydrocarbon ethylene (C_2H_4) is tested. Other promising candidates for EBID are chemical compounds like silane (SiH_4), metal hydrides or organometallic compounds. The concept of the project and first results will be discussed.

O 29.8 Wed 14:30 P2

Influence of pulsed laser light on gold triangles: Experiment vs. theory — ●JULIANE KÖNIG-BIRK¹, KEVIN SHUFORD², GEORGE SCHATZ², JOHANNES BONEBERG¹, and PAUL LEIDERER¹ — ¹Fachbereich Physik, LS Prof. Dr. Leiderer, Universität Konstanz, 78457 Konstanz — ²Chemistry Department, Northwestern University

The optical properties of nanostructures are a topic of current investigations. In analogy to the near-fields around a Hertz dipole we expect near-fields in the surrounding of all nanostructures. To visualize these near-fields we use a method called "optical near-field photography". In our experiments we use e.g. silicon as substrate. The nanostructures, in this case gold triangles, on the substrate are illuminated with femtosecond laserpulses. The intensity is adjusted such that no influence of the illumination is detectable on the bare substrate. When illuminating ARRAYS of nanostructures we observe ablation of the substrate below the gold triangles due to the local intensity enhancement in the optical near-field. Depending on the polarization of the laser light, two or one corner of the triangle show ablation holes. In contrast to simulations on single triangles these effects are rotated at 90°. When illuminating SINGLE nanostructures we observe good agreement with the simulation.

O 29.9 Wed 14:30 P2

Fabrication of Gold Nanoparticles using Nanosphere Lithography in Combination with Laser Tailoring — ●RODICA MORARESCU, FRANK HUBENTHAL, and FRANK TRÄGER — Institut für Physik and Center for Interdisciplinary Nanostructure Science and Technology- CINSaT, Universität Kassel, Heinrich-Plett Strasse 40

In order to overcome the classical limits of silicon technology the use of molecular circuits is a challenging new possibility. The idea behind this is to use molecular wires as active elements, thus reducing circuit dimensions to the molecular scale. As a possible approach to realize such structures, we describe exploratory experiments for the preparation of regular arrays of metal nanoparticles by nanosphere lithography (NSL) and their exploitation as anchor points for the formation of uni- and bidirectional molecular nanowires with a high degree of lateral orientation. Depending on the molecular species and length of the nanowires to be oriented on a substrate surface, the distance between the metal nanoparticles as well as their size and shape have to be chosen independently. For these purpose we apply nanosphere lithography in combination with laser based tailoring of the dimensions of the nanoparticles. In the past we have already achieved laser manipulation of the size and shape of gold and silver nanoparticles. Here we have further produced hexagonally close packed monolayers of latex spheres by the tilt coating method, gold atoms being deposited using electron beam evaporation under ultra high vacuum conditions. An array of triangularly shaped gold nanoparticles remains on the substrate, after the mask is removed. Subsequently, the interparticle spacing and particle shape are varied by laser tailoring.

O 29.10 Wed 14:30 P2

IR-spectroscopy of Pb films and nanowires — ●F. KOST¹, T. KOLB¹, R. LOVRINCIC¹, F. NEUBRECH¹, A. PUCCI¹, M. JALOCHOWSKI², and G. FAHSOLD¹ — ¹Kirchhoff-Institut für Physik, Ruprecht-Karls-Universität, 69120 Heidelberg, Germany — ²Institute of Physics, Maria Curie-Skłodowska University, 20031 Lublin, Poland

The conductivity of metal films and nanowires can be specified via IR spectroscopic measurements which allow analysing these structures in a non-contact mode. The experimental setup enables in-situ investigation in an UHV chamber and therefore, the growth during lead evaporation to a silicon substrate can be investigated. Since the mean free path of electrons at Fermi energy and at room temperature for lead is roughly ten nanometers, classical size effects occur as the film thickness is of this order of magnitude. Quantum size effects are expected as well since the diameter of the nanostructure reaches the range of several ten times the Fermi wavelength [1]. Using a model for charge transport, we describe the measured spectra and explore the development of relaxation rate and plasma frequency and hence get information about scattering effects, band structure and film morphology [2]. In order to obtain nanowires for IR spectroscopic studies, lead is evaporated onto a single-domain stepped silicon substrate. Thereby, solid like nanowires of Pb align parallel to the step edges of the silicon due to self-organization processes [3].

[1] Trivedi, N. and Ashcroft, N.W., *Phys. Rev. B* 38 (1988), 12298 [2] G. Fahsold and A. Pucci, *Adv. in Solid State Physics*, Vol. 43, ed. by B. Kramer (Springer, 2003) 833. [3] M. Jalochowski, M. Strozak, R. Zdyb, *Appl. Surf. Sci.* 211 (2003) 209-215.

O 29.11 Wed 14:30 P2

Angle-resolved photoelectron spectroscopy on self-assembled dysprosium-silicide nanowires on vicinal Si(001) — ●SYLVIA HAGEDORN¹, MARTINA WANKE¹, GERD PRUSKIL¹, MARIO DÄHNE¹, DENIS VYALIKH², FRIEDRICH SCHILLER², SERGEIJ MOLODTSOV², and CLEMENS LAUBSCHAT² — ¹Institut für Festkörperphysik, Technische Universität Berlin, D-10623 Berlin — ²Institut für Festkörperphysik, Technische Universität Dresden, D-01219 Dresden

Rare-earth silicide nanowires attract considerable interest due to their simple preparation and their anisotropic electronic properties. We report on angle-resolved photoelectron spectroscopy investigations of the electronic structure of dysprosium-silicide nanowires on vicinal Si(001) surfaces at BESSY II. Two types of nanowires are found depending on the specific preparation conditions. Different electronic properties of these nanowires depending on the wiretype will be presented. In nanowire direction strongly dispersing bands are found crossing the Fermi energy, while also a slight dispersion in perpendicular direction will be discussed in detail. Hence dysprosium-silicide nanowires could be interesting for contacting devices in future nanocircuit technologies.

This project was supported by DFG, project number DA 408/11.

O 29.12 Wed 14:30 P2

Electrochemically Fabricated Nanoscale Copper Wires: Investigation of Wire Morphology and Composition — ●THOMAS KOCH^{1,2}, SHENG ZHONG^{1,2}, EBERHARD NOLD³, TORSTEN SCHERER², HARALD ROESNER², HORST HAHN², STEFAN WALHEIM², MU WANG⁴, and THOMAS SCHIMMEL^{1,2} — ¹Institute of Applied Physics, University of Karlsruhe, D-76128 Karlsruhe, Germany — ²Institute of Nanotechnology (INT), Forschungszentrum Karlsruhe, D-76021 Karlsruhe, Germany — ³Institute for Materials Research I (IMF I), Forschungszentrum Karlsruhe, D-76021 Karlsruhe, Germany — ⁴National Laboratory of Solid-State Microstructures, Nanjing University, Nanjing 21009, China

Metallic nanostructures, especially made from copper, have attracted considerable attention in recent years due to their potential use both as interconnects and as components for future generations of electronics. Here we report on the investigation of electrochemically self-assembled copper wires by SEM, TEM and SAMS. The wires were found to be straight, regular, without branches and more than 100 micrometer long. These wires align spontaneously to form ordered arrays, covering the insulated substrate in large numbers. The thickness of the wires can be controlled by the experimental parameters down to 120 nm. The SAMS results show that the investigated stable structures consist of pure copper. The TEM results point out that the wires consist of stacked single crystalline copper lamellae, which have a thickness of down to a few monolayers. The SAMS depth profiles show that the wires are surrounded by an oxide layer with a thickness of less than 15 nm.

O 29.13 Wed 14:30 P2

Crescent-shaped noble-metal structures: preparation, optical properties and applications — ●NOELIA BOCCHIO, HEIKO ROCHHOLZ, JENIFFER SHUMAKER-PARRY, NATALIE HORN, and MAXIMILIAN KREITER — Max Planck Institut für Polymerforschung, Ackermannweg 10, D-55128, Mainz, Germany

Crescent-shaped metallic nanoparticles in the 60 nm - 400 nm size range were developed applying a combination of nanosphere lithography, metal deposition and ion-milling techniques. They were characterized by scanning electron microscopy and UV-Vis/NIR extinction spectroscopy (1). As expected from the symmetry of the system, the structure exhibits different responses to illumination polarised along the two symmetry axes. For both cases, distinct resonances are observed. A systematic study of the impact of variations of the most relevant geometrical parameters on the optical response is presented.

In the search for an explanation of these experiments and a full understanding of the optical response of the system, a first approach to the resonant responses through a simplified multipole model is presented and discussed.

Finally, single entity scattering and fluorescence measurements on the particles are introduced, laying the basis for applications in near-field enhanced spectroscopy.

(1) Adv. Mater. , 2005, 17, 2131 - 2134

O 29.14 Wed 14:30 P2

Surface Plasmon Polariton excitation on gratings with tunable grating constant — ●MICHAEL BERNDT^{1,2}, STEPHANIE REHWALD^{1,2}, FRANK KATZENBERG³, KLAUS SCHIERBAUM², and DOMINIC ZERULLA¹ — ¹UCD Dublin, School of Physics, Dublin 4, Ireland — ²Heinrich-Heine-Universität Düsseldorf, Materialwissenschaft, 40225 Düsseldorf, Germany — ³Universität Dortmund, Werkstoffe und Korrosion, 44227 Dortmund, Germany

For the excitation of Surface Plasmon Polaritons (SPP) grating couplers with tunable periodicity have been developed. Since the excitation of SPPs for a given grating period is restricted to a single, fixed wavelength at a certain angle of incidence, the possibility of adjusting the grating period provides much more flexibility to match resonance conditions, e. g. with respect to changes in the excitation wavelength.

Therefore the polymer based gratings present a well adapted substrate for extremely surface sensitive spectroscopic methods like Surface Plasmon Resonance (SPR) or Surface Enhanced Raman Scattering (SERS). The grating coupler consists of a polymer base upon which a sinusoidal structure is generated. Subsequently, the system is coated with a suitable metal (e.g. silver, gold, or aluminium).

Even though the metal stripes are separated by a nonconducting polymer, a strong surface plasmon resonance is observed. The experimentally obtained SPP dispersion relation is in good agreement with theoretical predictions with respect to an effective dielectrical constant for the metal-polymer surface.

O 29.15 Wed 14:30 P2

Optical Effects of Surface Plasmons Confinement in Planar Nanoparticles — ●MANUEL GONÇALVES, ANDRÉ SIEGEL, and OTHMAR MARTI — Department of Exp. Physics, University of Ulm, D-89069 Ulm, Germany

The scattering of light by metallic nanoparticles and nanostructures is intimately related with the surface plasmon-polaritons (SPP). Material, shape and size of the particles influence the confinement of the SPPs and their resonances. When the k-vector of the SPPs and the k-vector of light match a radiative process occurs. Small particles of the size of the wavelength, with sharp corners and edges, generate scattered waves with large k-vector and, therefore, are appropriate to study the scattering of light by SPPs.

We have investigated arrays of planar metallic particles of triangular shape, with different thicknesses and of different materials. The optical far-field characterization was done using a Total-Internal-Reflection illumination setup and a confocal microscope. The near-field was investigated using a SNOM microscope in illumination mode. It was observed that the scattering of laser light is strongly dependent on the material of the particle, on its orientation and on the polarization of light. We present an overview of the optical effects observed.

O 29.16 Wed 14:30 P2

Observation of Ferromagnetic Coupling in Eu/Gd(0001) by Spin-Resolved Photoelectron Spectroscopy — ●YURY DEDKOV¹, ELENA VOLOSHINA², THOMAS KLEISSNER¹, STEFFEN DANZENBAEHER¹, SERGUEI MOLODTSOV¹, and CLEMENS LAUBSCHAT¹ — ¹Institut für Festkörperphysik, Technische Universität Dresden, 01062 Dresden, Germany — ²Max-Planck-Institut für Physik komplexer Systeme, Nöthnitzer Str. 38, 01187 Dresden, Germany

We report on a magnetic analysis by means of spin-resolved photoelectron spectroscopy of an atomically flat heteromagnetic rare-earth interface of 1 ML Eu/Gd(0001). The measurements reveal a high net Eu magnetization at low temperatures reflected by a spin polarization of about +15% of the Eu 4f state. This magnetic Eu configuration is due to a strong ferromagnetic interlayer exchange coupling across the Eu/Gd interface which overcomes a weak negative intralayer coupling between Eu spins in the hexagonal two-dimensional lattice.

O 29.17 Wed 14:30 P2

Optical properties of ultrathin magnetic layers on Cu(110) — ●RICHARD DENK, ROBERT MITTERMAIR, MICHAEL HOHAGE, LIDONG SUN, and PETER ZEPPENFELD — Institut für Experimentalphysik, Johannes Kepler Universität Linz, A-4040 Linz, Austria

Magnetic thin films of Ni and Co on Cu(110)(2x1)O have been studied by means of Reflectance Difference Spectroscopy (RDS). The regular optical anisotropy signal has been used to monitor the morphology of the Co and Ni films during growth. In addition the magnetization of these films has been addressed by the RD-spectrometer via Magneto-Optical Kerr Effect (MOKE) measurements [1]. To perform the magnetic measurements the UHV chamber is equipped with an in-situ electromagnet. The present RD-MOKE setup allows conducting spectroscopic measurements of the magnetization of the films at photon energies between 1.5 eV and 5.5 eV. By applying the RD-technique at opposite magnetization (M^+ , M^-) of the film, the optical anisotropy signal $(\Delta r/r(M^+) + \Delta r/r(M^-))/2$ can be separated from the MOKE signal $(\Delta r/r(M^+) - \Delta r/r(M^-))/2$. Hysteresis curves at any desired photon energy between 1.5 eV and 5.5 eV can be recorded online. For characterization of the film morphology, the chamber is equipped with a STM and a LEED/AES system. A major focus of the study has been the temperature dependence of the magnetization of Ni on the oxygen precovered Cu(110) surface, as well as the way how the remanent polar magnetization develops within the ultrathin Ni films. References [1] M. Wahl, Th. Herrmann, N. Esser, and W. Richter, phys. stat. sol. 0, 3002 (2003)

O 29.18 Wed 14:30 P2

Monte Carlo simulations of small transition metal oxide clusters: a comparison of numerical efficiency — ●RALF GEHRKE and KARSTEN REUTER — Fritz-Haber-Institut, Faradayweg 4-6, D-14195 Berlin, Germany

Structural information is a key prerequisite to understand the peculiar chemical, optical, magnetic and materials properties of small transition metal oxide clusters. This concerns not only the ground state structure, but also all lowest-energy isomers within a thermally accessible energy range. Identification of these states requires proper sampling of the vast configurational space, suitably carried out by Monte Carlo (MC) based schemes. In order to make such simulations quantitative, they have to be based on reliable first-principles energetics, e.g. from density-functional theory. Due to the high computational cost of the latter techniques, utmost efficiency of the MC algorithms in terms of energy and force calls is mandatory.

As a prelude to targeted first-principles MC simulations, we therefore assess and optimize the efficiency of different MC schemes like basin hopping [1] or Wang-Landau sampling [2]. As representative test systems we use M_3O , M_5O_3 and M_7O_7 ($M = Ru, Pd$) oxide clusters described by a model Lennard-Jones potential. Since the evaluation of forces in first-principles methods is computationally more expensive than the calculation of energies, special emphasis is put on minimizing the number of required structural relaxations in the MC algorithms.

[1] D. Wales *et al.*, Science **285**, 1368 (1999).

[2] M. Scott Shell *et al.*, Phys. Rev. E **66**, 056703 (2002).

O 29.19 Wed 14:30 P2

DFT-Investigations of Coalescence Behaviour of small magic Si Clusters on Surfaces — ●WOLFRAM QUESTER and PETER NIELABA — Fachbereich Physik, Universität Konstanz, 78457 Konstanz

Experimental results indicate that small magic Si clusters do not form islands of bulk Si on weakly interacting surfaces (HOPG). For Si₄ this was confirmed in earlier calculations [1].

These investigations were extended to Si₇. Potential energy curves of two approaching Si₇ clusters were calculated for different reaction channels using Density Functional Theory implemented in the CPMD code available at [2]. It could be shown that there are fusion barriers higher than room temperature. This can be understood looking at the distribution of the electron density in the clusters.

The next step will be to model the graphite surface and investigate their influence on the cluster energetics.

[1] M. Grass, D. Fischer, M. Mathes, G. Ganteför and P. Nielaba, *Appl. Phys. Lett.*, **81**, 3810 (2002)

[2] www.cpmd.org

O 29.20 Wed 14:30 P2

Investigation of the morphology and electronic properties of small gold clusters and the impact of different organic ligands — ●MATHIS GRUBER^{1,2}, GEORG HEIMEL², LORENZ ROMANER^{1,2}, JEAN-LUC BRÉDAS², and EGBERT ZOJER^{1,2} — ¹Institute of Solid State Physics, Graz University of Technology, Petersgasse 16, A-8010 Graz, Austria — ²School of Chemistry and Biochemistry and Center for Organic Photonics and Electronics, Georgia Institute of Technology, Atlanta, Georgia 30332-0400

The synthesis and characterization of small metal clusters, both neutral and charged, have been the focus of vast experimental and theoretical efforts. Recently, small noble-metal clusters coated with a shell of organic ligands have received a lot of attention in the context of nanotechnology and molecular electronics. The motivation for the present theoretical study is to gain a basic understanding of the electronic structure of gold nanoclusters, its dependence on the geometric shape of the clusters, and the modification induced by organic ligands covalently bound to the particles. To that end, we performed density functional theory calculations on small gold clusters. We employed quantum-mechanical molecular dynamics simulations in order to find favored (low-energy) geometric structures with and without symmetry constraints. For all conformations, we performed a detailed analysis of the electronic properties focusing on the relation between morphology and total electronic spin. When studying clusters bearing conjugated organic ligands, we paid particular attention to the alignment of their molecular levels relative to the quasimetallic states of the gold nanoparticles.

O 29.21 Wed 14:30 P2

Calculation of radiation damping of plasmons in prolate gold nanoparticles — ●CHRISTIAN DAHMEN, STEFAN BECKER, and GERO VON PLESSEN — Nanostructure Optics Group, I. Physikalisches Institut (IA), RWTH Aachen, 52056 Aachen

Plasmon resonances of non-spherical noble-metal nanoparticles are of interest for possible applications in plasmon-enhanced spectroscopy, such as surface-enhanced Raman scattering. Theoretical work has mainly focussed on calculating the spectral position of the plasmon resonance and the optical field enhancement for irregularly shaped particles. In this work, we discuss how the radiation damping rate of prolate spheroidal gold nanoparticles depends on volume and shape of the particles. The separation of variables method [1] is employed to calculate their scattering cross sections. The contribution of the radiative plasmon decay to the total linewidth of the plasmon resonance is determined. We find that the radiative decay rate depends sensitively on both the particle volume and the aspect ratio.

[1] S. Asano and G. Yamamoto, *Appl. Opt.* **14**, 29-49 (1975)

O 29.22 Wed 14:30 P2

Fabrication and characterization of gold nanocrystals for use as probes in the diffracted x-ray tracking technique — ●ARMIN BRECHLING, JAWAD SLIEH, WIEBKE HACHMANN, ULF KLEINEBERG, and ULRICH HEINZMANN — University of Bielefeld, Molecular and Surface Science, D-33615 Bielefeld

Diffracted x-ray tracking (DXT), a new single molecule experiment, uses x-rays to monitor the rotating motions of a labeled nanocrystal. This technique has the potential to resolve intramolecular conformation changes in the scale of few picometers with a time resolution in the ms interval [1].

For this technique it is essential to prepare stable, highly ordered nanocrystals. Further it is advantageous to use a biocompatible material. Gold is a suitable material in biophysical studies because it can

be directly linked to the thiol groups of cystein in protein molecules [2].

We report the fabrication of dispersive gold nanocrystals using a vacuum evaporation technique. Gold has been evaporated under ultra high vacuum conditions on a freshly cleaved NaCl (100) surface at a substrate temperature of approximately 350°C. The substrate with the gold layer, grown in an island-type structure, was subsequently dissolved in an aqueous CHAPS-solution in order to get dispersed gold crystals.

The gold nanocrystals have been characterized by means of different techniques such as Atomic Force Microscopy (AFM), Transmission Electron Microscopy (TEM) and X-Ray Diffraction (XRD).

[1] Y. C. Sasaki et al. *Phys. Rev. Lett.* **87** (2001) 248102-1

[2] Y. C. Sasaki et al. *Biophys. J.* **72** (1997) 1842

O 29.23 Wed 14:30 P2

Scanning Tunnelling Microscopy and Photoemission of Clusters at Surfaces — ●MARKUS BIELETZKI¹, THOMAS IRAWAN¹, STEFANIE KRAUSE¹, HEINZ HÖVEL¹, CHUNRONG YIN², and BERND VON ISSENDORFF² — ¹Universität Dortmund, Experimentelle Physik I, 44221 Dortmund, Germany — ²Universität Freiburg, Fakultät für Physik, 79104 Freiburg, Germany

We study the electronic structure of cluster/surface systems and the nature of charge transfer processes between the cluster and the surface. STM/STS and UPS on size selected large clusters in contact with a surface will be combined with photoelectron spectroscopy on the same clusters in the gas phase. The direct comparison of the three different techniques is expected to improve the understanding of the cluster-surface interaction. For metal islands (gold and lead) on different surfaces (HOPG, Au(111) and Pb(111)) the electronic coupling to the surface and charging effects in the photoemission process were studied with UPS. We observed significant energetic shifts if the islands were decoupled from the surface by a thick rare gas layer and different materials for the substrate and the islands were used [1]. C₆₀ is a promising model system for STS on clusters at surfaces.

[1] T. Irawan, D. Boecker, F. Ghaleh, C. Yin, B. v. Issendorff and H. Hövel, "Metal Clusters on Rare Gas Layers - Growth and Spectroscopy", *Appl. Phys. A* (published online Sept. 2005)

O 29.24 Wed 14:30 P2

Oxidation of Au/Ag-nanoparticles and clusters on HOPG/SiO₂ surfaces — ●RAINER DIETSCHKE, DONG CHAN LIM, MORITZ BUBEK, IGNACIO LOPEZ-SALIDO, YOUNG DOK KIM, and GERD GANTEFÖR — Fachbereich Physik, Universität Konstanz, 78464 Konstanz

Au nanostructures were prepared on HOPG and SiO₂ surfaces. Size distribution was studied using STM. Oxidation and reduction of the particles was performed with atomic oxygen and carbonmonoxide under UHV conditions. XPS spectra of the Au 4f level show different behaviour depending on particle size.

On HOPG Au nanoparticles smaller than ~10 nm two different oxygen species were detected, suggested to be Au-oxide and subsurface oxygen. Both species show different reactivity towards CO.

On silica layers the oxidation/reduction behaviour of Au nanoparticles show a strong size dependency. Larger particles exhibit additional features of the Au 4f level. Whereas particles smaller than ~7 nm in height show a much less reactive type of Au-O bond.

Au and Ag clusters were deposited and studied with the same method. Small Au clusters on SiO₂ show a significant even-odd size dependency in CO oxidation.

[1] Lim, Lopez-Salido, Dietschke, Bubek and Kim, *Oxidation of Au nanoparticles on HOPG using atomic oxygen*, accepted for publication in *Surface Science*, 2005

[2] Lim, Lopez-Salido and Kim, *Size-selectivity for CO-oxidation of Ag nanoparticles on HOPG*, *Surface Science*, available on-line

[3] Lopez-Salido, Lim and Kim, *Surface Science*, **588** (1-3) 6-18, 2005

O 29.25 Wed 14:30 P2

Mo_nS_m- and W_nS_m-clusters: Nano-platelets and nano-wires — ●WILKO WESTHÄUSER, TIM FISCHER, NILS BERTRAM, JÖRN CORDES, RAINER DIETSCHKE, MORITZ BUBEK, and GERD GANTEFÖR — University of Konstanz, Department of Physics, D-78457 Konstanz

Clusters of the layered semiconductor materials MoS₂ and WS₂ may form fullerenes similar to carbon. Therefore, we used gas phase mass and photoelectron spectroscopy in combination with Density Functional Theory calculations in order to investigate small Mo_nS_m- and W_nS_m-clusters. E. g. the Mo₄S₆-clusters revealed a large HOMO-LUMO gap

(about 2eV) indicating to be a so-called “magic cluster” with a high stability and chemical inertness [1,2].

In mass spectra of $Mo_nS_m^-$ and $W_nS_m^-$ clusters with $n>5$ atoms the theoretically predicted stable 2-d triangular platelet structures were detected and 1-d chain-like clusters of the stoichiometry $Mo_{3n}S_{3n+2}$ were identified and characterised with PES. In addition, selected clusters were deposited in soft-landing mode on HOPG-, Au- and Ag- substrates in order to study the interaction of the clusters with the metal surfaces via XPS, AES and HREELS.

[1] N. Bertram, Y. D. Kim, G. Ganteför, Q. Sun, P. Jena, J. Tamuliene and G. Seifert, Chem. Phys. Lett. 396, 341 (2004).

[2] S. Gemming, J. Tamuliene, G. Seifert, N. Bertram, Y. D. Kim and G. Ganteför, Applied Physics A (2005), online available.

O 29.26 Wed 14:30 P2

Preparation of bimetallic AuAg/TiO₂ model catalysts — ●C. WEILACH, S. KIELBASSA, J. BANSMANN, and R.J. BEHM — Dept. of Surface Chemistry and Catalysis, University of Ulm

Studies on powder catalysts revealed, that using AuAg bimetallic particles instead of monometallic particles on metal oxides may enhance the performance and the stability of the catalytic system. Exploiting model catalysts with nm-sized bimetallic particles on flat TiO₂(110) single crystal surfaces will give new insights on the significance of particle composition and size with respect to catalyst activity and stability. Therefore, we examined the growth of AuAg nanoparticles by subsequent evaporation and the influence of substrate temperature and evaporation order on this process. Furthermore we developed a new preparation method resulting in samples with metal particles of different composition. This creates the opportunity to investigate the morphology with AFM and the catalytic activity with a newly designed scanning-mass spectrometer setup at chemically different regions on one substrate.

O 29.27 Wed 14:30 P2

Particle removal by laser-induced acoustic waves — ●TOBIAS GELDHAUSER, FLORIAN ZIESE, JOHANNES BONEBERG, and PAUL LEIDERER — University of Konstanz, Fach M676, Universitaetsstrasse 10, 78457 Konstanz

Different approaches can be used for particle removal from surfaces like ultra-/megasonics or Dry / Steam Laser Cleaning. Here we analyze an alternative approach where a laser pulse hits the back of a wafer and thereby initiates a bulk acoustic wave which travels towards the wafer surface, leading to surface displacements and particle removal. We relate the cleaning efficiency for colloidal contaminants of different diameters (measured by light scattering) to the surface expansion, and hence the acceleration, which is measured with a ns-time-resolved Michelson Interferometer. Furthermore the backside configuration is modified by sacrificial layers in order to enhance the intensity of the acoustic wave.

O 29.28 Wed 14:30 P2

Studying the dewetting behaviour of Ni-films on oxidized Si(001) by GISAXS — ●F. GARONE¹, ANDREA TOMA¹, FRANCESCO BUATIER¹, CORRADO BORAGNO¹, UGO VALBUSA¹, IAN K. ROBINSON², WEI ZHANG², NICOLE M. JEUTTER³, and ROBERTO FELICI³ — ¹Dipartimento di Fisica, Università di Genova, via Dodecaneso 33, 16146 Genova, Italy — ²Department of Physics, University of Illinois at Urbana-Champaign, 1110 West Green Street, Urbana, IL 61801-3080, USA — ³ESRF, 6 Rue Jules Horowitz, 38000 Grenoble France

The development of materials with new electronic and/or chemical properties is pushing the research through the study of nano-objects. For obtaining surfaces with morphology features on the nano-meters scale, we can take advantage of self-aggregation phenomena, which is generally easier to integrate in industrial processes. However the size uniformity and control, they offer, are more complex. A method for obtaining metal nano-objects at the surface of oxides is based on dewetting phenomena. In this case a thin metal film grown on an inert substrate is heated up at high temperatures, until the surface tension of the metal becomes higher than the adhesive force of the film onto the substrate. At this point the metal forms small droplets. In this study we present real-time in-situ studies of the nucleation and formation of Ni metal clusters starting from an uniform metal film deposited on an oxidized Si(001) substrate. Films of different thicknesses have been annealed at different temperatures in the range 400-800 K. By following in time the evolution of the grazing incidence small angle scattering pattern we gained unique information on the dynamics at the base of the nano-particles formation.

O 29.29 Wed 14:30 P2

Femtosecond Pump-Probe Measurements of Silver Nano-Clusters on Quartz (0001) — ●ALEXANDER GRUJIC, KONRAD VON VOLKMANN, and MARTIN WOLF — Fachbereich Physik der Freien Universität Berlin, Arnimallee 14, 14195 Berlin

We have measured the energy relaxation of supported silver nano-clusters by time resolved transient absorption spectroscopy. The clusters are prepared in UHV via VOLMER-WEBER growth by evaporation of silver on a single crystal quartz (0001) sample at room temperature, resulting in a mean cluster size of ≈ 12 nm. The sample was excited by 400-nm pump pulses with 40-fs duration, and the transmission was probed with a beam of the same wavelength. In-situ temperature, size and fluence dependent transmission measurements have been performed and a fast ($\approx 2 \dots 3$ ps) and a slow (≈ 150 ps) decay channel have been identified. They are attributed to the electron-phonon relaxation within the silver cluster and the much slower heat transfer of the cluster lattice to the quartz substrate.

O 29.30 Wed 14:30 P2

Oxidation of electrochemically deposited nanocrystalline aluminium — ●FABIAN BEBENSEE^{1,2}, WOLFGANG MAUS-FRIEDRICHS¹, and FRANK ENDRES² — ¹Institut für Physik und Physikalische Technologien, TU Clausthal, Leibnizstr. 4, D-38678 Clausthal-Zellerfeld — ²Institut für Metallurgie, TU Clausthal, Robert-Koch-Str. 42, D-38678 Clausthal-Zellerfeld

The applicability of nanocrystalline aluminium in semiconductor devices and corrosion protection is crucially dependent on the oxidation behaviour and interaction of nanocrystalline aluminium with molecules from the ambient atmosphere. Nanocrystalline aluminium with grain sizes around 20 nm was deposited onto Si(100)substrates via electrodeposition in the ionic liquid 1-butyl-1-methylpyrrolidinium-bis(trifluoromethylsulfonyl)imide, saturated with anhydrous AlCl₃. The interaction of nanocrystalline aluminium with oxygen was studied with Metastable Impact Electron Spectroscopy (MIES), Ultraviolet Photoelectron Spectroscopy (UPS) and X-Ray Photoelectron Spectroscopy (XPS). The oxidation behaviour of nanocrystalline aluminium is compared to the oxidation behaviour of aluminium films prepared by physical vapour deposition (PVD). The topography of the films being strongly dependent on the deposition parameters was investigated with microscopic techniques.

O 29.31 Wed 14:30 P2

Non-Destructive Trace Element Analysis of Presolar Stardust via XANES-PEEM — ●THOMAS BERG¹, PASQUAL BERNHARD¹, JOCHEN MAUL¹, NICOLE ERDMANN², CHRISTA SUDEK³, ULRICH OTT³, and GERD SCHÖNHENSE¹ — ¹Universität Mainz, Institut für Physik, D-55099 Mainz — ²Universität Mainz, Institut für Kernchemie, D-55099 Mainz — ³Max-Planck-Institut für Chemie, D-55128 Mainz

Meteorites contain small amounts of presolar dust that survived the formation of the solar system without being affected by the isotope homogenisation. Therefore the isotopic composition not only of bulk elements, but also of trace elements(1) is anomalous. Isotopic analysis via SIMS(2) / RIMS(3) often reveals the fingerprint of the nucleosynthetic s-process that occurred in the grain's origin star. The disadvantage of SIMS/RIMS, however, is that only a small number of isotopes can be investigated, because the sample grain is being destroyed. We present non-destructive synchrotron based XANES measurements using PEEM. Prior to isotopic analysis this technique is suitable for identification of interesting trace elements present in single stardust grains. In addition, XANES-PEEM provides information on the chemical environment in which the different elements occur within the particles. Supplementing TOF-SIMS measurements(4) confirming the XANES-PEEM results are also presented.

- (1) E.Zinner, Annu.Rev.Earth Planet.Sci.26(1998)147
- (2) K.K.Marhas, P.Hoppe, U.Ott, Meteorit.Planet.Sci.38(2003)A58
- (3) M.R.Savina et al., Geochim.Cosmichim.Acta67(2003)3201
- (4) T.Stephan, Planetary Space Sci.49(2001)859

O 29.32 Wed 14:30 P2

A Scanning Probe Microscope (SPM) with quasi in-situ Sample Treatment Capabilities — ●MARKUS HUND¹ and HANS HEROLD² — ¹Physikalische Chemie II, Universität Bayreuth, D-95440 Bayreuth — ²Elektronikwerkstatt der Universität Bayreuth, D-95440 Bayreuth

State-of-the-art SPMs have limited *in-situ* sample treatment capabilities. Aggressive treatments like plasma etching or etching in aggressive

liquids typically require to remove the sample from the microscope. In consequence, time consuming procedures are required if the same spot of the sample is to be imaged after successive processing steps. We have developed a first prototype of an SPM with quasi *in-situ* sample treatment capabilities based on a commercial atomic force microscope (AFM; Model Dimension 3100, Veeco Instruments Inc.). A sample holder is positioned in a special reactor chamber. The tip can be retracted by several millimeters such that the chamber can be closed for sample treatment. Most importantly, after the treatment the tip is moved back to sample with a lateral drift per process step in the 20 nanometer regime. We discuss recent experiments involving consecutive plasma etching of nanostructured polymer films.

O 29.33 Wed 14:30 P2

Two dimensional dopant profiling of semiconductor microdevices with high spatial resolution using High Speed Scanning Capacitance Spectroscopy — •MARTIN VON SPREKELSEN and ROLAND WIESENDANGER — University of Hamburg, Institute of Applied Physics and Microstructure Research Center, Jungiusstrasse 11, D-20355 Hamburg, Germany

For the analysis of semiconductor devices tools with high spatial resolution down to the nanometer scale become increasingly important. Scanning capacitance microscopy (SCM) is an established method to obtain 2D-dopant profiles of charge carrier concentrations. These profiles are usually taken at a constant bias voltage (V_{bias}).

However unavoidable side effects such as mobile surface charges or the strong influence of V_{bias} on the SCM profiles are limiting factors for the spatial resolution of SCM. To overcome these restrictions we modulate the V_{bias} voltage at a frequency in the kHz-range. The modulated electric field virtually traps mobile surface charges. We use High Speed Scanning Capacitance Spectroscopy (HSSCS) to obtain capacitance spectra for V_{bias} , by which we can analytically get rid of the influence of V_{bias} .

The method can be used on Si- and III-V-semiconductors. On ultrashallow junctions on Si-semiconductor samples a high spatial resolution down to 10 nm can be achieved. Examples of practical applications of HSSCS will be shown.

O 29.34 Wed 14:30 P2

Manipulation of nanometer-scale metallic islands in ultrahigh vacuum by dynamic force microscopy techniques — •DIRK DIETZEL¹, ANDRE SCHIRMEISEN¹, HARALD FUCHS¹, and UDO SCHWARZ² — ¹Institute of Physics, University of Münster, Münster, Germany — ²Department of Mechanical Engineering, Yale University, New Haven CT, USA

The fundamentals of friction are still insufficiently understood on the nanometer-scale. Recently, a new technique for systematic island manipulation using dynamic force microscopy (DFM) in air has been introduced by Ritter et al. [1], which allows the correlation between contact area, energy dissipation during motion, and crystalline structure. However, under ambient conditions, oxidation and contamination might influence the frictional properties of the interface. To avoid this, experiments have been performed entirely under UHV conditions. Metallic islands with diameters between 10-50 nm have been grown by thermal evaporation of aluminum on highly oriented pyrolytic graphite (HOPG). The experimental protocol by Ritter et al. was adapted to UHV conditions and frequency modulation detection by gradually reducing the frequency shift setpoint. This allows determining the threshold value for energy dissipation necessary to initiate manipulation. In addition, information about the dissipated energy can be obtained even during the lateral movement. First results show that the manipulation of the islands strongly depends on their size and on the strength of the interaction between the oscillating cantilever tip and the islands.

[1] Ritter et al., Phys. Rev. B 71, 085405 (2005)

O 29.35 Wed 14:30 P2

Design of a low temperature Tuning Fork Atomic Force Microscope combined with a Field Ion Microscope — •THOMAS KÖNIG¹, DANIEL BRAUN¹, JENS FALTER², ANDRÉ SCHIRMEISEN^{1,3}, HENDRIK HÖLSCHER³, MARCUS LIEBMANN⁴, UDO D. SCHWARZ², and HARALD FUCHS^{1,3} — ¹Institute of Physics, University of Münster, Münster, Germany — ²Department of Mechanical Engineering, Yale University, New Haven, CT, USA — ³Center of Nanotechnology (CeN-Tech), University of Münster, Münster, Germany — ⁴Institute of Physics, RWTH-Aachen, Aachen, Germany

The atomic force microscope (AFM) has been established as a tool for the imaging of surfaces with atomic resolution. However, an inter-

pretation of the forces which act between tip and surface atoms is only possible if the exact configuration of the tip apex atoms is known. The last atom layers of the tip can be analyzed by field ion microscopy (FIM). We have built a non-contact mode AFM by implementing a tuning fork as force sensor [1] in a low temperature, ultra high vacuum (UHV) design [2]. This setup allows us to choose an appropriate FIM material, such as tungsten for the tip, while maintaining atomic-scale resolution capabilities. The high stability of the setup has been proven by scanning tunneling microscopy investigations. Furthermore, we present a special home-built transfer design for the tuning fork exchange between the FIM and AFM chambers in the UHV system and first atomic resolution images of tungsten tips with the FIM are shown.

[1] F. J. Giessibl, Appl. Phys. Lett. 76 1470 (2000)

[2] W. Allers et al., Rev. Sci. Instrum. 69, 221 (1998)

O 29.36 Wed 14:30 P2

Towards Automatisation of Nanotomography Imaging — •CHRISTIAN DIETZ, NICOLAUS REHSE, MECHTHILD DÖRING, SABINE SCHERDEL, and ROBERT MAGERLE — Chemische Physik, TU Chemnitz, D-09107 Chemnitz

Nanotomography is a layer-by-layer imaging technique based on scanning probe microscopy. We present our approach to automate the process for successive etching and imaging. Thermal drift and non-linearities of the piezo scanners make it difficult to image exactly the same spot of the specimen. We correct this problem by applying an appropriate offset to the piezo scanners which is calculated from the offset between two successive images using the cross correlation coefficient. As an example, we image a thin film of polypropylene with tapping mode scanning force microscopy (SFM) and etch it successively with potassium permanganate. The etching and imaging is done *in-situ* in a liquid cell of a MultiMode SFM connected to reservoirs of etchants and water for flushing after each etching step. The flow of the different liquids is controlled with solenoid valves which allow for an automated measuring protocol. We will present first results and discuss our concepts for adjusting the imaging parameters to maintain a good imaging quality.

O 29.37 Wed 14:30 P2

Frequency Modulated Atomic Force Microscopy: Atomic Resolution and Force Spectroscopy — •GEORG SIMON, MARKUS HEYDE, HANS-PETER RUST, and HANS-JOACHIM FREUND — Fritz-Haber-Institute of the Max-Planck-Society, Faradayweg 4-6, D-14195 Berlin, Germany

Images with atomic resolution by frequency modulated atomic force microscopy (FM-AFM) on different materials have been presented. However, proper descriptions of the tip-sample interaction and contrast mechanisms are still under discussion. The understanding of these issues leads toward new insights of specific surface properties and to an extension of FM-AFM beyond topography measurements. In contrast to the simple relation connecting the static deflection of a cantilever to the interaction force, the corresponding relation for FM-AFM is significantly more complex and depends on both the spring constant and amplitude of oscillation. Here we present an experimental method for quantitative determination of the spring constant and the amplitude oscillation for a double tuning fork sensor operated at low temperature in ultra-high vacuum [1]. The quantitatively characterized measurements will be shown in combination with atomically resolved images.

[1] M. Heyde, M. Kulawik, H.-P. Rust, H.-J. Freund, Rev. Sci. Instrum. 75, 2446 (2004).

O 29.38 Wed 14:30 P2

Optimization of the preparation process for tips used in Scanning Tunneling Spectroscopy (STS) — •STEFAN ERNST¹, STEFFEN WIRTH¹, MICHAL RAMS^{1,2}, and FRANK STEGLICH¹ — ¹Max Planck Institute for Chemical Physics of Solids, 01187 Dresden, Germany — ²Institute of Physics, Jagiellonian University, 30-059 Kraków, Poland

Scanning Tunneling Spectroscopy (STS) is a powerful method to investigate the electronic structure of material surfaces. By means of STS, it is possible to probe the local density of states of a sample with sub-nanometre spatial resolution.

One prerequisite for high resolution and stability is a good tunneling tip. In our UHV STM systems, we plan on working predominantly with tips made of tungsten. A well-established way of producing tungsten tips is electrochemical etching. However, such tips are covered with a disturbing oxide layer and are usually not sufficiently sharp. Thus, facilities for further *in-situ* tip conditioning had to be added to our UHV-STM sys-

tems. The techniques for tip conditioning which have been investigated include direct annealing, electron beam heating and self-sputtering with light ions such as neon. Differently treated tips have been characterized by means of electron microscopy, field emission and STM experiments.

O 29.39 Wed 14:30 P2

Design of an UHV-STM with a Split Coil Magnet for Low Temperature Applications — •MIKE GYAMFI, OSWALD PIETZSCH, JULIAN C. CHEN, and ROLAND WIESENDANGER — Institute of Applied Physics, University of Hamburg, Jungiusstrasse 11, 20355 Hamburg

To study the spin dependent local electronic structure of single magnetic nanowires and nanoislands a new STM will be installed in a three chamber ultra high vacuum system. The STM will be operated in a liquid helium bath cryostat (expected base temperature 6 K) with a split-coil-magnet which assures good access for sample and tip exchange. A magnetic field of 5 T in z-direction will be available. A new feature of the system is a mechanism which will enable the controlled rotation of the magnetic tunnelling tip. It will provide the unique opportunity to tune the azimuth angle of an in-plane magnetised tip to a collinear configuration with the sample magnetisation in order to maximise the magnetic contrast. A further feature is the possibility to rotate the sample about the x-axis. This will allow evaporation onto the cold substrate and immediate STM measurements without loss of the microscopic position on the sample. We will discuss the design concept of the system.

O 29.40 Wed 14:30 P2

Digital Pulsed Force Mode in Ambient and Liquid Environment - Indentation of Soft Condensed Matter — •ALEXANDER GIGLER, CLAUDIA GNAHM, MICHAEL HOLZWARH, KATRIN HÜBNER, and OTHMAR MARTI — Department of Experimental Physics, Ulm University, D-89069 Ulm, Germany

AFM measurements can be conducted in every kind of environment, which makes it very suitable for material science investigations. The Digital Pulsed Force Mode (DPFM) allows the detailed investigation of the elastic and viscoelastic material parameters of samples. Thus, it is also a possible candidate for the determination of the mechanical properties of more difficult and complex structures such as biopolymers or even living cells. In this contribution the capability of the DPFM to investigate very delicate samples is demonstrated.

Due to the high volume of information acquired during the experiments, automated evaluation has been developed recently to allow a thorough physical testing of the sample materials. The possibilities of data evaluation of the force traces collected during these measurements will also be shown.

O 29.41 Wed 14:30 P2

Work function differences of C₆₀ on oriented metal surfaces — •ULRICH ZERWECK, CHRISTIAN LOPPACHER, and LUKAS M. ENG — Institute of Applied Photophysics, University of Technology Dresden, 01062 Dresden

Organic semiconductors have gained increased interest with respect to their use in organic light emitting diodes. For the efficient injection of charge carriers from the metal electrodes into the organic semiconductor, a low dipole barrier height is required. Similar to most organic molecules, C₆₀ also shows a linear dependence between the workfunction of the metal substrate and the dipole barrier formed between molecule and substrate. Such evidence stems from macroscopically measurements using UPS [1]. In this work, we compare these findings to microscopic inspections of local barrier heights investigating individual C₆₀ molecules by the use of Kelvin probe force microscopy.

In a previous publication [2] we showed the agreement between dipole barrier heights acquired with macroscopic UPS on one hand and, on the other hand, quantitative Kelvin probe force microscopy on the nanometer scale. Recently, we were able to push the lateral resolution forward down to ≈ 10 nm, still being quantitative.

[1] I. G. Hill et al., *Appl. Phys. Lett.* **73**, 662(1998)

[2] U. Zerweck et al., *Phys. Rev. B* **71**, 125424 (2005)

O 29.42 Wed 14:30 P2

Near-field-optical investigation of surface plasmons in metal-insulator-semiconductor tunnel junctions — •TINO GÖHLER¹, JAN SEIDEL¹, STEFAN GRAFSTRÖM¹, LUKAS ENG¹, BORIS CHICHKOV², and ALAIN DEREUX³ — ¹Institut für Angewandte Photophysik, TU Dresden, George-Bähr-Str. 1, 01069 Dresden, Germany — ²Laser Zentrum Hannover e.V., Hollerithallee 8, 30419 Hannover, Germany — ³Laboratoire de Physique de l'Université de Bourgogne, UMR CNRS 5027, 9 avenue Alain Savary, Boîte Postale 47870, F-21078 Dijon, France

In layered metal-insulator-semiconductor (MIS) structures electrons can excite surface plasmon (SP) oscillations in the metal layer via inelastic tunnelling [1]. In our experiments these structures consist of a silicon substrate covered by a thin oxide layer onto which a top metal electrode is deposited. This type of structure supports different SP modes for which the electromagnetic field is concentrated to different interfaces, namely the top metal-air interface and the bottom metal-oxide interface. SP excitation in the gap is supposed to be quite efficient with the inelastic tunnelling rate reaching $\sim 10\%$ of the elastic rate. Therefore, such MIS structures appear highly attractive as electrically pumped plasmon sources for integrated optoelectronic devices. We report here on SP emission directly investigated by scanning near-field optical microscopy (SNOM). Emphasis is placed on spectral characteristics of SPs in defined structures and at metal electrode edges.

[1] McCarthy, S. L., Lambe, J., *Appl. Phys. Lett.* **33**, 858 (1978)

O 29.43 Wed 14:30 P2

Dynamic Force Microscopy - Manifestations of Rare Atomic Jumps: Experiment and Simulation — •B. ITTERMANN¹, R. HOFFMANN¹, A. BARATOFF², L. KANTOROVICH³, T. TREVETHAN³, and H. v. LÖHNEISEN^{1,4} — ¹Physikalisches Institut und DFG-Center for Functional Nanostructures (CFN), Universität Karlsruhe, D-76128 Karlsruhe — ²NCCR on Nanoscale Science, Institute of Physics, University of Basel — ³Department of Physics, Kings College London — ⁴Institut für Festkörperphysik, Forschungszentrum Karlsruhe, D-76021 Karlsruhe

In recent non-contact scanning force microscopy experiments, jumps of the resonance frequency shift were observed below a critical tip-sample distance above specific atomic sites on a KBr (001) surface [1]. At the same distance additional energy dissipation related to the jumps sets in. The two branches of the frequency vs. distance curves between which the jumps occur are interpreted as the interaction of the surface with the tip being in two different configurational states. We proposed a model of the tip where an atom can hop from position A to position B in a double well potential. This proposal is checked with atomistic simulations for a small KBr cluster representing the tip and a KBr slab with a planar surface as sample [2]. The force as a function of distance obtained from the simulations is compatible with a double minimum potential for the different states A and B of the tip. Molecular dynamics simulations are planned in order to study the process at finite temperatures. [1] R. Hoffmann et al., to be published [2] R. Hoffmann et al., *Phys. Rev. Lett.* **92**, 146103 (2004)

O 29.44 Wed 14:30 P2

Imaging local potentials and thermovoltages with the STM — •J. HOMOTH, M. WENDEROTH, L. WINKING, T. DRUGA, and R. G. ULBRICH — IV. Physikalisches Institut der Universität Göttingen, Friedrich-Hund Platz 1, 37077 Göttingen

If tip and sample of an STM are at different temperatures, a thermovoltage arises which is correlated with the derivative of the sample's and tip's density of electronic states at the fermi level.

If the temperature difference between tip and sample is caused by a current parallel to the sample surface an additional potential component can be measured. The resulting tip-sample voltage is the sum of the local potential and the local thermovoltage.

This voltage is measured by a second interlaced feedback loop, which brings the average current from tip to sample to zero, while the tip height is kept constant. We show results for three different sample systems (semiconducting, semi-metallic and metallic) and distinguish between potential components caused by thermovoltage and the local potential.

In the case of a Si(111) surface the local thermovoltage represents the atomic corrugation in the Si(111)-7x7 reconstruction. Local potentials connected to the macroscopic field applied to the sample were measured in the case of thin metallic films. Potential components caused by ther-

movoltages were separated and potential gradients across grain boundaries and percolation structures are presented.

The work was financially supported by the SFB 602 TP A7.

O 29.45 Wed 14:30 P2

Improved design for a variable temperature scanning tunneling microscope — ●JAN WIENHAUSEN, GERMAR HOFFMANN, and ROLAND WIESENDANGER — Institut für Angewandte Physik und Zentrum für Mikrostrukturforschung, Universität Hamburg, 20355 Hamburg, Germany

Variable temperature scanning tunneling microscopy (VT-STM) is a versatile tool to study locally the growth of molecular systems on a carrier substrate. A recently installed VT-STM operated in ultra-high vacuum demonstrated high vertical and lateral stability down to 30 K sufficient for single molecule spectroscopy. To increase the available temperature range further we studied numerically the heat flow in the STM design. Whereas the rigid STM design itself is kept unmodified the design is optimized in terms of the heat balance. Heat transfer from a liquid helium flow cryostat is increased and heat losses to the environment are reduced. Here we will discuss the numerical results along with the detailed instrumental realization in comparison with its precursor. First applications to insitu prepared molecular films will be presented.

O 29.46 Wed 14:30 P2

The thermal resistance of a thermocouple tip in a scanning thermal microscope — ●ANDREAS KNÜBEL, ULRICH FLEISCHMANN-WISCHNATH, and ACHIM KITTEL — University of Oldenburg, D-26111 Oldenburg

The fabrication of a novel thermocouple sensor as a thermal profiler has enabled us to set up a very sensible scanning thermal microscope (SThM) based on a scanning tunnelling microscope (STM) under ultra-high vacuum conditions with high spatial resolution. This provides the possibility to an improved analysis of the frequently discussed near-field heat transfer on a nanometer scale. Because theory already provides a statement for the distance dependence of the heat transfer this quantity has to be determined experimentally for comparison. Therefore, it is essential to characterize the thermal resistance. By means of the thermal resistivity of the microscope tip its possible to quantify the heat transfer through the vacuum gap between the thermocouple tip and a cooled planar material surface from the measured temperatures. With a specially designed set-up we were able to evaluate the thermal resistance of the thermocouple.

O 29.47 Wed 14:30 P2

Video-rate Scanning Probe Microscopes: problems and solutions — ●M.J. ROST^{1,2}, G.J.C. VAN BAARLE^{1,2}, W.A. VAN LOO¹, L. CRAMA¹, P. SCHAKEL¹, E. VAN TOL¹, T.H. OOSTERKAMP¹, and J.W.M. FRENKEN¹ — ¹Kamerlingh Onnes Laboratory, Leiden University, P.O.Box 9504, 2300 RA Leiden, The Netherlands — ²Leiden Probe Microscopy, KOL, Leiden University, Niels Bohrweg 2, 2333 CA Leiden, The Netherlands

For a wide variety of surface and interface phenomena, in both fundamental and applied contexts, it is becoming increasingly important to visualize them with atomic or molecular resolution combined with high imaging speeds. We have recently developed a video-rate control system for scanning probe microscopes, including high-bandwidth amplifiers and fast data handling. From different tests, where we connected the new control electronics with several home-built and commercial instruments, we conclude that the current bottle neck in high-speed imaging is solely formed by the mechanical behaviour of the microscopes. We present new concepts and first, promising tests for high-frequency scanners, involving compact designs, new piezo geometries, and local damping solutions.

O 29.48 Wed 14:30 P2

A Besocke-type double-probe STM — ●PHILIPP JASCHINSKY, FRANZ-PETER COENEN, HELMUT STOLLWERK, GERHARD PIRUG, and BERT VOIGTLÄNDER — Institut für Schichten und Grenzflächen (ISG 3), Forschungszentrum Jülich, 52425 Jülich, Germany

A combination of a double-probe scanning tunnelling microscope (STM) with a scanning electron microscope (SEM) in ultrahigh vacuum (UHV) environment is presented. Due to a compact Besocke beetle-type design with two stages it was possible to integrate two independently driven STMs on small space. The positioning of the two tips can be controlled from macroscopic range down to 50 nm by an add-on electron column. This apparatus is a promising tool for manipulation and charac-

terizations of nanostructures on surfaces. The operation and performance of the instrument will be illustrated by several examples.

O 29.49 Wed 14:30 P2

Contact potential reading with a high-resolution tuning-fork AFM using a cantilever tip — ●SEBASTIAN TEICH, STEFAN GRAFSTRÖM, CHRISTIAN LOPPACHER, ULRICH ZERWECK, and LUKAS M. ENG — Institute of Applied Photophysics, University of Technology Dresden, 01062 Dresden

We report on a home-built tuning-fork non-contact atomic force microscope (AFM) operated with phase-sensitive electronics in the FM demodulation mode. One prong of the tuning fork is glued to a support mounted on the scanner piezo [1]. An ac voltage applied to the tuning fork electrodes induces a vibration of the free prong with an amplitude of 1-5 nm normal to the sample surface. We measure the oscillation amplitude by detecting the induced current using a lock-in amplifier. An electronic circuit compensates for the background signal originating from direct capacitive pick-up of the drive voltage. The probe-sample distance is controlled by a feedback loop such that the resonance frequency coincides with the given driving frequency. A second feedback keeps the mechanical oscillation amplitude constant, thereby providing information on the dissipation caused by the tip-sample interaction. As a probe, a commercial cantilever tip is glued to the tuning fork [2]. Various topographic structures with characteristic length scales down to 10 nm could be resolved. Furthermore, aiming for Kelvin probe force microscopy, we made the tip conductive and contacted it to one of the electrodes of the tuning fork by evaporating a metal layer onto the tip.

[1] F.J. Giessibl et al., *Nanotechnology* 15 (2004) S79

[2] S. Rozhok and V. Chandrasekhar, *Sol. Stat. Comm.* 121 (2002) 683

O 29.50 Wed 14:30 P2

Fluctuations and jump dynamics in atomic friction experiments — ●SABINE MAIER^{1,2}, YI SANG¹, TOBIN FILLETTER¹, MARTIN GRANT¹, ROLAND BENNEWITZ¹, ENRICO GNECCO², and ERNST MEYER² — ¹Department of Physics, McGill University, Montreal, Quebec, Canada — ²Department of Physics and Astronomy, University of Basel, Switzerland

We studied atomic stick-slip processes by means of friction force microscopy with high spatial and temporal resolution on KBr(100) in ultra-high vacuum. These processes are caused by the jump of the tip from one atomic position to the next. The occurrence of such stick-slip behavior is one-to-one related to energy loss in the sliding process. Thermal fluctuations in the combined system of tip, surface, and force sensor play a crucial role in the dynamics of the stick-slip behavior.

We characterized the influence of the tip-sample contact on the thermal fluctuations of the force sensor and on the dynamics of the stick-slip process. Results are compared with simulations based on an extended Tomlinson model including thermal fluctuations. A correlation between the duration of the atomic slip event and the atomic structure of the contact is established.

O 29.51 Wed 14:30 P2

Lateral and electrical forces during the manipulation of organic molecules — ●LARS ZIMMERLI, OLIVER PFEIFFER, THILO GLATZEL, SABINE MAIER, ENRICO GNECCO, ALEXIS BARATOFF, and ERNST MEYER — Institute of Physics, Klingelbergstr 82, 4056 Basel, Switzerland

The measurement of lateral forces between the tip of a force microscope and atomic scale features on a surface is an important issue in manipulation experiments. Feedback-controlled excitation of the torsional eigenmode of a rectangular cantilever beam forces the tip to oscillate parallel to the surface. We already reported the general capability to measure lateral forces using this technique [1, 2] at a step edge and we now observe these forces during the manipulation of organic molecules.

We have studied the lateral forces while manipulating single Cu-TBPP molecules on Cu[100]. Conservative and dissipative lateral interactions will be discussed while the tip is close or even directly above one porphyrine molecule. These results will be compared with those measured over a step edge or an impurity on the surface. We also studied Kelvin probe force microscopy which yields detailed information of topography and local work function on the nanometer scale. We identified distinct differences in energetics between the Cu-TBPP molecules and the substrate surface.

[1] O. Pfeiffer et al., *Phys. Rev. B* 65, 161403 (2002) [2] Ch. Loppacher et al., *Phys. Rev.* 90, 066107 (2003)

O 29.52 Wed 14:30 P2

Chirped-Pulse Two Photon Photoemission spectroscopy from surfaces — ●FELIX STEEB, STEFAN MATHIAS, MICHAEL BAUER, and MARTIN AESCHLIMANN — FB Physik, TU Kaiserslautern, Erwin-Schrödinger-Str. 46, 67663 Kaiserslautern

Two-Photon Photoemission (2PPE) with ultrashort laser pulses is a well-established technique which has been successfully applied to the investigation of the structure and dynamics of electron excitations at surfaces. In this paper, we show that the spectral chirp of the exciting laser pulse is an additional experimental parameter which can be utilised to gather further information on the electron states involved in the 2PPE process.

A well-defined amount of spectral chirp is applied to the ultrashort laser pulse. For a series of differently chirped pulses, the appropriate 2PPE spectra were recorded. In the case of a clean and a cesium covered Cu(111) surface, we observe significant energy shifts as large as 40 meV from the occupied shockley surface state and from the unoccupied cesium resonance respectively.

Model calculations within the framework of the Liouville-von-Neumann equations reproduce the experimental results for the photoexcited adsorbate and enable us to relate this shift to the finite lifetime of the adsorbate resonance. On the other hand, a lack of any energy shift of the shockley surface state in the simulations point to a need for further development of the theoretical model. The results and future prospects, e.g. the interaction of spectral chirp and adsorbate motion are discussed.

O 29.53 Wed 14:30 P2

Theoretical Study of the Electron Dynamics at the Silicon (100) 2x1-Surface — ●NORBERT BÜCKING^{1,2}, MARTIN SLOWIK¹, PETER KRATZER², MATTHIAS SCHEFFLER², and ANDREAS KNORR¹ — ¹Institut für Theoretische Physik, Nichtlineare Optik und Quantenelektronik, Technische Universität Berlin, Hardenbergstr. 36, 10623 Berlin, Germany — ²Fritz-Haber-Institut der Max-Planck-Gesellschaft, Abt. Theorie, Faradayweg 4-6, 14195 Berlin, Germany

Recent photoemission experiments call for a detailed study of the temporal surface dynamics on silicon surfaces. We use a model for the phonon based short-time dynamics where the electron-phonon interaction of both bulk and surface states is described by Density-Functional-Theory (DFT). The surface band structure of Si(100), including the surface states D^{up} and D^{down} , is calculated using a slab geometry in local density approximation (LDA). For the bands contributing to the surface dynamics, the corresponding Kohn-Sham wave functions are used to compute electron phonon coupling matrix elements. Density matrix formalism is used to evaluate the population dynamics of excited conduction band states. Different theoretical approaches, such as Markovian and time-convolutionless (TCL) methods are compared.

O 29.54 Wed 14:30 P2

Quasiparticle lifetimes of rare-earth elements, transition metals and noble metals — ●ALEXANDER MÖNNICH, JÖRG LANGE, MICHAEL BAUER, and MARTIN AESCHLIMANN — FB Physik, TU Kaiserslautern, Erwin-Schrödinger-Str. 46, 67663 Kaiserslautern

The dynamics of excited (hot) electrons play an important role in surface physics and chemistry. It is therefore important to address the question of how the bulk electronic structure influence the mean free path and the excited electron lifetimes. For excitation energies $> 10\text{ eV}$ the so called universal curve allows a rather good estimate of these quantities. However, at low excitation energies ($E - E_F < 10\text{ eV}$) there can be significant deviations from this approximation.

With the time resolved two-photon photoelectron spectroscopy (TR-2PPE) method we investigated the electron dynamics in various noble, transition and rare earth metals up to excitation energies $E - E_F = 3\text{ eV}$. The characteristics of the electronic structure of the respective metal classes responsible for energy dissipation processes of hot electrons will be analyzed by comparing our experimental data in to different theoretical results.

O 29.55 Wed 14:30 P2

ARUPS with higher harmonics using a 2D hemispherical energy analyser — ●STEFAN MATHIAS¹, RALF FRESE², MARTIN WIESENMAYER¹, SVEN PASSLACK¹, DOROTHEA HOFFMANN¹, MARTIN AESCHLIMANN¹, and MICHAEL BAUER¹ — ¹Department of Physics, TU Kaiserslautern, Erwin-Schrödinger-Str. 46, 67663 Kaiserslautern, Germany — ²Physics Department, University of Southern Denmark, Campusvej 55, 5230 Odense M, Denmark

Time-resolved UPS is an attractive experimental tool to study the ultra-fast dynamics of processes at surfaces [1]. Next to the photoelectron energy distribution also the time and angular dependence of the photoemission spectrum can contain important information, for instance the dynamics related to the coupling between molecules adsorbed on a surface. Short pulse EUV-light sources, such as higher harmonic generation (HHG), are typically driven at rather low repetition rates. Therefore, highly efficient parallel detection schemes are necessary to achieve time and angle resolved photoemission data (TR-ARUPS). Here we present first ARUPS experiments performed with a 1 kHz HHG light source using a hemispherical energy analyser, equipped with a 2D-detector for parallel energy and momentum detection. The HHG light source provides photon energies up to 45 eV and the photoelectrons are collected between $\pm 7^\circ$ ($k_{\parallel} = \pm 0,42\text{ 1/\AA}$ at 45 eV) with an angle resolution of better than $0,2^\circ$. We discuss limitations, advantages and disadvantages of this detection scheme in comparison to a time of flight electron analyser, typically used for this kind of experiments. [1] M. Bauer, J. Phys. D: Appl. Phys. 38 (2005) R1-R15

O 29.56 Wed 14:30 P2

TDDFT simulation of Si(001) dimer excitation by intense fs laser-pulses — ●ECKHARD PEHLKE and JAN VAN HEYS — Institut für Theoretische Physik und Astrophysik, Christian-Albrechts-Universität Kiel, 24098 Kiel

The surface band-structure of the Si(001) surface is characterized by either fully occupied or fully unoccupied dangling-bond orbitals located at the Si-dimer atoms. The population dynamics of the initially unoccupied states after laser excitation and the surface response has been studied by Weinelt *et al.* [1]. Here we present simulations of the dynamics of the Si(001) surface atoms, in particular the dimer-buckling angle, after very strong electron-hole pair excitation in the surface states by an intense fs laser-pulse. The dynamics of the electrons is described within time-dependent density functional theory while the nuclei follow classical Ehrenfest dynamics. The electric field representing the laser excitation is restricted to the direction perpendicular to the surface. Different laser-pulse shapes and intensities have been studied. The buckling angle decreases on a timescale of about 150 fs. A coupling between the dimer buckling angle and the total number of excited electrons is observed. Initial state contributions to the time-dependent surface core-level shifts have been calculated (screening effects, however, are still lacking). Additionally, the lifetime of the induced surface-atom vibrations has been investigated by molecular dynamics simulations on the Born-Oppenheimer surface.

[1] M. Weinelt *et al.*, Phys. Rev. Lett. **92**, 126801 (2004) and Appl. Phys. A **80**, 995 (2005).

O 29.57 Wed 14:30 P2

Description of femtosecond laser induced diffusion within the electronic friction model — ●J. GÜDDE¹, K. STEPAN¹, A.C. LUNTZ², and U. HÖFER¹ — ¹Fachbereich Physik und Zentrum für Materialwissenschaften, Philipps-Universität, D-35032 Marburg — ²Physics Department, Odense University, 5230 Odense M, Denmark

It has been recently shown that diffusion of atomic oxygen on a Pt(111) surface can be induced by femtosecond laser excitation [1]. The energy flow from the optical excitation to the adsorbate has been modeled in the same way as the well-studied process of desorption induced by femtosecond laser excitation is frequently described. Three coupled temperatures for electrons, substrate ions and the adsorbate are introduced and the electronic coupling between adsorbate and metal surface is represented by an electronic friction coefficient η_e . In this way a fast energy transfer to the adsorbate and a nonlinear dependence of the corresponding rate on laser fluence can be reproduced. We have made different approaches for η_e : Ab initio calculations give the correct order of magnitude for the response time, but cannot reproduce the extremely strong nonlinear fluence dependence of the hopping-rate, which has been observed in the experiment [1]. Satisfactory agreement with the experimental data can be achieved only if a strong dependence of η_e on electron temper-

ature is assumed, which is not supported by the ab initio calculations. We will discuss alternative excitation pathways including an anharmonic coupling between different vibrational modes, which may be responsible for an effective temperature dependence of the electronic friction.

[1] K. Stepan *et al.* Phys. Rev. Lett. **94**, 236103 (2005).

O 29.58 Wed 14:30 P2

Positron induced Auger electron spectroscopy — ●STEFAN LEGL and CHRISTOPH HUGENSCHMIDT — Technische Universität München, Lichtenbergstraße 1, 85747 München

Positron annihilation induced Auger electron spectroscopy (PAES) uses the annihilation of a positron with an electron of the inner shell of atoms whereas X-rays or high energy electrons are used in conventional AES for ionisation. Advantages of PAES are the higher surface sensitivity and the better signal to noise ratio. In order to benefit from PAES one has to use a low-energy positron beam of high intensity, which is available at NEPOMUC at FRM-II. However, the positron intensity amounts to a few picoampere whereas up to 1mA electron current is used in AES. To overcome this lack of intensity a novel time-of-flight spectrometer (TOF-PAES) was developed, which efficiently collects the emitted Auger electrons. In the TOF-PAES the energy of the Auger electrons is determined by the measurement of the electron flight time with an accuracy of 1eV. The detection of one annihilation quantum (511keV) delivers the start signal for the timing. After a flight of about 1.1m the Auger electron hits a micro channel plate detector which creates a stop signal. The features of this new spectrometer as well as first results will be presented.

O 29.59 Wed 14:30 P2

Electron Transfer Dynamics from Perylene to ZnO Semiconductor: A comparative study between TiO₂ and ZnO — ●CHARAF CHERKOUK, JODI SZARKO, LARS GUNDLACH, LIANA SOCACIU-SIEBERT, ANTJE NEUBAUER, and FRANK WILLIG — Hahn-Meitner-Institute, Department: Dynamics of Interfacial Reactions SE4, Glienickestrasse 100, 14109 Berlin

Heterogeneous electron transfer (ET) between different molecules adsorbed on semiconductor surfaces has been investigated mainly with TiO₂ as the substrate [1,2]. The (10-10) surface of ZnO was used here as a substrate in order to investigate the influence of the nature of the semiconductor on the injection and relaxation dynamics. For both substrates electron transfer and relaxation dynamics were measured using time resolved two-photon photoelectron spectroscopy (TR-2PPE). Angular dependent 2PPE intensity was measured in order to extract information on the orientation of the molecules on the surface of the semiconductor. Others techniques such as XPS, UPS, and LEED were used in addition to characterize the surface of the clean and the dye-covered ZnO (10-10) single crystal surface, respectively. These results are compared with measurements on identical systems using TiO₂ as a substrate.

[1] L. Gundlach, S. Felber, W. Störck, E. Galoppini, Q. Wei, and F. Willig, Res. Chem. Intermed. **31**, 39, 2005.

[2] R. Huber, J.-E. Moser, M. Grätzel, and J. Wachtveitl, J. Phys. Chem. B **106**, 6494, 2002.

O 29.60 Wed 14:30 P2

Design and Setup of a Butterfly X-Ray Reflectometer for the Investigation of Liquid Surfaces and Interfaces — ●VOLKER SCHÖN and PATRICK HUBER — Technische Physik, Universität des Saarlandes, 66123 Saarbrücken, Germany

We present the design and setup of a tabletop x-ray reflectometer suitable for the investigation of the microscopic structure of liquid surfaces and interfaces. First measurements from the bare surface of water and liquid hydrocarbons as well as polymer/lipid/vapor interfaces demonstrate its functionality.

O 29.61 Wed 14:30 P2

Experimental and theoretical studies of the structure and dynamics of the CaF₂(111) surface — ●A. GOTTE¹, M. BAUDIN¹, K. HERMANSSON¹, A. CABELLO², J. VOGT², and H. WEISS² — ¹Department of Materials Chemistry, The Ångström Laboratory, Box 538, 752 21 Uppsala, Sweden — ²Chemisches Institut der Universität Magdeburg, Universitätsplatz 2, 39106 Magdeburg, Germany

The structure and dynamics of the CaF₂(111) surface was investigated by means of low-energy electron diffraction (LEED) and molecular dynamics (MD) simulations at 300 K. LEED beam intensities were recorded as a function of electron energy and were analyzed with the tensor LEED

approach. Positions as well as mean square amplitudes (MSA) of the ions in the first layers were fitted to the experimental I(E) curves. The MD simulations were performed using a 2-dimensional slab representation of the surface. Short-range interactions were described by a Buckingham potential and long-range interactions were calculated using a 2-D Ewald summation technique. Ionic polarizations were included by the shell-model. All parameters of the force field were fitted to the experimental bulk structure and elastic and dielectric data. According to experiment and theory the structure of the CaF₂(111) surface is close to the bulk-terminated geometry with only small vertical displacements of the top-most ions. Moreover it is found that the MSAs of the anions are larger than those of the cations. Enhanced vibrational amplitudes of the ions in the surface layers are supported by both studies, although with different values of the respective MSAs.

O 29.62 Wed 14:30 P2

Jumping atom rows on Au(110) observed with video-rate STM — ●RICHARD VAN RIJN, JOOST W.M. FRENKEN, and MARCEL J. ROST — Kamerlingh Onnes Laboratory, Leiden University, P.O. Box 9504, 2300 RA Leiden, The Netherlands

When depositing gold on a Au(110) surface, we find the formation of atom rows with a width of only one atom and surprisingly large lengths up to hundreds of atoms. This length scale is roughly a factor ten larger than we expect on the basis of two-dimensional equilibrium shape theory (Wulff construction). In addition we observe a large spread in row lengths. Next to the unusual island form, we also find that these atom rows are mobile at room temperature. Using standard STM imaging speeds, we observe atom rows with lots of kinks. But at video rate it seems, as if the whole atom row jumps back and forth in the [001] direction via a collective movement of all (hundreds of) atoms. As this collective movement is highly unlikely, we suggest that the basic mechanism for the jumps is given by the creation and the diffusion of an individual kink within the row, but on a very fast time scale. This system is a perfect model for one-dimensional diffusion related to the 'classical ruin problem'. We analyze the row diffusion via the frequency and temporal correlations of kink passages, as a function of position along the row, row length and temperature.

O 29.63 Wed 14:30 P2

Surface conductivity induced by fullerenes on diamond — ●PAUL STROBEL, JÜRGEN RISTEIN, and LOTHAR LEY — Institut für Technische Physik, Universität Erlangen-Nürnberg, Germany

The surface conductivity of hydrogen terminated diamond under atmospheric conditions is a well known phenomenon. The atmospheric adsorbents induce a near-surface hole gas resulting in a surface conductivity of diamond. In the present work we investigated C60 and fluorinated derivatives C60F18, C60F36, and C60F48 as alternative electron acceptors on the diamond surface. The electron affinity of the fluorinated fullerenes increases with the number of F-atoms from 2.7eV for C60 up to 4.1eV for C60F48. As a consequence, the doping efficiency increases in the same order and reaches unity for C60F48, i.e. each adsorbed C60F48 accepts one electron from the diamond. With device applications in mind, we further investigated the thermal stability of fullerene induced surface conductivity on diamond. Due to the increasing vapour pressure of the fullerenes with increasing fluorination the desorption temperature in high vacuum decreases from 200°C for C60 to RT for C60F48. A notable improvement of thermal stability was achieved by passivation of fluorinated fullerenes by different dielectric layers (SiO, CaF₂). In the case of C60 we observed an auto stabilisation up to 350°C in high vacuum after light, air, and temperature promoted polymerisation.

O 29.64 Wed 14:30 P2

STM-investigations of metal films near the percolation threshold on GaAs(110) — ●J. HOMOTH, M. WENDEROTH, T. DRUGA, L. WINKING, and R. G. ULBRICH — IV. Physikalisches Institut der Universität Göttingen, Friedrich-Hund Platz 1, 37077 Göttingen

The resistance of thin Ag and Cu films on insulating GaAs(110) was measured in-situ during UHV deposition at different sample temperatures (80K - 300K). The onset of conductance is seen in the thickness range of d=2 monatomic layers (ML). At thicknesses of more than 2ML an increase of conductance as a function of d with a power law behaviour of an exponent grater 1 is found.

We present scanning tunnelling topographies of films near the percolation thickness. The overall film morphology resembles a 3D cluster growth. Spatially resolved scanning tunnelling spectroscopy reveals addi-

tional states in the band gap region of the clean GaAs(110) surface. The additional states are localised around the metal clusters with a lateral decay length of less than 5 Angstroms.

The work was financially supported by the SFB 602 TP A7.

O 29.65 Wed 14:30 P2

Structural and electronic analysis of Hf on Si(111) surface studied by angle-scanned photoelectron diffraction — ●M. F. CARAZZOLLE^{1,2}, M. SCHÜRMAN^{1,3}, U. BERGES³, C. FLÜCHTER^{1,3}, D. WEIER^{1,3}, A. DE SIERVO⁴, R. LANDERS^{2,4}, G. G. KLEIMAN², and C. WESTPHAL^{1,3} — ¹Experimentelle Physik 1 - Universität Dortmund, Otto-Hahn-Str. 4, D44221-Dortmund, Germany — ²Instituto de Fisica - Universidade Estadual de Campinas, C.P.6165, 1083-970-Campinas, SP, Brazil — ³DELTA-Dortmunder Elektronenspeicherring Test Anlage, Maria-Goeppert-Mayer-Str. 2, D44227-Dortmund, Germany — ⁴Laboratorio Nacional de Luz Sincrotron, C.P. 6192, 13084-971-Campinas, SP, Brazil

The development of alternative high-k gate dielectrics for future complementary metal-oxide-semiconductor (CMOS) devices is indispensable in achieving both low leakage current and small equivalent oxide thickness. HfO₂ is one possible candidate because of its high dielectric constant and high conduction band offset. On the other hand the formation of metallic Hf-silicide during the annealing process for activation is one of the most serious problems, because the electrical characteristics will be influenced drastically due to the leakage current. In this work we present a systematic electronic and structural study of the Hf-silicide formation upon annealing. We utilized XPS, LEED and angular XPD to study the surface of ultra-thin films of the Hf on Si(111). The work was performed at DELTA (Accelerator Facility at the University Dortmund) using an undulator beam line with a photon energy of 200 eV.

O 29.66 Wed 14:30 P2

A Photoelectron Diffraction Investigation of the SiO₂/4H-SiC(0001) Interface — ●MARK SCHÜRMAN, STEFAN DREINER, ULF BERGES, and CARSTEN WESTPHAL — Universität Dortmund, Experimentelle Physik 1, Otto-Hahn-Straße 4, 44227 Dortmund, Germany

In our study we used photoelectron diffraction to investigate ultrathin SiO₂-films on 4H-SiC(0001). Synchrotron radiation with high flux and sufficient spectral resolution of the U41-PGM beamline at BESSY 2 (Berlin) was used. It was possible to separate individual spectral components in the XPS spectra. These components display different diffraction patterns due to the different local atomic environments of the respective emitters. We present a comparison between experimental data of a thermally oxidized ultrathin oxide layer showing no long-range order and an ordered silicate layer. From the diffraction patterns of the Si⁺ component originating from silicon emitters at the interface it is possible to conclude that the local atomic structure at the interface is very similar for both samples. However, the diffraction of the SiO₂ component is different for both patterns and a comparison with simulations shows, that this difference is a result of the local order within the oxide film. Furtheron, an R-factor analysis of the Si⁺ diffraction reveals details about the local atomic structure of the interface between bulk SiC and non-ordered SiO₂.

O 29.67 Wed 14:30 P2

Initial stages of the graphite/SiC interface formation studied by photoelectron spectroscopy — ●K. EMTSEV¹, TH. SEYLLER¹, L. LEY¹, L. BROEKMAN², J.D. RILEY², and R.G.C. LECKEY² — ¹Lehrstuhl für Technische Physik, Universität Erlangen-Nürnberg, Erwin-Rommel-Str. 1, 91058 Erlangen — ²Department of Physics, La Trobe University, Bundoora, Victoria 3083, Australia

Nowadays graphite layers grown on SiC(0001) surface are widely accepted as an alternative to the samples of natural graphite. Single-crystalline graphite multilayers result from the decomposition of SiC upon annealing at high temperatures. As an initial stage of graphitization a complex ($6\sqrt{3} \times 6\sqrt{3}$)R30° surface reconstruction occurs after annealing of 6H-SiC(0001) at T=1150°C. The nature of this reconstruction is discussed controversially. Fingerprints of graphitization (π^* and σ^* bands) were observed in inverse photoelectron spectroscopy [1], while the energies of C1s surface shifted components differ from that of graphite [2]. The early models suggested a monolayer of graphite on top of either the unreconstructed surface or the ($\sqrt{3} \times \sqrt{3}$)R30° reconstructed surface. The latest model proposes that the surface is covered by the graphene-like islands arranged in a honeycomb structure [3]. In the present work we

analyze in detail the electronic structure of the $6\sqrt{3}$ reconstructed surface of 6H-SiC(0001) by means of angle-resolved photoelectron spectroscopy.

[1] I. Forbeaux et al., Phys. Rev. B, 58 16396 (1998)

[2] L.I. Johansson et al., Phys. Rev. B, 53 13793 (1996)

[3] W.Chen et al., Surf.Sci., in press (2005)

O 29.68 Wed 14:30 P2

Surface characterization of InN grown by PIMBE — ●MARCEL HIMMERLICH^{1,2}, VADIM LEBEDEV², STEFAN KRISCHOK^{1,2}, OLIVER AMBACHER², and JUERGEN A. SCHAEFER^{1,2} — ¹Institut für Physik, TU Ilmenau, P.O. Box 100565, 98684 Ilmenau, Germany — ²Zentrum für Mikro- und Nanotechnologien, TU Ilmenau, P.O. Box 100565, 98684 Ilmenau, Germany

Indium nitride (InN) layers were grown by plasma-induced molecular beam epitaxy using a conventional effusion cell for In and an rf nitrogen plasma source to supply active N radicals. The growth was monitored by a quadrupole mass spectrometer and reflection high energy electron diffraction (RHEED). After removal from the growth chamber, the samples were directly cut and loaded to a second UHV system to reduce the exposure to contaminants from ambient air. The InN layers were investigated using X-ray and ultra-violet photoelectron spectroscopy (XPS, UPS) and atomic force microscopy (AFM). Although the surface is quite rough (rms 4.5nm), surface steps with a height of 6Å can be observed. The amount of carbon and oxygen on the surface is relatively low compared to samples which have been exposed to air for a few days. Heating of the samples to 170°C-230°C resulted in a further reduction of oxygen along with a removal of the oxide related feature in the In3d and In4d core levels. However, this procedure did not succeed in removing any carbon. The binding energy of the InN related peaks are 443.9eV, 396.3eV and 17.4eV for In3d_{5/2}, N1s and In4d_{5/2}, respectively. Additionally, a structure in the valence band emerges at 3.1eV which can be attributed to a nitrogen related contribution.

O 29.69 Wed 14:30 P2

SiC Pore Surfaces: Surface Studies of 4H-SiC(1102) and 4H-SiC(1102) — ●U. STARKE¹, W.Y. LEE¹, M. HETZEL¹, C. VIROJANADARA¹, C. COLETTI², S.E. SADDOW², R.P. DEVATY³, and W.J. CHOYKE³ — ¹Max-Planck-Institut für Festkörperforschung, Stuttgart, Germany — ²University of South Florida, Tampa, USA — ³University of Pittsburgh, USA

Porous SiC has shown intriguing perspectives for a variety of possible applications in electronics, sensors, fuel cells and bio-technology. One important pore type found is a triangular shaped channel with surfaces inclined by about 62° with respect to SiC(0001). The respective single crystal surface, 4H-SiC($\bar{1}10\bar{2}$), and its isomorphous opposite, i.e. the 4H-SiC(1102) surface have been studied in this work using AFM, LEED, STM and AES. The mechanically polished samples were etched in hydrogen flux at about 1500°C which eliminates the polishing damage as monitored by AFM. Both surfaces immediately display a sharp LEED pattern of bulk-like periodicity. An apparent thin oxide layer termination is inferred from AES. Further annealing in UHV leads to the removal of oxygen after flashing to about 1200°C. Si deposition and subsequent annealing lead to a well ordered surface with the best LEED pattern obtained after heating to about 1120 and 1000°C, respectively. Also the Si/C composition ratio increases up to this temperature regime until it drops at higher temperatures. A tendency towards a (2×1) reconstruction is observed. The interpretation of LEED spot intensity curves indicates a different structure for the UHV treated surface as compared to the 'as-etched' surface condition.

O 29.70 Wed 14:30 P2

Temperature Induced Phase Transformation on the 4H-SiC(1120) Surface — ●U. STARKE¹, W.Y. LEE¹, and S. SOUBATCH^{1,2} — ¹Max-Planck-Institut für Festkörperforschung, Stuttgart, Germany — ²present address: International University Bremen, Germany

The demand for better SiC devices has initiated an increased focus the non-polar 4H-SiC(1120) surface which has a lower defect density than basal-plane surfaces and can serve as alternative growth orientation. In the present work, we have studied this surface after hydrogen etching as well as after Si deposition as a function of temperature using XPS, LEED, AES and AFM. Results show that despite having a smooth, featureless surface (as observed by AFM), the 'just-loaded' hydrogen etched surface exhibits a (1×1) LEED pattern, although weak. Chemically, the surface appears to be C-rich, indicated by XPS and AES spectra with an additional small amount of oxygen present. The oxygen peak vanishes upon

heating to about 1150°C. A well ordered surface can be obtained by Si deposition and subsequent annealing. The LEED pattern remains (1×1). However, the LEED intensities show a sharp change around 1000°C indicating a structural phase transformation. The chemical composition also changes during annealing, however in a more gradual manner. The results will be discussed in detail, focusing on the chemical and structural properties of the two distinct phases observed.

O 29.71 Wed 14:30 P2

Growth and morphology of ZnO on Fe(110) — ●CHRISTIAN TUSCHE, HOLGER L. MEYERHEIM, and JÜRGEN KIRSCHNER — MPI für Mikrostrukturphysik Halle, D-06120 Halle, Germany

The Fe/ZnO/Fe tri-layer system is a potentially promising system for tunneling magneto-resistance (TMR) and future spintronic applications. Since the tunneling properties sensitively depend on the details of the interface[1], the study of the growth, morphology and structure of ZnO on Fe and vice versa is of primary importance.

Ultrathin films of ZnO were deposited on Fe(110) from a ZnO-rod heated by electron bombardment and by pulsed laser deposition using a stoichiometric ZnO target. For the ZnO(0001)/Fe(110) epitaxy the lattice mismatch is 12% for $[11\bar{2}0]_{\text{ZnO}} \parallel [001]_{\text{Fe}}$. ZnO films up to 3 monolayers thickness exhibit a (1x1) pattern in low energy electron diffraction (LEED), although with reduced spot sharpness as compared to the clean Fe(110) surface. Structural order improves upon annealing to 520K, however at higher temperatures, the interface is subject to a reduction-oxidation reaction. Scanning tunneling microscopy on films in the same thickness range reveals a two dimensional growth of the ZnO.

For ZnO-deposition in ambient oxygen atmosphere ($p(\text{O}_2) = 10^{-7} \text{ mbar}$) photo electron spectroscopy indicates an oxidation of the Fe substrate. This goes in parallel with the observation of extra spots in the LEED-pattern, indicative for a relaxed ZnO adlayer (hexagonal a-axis = 3.25 Å).

[1] C. Tusche et al., Phys. Rev. Lett. **95** (2005) 176101

O 29.72 Wed 14:30 P2

Morphology and electronic structure of ultrathin manganese oxide films — ●MATHIAS NAGEL, LEI ZHANG, HEIKO PEISERT, and THOMAS CHASSÉ — Institute of Physical and Theoretical Chemistry, University of Tübingen, Auf der Morgenstelle 8, 72076 Tübingen, Germany.

Binary transition metal monoxides have been of basic scientific interest for many years. Due to their high electronic correlation they reveal interesting properties. Of particular interest besides their electronic properties are magnetic phenomena in layer systems which are already utilised in technical applications. As a consequence of the trend in miniaturising devices questions about the influence of the reduced dimensionality on the properties arise. In layered systems the influence of the morphology and the reactions directly at the specific interface have to be evaluated.

The MnO/Ag(100) is an interesting model system due to the lattice mismatch which is quite high (9 %). By choosing the optimal preparation method either pseudomorphic growth or relaxed growth of MnO on Ag(100) can be obtained. This defined growth method is giving the possibility of studying separately the interface strain and the effect of the reduced dimensionality. Ultrathin, epitaxial layers of MnO were prepared at Ag(100) and characterised in-situ by means of XPS, XPD and LEED. Additionally, in-situ grown samples were investigated with XES and XAS measurements. By combining these techniques a detailed understanding of the morphology and electronic structure of the evolving film can be obtained and is discussed.

O 29.73 Wed 14:30 P2

Growth, atomic structure and vibrational properties of thin MnO films on Pt(111) — ●STEFFEN SACHERT¹, CHRISTIAN HAGEDORF¹, KRASSMIR KOSTOV², and WOLF WIDDRA¹ — ¹Martin-Luther-Universität Halle-Wittenberg, FB Physik, D-06120 Halle (Salle) — ²Institute of General and Inorganic Chemistry, Bulgarian Academy of Science, BG-1113 Sofia

Thin MnO layers (from 0.2 to 4 monolayers) have been grown on Pt(111) by reactive deposition of Mn in an O₂ atmosphere. High-resolution electron energy loss spectroscopy (HREELS), low energy electron diffraction (LEED) and variable-temperature scanning tunneling microscopy (STM) have been used to investigate surface vibrational and structural properties of various thin manganese oxide films.

Submonolayer coverages of MnO grown at 375 K are characterized by strong Fuchs-Kliwer phonons. The corresponding MnO coverages

within the monolayer are estimated by CO adsorption at 85 K and thermal desorption. For the completed MnO monolayer on Pt(111) a well-ordered (19×1) superstructure is observed in LEED and in atomically resolved STM. The related HREEL spectrum shows a narrow Fuchs-Kliwer phonon at 365 cm⁻¹.

Further growth of MnO occurs layer-by-layer as found by STM. The layer-dependent vibrational properties and their changes with annealing to higher temperatures will be discussed: Heating the films to 700 K improves ordering in the 2D film. At 800 K, annealing leads to the well-defined monolayer with few, larger 3D MnO clusters, whereas at about 1100 K alloy formation takes place.

O 29.74 Wed 14:30 P2

Epitaxial Cobalt Oxide Films on Ir(100) — ●CHIARA GIOVANNARDI, LUTZ HAMMER, and KLAUS HEINZ — Lehrstuhl für Festkörperphysik, Universität Erlangen Nürnberg, Staudtstr. 7, D-91058 Erlangen

On various modifications of the Ir(100) surface (1×1, 5×1, 2×1-O) cobalt grows pseudomorphically up to several monolayers. Post-oxidizing a 2ML Co film grown on the 1×1 surface and subsequent annealing at around 500K leads to the formation of flat epitaxial CoO-films with rock-salt structure. In contrast to substrates like Fe(100) and Ag(100) [1,2] these CoO-films cannot grow in (100) orientation on the Ir(100) surface due to the large lattice misfit (2.72 Å vs. 3.04 Å). Instead, the film grows slightly distorted in (111) orientation giving rise to a c(10×2) superstructure. For other thicknesses and surface preparations fully relaxed CoO patches are found as well as patches with Co₂O₃ structure.

[1] S. Valeri et al., Surf. Sci. 423 (1999) 346

[2] Ch. Hagedorf et al., Surf. Sci. 532-535 (2003) 346

O 29.75 Wed 14:30 P2

Surface morphology of epitaxial lattice-matched Ba_{0.7}Sr_{0.3}O on the Si(001) surface — ●DIRK MÜLLER-SAJAK, JAN ZACHARIAE, and HERBERT PFÜR — Institut für Festkörperphysik, Abtl. Oberflächen, Universität Hannover, Appelstr. 2, 30167 Hannover

Recently we have shown that Ba_{0.7}Sr_{0.3}O as a high K gate dielectric offers an adequate band gap, an appropriate band alignment and an atomically sharp interface to the Si(001) substrate [1].

Here we will present a SPA-LEED (Spot Profil Analysis LEED) study of the Ba_{0.7}Sr_{0.3}O surface morphology. The vertical roughness was determined to be ≤ 2ML at up to 15 nm layer thickness. In addition, local variations of the lattice spacing due to fluctuations of the local composition were detected in our G(S) analysis.

Growth of Ba_{0.7}Sr_{0.3}O on vicinal Si(001)-[011]4° leads to stepped oxide surfaces. The spot splitting is 4% of the surface Brillouin zone for the oxide surface in contrast to 10% for vicinal Si(001). This indicates an uncorrelated mixture of terraces separated by triple steps and double steps in molecular units. This is mainly caused by a rearrangement of the vicinal Si(001) surface due to the preadsorbed Sr layers, which is necessary for the crystalline growth of Ba_{0.7}Sr_{0.3}O [1].

Pd chains which nucleate along these steps were investigated by ARUPS and SPA-LEED. The structure of this 1D electronic system will be discussed.

[1] J. Zachariae and H. Pfnür, Phys. Rev. B 72, 075410 (2005)

O 29.76 Wed 14:30 P2

Ultrathin vanadium oxide films on W(110) investigated by LEEM — ●BENJAMIN BORKENHAGEN, GERHARD LILIENKAMP, and WINFRIED DAUM — Institut für Physik und Physikalische Technologien, TU Clausthal, Leibnizstr. 4, D-38678 Clausthal-Zellerfeld

Vanadium oxide films with thicknesses in the range between submonolayer and several monolayers were epitaxially grown on a W(110) single crystal under UHV conditions. Depending on the growth conditions, LEED investigations revealed various well-ordered superstructures, e. g. with 2x2 symmetry, and a hexagonal film in Kurdjumov-Sachs orientation. Cleanliness and composition of the films were checked by Auger spectroscopy. Low energy electron microscopy (LEEM) of the vanadium oxide-covered tungsten surface showed a flat surface with monoatomic steps. Dark field images using one or more diffraction spots revealed the growth process and the distribution of different domains of the vanadium oxide. The sample was also investigated in situ during annealing under oxidizing and reducing conditions, respectively. Structural transitions are correlated with the oxygen content in the film and alloying of vanadium with the tungsten substrate.

O 29.77 Wed 14:30 P2

Thermally and Electron-Induced Processes in Condensed Acetic Acid–Water Films between 80 and 200K studied with MIES, UPS(HeI and II), FTIR and TPD — ●S. BAHR¹, O. HÖFFT¹, A. BORODIN¹, V. KEMPTER¹, F. BORGET², T. CHIAVASSA², and A. ALLOUCHE² — ¹Institut für Physik und Physikalische Technologien, TU Clausthal, Leibnizstr. 4, D-38678 Clausthal-Zellerfeld — ²Physique des Interactions Ioniques et Moléculaires, CNRS-UMR6633 Campus Universitaire de Saint Jérôme, Marseille, France

Thermally and electron-induced processes in condensed acetic acid (AA)-water films, deposited on tungsten and gold at 80K and 120K, were studied with Metastable Impact Electron Spectroscopy (MIES), UPS(HeI and II), FTIR-Spectroscopy and TPD in a temperature range between 80K (120K) and 200K. The results are interpreted with the help of cluster DFT calculations. The prepared interfaces, namely AA layers on thin films of solid water and H₂O adlayers on thin AA films, were characterised with the above mentioned techniques at 80K (120K) and additionally with TPD during annealing. By the combination of electron spectroscopy with FTIR and TPD we are able to get informations about inter and intra species binding strengths in addition to structural changes (in the case of AA from cyclic dimers to chain like structures at 150K) and desorption behaviour of both species in the films during annealing. Currently, we study the electron-induced modification of the AA film structure as well as processes initiated by the radiation-induced H₂O fragments (OH, H₃O⁺ etc).

O 29.78 Wed 14:30 P2

Segregation of salt ions at surfaces of polar liquids and the corresponding amorphous solids — ●O. HÖFFT¹, U. KAHNERT¹, V. KEMPTER¹, P. JUNGWIRTH², and L.X. DANG³ — ¹Institut für Physik und Physikalische Technologien, TU Clausthal, Leibnizstr. 4 38678 Clausthal-Zellerfeld — ²Institute of Organic Chemistry and Biochemistry, Czech Academy of Sciences, Prague — ³EMSL, Pacific Northwest National Lab

Surface segregation of iodide, but not of fluoride, or cesium, is observed by a combination of metastable impact electron spectroscopy (MIES) and ultraviolet photoelectron spectroscopy (UPS(HeI)) of amorphous solid water exposed to CsI and NaI on one side and NaF and CsF vapour on the other side. The same surface ionic behavior is also derived from molecular dynamics (MD) simulations of the analogous aqueous salt solutions. These results give a strong support to the suggested surface propensity of heavier halides (iodide, bromide) in water and confirm the structural similarity between the amorphous solid and the corresponding liquid. In contrast, no appreciable surface segregation of ions is observed in methanol, neither in the experiment nor in the simulation, which points to the remarkable surface properties of water among polar solvents. The propensity of heavier halides for the air/solution interface has important implications for heterogeneous chemical processes, particularly in the atmosphere.

O 29.79 Wed 14:30 P2

The structure of ordered iodine layers on Pt(100) in electrolyte and air — ●BJÖRN BRAUNSCHWEIG and WINFRIED DAUM — Institut für Physik und Physikalische Technologien, TU Clausthal, Leibnizstrasse 4, D-38678 Clausthal-Zellerfeld

Well-defined iodine adlayers, prepared by flame annealing and subsequently quenching in iodine vapor, were studied by scanning tunneling microscopy (STM) in air and a 0.1M HClO₄ electrolyte with atomic-resolution. The I-Pt(100) surface showed atomically flat terraces with monoatomic steps mainly along the [010] direction. At low iodine coverage STM in air reveals domains of clean reconstructed Pt(100)-hex and domains of an ordered ($\sqrt{2} \times 5\sqrt{2}$)R45°-I adlattice on Pt(100)-(1x1). At high coverage iodine forms a complete ($\sqrt{2} \times 5\sqrt{2}$)R45° layer on the Pt(100) surface which consists of a defect-free phase with iodine rows perpendicular to the main direction of the terrace steps, and a defect-rich phase with iodine rows parallel to the steps and with quasi-one-dimensional defects along the [010] direction. The boundary between the two phases is found to be atomically abrupt. Contrary to our STM data in 0.1M HClO₄ which are in agreement with previous work [1], STM imaging in air reveals buckled iodine double-rows. The strength of buckling depends on tunneling resistance and on the orientation of the ($\sqrt{2} \times 5\sqrt{2}$)R45° domains.

[1] R. Vogel and H. Baltruschat; Surf. Sci. Lett. 259,L739-42(1991)

O 29.80 Wed 14:30 P2

Reactivity studies of formic acid oxidation on the bare and the Cu modified Pd(111) surface — ●KLAUS WANDEL, KATRIN BRANDT, and MARCO STEINHAUSEN — Institute of Physical and Theoretical Chemistry, University of Bonn, Wegelerstr. 12, D-53115 Bonn, Germany

FTIRS, CV and AES have been used to investigate the reactivity of formic acid oxidation on the bare and the Cu modified Pd(111) surface as a function of potential, electrolyte and surface composition. This reaction has thus been studied in pure formic acid as well as in 10 M and 5 mM aqueous formic acid solution. Carbon dioxide evolution which was characterised by the asymmetric O=C=O stretching vibration at 2345 cm⁻¹ has been employed as "probe" for the surface reactivity.

The spectroscopic characterisation of HCOOH/Pd(111) points to an extraordinary acceleration of CO₂ evolution at the electrode as the potential is increased above 0.45 V. Analysis of IR-measurements at constant potentials lead to the assumption that the electronic state of the solid/liquid interface in the open-circuit HCOOH/Pd(111)-H₂SO₄-system corresponds to that at about 0.4 V vs. RHE. Water as solvent plays an important role in formic acid oxidation as a decrease in formic acid concentration in the electrolyte results in an augmentation of the relative reactivity normalized to the number of formic acid molecules in solution. Depending on the direction of the potential scan the rate of formic acid oxidation is inhibited or accelerated by electrochemically deposited Cu on the Pd(111)-surface.

O 29.81 Wed 14:30 P2

Immobilization of cationic porphyrins (H2TMPyP) on sulfate modified Cu(111): An ECSTM study — ●MINH HAI NGUYEN THI, KLAUS WANDEL, and PETER BROEKMANN — Institut für Physikalische und Theoretische Chemie, Universität Bonn, Wegelerstr. 12, D-53115 Bonn, Germany

The immobilization of cationic porphyrins (Meso-Tetra (N-methyl-4-pyridyl) Porphyrine Tetratosylat (H2TMPyP)) on sulfate modified Cu(111) surface has been studied by means of Cyclic Voltammetry (CV) and in-situ Scanning Tunnelling Microscopy (STM). Therefore a Cu(111) electrode surface was exposed to dilute sulfuric acid (5 mM H₂SO₄). Sweeping the electrode potential into the anodic direction starting from the regime of hydrogen evolution initiates the adsorption and subsequent ordering of a hydrophilic sulfate/water coadsorption layer. This adlayer formation follows a nucleation and growth mechanism so that even submonolayer coverages of this sulfate/water can be obtained depending on the applied electrode potential. Adsorption and immobilization of the cationic porphyrins takes place exclusively on the negatively charged sulfate/water coadsorption layer but not on the bare sulfate-free copper surface. This preferential adsorption is explained in terms of enhanced electrostatic interactions between the anion/water layer on the one hand and the cationic porphyrins layer on the other hand.

O 29.82 Wed 14:30 P2

Organized Chirality at the Solid/Liquid Interface: An In-Situ STM Study — ●MINH HAI NGUYEN THI¹, NAKCHEOL JEONG², BARBARA KIRCHNER¹, MAKUS REIHER³, CHRISTOPH A. SCHALLEY⁴, KLAUS WANDEL¹, and PETER BROEKMANN¹ — ¹Institut f. Physikalische und Theoretische Chemie, Universität Bonn — ²Department of Chemistry and Division of Molecular Engineering and Chemistry, Korea University — ³Institut f. Physikalische Chemie, Universität Jena — ⁴Institut f. Chemie und Biochemie, Freie Universität Berlin

The phase behavior of chiral metallo-supramolecular rhomboids of the Fujita type has been studied under electrochemical conditions by means of in-situ STM. A Cu(100) electrode which is pre-covered by a well ordered c(2 x 2) chloride layer served as substrate for the subsequent adsorption of positively charged metal complexes of the Fujita type. Characteristically, these metallo-supramolecular cages exhibit a molecular cavity of about 1.6 nm diameter and can therefore be regarded as potential model systems for the inclusion of small aromatic molecules in terms of supramolecular host/guest chemistry. On the c(2 x 2) chloride lattice these rhomboids adsorb flat lying with their cavity oriented to the solution phase. The racemic mixture of the chiral rhomboids spontaneously separates at the surface into two laterally well ordered mirror domains of enantiomerically pure rhomboids. When only one of both enantiomers is added to the supporting electrolyte we consequently observe only one of both mirror domains leading to a truly chiral electrode surface. Submolecular features of the chiral rhomboids in the STM experiment can be understood with the help of additional DFT calculations.

O 29.83 Wed 14:30 P2

Solid-liquid surfaces under potential control studied by X-ray diffraction — ●FRANK UWE RENNER, YVONNE GRÜNDER, and JÖRG ZEGENHAGEN — ESRF, BP220, 38043 Grenoble, France

At modern synchrotron radiation sources (e.g. ESRF in Grenoble) it is possible to study structures of surfaces in contact with liquids or electrolytes by in-situ X-ray diffraction with atomic resolution. On a conducting (metal or semiconductor) surface in contact with electrolyte it is possible to control the chemical potential of surface atoms by adjusting the electrical potential. Thus adsorption and desorption processes as well as structural phase changes of the bare crystal surfaces can be initiated close to or far from the equilibrium depending on the choice of potential. At the X-ray Standing Waves Surface Science Beamline ID32 at the ESRF we are studying these phenomena with newly developed electrochemical cells in-situ with X-ray diffraction and X-ray standing waves. Especially for metal alloy and semiconductor systems that have to be prepared by surface science vacuum methods a new UHV transfer electrochemical cell for in-situ X-ray diffraction has been developed using and controlling a droplet of electrolyte solution on the sample surface. We will present latest results for potential induced corrosion of low-index single crystal surfaces of the metal alloy systems Cu-Au and Cu-Pd, as well as metal deposition on semiconductors.

O 29.84 Wed 14:30 P2

Video STM Observation on A(111) Surface and Cu upd Layer in Aqueous Solution — ●KOJI SUTO and OLAF MAGNUSSEN — Institut für Experimentelle und Angewandte Physik, Universität Kiel

Dynamics of atom or ion on the electrified interface has been a hot topic on physics and nanotechnology over decades, but there are only a few reports on electrochemical systems. This time we will present some investigation on Au(111) surface in aqueous solution by Video STM (acquiring up to 30 images/s). First, electrochemically induced lifting of reconstruction was investigated in sulfuric acid. Herringbone structure was observed to disappear line by line, and its decay rate was analysed quantitatively. Next, Cu electrodeposition was investigated. It is well known that, by under potential deposition (upd), submonolayer of Cu is formed on Au(111) reductively at slight positive potential towards bulk deposition. Sulfate ($\sqrt{3} \times \sqrt{3}$) structure, which covered Cu upd layer was seen and the motion of the boundary fluctuating in between two parallel ($\sqrt{3} \times \sqrt{3}$) domains was observed by Video STM. Dynamic state of bulk deposition was also considered.

O 30 Invited talk Dujardin

Time: Thursday 09:30–10:15

Room: TRE Phys

Invited Talk

O 30.1 Thu 09:30 TRE Phys

Electronic control of molecular dynamics inside a single molecule; towards molecular nano-machines — ●GÉRALD DUJARDIN, GENEVIÈVE COMTET, MATHIEU LASTAPIS, MARTA MARTIN, and DAMIEN RIEDEL — Laboratoire de Photophysique Moléculaire, Bât. 210, Université Paris-Sud, Orsay, France

The use of a single molecule as a functionalized nano-machine requires being able to power and to control numerous dynamical processes at the

atomic-scale. We have found that tunneling electrons from a low temperature (5 K) scanning tunneling microscope (STM) can be used to control, through resonant electronic excitation, different molecular movements of a single molecule. Both the energy dependence and the spatial selectivity of the electronic excitation inside the molecule demonstrate the feasibility of controlling the reversible dynamics (diffusion, isomerization, bistable state and transient state movement) of a single molecule with precision.

O 31 Invited talk Repp

Time: Thursday 10:15–11:00

Room: TRE Phys

Invited Talk

O 31.1 Thu 10:15 TRE Phys

Scanning Tunneling Microscopy of Adsorbates on Insulating Films: From the Imaging of Individual Molecular Orbitals to the Manipulation of the Charge State — ●JASCHA REPP — IBM Research, Zurich Research Laboratory, 8803 Rüschlikon, Switzerland

Ultrathin insulating films on metal substrates are unique systems to use the scanning tunneling microscope to study the electronic properties of single atoms and molecules, which are electronically decoupled from the metallic substrate.

Individual gold atoms on an ultrathin insulating sodium chloride film supported by a copper surface exhibit two different charge states, which

are stabilized by the large ionic polarizability of the film. The charge state and associated physical and chemical properties such as diffusion can be controlled by adding or removing a single electron to or from the adatom with a scanning tunneling microscope tip. The simple physical mechanism behind the charge bistability in this case suggests that this is a common phenomenon for adsorbates on polar insulating films.

In the case of molecules on ultrathin NaCl films the electronic decoupling allows the direct imaging of the unperturbed molecular orbitals, as will be shown in the cases of individual pentacene and oligothiophene molecules. Scanning tunneling spectroscopy of these double-barrier tunneling junctions reveals strong electron-phonon coupling to NaCl phonons.

O 32 Adsorption IV

Time: Thursday 11:15–13:00

Room: TRE Phys

O 32.1 Thu 11:15 TRE Phys

Organic molecules on surfaces: Structural and dynamical properties — ●MARTIN PREUSS¹, KAORI SEINO¹, WOLF GERO SCHMIDT², and FRIEDHELM BECHSTEDT¹ — ¹Institut für Festkörpertheorie und -optik, Friedrich-Schiller-Universität Jena, Germany — ²Fakultät für Naturwissenschaften, Department Physik, Universität Paderborn, Germany

For the microscopic control of organically functionalized surfaces an understanding on the atomic scale can only be achieved by combined experimental and theoretical studies. For the elucidation of interface structures infrared (IR) and high-resolution electron energy loss spectroscopy (HREELS) are among the most prominent methods due to the sensitivity towards subtle changes in geometry and, hence, vibrational properties. The determination of normal-mode and phonon frequencies belongs to the standard repertoire of density-functional theory (DFT)

calculations whereas the corresponding intensities are seldomly reported. We have recently implemented a simple but accurate method into an existing plane-wave DFT code that allows for the calculation of the dynamical dipoles, and thus of IR intensities, for extended systems. For test purposes, the procedure is applied to small isolated molecules (NH₃, AlH₃, H₂O) and to benzene (C₆H₆) adsorbed on the Si(001) surface. For the system of perylene (C₂₀H₁₂) on Si(001) studied lately we scrutinize a number of possible adsorption configurations and single out the most probable one by comparison of the calculated and the measured vibrational spectrum.

O 32.2 Thu 11:30 TRE Phys

Observation of the Dynamical Change in a Water Monolayer Adsorbed on a ZnO Surface — ●B. MEYER¹, O. DULUB², and U. DIEBOLD² — ¹Lehrstuhl für Theoretische Chemie, Ruhr-Universität Bochum — ²Department of Physics, Tulane University, New Orleans, USA

A combined density functional theory (DFT) and scanning tunneling microscopy (STM) study shows a rich structure of water monolayers adsorbed on the ZnO(10 $\bar{1}$ 0) surface at room temperature. Most of the water is in a lowest-energy configuration where every second molecule is dissociated. It co-exists with an energetically almost degenerate configuration, consisting of a fully molecular water monolayer. Parts of the layer continuously switch back and forth between these two states. DFT calculations reveal that water molecules repeatedly associate and dissociate in this sustained dynamical process.

[1] O. Dulub, B. Meyer, U. Diebold, Phys. Rev. Lett. **95**, 136101 (2005)

O 32.3 Thu 11:45 TRE Phys

Wetting behavior of low-index cubic SiC surfaces — ●ALESSANDRA CATELLANI¹, GIANCARLO CICERO^{2,3}, and GIULIA GALLI³ — ¹CNR-IMEM, Parco Area delle Scienze 37a, I-43010 Parma, Italy — ²Physics Department, Torino Polytechnic, C. Duca degli Abruzzi, 24, I-10129 Torino, Italy — ³Lawrence Livermore National Laboratory, P.O. Box 808, Livermore, California 94550, USA

We report on the interaction of water molecules with polar and non polar stoichiometric surfaces of cubic silicon carbide, as described by ab initio molecular dynamics at finite temperature. Our calculations show that, irrespective of coverage, in the gas phase water spontaneously dissociates on both polar Si-terminated (001) and non-polar (110) surfaces, following similar mechanisms. The specific geometric arrangement of atoms on the outermost surface layer is responsible for water orientation and coordination and thus plays a major role in determining surface reactivity. The ability of the crystalline surfaces with different polarity to induce water dissociation can be related to the similarities of their ionization potentials.

O 32.4 Thu 12:00 TRE Phys

Ab initio study of chemisorption reaction of Carboxylic group on Hydrogenated Silicon — ●ALESSANDRA CATELLANI^{1,2}, CLOTILDE S. CUCINOTTA^{2,3}, ALICE RUINI^{2,3}, MARILIA J. CALDAS^{4,2}, and ELISA MOLINARI^{2,3} — ¹CNR-IMEM, Parco Area delle Scienze 37a, 43010 Parma, Italy — ²CNR-INFM 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 — ⁴Instituto de Física, Universidade de Sao Paulo, Cidade Universitaria, 05508-900 Sao Paulo, Brazil

We studied the reactivity of the dihydrogenated Si(001) surface exposed to propionic acid [1]. The NEB method has been applied to predict energy barriers for chemisorption through the diverse O atoms pertaining to the -COOH group; the different paths to double Si-O bond formation are compared, and discussed in the light of grafting probability and functionalization stability.

[1] C. S. Cucinotta, A. Ruini, M. J. Caldas, and E. Molinari, J. Phys. Chem. B **108**, 17278 (2004).

O 32.5 Thu 12:15 TRE Phys

Conformational changes in adsorbed molecules — ●PHILIPP MARTIN SCHMIDT, THORSTEN U. KAMPEN, J. HUGO DIL, and KARSTEN HORN — Fritz-Haber-Institut der Max-Planck-Gesellschaft, Faradayweg 4-6, 14195 Berlin, Germany

Stilbene is the monomer building block of phenylenevinylene-type oligomers and polymers. It undergoes an interconversion around the central C=C double bond upon irradiation with UV-light of 250-320nm

wavelength. This cis-trans-isomerization of the free molecule follows an in-plane hula-twist mechanism whose pathway can be assumed to work also in constraint systems as on surfaces - thus assessing a 'molecular switch'. To investigate the isomerization of stilbene-molecules on surfaces, planar trans(t)-stilbene has been studied on Si(100) surfaces at ~90 K by means of UPS and NEXAFS. Valence band spectra show that t-stilbene adsorbs undissociated onto the Si(100) surface. Neither Si2p nor C1s core level spectra show an energy shift upon coverage of the surface with t-stilbene, suggesting that the interaction is weak. Intensity changes of different components of the Si2p and C1s reveal that bonding takes place between Si dimers and the carbon atoms in the central C=C double bond. NEXAFS spectra indicate that the first layer of t-stilbene adsorbs in a flat orientation with the benzene rings being parallel to the substrate surface. Multilayers, on the other hand, physisorb highly disordered. A comparison of valence band spectra of trans- with cis-stilbene reveal significant differences which may permit an identification of both isomers for a further investigation of the isomerization process.

O 32.6 Thu 12:30 TRE Phys

Nano-ordering of defect structures in disordered Au/Si(111)-(5x2) — ●CHRISTOPH SEIFERT, CHRISTIAN WIETHOFF, FRANK MEYER ZU HERINGDORF, and MICHAEL HORN-VON HOEGEN — Universität Duisburg-Essen, Duisburg, Germany

Au adsorption at elevated temperatures in the Au coverage regime of up to 0.4 ML on Si(111) leads to the formation of (5x2) reconstructed domains. The electron diffraction pattern of this surface resembles that of a (5x1) reconstructed surface with additional pronounced lines at 50% Brillouin-Zone. These lines are well known to be caused by a random phase-shift of adjacent rows of the reconstruction in the two-fold direction[1].

Preparation at temperatures above 500°C - in combination with an increased Au coverage - yields a pronounced wavy modulation of these lines with a 20% BZ periodicity, which is visible after cool-down to room-temperature. This modulation is caused by an ordering of neighbouring phase-shifts and thus of the antiphase translational domains as well. A simple model, that qualitatively explains the resulting electron diffraction pattern, will be presented.

[1] Lipson et al. J. Phys. C **7**, p.12 (1974)

O 32.7 Thu 12:45 TRE Phys

Friction and adhesion mechanisms of the hairy attachment systems in spiders — ●MICHAEL SCHUCH¹, WOLFRAM HILD¹, KATHRIN CARL², YONGHE LIU¹, MATTHIAS SCHERGE³, and JUERGEN A. SCHAEFER¹ — ¹TU Ilmenau, Institut für Physik und Zentrum für Mikro- und Nanotechnologien, Postfach 100565, 98684 Ilmenau, Germany — ²TU Ilmenau, Fakultät für Maschinenbau, Postfach 100565, 98684 Ilmenau, Germany — ³IAVF Antriebstechnik AG, Im Schleherth 32, 76187 Karlsruhe, Germany

Biological attachment systems, such as the foot of geckos and spiders show a rich variety of shape and structure. Easy deformable attachment pads, hierarchical hairy structures with dimensions in the range of some hundred nm up to some μm lead to an enormous attachment ability. It has been proposed that attachment is achieved by the interaction between the attachment system and substrate, and by visco-elastic deformation. Both mechanisms are closely related with the contact area, which changes in the motion process. This work examines the contact area of spider feet on glass substrate and measures the friction and detachment forces. A living spider moving on a transparent glass substrate is observed by an optical microscope directly. The motion process recorded by a CCD-camera is examined to determine how the attachment and detachment are related with contact area of the spider feet. The foot prints obtained by a dyeing method are observed by a scanning electron microscope and correlated with the optical observations. Friction and detachment forces are measured with a microtribometer. The relationship between the friction and detachment forces and the contact area is discussed.

O 33 Scanning probe techniques III

Time: Thursday 11:15–13:00

Room: PHY C213

O 33.1 Thu 11:15 PHY C213

Combined Frequency Modulated Atomic Force and Scanning Tunneling Microscope: Basic Concept, Experimental Design, Signal Electronics, Atomic Resolution — ●GEORG SIMON, MARKUS HEYDE, HANS-PETER RUST, and HANS-JOACHIM FREUND — Fritz-Haber-Institute of the Max-Planck-Society, Faradayweg 4-6, D-14195 Berlin, Germany

A low temperature (5 Kelvin) ultra-high vacuum system has been supplemented with a new double tuning fork sensor for frequency modulated atomic force microscopy (FM-AFM) and scanning tunneling microscopy (STM) measurements [1]. Here the experimental set-up of the whole microscope will be presented, e.g. vacuum chamber, vibrational isolation, cryostat, microscope head, force sensor and signal electronics. The combined FM-AFM/STM set-up has been tested successfully. It shows atomic resolution in both modes. For detailed analysis and interpretation of surface structures, we benefit from the capability of our sensor to record FM-AFM and STM images as well as spectroscopic data at the same surface area. Atomically resolved images obtained on thin oxide films will be presented [2].

[1] M. Heyde, M. Kulawik, H.-P. Rust, H.-J. Freund, *Rev. Sci. Instrum.* 75, 2446 (2004).

[2] M. Heyde, M. Sterrer, H.-P. Rust, H.-J. Freund, *Appl. Phys. Lett.* 87, 083104 (2005).

O 33.2 Thu 11:30 PHY C213

Computing scanning tunneling spectroscopy by the layer-KKR real-space method — ●KAMAL K. SAHA, JÜRGEN HENK, ARTHUR ERNST, and PATRICK BRUNO — Max-Planck-Institut für Mikrostrukturphysik, Halle/Saale, Germany

Often, the computation of scanning tunneling spectroscopy (STS) relies on severe approximations. For example in the Tersoff-Hamann model, the electronic structure of the STM tip is taken into account rather imprecisely. Or in a supercell approach, the periodicity may lead to artifacts.

In this contribution, a new approach to compute STS from first principles is proposed. Applying a self-consistent real-space multiple-scattering theory (here: spin-polarized relativistic layer-KKR) for the Green function of the tunnel junction, the abovementioned shortcomings can be avoided. The conductance is obtained within the Landauer-Büttiker theory.

After introducing key issues of the proposed approach, its application to the Co(0001) surface will be discussed, with a focus on the tunnel magnetoresistance due to spin-polarized surface states.

O 33.3 Thu 11:45 PHY C213

Calibration and optimization of scanning conditions in combined scanning thermal microscopy and scanning thermoelastic microscopy — ●DIRK DIETZEL¹, SUTHARAT CHOTIKAPRAKHAN², RALF MECKENSTOCK², DETLEF SPODDIG², and JOSEF PELZL² — ¹Physikalisches Institut, Universität Münster, 48149 Münster — ²Experimentalphysik 3, Ruhr Universität Bochum, 44780 Bochum

In this contribution we will present a combined experimental set-up for the simultaneous detection of the thermal and thermoelastic signal of electrically heated semiconductor devices by scanning probe techniques. The simultaneously obtained signal profiles of the Scanning Thermal Microscope (SThM) and the Scanning Thermoelastic Microscope (SThEM) give information on the shape and position of heat sources, where the combination of the two detection schemes gives a more precise set of parameters describing the heat sources and the temperature distribution in the sample. Additionally, two new techniques related to SThEM are presented: 1) a simple and straightforward calibration technique for the modulated surface expansion by force distance spectroscopy measurements using an electrically heated tip and 2) the optimisation of the scanning conditions by performing SThEM measurements on the 2nd harmonic resonance frequency of the cantilever. Using this technique on a high power capacitor structure a significant increase of the sensitivity can be achieved, which allows faster scanning or the detection of smaller surface oscillations (e.g. from subsurface heat sources).

O 33.4 Thu 12:00 PHY C213

Development of an ultra-low cost scanning tunneling microscope for high-school education — ●GRIT PETSCHICK¹, HOLGER EISELE¹, ROBERT KASTL², KAI HODECK¹, VOLKHARD NORDMEIER², and MARIO DÄHNE¹ — ¹Technische Universität, Festkörperphysik, Hardenbergstr. 36, 10623 Berlin — ²Freie Universität, Didaktik der Physik

25 years ago we learned in school that atoms cannot be optically imaged. But nowadays, since the invention of the scanning tunneling microscope (STM) in the early 1980th it is possible to map surfaces on the atomic scale. Today, a various number of microscopic possibilities exist to image atoms, still none is as simple and trouble-free as the scanning tunneling microscope itself. As schools funds are strictly limited it is mostly not possible to equip them with commercial microscopes and thus to gain experience about the nano-world of atoms at the state of the art of modern physics in the 21st century.

We report on the development and construction of an ultra-low cost scanning tunneling microscope setup, which is designed especially for high-school education requirements. A special challenge was to comply with safety requirements, requiring a special design of the piezo-based coarse approximation. Yet, another requirement towards capability was the possibility to image actual solid surfaces at the atomic scale. The aim towards school application is to get pupils to independently prepare and analyse surfaces of graphite and mica.

O 33.5 Thu 12:15 PHY C213

Little Changes - big Effects! Molecular Self-Organization probed by STM. — ●B. A. HERMANN¹, L. J. SCHERER², C. E. HOUSECROFT², and E. C. CONSTABLE² — ¹Dept. of Physics / CeNS, LMU Munich and WMI, Walther-Meissner-Str. 8, 85748 Garching, Germany — ²Dept. of Chemistry, Uni. of Basel, Spitalstrasse 51, 4056 Basel, Switzerland

Aromatic-rich Fréchet-type dendrons are ideally suited to visualisation by scanning tunnelling microscopy (STM) and guarantee excellent self-organization on graphite. Here, asymmetric dendritic wedge-functionalised terpyridine ligands, are studied in a careful comparison of highly resolved 2-D self-organized monolayers on graphite using scanning tunnelling microscopy (STM) and x-ray analysis of crystals of the same molecules. The (sometimes) near atomic resolution in conjunction with x-ray analysis of 3-D crystals allowed us to assign the observed molecular arrangements. The observed molecular pattern appears like being knitted row by row. As the octyl chains of the Fréchet-type dendrons, play a major role in the process of molecular organisation, we also synthesised compounds without the octyl chains but otherwise similar molecular structure. Omitting the octyl chains led to no longer opposing Fréchet wedges. Replacing additionally the inner oxygen atom by a sulphur atom and thus changing an inner bond angle caused completely different symmetric properties in the observed self-organized monolayers. Deposition of dendritic wedge-functionalised terpyridine ligands on HOPG resulted in the formation of well-defined monolayers exhibiting different arrangements depending on small changes in the studied molecules.

O 33.6 Thu 12:30 PHY C213

High-ordered arrays of single molecular magnets on Cu(111) — ●LUCIA VITALI¹, M.ALEXANDER SCHNEIDER¹, MARIO RUBEN², ADRIANO MOSCA CONTE³, STEFANO FABRIS³, STEFANO BARONI³, and KLAUS KERN¹ — ¹Max-Panck-Institute for solid state research Stuttgart — ²Institute of Nanotechnology Karlsruhe — ³INFN CNR DEMOCRITOS National Simulation Center Trieste

Molecular magnets are promising candidates for the realization of molecule-based information storage media within the nanometer regime. So far, the difficulty of forming ordered structures on surfaces prevented their application. Here we report on the formation of long-range ordered layers of a recently discovered class of single-molecular-magnets (SMMs), called lanthanide double-deckers, on the Cu(111) surface. These, consisting of a single lanthanide ion located between two phthalocyanine units, act as isolated magnetic domains exhibiting a magnetization hysteresis below a characteristic blocking temperature of 40K[1]. The highly-ordered hexagonal networks have been imaged and analyzed in situ by Scanning Tunneling Microscopy and Spectroscopy at 6K. The direct comparison of the spectroscopic results with density-functional-theory calcu-

lations of the molecule in the gas phase suggests that the molecules are not affected by the deposition and contact to the metallic substrate.

[1] N. Ishikawa et al., J. Am. Chem. Soc. 125, 8694 (2003)

O 33.7 Thu 12:45 PHY C213

Quantitative Dynamic Mode Force Spectroscopy on a Type-II Superconductor Using a Magnetic Tip: Meissner Force, Magnetostatic Tip-Vortex Interaction and Lateral Dragging Force

— ●ALEXANDER SCHWARZ¹, UNG HWAN PI¹, MARCUS LIEBMAN², ZHEONG GU KHIM³, DONG HO KIM⁴, and ROLAND WIESENDANGER¹ — ¹University of Hamburg, IAP, Jungiusstr. 11, 20355 Hamburg — ²Present Address: RWTH Aachen, Department of Physics, 52056 Aachen — ³School of Physics, SNU, Seoul 151-742, South Korea — ⁴Dept. of Physics, Yeungnam University, Kyongsan, South Korea

In the mixed phase of type II superconductors quantized flux can pen-

etrate the specimen in the form of vortices with a normal conducting core. Using magnetic tips, such samples can be investigated by magnetic force microscopy. We used the frequency modulation technique to study the glass-like flux solid state of a $\text{Bi}_2\text{Sr}_2\text{CaCu}_2\text{O}_{8+\delta}$ single crystal in the low flux density regime, where neighboring vortices do not overlap. To quantify the distance dependence of the relevant tip-sample interactions, force spectroscopy has been utilized. On top of a vortex, the maximum attraction 18 nm above the surface was determined to be about 5.4 pN. Far away from vortices the Meissner repulsion of about 4.0 pN between the magnetic tip and the superconducting phase dominates the interaction. By taking several force spectroscopy curves across a vortex, the lateral dragging force exerted by a scanning tip on a vortex could be determined to be about 1.5 pN [1]. These results agree well with theoretical predictions.

[1] U. H. Pi *et al.*, Appl. Phys. Lett. **85**, 5307 (2004).

O 34 Particles and clusters II

Time: Thursday 11:15–13:00

Room: WIL A317

O 34.1 Thu 11:15 WIL A317

Supported Ag clusters deposited on insulating substrates studied by reflectance-difference spectroscopy and ellipsometry — ●J.M. FLORES-CAMACHO, L.D. SUN, M. HOHAGE, K. SCHMIDEGG, N. SAUCEDO-ZENI, G. WEIDLINGER, and P. ZEPPENFELD — Institute of Experimental Physics, Johannes Kepler University Linz, Altenberger str. 69, A4040 Linz, Austria

Metal clusters were formed during the deposition of nominally few nanometer thick Ag layer on insulating substrates, i.e., poly(ethylene terephthalate) (PET) and amorphous quartz. Depending on the cluster size, substrate crystallinity, and substrate dielectric properties, the metal clusters exhibit different plasmon related optical responses with out-of-plane and even in-plane anisotropy. In the case of clusters deposited on biaxially drawn PET substrates, reflectance-difference spectroscopy (RDS) provided a tool for the study of anisotropic plasmon resonances lying in the plane of the substrate. On the other hand, since Ag clusters on amorphous substrates such as quartz do not show in-plane anisotropy, then the out-of-plane anisotropy plays a prominent role in the determination of the cluster properties, therefore, the employment spectroscopic ellipsometry (SE) is proposed to accomplish such a task. This enables us to study plasmon resonances along both parallel and perpendicular directions to the substrate surface normal.

O 34.2 Thu 11:30 WIL A317

Photodesorption NO from silver nanoparticles on a thin alumina film — ●KAZUO WATANABE¹, KI-HYUN KIM¹, DIETRICH MENZEL^{1,2}, and HANS-JOACHIM FREUND¹ — ¹Fritz-Haber-Institut der Max-Planck-Gesellschaft, Faradayweg 4-6, 14195 Berlin, Germany — ²Physik-Department E20, Technische Universität München, 85747 Garching, Germany

The photodesorption (PD) of NO adsorbed on Ag nanoparticles supported on a thin Al_2O_3 film has been studied by a mass selected time-of-flight method (MS-TOF) and by temperature programmed desorption (TPD). NO was adsorbed on 0.5-nm deposited Ag nanoparticles (~ 8 nm particle diameter) at 75 K. NO TPD showed two peaks at 75 K and 96 K due to desorption from NO dimers. NO adsorbates were photodesorbed by nanosecond laser pulses at $h\nu = 3.5$ and 4.0 eV. PD cross sections were obtained from the fluence dependence of the integrated TOF signals of desorbing NO. By fitting the data with a single exponential, cross sections of 7.1×10^{-17} and 8.4×10^{-17} cm^2 were obtained for the two energies. This corresponds to enhancement factors of 37 and 1.6 compared to those on Ag(111) at $h\nu = 3.5$ and 4.0 eV, respectively. The large enhancement at 3.5 eV is explained by resonant excitation of the Mie plasmon of the Ag nanoparticles. Mean translational energies of NO were 700 K and 800 K at $h\nu = 3.5$ and 4.0 eV, respectively; they increased to more than 1000 K for extended photoirradiation. These values are considerably larger than that from Ag(111): ~ 490 K at $h\nu = 3.5$ eV. The increase of translational energies of photodesorbed NO from silver nanoparticles may be attributed to longer lifetimes of the active excited states of NO.

O 34.3 Thu 11:45 WIL A317

Plasmon excitations in clusters in the vicinity of metal surfaces — ●YAROSLAV PAVLYUKH and WOLFGANG HÜBNER — Department of Physics, Kaiserslautern University, Box 3049, D-67653, Kaiserslautern, Germany

We study the collective excitations of metal clusters approaching a metal surface. Using a simple model for the frequency-dependent dielectric constant $\epsilon(\omega)$ and the multiple scattering method we numerically investigate the shift in the plasmon resonance due to the coupling of the collective modes of the sphere with those of its mirror image. Results of the model calculation are verified by means of *ab initio* theory. As a prototypic system we study Na_9^+ cluster on the Cu (100) surface. The representation of the solid surface by a cluster of several, typically 54 substrate atoms is used in the combination with a high level configuration interaction (CI) calculation.

O 34.4 Thu 12:00 WIL A317

Radiation damping of plasmons in metal nanoparticle pairs — ●CHRISTIAN DAHMEN, BENJAMIN SCHMIDT, and GERO VON PLESSEN — Nanostructure Optics Group, I. Physikalisches Institut (IA), RWTH Aachen, 52056 Aachen

The optical properties of electromagnetically coupled metal nanoparticles have received much interest. This interest is partially fuelled by the large local-field enhancement near coupled nanoparticles, which plays an important role in surface-enhanced Raman scattering. Another point of interest are the spectral properties of the coupled particle-plasmon resonances. They show large frequency shifts when the particle spacing is sufficiently small for near-field coupling to occur. Less attention has been devoted to the issue of radiation damping in coupled nanoparticles. Here we calculate the radiation damping rates of plasmon resonances in metal nanoparticle pairs using Generalized Mie theory, which takes retardation effects into full account. The radiation damping of the coupled particle-plasmon mode alternates between superradiative and subradiative behavior when the particle spacing is varied. The damping thus depends on the phase difference between the dipole of one particle and the field scattered by the other particle. At small particle spacings where near-field coupling sets in, the radiation damping rate lies far below that of an isolated particle. This reduction of radiation damping implies a reduced dephasing of the coupled plasmon mode and thus tends to increase the local field enhancement in the space between the particles.

O 34.5 Thu 12:15 WIL A317

Optical and structural changes of embedded silver nanoparticles during photochromic transformation — ●CHRISTIAN DAHMEN, ALEXANDER N. SPRAFKE, HENNING DIEKER, FLORIAN HALLERMANN, MATTHIAS WUTTIG, and GERO VON PLESSEN — I. Physikalisches Institut (IA), RWTH Aachen, 52056 Aachen

Photochromic materials reversibly change their color under light illumination. We have recently reported that dc-sputter deposition can be employed to prepare a multicolor photochromic material consisting of silver nanoparticles embedded in TiO_2 . The explanation for photochromism in this system is spectral hole burning in the inhomogeneously broadened particle-plasmon band, which is probably caused by photoemission of electrons from the Ag nanoparticles. In this work, we investigate how

the particle-plasmon line of optically excited silver nanoparticles is modified to give rise to the photochromic effect. We find that the spectral hole is mainly due to a reduction of the plasmon extinction peak of the excited nanoparticles. From a comparison with x-ray diffraction experiments we conclude that this decrease of the extinction peak is caused by a photoinduced reduction of the mean size of the silver nanocrystals.

O 34.6 Thu 12:30 WIL A317

Characterisation of silver nanoparticles on magnesium oxide — ●M. ALSCHINGER¹, Y. CHEN², M. DI VECE², F. HUBENTHAL¹, R.E. PALMER², and F. TRÄGER¹ — ¹Institut für Physik, Universität Kassel, Kassel — ²Nanoscale Physics Research Laboratory, The University of Birmingham, Birmingham, UK

Determination of the dimensions of supported nanoparticles has long been a very important issue that can most reliably be accomplished by transmission electron microscopy (TEM). Such measurements are, however, time consuming and require laborious preparation of the samples. In order to develop a more straightforward, easy to apply and accurate alternative, optical spectroscopy and its potential for the determination of the particle size and shape has been examined in detail here. The results were complete by AFM images and compared to data derived from TEM pictures. First, Ag nanoparticles have been prepared in vacuum by deposition and nucleation of silver atoms on magnesium oxide substrates. Subsequently, the optical spectra were recorded and compared to theoretical spectra based on the quasistatic approximation in order to establish a relation between the size and shape of the particles. AFM has been used to measure the size and the size distribution of the particles.

In a second step the same kind of particles was prepared for TEM experiments from which we could obtain precise data for comparison. The most important result is that modelling of the optical spectra revealed a relation between the size and shape of the particles that is in accord with the TEM results and therefore forms a basis for reliable determination of the dimensions of nanoparticles by measuring their optical spectra.

O 34.7 Thu 12:45 WIL A317

Setup for the Study of Mass Selected Clusters at Surfaces with Low-Temperature STM and UPS — ●STEFANIE KRAUSE¹, THOMAS IRAWAN¹, MARKUS BIELETZKI¹, HEINZ HÖVEL¹, CHUNRONG YIN², and BERND VON ISSENDORFF² — ¹Universität Dortmund, Experimentelle Physik I, 44221 Dortmund, Germany — ²Universität Freiburg, Fakultät für Physik, 79104 Freiburg, Germany

We measure mass spectra of size selected Ag clusters with a cluster machine consisting of a magnetron sputter gas aggregation source [1], a differential pumping stage with a cryo pump and a high transmission infinite range mass selector [2]. In current experiments we extend these studies to the deposition of mass selected clusters on rare gas layers and different substrate systems. For these samples low-temperature STM and UPS [3] will be compared with photoelectron spectroscopy for the same clusters in a free cluster beam.

[1] H. Haberland, M. Mall, M. Moseler, Y. Qiang, Th. Reiners and Y. Thurner, *J. Vac. Sci. Technol. A* **12**, 2925 (1994).

[2] B. von Issendorff and R. E. Palmer, *Rev. Sci. Instr.* **70**, 4497 (1999).

[3] H. Hövel, T. Becker, D. Funnemann, B. Grimm, C. Quitmann and B. Reihl, *J. Electron Spectros. Rel. Phenom.* **88-91**, 1015 (1998).

O 35 Organic films III

Time: Thursday 11:15–13:00

Room: WIL B321

O 35.1 Thu 11:15 WIL B321

HREELS study of thin NTCDA/Ag(111) films upon different — ●DOMINIQUE HÜBNER¹, V. SHKLOVER¹, C. STADLER¹, R. FINK², and E. UMBACH¹ — ¹Univ. Würzburg, Exp. Phys. II — ²Univ. Erlangen, Phys. Chem. II

High Resolution Electron Energy Loss Spectroscopy is a well established tool to investigate both electronic and vibronic excitation of thin films of large organic molecules. In addition to the vibronic and electronic properties, HREELS can provide structural information due to its sensitivity to molecular orientation. We investigated thin NTCDA films on Ag(111) surface with respect to different growth conditions (i.e. film thickness, growth rate, substrate temperature). The results are compared to FTIR, NEXAFS, and SPA-LEED measurements. For room temperature a Stranski-Krastanov growth with well ordered islands is observed whereas on cooled substrates a less well ordered Frank van der Merwe growth is observed.

O 35.2 Thu 11:30 WIL B321

Morphology of Sexiphenyl thin films — ●GREGOR HLAWACEK¹, ANDREI ANDREEV¹, CHRISTIAN TEICHERT¹, PAUL FRANK², ADOLF WINKLER², ROLAND RESEL², and MICHAEL RAMSEY³ — ¹Institut of Physics, University of Leoben, 8700 Leoben, Austria — ²Department of Solid State Physics, Graz Technical University, A-8010 Graz, Austria — ³Department of Experimental Physics, University of Graz, A-8010 Graz, Austria

Understanding and controlling the growth of organic thin films is vital for the production of high quality organic devices. Small organic molecules have shown a high potential for applications like organic lasers, organic light emitting devices and organic thin film transistors.

Here, para-sexiphenyl has been grown under UHV conditions at different growth temperatures. The used substrates include Si(001), mica(001), BaF₂(111) and KCl(001). Ex-situ as well as in-situ atomic-force microscopy (AFM) has been used to characterize the film morphology. Phase imaging has shown to be a useful tool to analyse the growth of the first few monolayers. In addition, some of the films have been analysed by different X-ray methods.

The molecular orientation (upright or parallel to the substrate) can be controlled by using the right combination of substrate and growth temperature. The films formed from lying molecules usually show a higher anisotropy that is mediated by the underlying substrate.

O 35.3 Thu 11:45 WIL B321

Transition from layer-by-layer to rapid kinetic roughening in organic semiconductor DIP films on SiO₂ — ●XUE NA ZHANG¹, ESTHER BARRENA², 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

Over the past two decades, organic semiconductors have widely investigated, due to their exciting optical, electronic, and optoelectronic properties. Recently, thin films of diindenoperylene (DIP) have been studied showing an extraordinarily high structural order on silicon dioxide making this molecule a prospective candidate for application in electronic devices [1][2]. Here we present a study of the structure and growth in the early stages of the DIP film formation on SiO₂ by Atomic Force Microscope and in-situ x-ray diffraction. We show that a transition from perfect layer-by-layer to rapid kinetic roughening occurs at a critical thickness of about 4-5 ML. In addition, our results reveal that significant changes in the lateral structure take place during these first stages of the DIP growth. Different aspects of the growth are discussed in relationship with the observed structural data.

[1]A.C. Dürr, et al. *Applied Physics Letters* **81**, 2267 (2002).

[2]A.C. Dürr, et al. *Physical Review Letters* **90**, 016104 (2003).

O 35.4 Thu 12:00 WIL B321

Influence of the substrate morphology on the organic layer growth of PTCDA/Ag(111) — ●THOMAS SCHMIDT¹, HELDER MARCHETTO², ULLRICH GROH¹, HELMUT KUHLENBECK², RAINER FINK³, HANS-JOACHIM FREUND², and EBERHARD UMBACH¹ — ¹Experimentelle Physik II, Universität Würzburg — ²Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin — ³Physikalische Chemie II, Universität Erlangen-Nürnberg

Using UV-excited photoelectron emission microscopy (UV-PEEM) we investigated the microscopic growth behavior of organic thin films (here PTCDA) on a Ag(111) single crystal substrate. Real time observation allows to correlate the growth mode (and related kinetic parameters) with substrate properties like terrace width (step density) and step bunches for the initial film formation, i.e., from the submonolayer range up to 5 monolayers. Above room temperature PTCDA (3,4,9,10-perylene-tetracarboxylic acid dianhydride) grows in a Stranski-Krastanov like fashion: after completion of the first two stable layers three dimensional islands are formed. The nucleation density depends drastically on

the substrate morphology and thus affects the structural and morphologic properties of the organic film. Funded by BMBF under contract no. 05KS4WWB/4.

O 35.5 Thu 12:15 WIL B321

Optical Evidence for Substrate Induced Growth of Ultra-thin Hexa-*peri*-hexabenzocoronene Layers on HOPG — ●ROMAN FORKER¹, THOMAS DIENEL¹, KLAUS MÜLLEN², and TORSTEN FRITZ¹ — ¹Institut für Angewandte Photophysik, TU Dresden, Germany — ²MPI für Polymerforschung, Ackermannweg 10, 55128 Mainz, Germany

We report on the influence of the substrate on the optical properties of ultra-thin hexa-*peri*-hexabenzocoronene (HBC) layers deposited by organic molecular beam epitaxy (OMBE). For that purpose, the *in situ* differential reflectance spectroscopy (DRS) was employed, providing unsurpassed sensitivity for the thickness-dependent optical analysis. From the DR spectra, the optical constants were extracted using a novel numerical algorithm [1]. It turns out that HBC films on different substrates exhibit different growth modes which could be confirmed by structural examinations.

While HBC shows polycrystalline island structures on mica and on fused quartz, layer-by-layer growth along with the formation of one-dimensional stacks on HOPG could be demonstrated optically. The observed monomer → dimer → oligomer transition was related to the well-known findings for perylenetetracarboxylicdianhydride (PTCDA) layers on mica [2, 3].

[1] R. Nitsche et al., Phys. Rev. B **70** (2004), 195432

[2] H. Proehl et al., Phys. Rev. Lett. **93** (2004), 097403

[3] H. Proehl et al., Phys. Rev. B **71** (2005), 165207

O 35.6 Thu 12:30 WIL B321

***In situ* study of the Growth of Titanylphthalocyanine (TiOPc) on Au(111)** — ●T. DIENEL¹, S.C.B. MANNSFELD², K. WALZER¹, and T. FRITZ¹ — ¹Institut für Angewandte Photophysik, TU Dresden, Germany — ²Department of Chemical Engineering, Stanford University, USA

We present a combined optical and structural investigation of the growth of TiOPc molecules on Au(111). Many different crystallographic

polymorphs are known for TiOPc, exhibiting very distinct optical properties. Highly ordered TiOPc films were prepared by means of OMBE with submonolayer to multilayer coverage. The structural analysis was done by Scanning Tunneling Microscopy (STM) and was confirmed by Low Energy Electron Diffraction (LEED) [1].

The recently implemented Differential Reflectance Spectroscopy (DRS) in combination with Photoluminescence measurements [2] were used to observe the change of the optical properties of the molecular layer *in situ*, which means during the actual growth of the film. The influence of the substrate temperature on the formation of different crystallographic polymorphs will be discussed as well as the strong quenching of the emission properties of the TiOPc film due to the metal substrate.

[1] S.C.B. Mannsfeld and T. Fritz, Phys. Rev. B **71**, 235405 (2005).

[2] H. Proehl et al., Phys. Rev. B **71**, 165207 (2005).

O 35.7 Thu 12:45 WIL B321

Nanostructured organic templates for the directed self-assembly of gold nanoparticles into confined domains — ●DANIEL DAHLHAUS, STEFFEN FRANZKA, NILS HARTMANN, and ECKART HASSELBRINK — Universität Duisburg-Essen, Campus Essen, Fachbereich Chemie, Universitätsstr. 5, 45141 Essen

A new procedure for the preparation of ordered arrays of gold nanoparticles is demonstrated. Octadecylsiloxane monolayers are grown on native silicon substrates. Subsequently these coatings are patterned using a focused beam of an argon ion laser [1]. The method allows for a well-confined decomposition of the monolayer with a lateral resolution which is significantly below the laser spot diameter. In particular, at a spot diameter of about 2.5 microns, structures with a width of 100 nm and below have been prepared. After patterning the remaining domains of the monolayer are chemically functionalized via amination of the hydrocarbon tails. The chemically functionalized patterns are suitable to direct the adsorption and self-assembly of citrate-coated gold nanoparticles. In particular, gold nanoparticles with an average diameter of 16 nm are shown to self-assemble into quasi one-dimensional structures.

[1] T. Balgar, S. Franzka and N. Hartmann, Appl. Phys. A, in press

O 36 Structure and dynamics

Time: Thursday 11:15–13:00

Room: WIL C207

O 36.1 Thu 11:15 WIL C207

Living on the Edge: Life and Death of Vacancies in Cu(100) — ●KOEN SCHOOTS, THOMAS H. BEUMAN, MARCEL J. ROST, and JOOST W.M. FRENKEN — Leiden Institute of Physics, Universiteit Leiden, Leiden, The Netherlands

We have used STM to investigate where surface vacancies originate and annihilate on Cu(100).

Because of the extremely high mobility of the surface vacancies, we have been forced to use tracer particles to follow the vacancy motion, in the form of In atoms, incorporated in the top layer. The "slide-puzzle"-diffusion of the vacancies makes the In atoms move through the surface, as has been reported in [1,2].

In the present study, we have employed tailor-made geometries, in which the In atoms were surrounded exclusively by upward or by downward steps. Our STM movies show a striking difference between these two cases, with differences in jump frequencies and average jump lengths of more than one order of magnitude. These results show that vacancies are primarily created at the upper side of a step and can be formulated in analogy with the energetics of ad-atoms, in terms of an Ehrlich-Schwöbel barrier [3] for surface vacancies.

[1] R. van Gastel et al., Nature **408** (2000) 665, Phys. Rev. Lett. **86** (2001) 1562, Surf. Sci **521** (2002) 10, Surf. Sci. **521** (2002) 26.

[2] M.L. Grant et al., Phys. Rev. Lett. **86** (2001) 4588.

[3] G. Ehrlich et al., J. Chem. Phys. **44** (1966) 1039.

O 36.2 Thu 11:30 WIL C207

Lattice dynamics of an iron monolayer — ●MARCEL SLADECEK¹, A. CHUMAKOV², P.T. JOCHYM³, J. KORECKI^{4,5}, J. LAZEWSKI³, K. PARLINSKI³, R. RÖHLSBERGER⁶, R. RÜFFER², B. SEPIOL¹, T. SLEZAK^{4,5}, N. SPIRIDIS⁵, S. STANKOV^{1,2}, and G. VOGL¹ — ¹Institut für Materialphysik der Universität Wien, Wien, Austria — ²ESRF, F-38043 Grenoble, France — ³Department of Materials Research by Computers, Institute of Nuclear Physics, Polish Academy of Sciences, Cracow, Poland — ⁴Faculty of Physics and Nuclear Techniques, AGH University of Science and Technology, Cracow, Poland — ⁵Institute of Catalysis and Surface Chemistry, PAS, Cracow, Poland — ⁶HASYLAB at DESY, Hamburg, Germany

Nuclear resonant scattering (Mössbauer spectroscopy with synchrotron radiation) allows the direct observation of the phonon density of states (DOS). The resonant feature of the method enables the selective investigation of the dynamics of an iron layer deposited at the surface or at an interface. The results of a systematic investigation of iron layers with thicknesses in the range from 40 ML down to 1 ML deposited on a W(110) substrate are presented and compared with bulk DOS and ab-initio calculations. The observed spectra, which are the first DOS spectra of an uncoated iron monolayer, show a phonon softening due to the broken translational symmetry and an inplane anisotropy.

Supported by: Austrian ministry of science bm:bwk (GZ45.529/2-VI/B/7a/2002 "Materials Dynamics Network") and European Community under the STREP Project Contract No. NMP4-CT-2003-001516 (DYNASYNC).

O 36.3 Thu 11:45 WIL C207

Dynamics of Heat Transport in Ultrathin Bi-Films on Si(001) Studied by Ultrafast Electron Diffraction — ●ANDREAS JANZEN, BORIS KRENZER, PING ZHOU, DIETRICH VON DER LINDE, and MICHAEL HORN-VON HOEGEN — Universität Duisburg-Essen, Institut für Experimentelle Physik, 47057 Duisburg

We used Ultrafast Electron Diffraction to study the surface temperature evolution following the intense fs-laser excitation (800 nm, 45 fs, 1.3 mJ/cm²) of thin, epitaxial Bi(111)-films deposited onto Si(001)-substrates. Reflection high-energy electron diffraction patterns at 7 keV have been recorded in a laser pump-electron probe experiment with ps-time resolution. The transient surface temperature is determined utilizing the intensity drop due to the Debye-Waller effect and comparing the transient diffraction spot intensity with a static calibration measurement. The cooling of a 6 nm thick Bi-film is much slower ($\tau = 640$ ps) than expected for purely diffusive bulk-heat conduction. For the smooth, abrupt Bi/Si-interface, the acoustic mismatch model explains this effect in terms of total internal reflection of phonons at the interface: the phonons are trapped in the Bi-film. The dependence of the cooling rate on the Bi-film thickness and the transition to the regime of diffusive heat transport will also be addressed.

O 36.4 Thu 12:00 WIL C207

First-principles based ground-state analysis of Co subsurface segregation in CoAl(111) — ●CHRISTIAN RIEDL, OLE WIECKHORST, STEFAN MÜLLER, LUTZ HAMMER, and KLAUS HEINZ — Lehrstuhl für Festkörperphysik, Universität Erlangen-Nürnberg, Staudtstr. 7, D-91058 Erlangen

As recently shown [1,2], the segregation profile of B2-ordered CoAl surfaces is controlled by tiny off-stoichiometries (Co antisite atoms). By applying the combination of density functional theory with the cluster expansion method and genetic algorithms we present the surface stability diagram of CoAl(111) considering the energetics of thousands of geometrically fully relaxed surface structures. It turns out that Al-Co-Co layer stacking is clearly the most stable configuration in agreement with our earlier DFT and quantitative LEED analysis [2]. We discuss the electronic structure providing reasons for the stability of the Al-Co-Co layer stacking. Furthermore, subsequent Monte-Carlo-simulations allow for the determination of the temperature dependent segregation profile up to the 7th layer as well as for an analysis of substitutional ordering at the surface.

[1] V. Blum et al, Phys. Rev. Lett. **89**, 266102 (2002)

[2] L. Hammer et al., Phys. Rev. B **71**, 075413 (2005)

O 36.5 Thu 12:15 WIL C207

Preparation and characterization of bimetallic AuPt/Pt(111) surface alloys - a quantitative STM study — ●ANDREAS BERGBREITER, HARRY E. HOSTER, ELEONORA FILONENKO, and ROLF J. BEHM — Department of Surface Chemistry and Catalysis, University of Ulm, D-89069 Ulm

Structures of atomically smooth and laterally equilibrated AuPt/Pt(111) surface alloys have been studied by UHV-STM. The alloys were prepared by Au island deposition onto a Pt(111) single crystal

followed by annealing at 1000K. The Au fraction visible by atomically resolved STM images with chemical contrast is correlated to the respective amount of Au deposited on the Pt(111) single crystal prior to annealing. The known bulk immiscibility of AuPt is reflected in a tendency towards phase separation also in two dimensions. Across the whole concentration range, homoatomic bonds dominate the structure and cause the formation of larger homoatomic ensembles. For comparison with other systems, the short range order (SRO) was quantified by Warren-Cowley-parameters. In order to correlate the atomic distribution with adsorption properties and catalytic behaviour in further studies, the surface density of selected homoatomic adsorption sites were calculated.

O 36.6 Thu 12:30 WIL C207

First Principles based prediction of short range order at the Pt₂₅Rh₇₅ (111) surface — ●MARKUS STÖHR, OLE WIECKHORST, and STEFAN MÜLLER — Universität Erlangen-Nürnberg, Lehrstuhl für Festkörperphysik, Staudtstr. 7, D-91058 Erlangen, Germany

The disordered Pt₂₅Rh₇₅(111) alloy surface shows a strong tendency towards Pt segregation. Although the segregation profile and atomic position in the near surface layers are well known by earlier STM and LEED studies [1,2], the reasons for the observed behaviour are widely unknown. We have used the combination of density functional theory (DFT) with cluster expansions and Monte-Carlo-simulations to model the substitutional ordering behaviour of the Pt₂₅Rh₇₅ (111) surface. This approach allows for the determination of the segregation profile, being in good agreement with the experimental data [1,2]. Moreover our approach gives access to the detailed short range order behaviour of the surface, as well as to the geometric structure of the surface.

[1] E. Platzgummer, M. Sporn, R. Koller, S. Forsthuber, M. Schmid, W. Hofer, P. Varga, Surf. Sci. **419** (1999) 236.

[2] E. L. D. Hebenstreit, W. Hebenstreit, M. Schmid, P. Varga, Surf. Sci. **441** (1999) 441.

O 36.7 Thu 12:45 WIL C207

Investigation of kinetic effects in the PtAu/Ru system. — ●ELEONORA FILONENKO, HARRY HOSTER, and R.J. BEHM — Department of Surface Chemistry and Catalysis

In order to explain the catalytic properties of well defined PtAu films, the behaviour of both metals was investigated in PtAu films deposited on the Ru(0001) monocrystal surfaces. The effect of heating temperature, ratio of both metals and sequential evaporation on the kinetic processes were studied in the model system PtAu/Ru by means of STM analysis. PtAu films were prepared by means of sequential evaporation and annealed. The non-miscibility of Pt and Au on Ru was proved by the carried out experiments, which agrees with the behavior of PtAu alloy in volume. Results are compared with a system PtAu/Pt(111) and discussed.

O 37 Invited talk Rostrup-Nielsen

Time: Thursday 14:00–14:45

Room: TRE Phys

Invited Talk

O 37.1 Thu 14:00 TRE Phys

Fuel Cells linking Catalysis and Electrochemistry. A challenge to Surface Science — ●JENS R. ROSTRUP-NIELSEN and N. CHRISTIANSEN — Topsoe Fuel Cells A/S, Lyngby, Denmark

Fuel cells represent a challenging overlap of catalysis and electrochemistry. This is illustrated by anode reactions in a solid oxide fuel cell. The fuel (methane, hydrogen..) is activated by chemisorption on the nickel surface of the anode. This is linked to the electrochemical reaction at the interface of the electrolyte and the nickel crystals converting oxygen

ions into electrons and water by reaction with adsorbed hydrogen atoms resulting from the activation of the fuel. The sites for these reactions appear not to be the same. This is reflected by different sensitivities of the two steps to poisoning. The role of different sites on the nickel surface for the steam reforming reaction is well understood in terms of impact on activity for methane activation, carbon formation and sintering. This knowledge is applied in an analysis of anodes having been exposed to 13000 hours of operation using an number of characterization methods.

O 38 Adsorption V

Time: Thursday 15:00–18:00

Room: TRE Phys

O 38.1 Thu 15:00 TRE Phys

Scanning Tunneling Microscopy and Spectroscopy of Cobalt Phthalocyanine on Cu(111) — ●XIN GE, CARLOS MANZANO, and RICHARD BERNDT — Institute für Experimentelle und Angewandte Physik, Christian-Albrechts-Universität zu Kiel, Olshausenstr. 40, D-24908 Kiel, Germany

The adsorption morphology and electronic properties of Cobalt Phthalocyanine (CoPc) adsorbed on Cu(111) substrate were investigated

by scanning tunneling microscopy and spectroscopy (STM/STS) at 5 K in ultrahigh vacuum. While CoPc has four fold symmetry in the gas phase, STM images acquired at submonolayer coverages show that two opposite lobes of a molecule appear higher than the other two, and they are oriented along the close-packed $\langle 1\bar{1}0 \rangle$ directions. Tunneling spectra recorded over center and lobes of the molecule are different. Four different CoPc superstructures were observed at ~ 1 ML coverage. Spectral features of CoPc in the superstructures are observed to differ with respect

to those of single adsorbed CoPc. We discuss these findings in terms of the different adsorption geometries and intermolecular interactions.

O 38.2 Thu 15:15 TRE Phys

Toward direct structure determination of adsorbed molecules: D and L cysteine on Cu(17 11 9)^s — ●RICHARD SCHILLINGER^{1,2} und THOMAS GREBER¹ — ¹Universität Zürich, Winterthurerstrasse 190, CH 8057 Zürich, Schweiz — ²Paul Scherrer Institut, CH 5232 Villigen PSI, Schweiz

Adsorption of biomolecules on metal surfaces finds an increasing number of applications from biocompatibility to chemical sensing.

The Cu(17 11 9) is a chiral vicinal (111) surface with 14 atoms in the unit cell. Upon adsorption of cysteine already in the monolayer (coverage 4 to 5 molecules per unit cell) find we hints for a change in conformation or ordering of the molecules from core level shifts and from angle scanned X-ray photoelectron diffraction (XPD). Further on, the XPD data point toward a pairing of the molecules in the (17 11 9) unit cell. This finding is in contrast to the situation on the also chiral Au(17 11 9)^s surface, where we observe ordered single orientation adsorption with a different conformation for the D and L enantiomer. In the monolayer cysteine takes the neutral acidic (SCH₂CH(NH₂)-COOH) state. Upon multilayer formation the molecule takes the zwitterionic (HSCH₂CH(NH₃⁺)-COO⁻) state, identified by appearance of the respective components in the C1s, N1s, S2p, and O1s core level spectra. The experiments were performed on enantiopure systems i.e. only D or L cysteine was evaporated at one time.

O 38.3 Thu 15:30 TRE Phys

STM-manipulation of HB-HPB molecules: transport of adatoms and rotation along the edge of a molecular island — ●FRANCESCA MORESCO, LEO GROSS, FRANCO CHIARAVALLOTI, and KARL-HEINZ RIEDER — Institut für Experimentalphysik, Freie Universität Berlin, Arnimallee 14, 14195 Berlin

A specially designed six-legs molecule called HB-HPB (hexa-tert-butyl-hexaphenylbenzene), is manipulated on the Cu(111) surface by Scanning Tunneling Microscopy (STM) at low temperature. The molecule is able to aggregate and move Cu adatoms when moved with a STM tip. A single molecule accommodates up to six copper adatoms forming a 2D cluster. The molecule-atoms complex is then further STM manipulated on the surface to bring the Cu freight to a chosen position on the surface and the atoms alone can be released [2]. Moreover, the molecules form well-ordered monolayer structures by self-organisation on Cu(111) [3]. The manipulation of the molecules along the edge of such molecular ordered islands results in the movement between stable positions within the molecular monolayer structure. By marking one of the six molecular legs by substituting a phenyl side ring by a pyrimidine ring, we demonstrate that the molecule rotates along the edge of the monolayer in 60° steps.

[1] L. Gross, K.-H. Rieder, F. Moresco, S. Stojkovic, A. Gourdon, C. Joachim, *Nature Materials*, in press

[2] L. Gross, F. Moresco, P. Ruffieux, A. Gourdon, C. Joachim, K.-H. Rieder, *Phys. Rev. B* 71, 165428 (2005)

O 38.4 Thu 15:45 TRE Phys

Absorption of π -conjugated molecules on Cu(111) studied by X-ray standing waves — ●A. GERLACH¹, S. SELNER^{1,2}, F. SCHREIBER¹, N. KOCH³, T.-L. LEE⁴, and J. ZEGENHAGEN⁴ — ¹Institut für Angewandte Physik, Universität Tübingen, Auf der Morgenstelle 10, 72076 Tübingen, Germany — ²Max-Planck-Institut für Metallforschung, Heisenbergstr. 3, 70569 Stuttgart, Germany — ³Institut für Physik, Humboldt-Universität zu Berlin, Newtonstr. 15, 12489 Berlin, Germany — ⁴ESRF, Rue Jules Horowitz, B.P. 220, 38043 Grenoble Cedex 9, France

We study the adsorption of different aromatic molecules such as phthalocyanines and perylene derivatives on Cu(111) using the X-ray standing wave (XSW) technique. Element specific structural information of high precision is derived from the analysis of XSW yield measurements. Using the C(1s), N(1s), and F(1s) photoelectron signals we show that the molecules adsorb in a lying-down configuration, but with different distances relative to the metal substrate.

The binding distances between the aromatic ring structure and the metal substrate is generally found to be larger than covalent bond lengths. Furthermore, we discuss more subtle effects as e.g. deformations of the adsorbed molecules that are related to the charge (re)distribution at the interface.

[1] A. Gerlach, F. Schreiber, S. Sellner, H. Dosch, I. A. Vartanyants, B. C. C. Cowie, T.-L. Lee, J. Zegenhagen, *Phys. Rev. B* 71 (2005) 205425
[2] M. Preuss, W. G. Schmidt, and F. Bechstedt, *Phys. Rev. Lett.* 94, 236102 (2005)

O 38.5 Thu 16:00 TRE Phys

Fullerene nanowires on a vicinal gold surface — ●NÉEL NICOLAS, KRÖGER JÖRG, and BERNDT RICHARD — Institut für Experimentelle und Angewandte Physik, CAU Kiel

Submonolayer coverages of fullerene molecules on vicinal gold surface were investigated by low-temperature scanning tunneling microscopy. Straight fullerene stripes of few nanometers width and extending over hundreds of nanometers have been fabricated on the gold surface by utilizing faceting of Au(433) substrates upon C₆₀ adsorption and subsequent annealing. The observed step bunching is attributed to a lowering of the facet free energy. This surface morphology is a promising template candidate for subsequent deposition of functional units.

O 38.6 Thu 16:15 TRE Phys

Probing and Modifying Locally the Intrinsic Electronic Structure and the Conformation of Supported Non-Planar Molecules — ●WOLF-DIETER SCHNEIDER, MARIE-CHRISTINE BLÜM, MARINA PIVETTA, and FRANÇOIS PATTHEY — Institut de Physique des Nanostructures, Ecole Polytechnique Fédérale de Lausanne, CH-1015 Lausanne, Switzerland

The supramolecular self-assembly of rubrene (C₄₂H₂₈) on Au(111) results in different adsorption conformations of the physisorbed molecules. Owing to the three-dimensional geometry of the molecule providing an inherent decoupling of the molecular π -states from the substrate, the conformers are distinguished by their submolecular appearance in the scanning tunneling microscopy (STM) images and by the corresponding position of the highest occupied molecular orbital (HOMO) in the differential conductance (dI/dV) spectra. The application of an electric field induces an irreversible switching of the electronic and geometric conformation of the self-assembled molecules.

O 38.7 Thu 16:30 TRE Phys

Adsorbate Properties of single PTCDA-Molecules on Ag(111) — ●ROLF ÖTTLING¹, WERNER A. HOFER², WICHARD J.D. BEENKEN¹, ERICH RUNGE¹, and JUERGEN A. SCHAEFER¹ — ¹Institut für Physik und Zentrum für Mikro- und Nanotechnologien, Technische Universität Ilmenau Postfach 100565, 98684 Ilmenau — ²Surface Science Research Centre, The University of Liverpool, Liverpool L69 3BX

We present structural, charge and bonding properties of the initial adsorption state of the organic molecule (3,4,9,10)-perylene-tetracarboxylic dianhydride (PTCDA) on highly coordinated silver Ag(111) surfaces derived from first-principles- (DFT-) calculations using projector-augmented waves (PAW-) pseudopotentials and a plane wave basis set. The substrate was taken to be a 11.5Å×20.0Å 4-layer slab with the PTCDA- adsorbate with dimensions of ~11.3Å×6.8Å planar placed on top. After structural relaxation, performed along the Hellmann-Feynman-Forces, the molecule shows a bent structure with radius of curvature of ~20Å. The oxygen-atoms point downwards with a height difference of ~0.17Å to the silver surface plane between the carboxylic (corner) and the anhydride oxygen atoms. From a Bader analysis we derive a net charge transfer of ~1 electron charge from delocalised states of the two topmost silver layers into the adsorbate LUMO. In addition, binding orbitals and Ag 3d_{5/2} core level shifts were determined.

O 38.8 Thu 16:45 TRE Phys

Robust hydrogen bonding plus molecular backbone flexibility: step-crossing allowed! — ●JOACHIM SCHNADT^{1,2}, EVA RAULS¹, WEI XU¹, JAN KNUDSEN¹, RONNIE T. VANG¹, BJØRK HAMMER¹, and FLEMMING BESENBACHER¹ — ¹Interdisciplinary Nanoscience Center and Department of Physics, University of Aarhus, Building 1520, Ny Munkegade, 8000 Aarhus C, Denmark — ²Department of Synchrotron Radiation Research, Lund University, Box 118, 221 00 Lund, Sweden

On perfect single crystal surfaces small organic molecules can self-assemble to form extended one- or two-dimensional networks using hydrogen bonding as the network-determining interaction. Real surfaces, however, are defect-afflicted and often it will be desirable that the self-assembled structures are tolerant with respect to the defects, a subject which has not been explored in detail to-date.

We have studied the self-assembly of 2,6-naphthalene-dicarboxylic acid (NDCA) on a Ag(110) surface by STM and XPS. We find that NDCA

forms macroscopic-scale one-dimensional hydrogen-bonded structures up to the μm range. These structures extend over the step edges, which can be regarded as surface defects. We have used DFT to investigate the detailed structure of the assembly on both the terraces and at the step edges. The results show that NDCA indeed can form hydrogen bonds across the step edges, with the assembly having similar binding energies and geometries on the terraces and at the step edges. This behaviour can be traced back to an appropriate balance of the different interactions as well as a combination of molecular backbone flexibility and directionality of the hydrogen bonds.

O 38.9 Thu 17:00 TRE Phys

Complex formation and proton transfer between formic acid and water on Au(111) surfaces under UHV conditions — ●MICHEL KAZEMPOOR and GERHARD PIRUG — Institut für Schichten und Grenzflächen (ISG3), Forschungszentrum Jülich GmbH, 52425 Jülich

The coadsorption of formic acid (HCOOH) and water (H_2O) on Au(111) single crystal surfaces has been investigated by means of vibrational spectroscopy (HREELS), photoelectron spectroscopy (XPS) and low energy electron diffraction (LEED). Formic acid adsorbs at 90 K molecularly with vibrational modes characteristic for flat lying zig-zag chains and solid formic acid in the monolayer and physisorbed multilayer regime, respectively. Annealing results in a complete desorption at 190 K without any detectable formation of intermediates like formates. Sequential adsorption of formic acid and water at 90 K shows no significant chemical interaction in the vibrational signatures and the core level photoelectron binding energies. Upon annealing the coadsorbed layer to 140 K new vibrational losses appear in the HREEL-spectrum at 190, 590 and 1000 cm^{-1} . Using isotopically labelled adsorbates such as D_2O and H^{13}COOD we were able to identify a hydrogen-bonded complex between formic acid and water with a molecular ratio of one. Upon further annealing this complex decomposes leaving only molecularly adsorbed formic acid on the surface at 160 K. This process is accompanied by a proton exchange between formic acid and water. The results will be discussed in the light of recent findings for the electrochemical oxidation of formic acid on Au surfaces.

O 38.10 Thu 17:15 TRE Phys

Isomerization of an azobenzene derivative on Au(111) by scanning tunneling microscopy — ●MICOL ALEMANI, LEONHARD GRILL, KARL HEINZ RIEDER, and FRANCESCA MORESCO — Inst. für Exp.physik, FU Berlin, Armimallee 14, D-14195 Berlin

Azobenzene molecules are of great interest because they have in the gas phase two stable isomers (cis and trans) and can switch reversibly from one configuration to the other by photo-excitation. An azobenzene derivative, equipped with four tert-butyl groups, has been investigated on Au(111) with a scanning tunnelling microscope (STM) at low temperature (5K).

The molecules result mobile after preparation at room temperature and form islands. From the STM images, the exact molecular orientation and configuration have been extracted. All the molecule are found in the trans configuration, as it is in the gas phase the more energetically favoured one.

By applying voltage pulses with the STM tip on molecular islands, the isomerization of single molecules from the trans configuration to the cis and backwards has been realized. The process is characterized by changing the applied voltage. A model is proposed for the cis isomer adsorbed on the surface which is in accordance with its chemical properties.

O 38.11 Thu 17:30 TRE Phys

Porous Network Structure of Octacyano-metal free Phthalocyanine on HOPG Surface — ●THIRUVANCHERIL G. GOPAKUMAR¹, WERNER R. THIEL², and MICHAEL HIETSCHOLD¹ — ¹Chemnitz University of Technology, Institute of Physics, Solid Surfaces Analysis Group, D-09107 Chemnitz, Germany. — ²Technical University Kaiserslautern, Department of Chemistry, Inorganic Chemistry, D-67663 Kaiserslautern, Germany.

The molecule-molecule interaction in the thin films of Phthalocyanine is the reversible weak van der Waals interaction. The use of functional groups in these molecular systems open the possibility to introduce strong molecule-molecule interaction and thereby a supra-molecular engineering. In this work we report the porous-network structure formation in Octacyano-metal free Phthalocyanine ($\text{H}_2\text{Pc}(\text{CN})_8$) on HOPG surface. The molecular layers forming quadratic packing with one void per unit cell with an average void area of 2 nm^2 . Simple molecular dynamics calculation of different type of quadratic molecular unit cells shows the minimum energy structure has only one void per unit cell and show good agreement with the experiments. Beyond these porous structures there has been observed another phase of molecules, where highly close packed structures were found. Moreover typical point defects of filling of pore-structures are found which suggest this molecular layer to be used as a template for other organic molecules to elaborate the understanding of co-adsorption, site-selectivity, sensing etc. Finally we show that these defects can be induced and repaired by a tip-induced process.

O 38.12 Thu 17:45 TRE Phys

In-situ Alteration of Bimolecular Hydrogen-bond Networks — ●LORENZ KAMPSCHULTE^{1,2}, MARKUS LACKINGER¹, TOVA ADLERSTEIN², STEFAN GRIESSL¹, GEORGE W. FLYNN², and WOLFGANG M. HECKL^{1,3} — ¹Dept. Earth and Environmental Sciences, LMU München, Theresienstr. 41, 80333 Munich, Germany — ²Dept. of Chemistry, Columbia University, New York, New York 10027, USA — ³Deutsches Museum, Museumsinsel 1, 80538 Munich, Germany

Bimolecular monolayers were grown by spontaneous self-assembly from solution at the liquid-solid interface and subsequently investigated by Scanning Tunneling Microscopy (STM). The co-adsorption of two different molecules, BTB (1,3,5-benzenetribenzoic acid) and TMA (trimesic acid) in open (loosely packed) networks was studied in two different solvents (heptanoic and nonanoic acid). Altering the absolute and relative concentrations of the two compounds in binary solutions resulted in phases with six different structures. Their cavity size ranges from 1.1 nm for a structure solely composed of the smaller TMA molecules up to 2.8 nm for a pure BTB network. All structures are stabilized by twofold intermolecular hydrogen bonding between the carboxylic acid head groups. Moreover, in-situ dilution of liquid mixtures induced phase transitions of the monolayer structures, accompanied by an alteration of the size and shape of cavity voids in the 2-dimensional molecular assembly.

O 39 Nanostructures III

Time: Thursday 15:00–18:00

Room: PHY C213

O 39.1 Thu 15:00 PHY C213

Spin-dependent excitation of surface states on ultrathin ferromagnetic films — ●MARTIN PICKEL¹, ANKE B. SCHMIDT², MARTIN WEINELT², and MARKUS DONATH¹ — ¹Physikalisches Institut, Universität Münster, Wilhelm-Klemm Str. 10, 48194 Münster — ²Max-Born-Institut, Max-Born-Str. 2A, 12489 Berlin

Studying image-potential states with time-resolved two-photon photoemission (2PPE) has provided new insight into electron dynamics at surfaces. Recent spin-resolved measurements of electron dynamics in front of ultrathin iron films [1] even allow for the distinction between majority- and minority-spin electron scattering channels.

In this talk we discuss the initial, pump-induced spin polarization of the image-potential states in front of ultrathin iron and cobalt films on Cu(001). Following the argument of spin-integrated studies for the $n=1$ image-potential state [2], the spin polarization can be ascribed to the ini-

tial bulk states and the dipole selection rules governing the pump process. Additionally, we observe linear dichroic effects with 2PPE.

Therefore, by 2PPE we do not only obtain information about image-potential states itself but also about the initial states. They must have a considerable overlap with the image-potential states which makes this method very surface sensitive.

[1] A. B. Schmidt et al., Phys. Rev. Lett. **95**, 107402 (2005)

[2] U. Thomann et al., Appl. Phys. B **68**, 531 (1999)

O 39.2 Thu 15:15 PHY C213

Embedded foreign atom interactions and cluster configurations: Co/Cu(001) — ●BENE POELSEMA, NURI ÖNCEL, RONALD VAN MOERE, and HAROLD J.W. ZANDVLIET — Solid State Physics; MESA+ Institute for Nanotechnology, University of Twente, P.O.Box 217; 7500 AE Enschede; The Netherlands

At low coverages (~ 0.03 ML) of Co on Cu(001) and intermediate temperatures (300-380K), small clusters composed of embedded Co atoms coexist with larger adatom islands. The configurations and concentrations of the former have been analyzed, assuming (local) equilibrium. The observations of fluctuations of the shape/configurations of small embedded clusters encourage this assumption. Taking into account configuration entropy and assuming pairwise interactions leads to a surprisingly accurate description of the relative occurrence of monomers, dimers, trimers and tetramers. The same applies for the probability distribution of the various configurations of dimers, trimers and tetramers. These findings suggest an *a posteriori* confirmation of local equilibrium. The embedded Co-Co interactions have been found attractive for both nearest neighbour (NN) and next nearest neighbour (NNN) interactions. The latter (-93+/-5 meV) is twice as strong as the NN-interaction (-45+/-10 meV), which explains the predominance of observed c(2x2) building blocks in the clusters. With inclusion of NN- and NNN-interactions only moderate agreement between calculations and experiments is achieved. Adding a next-next nearest neighbour (NNNN) interaction term of -20+/-10 meV results in a very convincing fit of the configuration distributions of both trimers and tetramers.

O 39.3 Thu 15:30 PHY C213

Spin-resolved STM measurements of Co nanostructures on Pt(111) — ●FOCKO MEIER, KIRSTEN VON BERGMANN, JENS WIEBE, MATTHIAS BODE, and ROLAND WIESENDANGER — Institute of Applied Physics, Hamburg University, D-20355 Hamburg, Germany

The Co/Pt(111) sample system has been studied quite intensively in the past to investigate fundamental magnetic properties: using spatially-averaging optical techniques the direction and magnitude of the anisotropy of 2-dimensional Co nanostructures, chains at step edges and single atoms on Pt(111) have been probed.[1] We performed spin-resolved scanning tunneling microscopy measurements on Co nano-structures on Pt(111) to gain further insight into the electronic and magnetic properties of this system. The measurements were done in a LT-UHV-STM system below 13 K. Using magnetically sensitive tips (Fe- or Cr-coated W tips) we measured the electronic structure of ML and DL high Co with spatial and spin resolution to get access to the energy dependence of the spin polarization. Additionally we probed the response of Co nanostructures to an external magnetic field. The spatial resolution reveals the different switching mechanisms of multi-domain Co-nanowires and single-domain Co islands.

[1] Rusponi et al. *nature materials*, Vol 2, p546, 2003; Gambardella et al. *Nature*, Vol 416, p301, 2002; *Science*, Vol 300, p1130, 2003

O 39.4 Thu 15:45 PHY C213

Spin-polarized unoccupied states in Cu/Co/Cu(001) and Cu/Ni/Cu(001) thin-film structures — ●VOLKER RENKEN¹, DEHONG YU², GEORGI RANGELOV¹, and MARKUS DONATH¹ — ¹Physics Institute, University of Münster, Wilhelm-Klemm-Str. 10, 48149 Münster, Germany — ²Bragg Institute, Australian Nuclear Science and Technology Organisation, PMB 1, Menai NSW 2234, Australia

Ultrathin Cu films on thin fcc Co and Ni films grown on Cu(001) have been investigated by spin- and angle-resolved inverse photoemission. For no Cu overlayers but for increasing Co [1] and Ni film thickness on Cu(001), spin-polarized quantum-well states shift to higher energies and finally converge toward the lower band-gap boundary at the top of the sp-band. With little Cu overlayer coverage, the quantum-well states within the Co and Ni layers are still observed. With increasing Cu overlayer thickness, spin-polarized quantum-well states within the Cu layers are identified and eventually the Cu bulk sp-band is formed. Because the top of the sp-band is lower in energy for Cu compared to Co and Ni, a seemingly negative dispersion of the observed features with increasing Cu overlayer thickness appears. As a function of the electron momentum parallel to the surface, the quantum-well states develop into a surface resonance [2]. The loss of spin polarization of this surface resonance as a function of the Cu overlayer thickness reflects the penetration depth of the electron wave function.

[1] D.H. Yu et al., *Phys. Rev. B* 68 (2003) 155415,

[2] D.H. Yu and M. Donath, *Europhys. Lett.* 63 (2003) 729.

O 39.5 Thu 16:00 PHY C213

New methods to determine the sputtering yield at step edges — ●ALEX REDINGER, HENRI HANSEN, and THOMAS MICHELY — I. Physikalisches Institut, RWTH Aachen University, 52056 Aachen, Germany

STM investigations on pattern formation at grazing incidence ion bombardment are used to determine the sputtering yield at step edges. A Pt(111) crystal is bombarded with 5 keV Ar^+ ions at angles of incidence between 79° and 86° to the surface normal. A series of experiments at 83° and 550K sample temperature is used to determine the amount of removed material as a function of ion fluence. Relating for this series the number of ascending steps with the removed amounts allows to establish the sputtering yield at ascending steps.

At 86° ion incidence and 550K sample temperature the step edge motion of preexisting steps due to ion bombardment is used to determine the step edge velocity. By taking into account the damage created by ion bombardment below the surface we could again determine the sputtering yield at an ascending step edge. Both methods led to similar results and are in good agreement with earlier experiments and MD simulations [1]. [1] Hansen et al. *PRL* 92, 246106 (2004)

O 39.6 Thu 16:15 PHY C213

Low-dimensional Supramolecular Structures by Design — ●NIAN LIN, SEBASTIAN STEPANOW, DIETMAR PAYER, STEVE TAIT, and KLAUS KERN — Max-Planck-Institute for Solid State Research

Supramolecular chemistry provides powerful methodologies for the controlled generation of nanostructures following bottom-up fabrication principles. Here we present our systematic studies using surfaces as platforms to direct the assembly of novel low-dimensional supramolecular structures. The flexibility of the underlying non-covalent interactions, e.g., H-bond, ionic bond and metal-coordination, facilitates the formation of thermal equilibrium structures. We demonstrate that the information stored in the individual molecular building blocks, e.g., end groups, backbone symmetry, geometry and chemistry, can be transferred to the supramolecular organization level. As the first example we will show that by specific element substitution at the molecular backbones, one may steer 1D vs. 2D growth. Furthermore chiral organization can be controlled by modifying the molecular backbone symmetry. Then we will demonstrate that open network structures of tunable pore geometry can be obtained through careful selection of molecular structure and intermolecular binding modes. The chemistry and morphology of the supporting surfaces are found to be important in determining the final structures. The surface-supported supramolecular systems represent promising materials for potential applications, e. g., in nano-patterning, surface templating, low-dimensional magnetic systems, heterogenous catalysis, sensing or molecular recognition.

O 39.7 Thu 16:30 PHY C213

Nanopatterning by a Combination of Micellar and Conventional Lithographic Techniques — ●CHRISTIAN PFAHLER, SABRINA BRIEGER, OLIVER DUBBERS, ACHIM MANZKE, ALFRED PLETTL, and PAUL ZIEMANN — Solid State Physics, University of Ulm, D-89069 Ulm, Germany

Diblock copolymers of PS-b-P2VP, dissolved in toluene, form reverse micelles comprised of a P2VP core and a PS corona. The core can be loaded with e.g. H₂AuCl₄. By dip coating, these micelles are deposited onto substrates. Subsequently the polymer is removed and Au-nanoparticles are created in an isotropic Hydrogen plasma. This micellar technique was used to produce 14 nm Au nanoparticles with spacings of 100 nm, which form hexagonally well ordered arrays on Si. Some lithographic applications of these particles will be demonstrated: Deposited on Si wafers, they can be used directly as an etching mask for pillar fabrication by an anisotropic plasma etching process with a CF₄/CHF₃ gas mixture. In this way, heights of more than 100 nm and aspect ratios of 10 were achieved. It will further be demonstrated that the array of pillars can be transferred into a corresponding array of cylindrical holes which offer additional applications. A typical diameter of the cylindrical holes is less than 20 nm with an aspect ratio of 10. Both preparation techniques can be applied to amorphous Si films as well, which can be evaporated onto any insulating substrates or metallic films. By combining this approach with conventional ebeam lithography, one can position the micelles on the nanoscale. For this purpose, first metal or, in a new process route, resist templates have to be prepared lithographically.

O 39.8 Thu 16:45 PHY C213

Production of ordered nanometer sized pits with Focused Ion Beams (FIB) — •F. GHALEH¹, R. KÖSTER¹, H. HÖVEL¹, L. BRUCHHAUS², J. THIEL², and R. JEDE² — ¹Universität Dortmund, Experimentelle Physik I, 44221 Dortmund, Germany — ²Raith GmbH, Hauert 18, Technologiepark, 44227 Dortmund, Germany

Nanometer sized pits on HOPG substrate can be used as nucleation centers to produce clusters with a narrow size distribution. In previous experiments [1] nanometer sized pits were produced by sputtering and oxidizing of the sample. As result we get nanopits which are a few nanometers wide and just one monolayer deep. The pits are distributed at random locations on the surface.

In the present study a focused beam of gallium ions is used to produce the defects at localized positions on the substrate. The Focused Ion Beam (FIB) facility used here was developed within the NanoFIB Project [2]. It can achieve a resolution of about 10 nm [3]. The oxidation of a sample structured with FIB allows to measure areas structured with very small ion intensity or the penetration depth of the incident ions.

[1] H. Hövel, Appl. Phys. A **72**, 295 (2001).

[2] <http://www.nanofib.com>.

[3] J. Gierak, D. Maily, P. Hawkes, R. Jede, L. Bruchhaus, L. Bardotti, B. Prével, P. Mélinon, A. Perez, R. Hyndman, J.-P. Jamet, J. Ferré, A. Mougin, C. Chappert, V. Mathet, P. Warin, J. Chapman, Appl. Phys. A **80**, 187 (2005).

O 39.9 Thu 17:00 PHY C213

Influence of STM measurements during MOVPE — •BERT RÄHMER¹, MARKUS PRISTOVSEK¹, RAIMUND KREMWOW¹, MARKUS BREUSING², and WOLFGANG RICHTER² — ¹TU-Berlin, Institut für Festkörperphysik, Hardenbergstr. 36, 10623 Berlin — ²Università degli Studi di Roma "Tor Vergata", Via della Ricerca Scientifica 1, 00133 Roma, Italy

We developed a Scanning Tunneling Microscopy (STM) and its deviate Atomic Force Microscopy (AFM) that measures *in-situ* the surface topography in real time and real space with high spatial resolution during Metal-Organic Vapour Pressure Epitaxy (MOVPE) growth. The set-up of STM is simpler for good resolution. AFM has the advantage, to be able to measure also on semi-isolating substrates like sapphire. Last year we described the set-up and presented first measurements of a step-bunched GaAs sample at 500 °C. Additionally we showed measurements with the *in-situ*STM during the growth of InAs quantumdots on GaAs, which show different growth regions in the proximity on the scanning region. We measured the sample *ex-situ* with a Atomic Force Microscope (AFM), with Scanning Electron Microscopy (SEM) and Energy Dispersive X-Ray Diffraction (EDX). The origin of different areas is a temperature reduction by the STM tip. This can be compensating by adjusting the growth conditions accordingly.

O 39.10 Thu 17:15 PHY C213

A Two-dimensional Porphyrin-based Porous Network Featuring Communicating Cavities — •NIKOLAI WINTJES¹, HANNES SPILLMANN¹, ANDREAS KIEBELE¹, MEIKE STÖHR¹, THOMAS JUNG², DAVIDE BONIFAZI³, FUYONG CHENG³, and FRANÇOIS DIEDERICH³ — ¹Department of Physics, University of Basel, CH-4056 Basel — ²Paul Scherrer Institute, CH-5232 Villigen PSI — ³Laboratory for Organic Chemistry, ETH-Zürich, CH-8093 Zürich

The unique electrochemical and photophysical properties of porphyrin and [60]fullerene compounds make them promising candidates for the construction of two- and three-dimensional organic-based materials. Therefore, a detailed understanding of these molecular systems is crucial for a further and targeted development of new molecularly based materials. Metallo-porphyrins and their derivatives have been shown to be exceedingly useful building blocks for the construction of 3D supramolecular functional networks due to their excellent thermal and chemical stability

and synthetic versatility. Nonetheless, no 2D analogon has been reported so far, although these could be interesting for various potential applications such as catalysts, molecular sieves, or chemical sensors. Herein we report on an unprecedented two-dimensional porphyrin network featuring dynamic pores capable of hosting fullerenes following a bottom-up approach at a single crystal silver surface. Surface- and porphyrin-driven long-range interactions between the C60 guest molecules and porphyrin layer resulted in the formation of exceptionally large supramolecular hybrid chains and islands as evidenced by Scanning Tunneling Microscopy (STM).

O 39.11 Thu 17:30 PHY C213

Intermixed patterns of perylene derivatives on Ag(111) — •MEIKE STÖHR¹, MARKUS WAHL¹, TOMAS SAMUELY¹, TILL RIEHM², THOMAS A. JUNG^{1,3}, and LUTZ H. GADE² — ¹Institute of Physics, University of Basel — ²Institute of Inorganic Chemistry, University of Heidelberg — ³Laboratory for Micro- and Nanostructures, Paul-Scherrer-Institute

Self-assembled systems are in the focus of nanotechnology research because of their potential use in the bottom-up creation of functional supramolecular structures. Potential applications of such systems include several functional groups. Therefore, the intermixing of different molecular compounds will become a key issue. In our approach we made use of H-bonding to form well-ordered intermixed patterns of two different perylene derivatives. These are PTCDA (3,4,9,10-perylene-tetracarboxylicdianhydride) and DPDI (4,9-diaminoperylenequinone-3,10-diimine) [1]. In an UHV-setup consisting of different chambers for sample preparation and characterization thin films of DPDI and PTCDA were prepared by evaporation on Ag(111). The sample characterization was carried out with a homebuilt STM. For a ratio of 1:1 and a total coverage of about one monolayer, an ordered intermixed pattern was observed. We assume that each PTCDA molecule is interacting via H-bonding with four neighbouring DPDI molecules and vice versa. Furthermore, different intermixed patterns were observed depending on the ratio of the molecules and on the total coverage. [1] Gade et al., Angew. Chem. Int. Ed. **42** (2003) 2677

O 39.12 Thu 17:45 PHY C213

Thermal boundary conductance of solid-solid interfaces — •BORIS KRENZER, ANDREAS JANZEN, ANJA HANISCH, MATTHIAS WIELENS, and MICHAEL HORN-VON HOEGEN — Universität Duisburg-Essen, Fachbereich Physik, Lotharstr. 1, 47057 Duisburg

With decreasing size the thermal properties of nanoscale devices become more and more important. The thermal conductivity of such devices is drastically altered compared to simple heat diffusion given in bulk material. Especially the cross plane thermal conductivity in layered structures is determined by the thermal conductivity of the interface between the neighboring layers. The microscopic picture of this situation is that phonons only have a certain probability to cross the interface and carry energy from one material to the other. The most two basic models for the calculation of the phonon transmission probability are the acoustic mismatch model (AMM) and the diffusive mismatch model (DMM). For low temperatures when the dominant phonon wavelength is much larger than the interface roughness the AMM is used for the calculation. With increasing temperature the dominant phonon wavelength becomes comparable to the interface roughness and the transmission probability is calculated within the DMM. In the past the models explained the observed TBC at low temperatures but failed at higher temperatures where the experimental TBC was found to be orders of magnitude higher than the prediction. Recently we measured the TBC of the Bi/Si-interface which is in good agreement with the predictions. In this talk the AMM and DMM are presented in general and the results of the calculations will be applied to the Bi/Si-system.

O 40 Oxides and insulators

Time: Thursday 15:00–18:00

Room: WIL A317

O 40.1 Thu 15:00 WIL A317

Thin oxide films: analysis of finite-size effects — •CHRISTOPH FREYSOLDT, PATRICK RINKE, and MATTHIAS SCHEFFLER — Fritz-Haber-Institut der MPG, Berlin

Oxide surfaces have attracted considerable interest over the last years. In order to employ surface science tools, oxides are often grown epitaxially on metals. Recent findings for SiO₂ on Mo(112) indicate that

well-ordered films are only 2-3 atomic layers thick – less than previously thought [1,2]. But is the surface of the films characteristic for the surface of a bulk oxide? Not only the structure may differ from any known bulk structure, but also the metal might alter the electronic structure. Also, sizeable quantum effects are expected at these dimensions. We present DFT simulations for oxide films of various thicknesses for α -quartz SiO₂, α -alumina Al₂O₃ and cubic hafnia HfO₂. In order to separate the thick-

ness from the substrate dependence, free-standing films are considered. We find that the electronic structure at the DFT level becomes bulk-like for very few atomic layers. The case of silica is discussed in detail. The film structure on Mo(112) corresponds to the most stable quartz(0001) surface. The electronic structure is essentially bulk-like and independent of the film thickness. The presence of the substrate does not alter these findings. For the electronic response of the thin film, however, the quasiparticle picture predicts a thickness-dependent band gap due to the dielectric discontinuity at the interface. Likewise, the chemistry and stability of defects is expected to be influenced by the substrate.

[1] L. Giordano *et al.*, Surf. Sci. 584, 225 (2005).

[2] J. Weissenrieder *et al.*, Phys. Rev. Lett. 95, 076103 (2005).

O 40.2 Thu 15:15 WIL A317

A Combined DFT/LEED-Approach for Complex Oxide Surface Structure Determination: $\text{Fe}_3\text{O}_4(001)$ — ●R. PENTCHEVA¹, J. RUNDGREN², S. FRANK¹, D. SCHRUPP³, M. SCHEFFLER⁴, and W. MORITZ¹ — ¹Section Crystallography, University of Munich — ²Physics Dept., Royal Institute of Technology, Stockholm — ³Dept. of Physics, University of Augsburg — ⁴Fritz-Haber-Institut der MPG, Berlin

The structural determination of complex oxide surfaces is a challenge for quantitative analysis techniques such as XRD or LEED. Density functional theory (DFT) total energy calculations provide a mean to compare the stability of different configurations. Still, for complex structures, when many atoms relax (e.g. 50-100 degrees of freedom) the energy landscape may be rather flat and/or corrugated. In this paper we show that a multi-technique approach (employing DFT→LEED→DFT) is indeed most useful: In the framework of *ab initio thermodynamics* we compiled a surface phase diagram of $\text{Fe}_3\text{O}_4(001)$ for a variety of surface terminations. The novel (so far ignored) Jahn-Teller distorted, oxygen-rich surface structure predicted from the DFT-calculations [1] is confirmed by a LEED I/V (and XRD) analysis. Only the here put forward combined DFT-LEED-DFT approach where the atomic positions obtained from DFT were used as input for the LEED structural refinement and vice versa enables us to achieve a *quantitative* agreement between the different methods. Furthermore, we explored the influence of phase shifts obtained from the DFT-electron density for magnetite bulk and surface as opposed to conventional phase shifts.

[1] R. Pentcheva, et al., Phys. Rev. Lett. 94,126101 (2005).

O 40.3 Thu 15:30 WIL A317

Frequency Modulated Atomic Force Microscopy and Scanning Tunneling Microscopy of the Ultrathin Aluminum Oxide Film on NiAl(110) — ●MARKUS HEYDE, GEORG SIMON, HANS-PETER RUST, and HANS-JOACHIM FREUND — Fritz-Haber-Institute of the Max-Planck-Society, Faradayweg 4-6, D-14195 Berlin, Germany

Metal oxides are of great technological importance because they are involved in a variety of applications, such as microelectronics or heterogeneous catalysis. The characterization of their properties on the atomic scale is therefore of special interest. The thin aluminum oxide film grown on NiAl(110) serves as an often used model system in catalysis [1]. We have started a detailed analysis by low temperature (5 Kelvin) ultra-high vacuum frequency modulated atomic force microscopy (FM-AFM) and scanning tunneling microscopy (STM) [2] of the thin aluminum oxide film grown on NiAl(110). A model of the structure of this film has been recently published by Kresse et al. [3]. Here we compare our combined FM-AFM and STM measurements with the model of the thin aluminum oxide film.

[1] M. Bäumer and H.-J. Freund, Progress in Surface Science 61, 127 (1999).

[2] M. Heyde, M. Kulawik, H.-P. Rust, H.-J. Freund, Rev. Sci. Instrum. 75, 2446 (2004).

[3] G. Kresse et al., Science 308, 1440 (2005).

O 40.4 Thu 15:45 WIL A317

Ordered alumina film on NiAl(110): Structure of the antiphase domain boundaries and of metallic clusters — ●EVELYN NAPETSCHNIG¹, MICHAEL SCHMID¹, GEORG KRESSE², LUKAS KÖHLER², MAXIM SHISHKIN², and PETER VARGA¹ — ¹Institut f. Allgemeine Physik, Vienna University of Technology, Austria — ²Institut fuer Materialphysik, University of Vienna, Austria

Transition metal clusters on alumina support are one of the most frequently used model systems for investigations of heterogeneous catalysis. When NiAl(110) is oxidized at elevated temperatures an alumina film of uniform thickness and structure [1,2] with a network of domain bound-

aries is formed. The domain boundaries act as nucleation centers for metal clusters. We could determine the structure of the antiphase domain boundary by combining STM images and density-functional theory calculations [3]. Our measurements of the morphology of Co, Pd and bimetallic Co-Pd clusters on the alumina film show that for Pd and Co non-crystalline clusters with a steep slope and a round top are thermodynamically favourable. For the bimetallic Pd-Co clusters we proof that Pd is covering pre-deposited Co clusters like a shell whereas for deposition in the reverse order Pd is segregating to the cluster*s surface and intermixes with the added Co.

[1] M. Bäumer and H.J. Freund, Prog. Surf. Sci. 61 (1999) 127

[2] G. Kresse M.Schmid, E.Napetschnig, M.Shishkin, L.Köhler and P.Varga, Science 308 (2005) 1440

[3] M. Schmid, G. Kresse, M. Shishkin, E.Napetschnig, M. Kulawik, N. Nilius, H.J. Freund and P. Varga, to be published

O 40.5 Thu 16:00 WIL A317

Structural investigation of the ultra-thin gallium oxide grown on the CoGa(100) surface — ●ALINA VLAD¹, ANDREAS STIERLE¹, REINHARD STREITEL¹, GEORG KRESSE², MARTIJN MARSMAN², and HELMUT DOSCH¹ — ¹Max-Planck Institut für Metallforschung, Heisenbergstraße 1, 70569 Stuttgart — ²Institut für Materialphysik and Centre for Computational Materials Science, Universität Wien, A-1090 Wien, Austria

Understanding the oxidation of metallic alloy surfaces is not only of fundamental interest, but is also a important for industrial applications in sectors like heterogeneous catalysis, microelectronics, high-density data storage technologies. Beside having the desired properties, one of the requirements for practical applications is that the oxide layer should be reproducible in thickness and composition. Also, a detailed knowledge of the structural aspects is often important. The formation of a well-ordered ultra thin surface gallium oxide was previously observed when exposing the CoGa(100) surface at 450°C and an oxygen pressure of $5 \cdot 10^{-7}$ mbar. The aim of this study was to determine the structure of the oxide film by means of Surface X-ray Diffraction (SXRD) and DFT calculations. The set of experimental data (surface rods and CTR's) were measured at the ID32 beamline at ESRF, Grenoble. A trilayer O-Ga-O model for the surface oxide is proposed. The overall stoichiometry of the film does not correspond to that of the stable bulk $\beta\text{-Ga}_2\text{O}_3$ but it is Ga_2O .

O 40.6 Thu 16:15 WIL A317

Composition, structure, and catalytic activity of sulfated c-ZrO₂(111) films on Pt(111) — ●STEFAN FÖRSTER¹, KLAUS MEINEL¹, ALEXANDER HOFMANN², RALF KULLA¹, KARL-MICHAEL SCHINDLER¹, HENNING NEDDERMEYER¹, JOACHIM SAUER², and WOLF WIDDRA¹ — ¹Martin-Luther-Universität Halle-Wittenberg, FB Physik, D-06099 Halle, Germany — ²Humboldt-Universität zu Berlin, Institut für Chemie, D-10099 Berlin, Germany

Sulfated zirconia catalysts are very active in the low-temperature isomerization of n-alkanes. Single crystalline sulphated c-ZrO₂(111) films of the cubic (c) type have been prepared as a model catalyst by reactive deposition of Zr onto Pt(111) in an O₂ atmosphere and subsequent exposition to a SO₃ atmosphere. Structure and composition of the film surface have been examined by scanning tunneling microscopy, low-energy electron diffraction (LEED), Auger electron spectroscopy, and density functional theory (DFT) calculations. The clean c-ZrO₂(111) films display a (2x2) surface structure. During SO₃ exposure, a clear ($\sqrt{3} \times \sqrt{3}$)R30° structure develops. At about 700 K, the ($\sqrt{3} \times \sqrt{3}$)R30° structure disappears and the bright LEED pattern of the clean ZrO₂ films reappears. The energies of plausible c-ZrO₂(111)/SO₃ structures have been examined by DFT. The ($\sqrt{3} \times \sqrt{3}$)R30° structure found in the experiments turned out to be the most stable one for temperatures below 700 K. During reaction with n-butane, the ($\sqrt{3} \times \sqrt{3}$)R30° sulfation structure is stable and its chemical activity is indicated by the formation of surface carbon.

O 40.7 Thu 16:30 WIL A317

Formation and splitting of paired hydroxyl groups on reduced TiO₂(110) — ●STEFAN WENDT, JESPER MATTHIESEN, RENALD SCHAUB, EBBE K. VESTERGAARD, ERIK LAEGSGAARD, FLEMMING BESENBACHER, and BJØRK HAMMER — Interdisciplinary Nanoscience Center (iNANO)

A combination of high-resolution scanning tunneling microscopy and density functional theory is utilized in order to study the interaction of water with the reduced TiO₂(110)-(1 × 1) surfaces. As the direct prod-

uct of water dissociation at oxygen vacancies, paired hydroxyl groups are formed. The pairs are immobile and stable at the surface unless they interact with adsorbed water molecules. As a result of these interactions, one proton per paired hydroxyl group is net transferred to the next oxygen row, thereby forming single hydroxyl groups. Furthermore, we find that hydroxyl groups on the bridging oxygen rows facilitate water diffusion in the $[1\bar{1}0]$ direction.

O 40.8 Thu 16:45 WIL A317

Photon emission from MgO thin films on Mo(100) — ●HADJ-MOHAMED BENIA¹, STEFANIA BENEDETTI², NIKLAS NILIUS¹, and HANS-JOACHIM FREUND¹ — ¹Fritz-Haber-Institut der Max-Planck-Gesellschaft, Faradayweg 4-6,14195 Berlin — ²Università di Modena e Reggio Emilia, Dipartimento di Fisica and INFM-CNR National Research Center on nanoStructures and bioSystem at Surface (S3), Via G. Campi 213/a, 41100 Modena, Italy

MgO is a prototype material which exhibits color centers (oxygen vacancies). Such centers dominate the optical properties as well as the catalytic behavior of the MgO surface. The aim of our experiment is to locally characterize the optical properties of surface color centers by employing STM in combination with photon emission spectroscopy (PSTM). For this purpose, we have grown MgO films on Mo(100) with varying thicknesses ranging from 2-10 monolayers. Depending on the MgO deposition temperature we have found different morphological and structural properties of the film by LEED and STM. The optical spectra are dominated by two emission peaks located at around 300 and 400 nm with intensities depending on preparation procedure and film thickness. We tentatively attribute these peaks to excitonic and defect-mediated recombination processes within the oxide film.

O 40.9 Thu 17:00 WIL A317

LASER DESORPTION OF METAL ATOMS BY SITE-SPECIFIC EXCITATION OF METAL OXIDE SURFACES

— ●MATTHIAS HENYK¹, KENNETH M. BECK¹, CHONGMIN WANG¹, PAOLO E. TREVISANUTTO², PETER V. SUSHKO², ALEXANDER L. SHLUGER², and WAYNE P. HESS¹ — ¹Pacific Northwest National Laboratory, EMSL, P.O. Box 999, Richland, WA 99352, USA — ²Department of Physics and Astronomy, University College London, Gower Street, London WC1E 6BT, UK

Mg-atom emission is studied at MgO by using laser light tuned to excite specific surface sites at energies well below the excitation threshold of the bulk material. We find that at 4.66 eV laser excitation MgO nanocrystalline films and nanocube samples desorb neutral Mg-atoms with multi-modal distributions of kinetic energy (0.11, 0.18, 0.25 eV). Time-resolved desorption measurements reveal two distinct decay components (1.2, 100 ps) in addition to the typically observed coherence feature (80 fs, FWHM). These results are consistent with Mg-atom desorption driven by multiple electronic transitions, including an ultra-fast correlated 2-electron-transfer as well as the rapid decay of Mg⁺ surface states. Our ab initio calculations suggest an electron plus exciton mechanism, involving both excitation and trapping of electrons and surface excitons at 3-coordinated Mg surface sites. The proposed mechanism exemplifies a scheme of atomic scale modification of a metal oxide surface and can be useful for the further understanding of photo-induced desorption of more complex metal oxide materials.

O 40.10 Thu 17:15 WIL A317

Thin Manganese Oxide Films on Ag(001) — ●MICHAEL HUTH¹, KARL-MICHAEL SCHINDLER¹, CHRISTIAN HAGENDORF¹, JIAN WANG¹, RICHARD BÖRNER¹, STEPHAN GROSSER¹, STEFFEN SACHERT¹, WOLF WIDDRA¹, FRANCESCO ALLEGRETTI², MARTIN POLCIK², DAVID SAYAGO², and EMILY KRÖGER² — ¹Martin-Luther-Universität Halle-Wittenberg, FB Physik, D-06120 Halle — ²Fritz-Haber-Institut der MPG, Faradayweg 4-6, D-14195 Berlin

Thin films of MnO (4 ML) were grown on a Ag(001) substrate by reactive evaporation of Mn in an O₂ atmosphere and investigated with XPS and NEXAFS spectroscopy at the UE56/2 BESSY beamline. The identity of the MnO film was assessed using the exchange splitting (6.2 eV) of the Mn 3s photoemission line which is highest for stoichiometric MnO. After annealing such a film to 720 K the exchange splitting is reduced to 5.6 eV pointing to a composition of MnO_{1-x}. NEXAFS spectra of the O K-edge in normal and grazing incidence are very similar for MnO due to its cubic structure, but for MnO_{1-x} they show a strong dependence on the angle of incidence and nearly twice as many resonances. O 1s photoelectron diffraction (PED) curves were recorded in energy scan mode for both films. The intensity modulations of the MnO film are much stronger than the ones of the MnO_{1-x} films. We attribute this again to the lower symmetry of the MnO_{1-x} films. Finally, the intensity ratio of the two exchange split Mn 3s photoemission lines varies for kinetic energies which indicate the presence of a local magnetic ordering above the Neel temperature.

O 40.11 Thu 17:30 WIL A317

Local differential conductance of thin CoO films on Ag(001) at low temperatures — ●STEPHAN GROSSER, CHRISTIAN HAGENDORF, and WOLF WIDDRA — Martin-Luther-Universität Halle-Wittenberg, FB Physik, D-06120 Halle(Saale)

Scanning tunneling microscopy (STM) and scanning tunneling spectroscopy (STS) have been applied to study simultaneously the local electronic and geometric structure of thin CoO films on Ag(001). CoO has been grown by reactive deposition of Co in an O₂ atmosphere. Growth at 480 K substrate temperature leads to precursor or unordered phases and subsequent annealing to ordered CoO(001) films.

dI/dV spectra for structurally well-characterized different precursor phases, CoO bilayer and layers up to 5 ML show distinct differences. The region of the unoccupied states up to 5 eV is dominated by the local density of states within the oxide film. Especially for 2 ML islands and thicker films, a strong and well-resolved unoccupied Co d-state at about 2.3 eV is found. For higher bias voltages between 5 and 10 V the spectra exhibit strong field emission resonances which are characteristically modified by the different oxide structures as compared to the bare metal substrate. Topographic and simultaneous measured spectroscopic maps reveal details of the lateral electronically homogeneity and defect distribution down to atomic resolution. The results will be compared with spectra for Ag(001) and first results of NiO on Ag(001).

O 40.12 Thu 17:45 WIL A317

In-situ investigation of the Nb(110)/oxygen interface —

●MELISSA DELHEUSY^{1,2}, ANDREAS STIERLE¹, CLAIRE ANTOINE², and HELMUT DOSCH¹ — ¹Max-Planck-Institut für Metallforschung, Heisenbergstr. 3, D-70569 Stuttgart, Germany — ²Commissariat à l'énergie atomique, Dapnia/SACM- Centre d'étude Saclay F-91191 Gif-sur-Yvette

Interstitial oxygen impurities are known to affect strongly the physical properties of Nb. This is of first importance for numerous superconducting high technology applications and in particular, for the future improvement of radio-frequency (RF) accelerating cavities. In-situ surface sensitive x-ray studies during oxidation and mild thermal treatments (RT-300°C, UHV) of Nb(110) have been performed. Different aspects of the interaction oxygen/Nb were investigated in the first 50-100 nm below the surface, corresponding to the penetration length of a RF field in Nb. The oxide layer has been characterised by x-ray reflectivity; the depth-distribution of interstitial oxygen was studied with a nm-resolution by depth-resolved grazing incidence x-ray diffuse scattering; finally, the structure of the Nb/oxide interface was investigated by crystal truncation rods measurements. The experiments were realised at the Max-Planck-Institute surface diffraction beamline at the synchrotron source ANKA, and reveal an ordering of the interstitial oxygen atoms below the metal/oxide interface at 300°C parallel to the dissolution of the oxide layer.

O 41 Electronic structure III

Time: Thursday 15:00–17:30

Room: WIL B321

O 41.1 Thu 15:00 WIL B321

Focusing effect on surfaces due to scattering of bulk electrons at subsurface impurities — ●SAMIR LOUNIS, PHIVOS MAVROPOULOS, PETER H. DEDERICHS, and STEFAN BLÜGEL — Institut für Festkörperforschung, Forschungszentrum Jülich, D-52425 Jülich, Germany

An impurity placed below the surface of a noble metal acts as a scatterer of bulk electrons which can lead to short wavelength patterns at the surface as recently found in STM experiments [1]. As explained by these authors the scattering intensity is focused in special directions being determined by regions of low curvature on the Fermi surface. Motivated by this, we carried out a systematic theoretical investigation on the scattering effect of a Co impurity buried at different positions below the (001), (110) and (111) surfaces of noble metals. The wavelength patterns which are related to the curvature of the Fermi surface of the host have different shapes depending on the orientation of the surface. In addition we discuss typical anomalies arising from the reflection of the scattered waves at buried interfaces. The calculations were performed using the full-potential scalar-relativistic Korringa-Kohn-Rostoker Green-function method within Density Functional Theory.

–Work supported by the DFG Schwerpunktsprogramm “Clusters on Surfaces” (SPP 1153).

[1] A. Weismann, M. Wenderoth, N. Quaas, and R. G. Ulbrich, *Verhandlungen der Deutschen Physikalischen Gesellschaft*, O 36.13, 502 (2005) (unpublished).

O 41.2 Thu 15:15 WIL B321

Electronic structure of molybdenum dioxide. Periodic and cluster DFT quantum chemical studies. — ●RENATA TOKARZ-SOBIERAJ, MALGORZATA WITKO, and ROBERT GRZYBOS — Institute of Catalysis and Surface Chemistry, PAS, Cracow, Poland

DFT method is used to describe the electronic structure of bulk and catalytically interesting (011) surface of molybdenum dioxide. MoO₂ exists in literature mainly as a product of MoO₃ reduction; however, the problem of its role in catalytic processes is still unsolved. The electronic structure of bulk system is calculated using periodic approach (VASP code), whereas the information of monoclinic (011) surface is obtained from the cluster method (StoBe code). In both calculations the gradient corrected functionals are used. Detailed analyses of total and atom projected density of states (DOS, PDOS) yield metallic behavior for MoO₂ bulk material. The band around the Fermi level is mainly of Mo 4d character, whereas directly below - there are the O 2p bands (up to -3eV). Further, below EF there is a band (from -3 to -8 eV) identified as Mo-O bonding molecular orbitals. Local properties of different surface sites that are exposed at (011) surface, namely five- and six- fold coordinated Mo atoms, and nucleophilic O sites with different coordination numbers are discussed using charge densities, bond orders indices and molecular orbital diagrams. The discussed surface is characterized by DOS spectra similar to the bulk. Pairs of metallic sites and isolated oxygen centers are identified.

O 41.3 Thu 15:30 WIL B321

Theoretical investigations of molecule-metal interfaces — ●LORENZ ROMANER^{1,2}, GEORG HEIMEL², PETER PACHER^{1,2}, MATHIS GRUBER^{1,2}, JEAN-LUC BRÉDAS², and EGBERT ZOJER^{1,2} — ¹Institute of Solid State Physics, Graz University of Technology, Petersgasse 16, A-8010 Graz, Austria. — ²School of Chemistry and Biochemistry and Center for Organic Photonics and Electronics, Georgia Institute of Technology, Atlanta, Georgia 30332-0400.

We present a theoretical investigation of π -conjugated molecules bound to metallic surfaces. The physical properties of organic/metal interfaces are of high interest for the understanding of self-assembled monolayer formation, workfunction modification of metals, injection barrier tuning in electronic devices, chemical sensing, and molecular electronics. By means of band-structure calculations based on density functional theory, we discuss the interplay between: i) the formation of the bond between metal atoms and atoms of the molecular docking groups; ii) the hybridization and alignment of the molecular states with the Bloch states of the metal; and iii) the charge redistribution between metal and molecule. To that purpose, we systematically varied the molecular structure by exchanging the docking groups, attaching different donor/acceptor groups

to the molecule and varying the conjugation length. We also analyze the reversal of interface formation by mechanically stretching a metal-molecule-metal structure and focusing on stretching forces and structural deformations.

O 41.4 Thu 15:45 WIL B321

Stability of different V2O5 surfaces - theoretical studies — ●MALGORZATA WITKO, JAKUB GOCLON, and ROBERT GRZYBOS — Institute of Catalysis and Surface Chemistry, PAS, Cracow, Poland

Vanadia-based catalysts have a well established position both for large-scale applications and as laboratory research material. Experimental studies on vanadia crystallites point out the presence of only (010) surface. On the other hand, a wide spectrum of reactions, which are catalyzed by vanadia-based materials, suggests an important role of other low-index surfaces such as (001) and (100). Therefore, the relative stability of 3 stoichiometric surfaces (010), (100) and (001)V₂O₅ is studied and compared. Surface energy of low-index terminations is calculated using the periodic DFT approach employing the VASP code. V₂O₅ has a structure of weakly interacting layers stacked along [010] direction, therefore the (010) surface can be modeled by only one layer, whereas the (001) and (100) surfaces need models containing larger number of layers. It is found that the relative stability of surfaces changes in the following order: (010) > (001) > (100). For all surfaces, ionic positions are optimized. Only for the (001) surface a considerable energetic effect of relaxation is found. Surface free energies obtained from DFT calculations are used to make the Wulff construction for V₂O₅ crystal.

O 41.5 Thu 16:00 WIL B321

Reactivity of different V2O5 surfaces - cluster DFT studies — ●PAWEŁ HEJDUK¹, MALGORZATA WITKO¹, and KLAUS HERMANN² — ¹Institute of Catalysis and Surface Chemistry, PAS, Cracow, Poland — ²Fritz-Haber Institut der MPG, Berlin, Germany

The wide application of vanadium oxides as catalysts follows from the fact that their crystallites may exhibit two structurally different types of faces: surfaces built of chemically saturated atoms and those built of unsaturated cations and anions. Both show different behavior in catalytic reactions by performing a complex multi-step operation on the reacting molecule through activation of some of the reactant bonds and hindering those interactions which could result in unwanted product. In this study the reactivity of saturated (010) and unsaturated (001) and (100) surfaces is determined by ab initio DFT cluster methods where electron exchange and correlation is approximated by the gradient corrected RPBE functional. Detailed electronic structure analyses are performed using Mulliken populations and Mayer bond indices, electrostatic potentials, total and partial (atom projected) densities-of-states. Further, adsorption of one and two hydrogen atoms as an atomic/molecular probe at the different surfaces, which leads to surface OH and H₂O or two OH species, will be discussed in detail.

O 41.6 Thu 16:15 WIL B321

Coverage-dependent evolution of plasmon modes in adsorbed Cs layers on Si(111) — ●VOLKMAR ZIELASEK^{1,2}, NEELE RÖNITZ³, EDDY PATRICK RUGERAMIGABO¹, MARTIN HENZLER¹, and HERBERT PFNÜR¹ — ¹Universität Hannover, Institut für Festkörperphysik, Appelstr. 2, 30167 Hannover — ²Universität Bremen, Institut für Angewandte und Physikalische Chemie, Leobener Straße, NW II, 28359 Bremen — ³Philips Semiconductors, Stresemannallee 101, 22529 Hamburg

The transition between substrate and overlayer metalization with varying alkali metal coverage has been studied for Si(111) (7 × 7)-Cs by EELS with ultra-high momentum resolution and measurements of electrical conductance at low temperatures. As the Cs coverage is increased from 0.5 to 1.2 ML coverage, the predominant surface plasmon transforms from a monopole mode, representing metallicity in substrate surface states modified by Cs, to an overlayer multipole mode, which indicates metallicity within a Cs adlayer. The multipole mode continuously shifts in energy from 1.4 to 2.2 eV until a continuous Cs wetting layer is formed. In contrast to previous conventional EELS experiments, the multipole plasmon is clearly identified by an extremely narrow angular distribution of the inelastic electron scattering, unaccounted for by standard dipole scattering theory. Its observation provides evidence for luminescence from atomic Cs layers on Si(111) which can be tuned from infrared to the visible energy range by adjusting Cs coverage.

O 41.7 Thu 16:30 WIL B321

Quantum Size Effects in a decoupled Pb slab on graphitized SiC — ●HUGO DIL¹, THORSTEN KAMPEN¹, THOMAS SEYLLER², and KARSTEN HORN¹ — ¹Department of Molecular Physics, Fritz-Haber-Institut der Max-Planck-Gesellschaft, Faradayweg 4-6, 14195 Berlin, Germany — ²Institute of Technical Physics, University of Erlangen-Nürnberg, Erwin-Rommel-Straße 1, 91058 Erlangen, Germany

Quantum size effects (QSE) which occur in metal overlayer when the dimensions become comparable to the de Broglie wavelength, are responsible for a wide variety of novel effects. In almost all previous work on this subject the influence of the substrate is not negligible. The preferred height of Pb layers on Si(111), for example, changes from 8 to 6 monolayers when depositing on either the 7x7 or sqrt3 x sqrt3. This can be either due to the interface atomic or electronic structure.

To study QSE in films decoupled from the substrate, one has to create a quasi free standing metal slab. We have accomplished this by depositing lead at low temperature on a single domain graphite substrate which shows very little interaction with the metal film. This substrate was prepared, according to a recently developed procedure, from H-etched SiC. The measured band structure of the Pb quantum well states shows an almost perfect match to density functional theory calculations for free standing lead slabs. The observed heights corresponds well to those expected from a simple total energy minimization principle.

O 41.8 Thu 16:45 WIL B321

Unusual temperature dependence of the surface state lifetime on Al(001) — ●M. F. JENSEN¹, T. K. KIM¹, S. BENGIÒ¹, PH. HOFMANN¹, I. YU. SKLYADNEVA², A. LEONARDO², and E. V. CHULKOV² — ¹Institute for Storage Ring Facilities and iNano Center, University of Aarhus, 8000 Aarhus C, Denmark — ²Donostia International Physics Center (DIPC), 20018 San Sebastián / Donostia, Basque Country, Spain

The influence of many-body effects on surface state lifetimes, and in particular the role of the electron-phonon coupling, has recently attracted considerable attention. For temperatures higher than the surface Debye temperature, the situation is expected to be very simple: The inverse surface state lifetime depends linearly on the temperature with the slope mainly given by the electron-phonon mass enhancement parameter λ . Here we present results for the surface state on Al(001) which turns out to behave differently: for high temperatures a stronger than linear increase of the inverse lifetime is observed. The experimental results are compared to first-principles calculations and possible reasons for the unexpected temperature dependence are discussed.

O 41.9 Thu 17:00 WIL B321

Ab initio study of non-reconstructed clean and H-passivated SiC(0001) surfaces — ●TASSILO DANNECKER, ALEXANDER MATTAUSCH, and OLEG PANKRATOV — Theoretische Festkörperphysik, Staudtstr. 7, 91058 Erlangen

The SiC(0001) surface is regarded as a two-dimensional Mott-Hubbard insulator [1]. Up to now mostly the reconstructed $\sqrt{3} \times \sqrt{3}R30^\circ$ -surface has been studied, whereas the 1×1 -surface was considered as unstable. However, recently the 1×1 -structure was stabilized by H-passivation. Moreover, after the hydrogen removal the surface remains metastable [2]. Early DFT-LDA calculations suggested a metallic character of both 1×1 - and $\sqrt{3} \times \sqrt{3}R30^\circ$ -surfaces [3]. However, experimentally the surfaces are semiconducting. For the $\sqrt{3} \times \sqrt{3}R30^\circ$ -surface it was suggested that the Hubbard correlations are responsible for its semiconducting state [1]. In this work we focus on the Si-terminated (0001) as well as the C-terminated (000 $\bar{1}$) side. We consider both clean and H-passivated surfaces. In particular, we study the nature of the surface electron states and in case of the H-passivated surface we discuss the resonant surface states, which are induced by the hydrogen-surface interaction.

[1] V.I. Anisimov *et al.*, Phys. Rev. B, **61** (2000) 1752.[2] T. Seyller, J. Phys.: Condens. Matter, **16** (2004) 1755.[3] M. Sabisch, P. Krüger and J. Pollmann, Phys. Rev. B **55** (1997) 10561.

O 41.10 Thu 17:15 WIL B321

Scattering of electrons in image-potential bands on Cu(001) by Co-Adatoms — ●MICHAELA HIRSCHMANN, KLAUS BOGER, and THOMAS FAUSTER — Lehrstuhl für Festkörperphysik, Universität Erlangen-Nürnberg, Staudtstr. 7, 91058 Erlangen

Energy-, time- and angle-resolved two-photon photoemission has been used to study the various scattering processes induced by adsorbate atoms. We have examined the dynamics of electrons in image-potential states on the Cu(001) surface covered by statistically distributed Co-Adatoms.

From the measured data the scattering probabilities of the inelastic and quasielastic, interband and intraband scattering processes can be determined. The results are discussed in relation to previous work for Cu on Cu(001) [1,2].

[1] K. Boger, M. Weinelt, Th. Fauster, Phys. Rev. Lett. **92** (2004) 126803[2] K. Boger, Th. Fauster, M. Weinelt, New J. Phys. **7** (2005) 110

O 42 Symposium Electron transfer processes II

Time: Thursday 15:00–17:30

Room: WIL C207

Keynote Talk

O 42.1 Thu 15:00 WIL C207

Inter- and intraband scattering of electrons at surfaces — ●THOMAS FAUSTER — Lehrstuhl für Festkörperphysik, Universität Erlangen-Nürnberg, Staudtstr. 7, 91058 Erlangen

Time-resolved two-photon photoemission is the method of choice to study the electron dynamics at surfaces. With high energy and angular resolution various scattering processes (interband vs. intraband and inelastic vs. elastic) can be unraveled in detail. For image-potential states at Cu(001) surfaces it is shown [1], that adatoms induce mainly elastic scattering. Inelastic scattering processes are attributed to electron-electron scattering which is not significantly influenced by adatoms. The detailed study of scattering processes is particularly important to understand the electron dynamics at semiconductor surfaces [2].

[1] K. Boger, M. Weinelt, and Th. Fauster: Phys. Rev. Lett. **92**, 126803 (2004); New J. Phys. **7**, 110 (2005).[2] M. Weinelt, M. Kutschera, Th. Fauster, and M. Rohlfing: Phys. Rev. Lett. **92**, 126801 (2004).

Keynote Talk

O 42.2 Thu 15:30 WIL C207

Image potential states on a finite size adsorbate island — ●J.P. GAUYACQ and A.G. BORISOV — Université Paris-Sud, 91405 Orsay Cedex, France

When adsorbate islands are grown on a metal surface, image potential states can appear localized at two different places: on the adsorbate islands and on clean substrate patches. Confinement of the image states on islands leads to two phenomena deeply influencing their dynamical be-

haviour: quantisation on the finite size object and scattering at the island edges. This provides a very appealing opportunity to study finite size effects on a 2D-continuum of states. Results of a theoretical parameter-free study of this problem in the case of Ar islands on a Cu(100) substrate will be presented. Two main points will be addressed: i) quantisation of the image state continuum on the Ar island leading to a series of resonance states and ii) scattering at the edges of the island that results in reflection, or transmission into the image states continua of the clean part of the surface, or decay into the substrate bulk states. Transmission at the island edges is highly probable making the image states on small islands very short-lived. The variation of the image state characteristics (energy and lifetime) with the island size will be presented. The question of the observability of finite size effects and the related question of the minimum island size for an image state to 'look like' on an infinite layer will be addressed.

Keynote Talk

O 42.3 Thu 16:00 WIL C207

Dynamics of surface-localised electronic excitations studied with the scanning tunnelling microscope — ●J. KRÖGER — Institut für Experimentelle und Angewandte Physik, Christian-Albrechts-Universität zu Kiel, D-24098 Kiel, Germany

The dynamics of surface-localised electronic states can be influenced by confinement, by the presence of single adsorbed atoms, and, in the case of superstructures, by Brillouin zone backfolding.

On Ag(111) monatomically deep vacancy islands were fabricated to confine the electronic surface state. Depending upon the size of the vacancy island the dominant lifetime-limiting process can be lossy scat-

tering of the electron waves at the vacancy boundary. An analytic expression is derived to take this effect into account. Further, a corrected analysis of the spatial decay of electron interference patterns is presented, which leads to a more consistent description of the Ag(111) surface state lifetime.

Single adsorbed Ag, Cu, and Co atoms on Ag(111) and Cu(111) induce an electronic resonance, which is split off from the bottom of the surface state band. Whereas Ag atoms on Ag(111) and Cu atoms on Cu(111) decrease the surface state lifetime, the impact of Co atoms on the surface state dynamics is found to be negligible.

The role of elastic scattering in the dynamics of quantum well states on Cu(111)-p(2x2)Cs is addressed. We find that elastic scattering is enhanced by Brillouin zone backfolding and contributes appreciably to the observed quantum well state linewidth: Calculations show that 50% of the linewidth are due to the backfolding mechanism.

Keynote Talk

O 42.4 Thu 16:30 WIL C207

Electron induced isomerization — ●KARINA MORGENSTERN — Universität Hannover, Institut für Festkörperphysik, Appelstr. 2, 30167 Hannover

With the scanning tunneling microscope (STM) it is possible to induce chemical reactions on a single molecule basis by electrons tunneling inelastically from the STM tip into a molecule. The method is based on high-resolution imaging at low-temperature (5K) that allows us to identify different groups within the molecule. Chemical reactions are induced by injecting selectively electrons into specific parts of the molecule. The success of the manipulation is visualized in the recorded tunneling current during the manipulation and in STM images taken afterwards.

We will present isomerization for two molecules of different complexity, specifically substituted benzene molecules (chloronitrobenzene), and photochrome molecules (azobenzene derivate). The energies needed for the reactions are remarkably low and can be best understood in terms of weakened bonds on the surface in connection with direct reformation of a new bond.

Keynote Talk

O 42.5 Thu 17:00 WIL C207

Non-adiabatic Surface Dynamics: Electron Transfer and Femtochemistry at the Adsorbate/Metal Interface — ●MARTIN WOLF — Dept. of Physics, Freie Universität Berlin, 14195 Berlin, Germany

One of the key goals in surface physics is to obtain a microscopic understanding of elementary excitations in surface reaction dynamics. At metals the dynamics of gas surface interactions are governed by ultrafast charge and energy transfer to the substrate, leading to non-adiabatic couplings between electronic and nuclear degrees of freedom. As a consequence electronic excitation of the substrate by ultrafast laser pulses can induce efficiently non-thermal reactions of adsorbed species. In this talk we present recent progress in the application of femtosecond time-resolved laser spectroscopy to investigate electron thermalization dynamics in metals, electron transfer at the adsorbate metal interface as well as surface femtochemistry induced by photoexcited hot electrons. We show that time-resolved photoemission spectroscopy allows to analyze directly the transient non-equilibrium electron distribution in Ru(001) and discuss the role of electronic friction and energy partitioning between various degrees of freedom in the associative formation of hydrogen and CO on Ru(001).

O 43 Time-resolved spectroscopy I

Time: Thursday 17:30–18:30

Room: WIL C207

O 43.1 Thu 17:30 WIL C207

Nanoscope ultrafast space-time-resolved spectroscopy — ●W. PFEIFFER¹, T. BRIXNER¹, C. SPINDLER¹, and F.J. GARCÍA DE ABAJO² — ¹Physikalisches Institut, Universität Würzburg, Am Hubland, 97074 Würzburg, Germany — ²Centro Mixto CSIC-UPV/EHU, Apartado 1072, 20080 San Sebastián, Spain

We analyze a recently proposed new scheme for ultrafast spectroscopy with nanometer spatial and femtosecond temporal resolution [1] that enables the direct spatial probing of nanoscale energy transfer or charge transfer processes. The interaction of polarization-shaped laser pulses with a nanostructure allows us to control the spatial and temporal evolution of the optical near-field. Employing a learning algorithm, the field is tailored such that pump and probe excitation occur at different positions. Both excitations can be restricted to sub-diffraction extensions and are separable on a nanometer length scale. Substantial control according to different goals is demonstrated and the limits of controllability are investigated. The dominating control mechanism is local interference of near-field modes that are excited with the two independent polarization components of the incident light pulses and hence polarization pulse shaping is essential to achieve substantial control in the optical near-field. The influence of other control mechanisms is discussed and a number of possible applications using different nanostructures such as planar and three-dimensional arrangements of nanoparticles are presented.

[1] T. Brixner, F. J. García de Abajo, J. Schneider, and W. Pfeiffer, Phys. Rev. Lett. 95, 093901 (2005).

O 43.2 Thu 17:45 WIL C207

Competing Processes at Ice-Metal Interfaces: Ultrafast Electron Transfer and Solvation Dynamics — ●JULIA STÄHLER, CORNELIUS GAHL, UWE BOVENSIEPEN, and MARTIN WOLF — Freie Universität Berlin, Fachbereich Physik, Arnimalle 14, 14195 Berlin, Germany

The ultrafast dynamics of excess electrons photo-injected into ultrathin amorphous D₂O layers on Ru(001) and Cu(111) are investigated using time-resolved two-photon photoelectron spectroscopy. On both substrates we observe electron localization and solvation in the ice films, competing with back relaxation to the metal. We identify two regimes of back transfer: (i) For $t < 300$ fs the initial back transfer rate is four times higher on Ru(001) ($\tau_1^{Ru} = 34$ fs) compared to Cu(111) ($\tau_1^{Cu} = 140$ fs). (ii) At $t > 300$ fs we observe a slower back transfer, which is comparable for both systems ($\tau_2^{Ru} = 302$ fs, $\tau_2^{Cu} = 316$ fs). By an empirical model calculation based on rate equations, which nicely reproduces our data,

we show that the back transfer is initially determined by the electronic surface band structures of the two substrates, whereas the population decay at later times is dominated by tunneling through a potential barrier at the interface, which arises from the rearrangement of the surrounding polar molecules during solvation.

O 43.3 Thu 18:00 WIL C207

Time-Resolved Two-Photon Photoemission study of C₆₀ — ●ARNE ROSENFELDT, BENJAMIN GÖHLER, and HELMUT ZACHARIAS — University of Münster, 48149 Münster, Germany

Up to 200 ML of C₆₀ on Cu(111) are illuminated by tunable 365 to 415 nm (3.40 to 2.99 eV) radiation of 50 ps pulse duration. Delayed 263 nm (4.71 eV) photons have sufficient energy to probe half of the LUMO and the LUMO+1. A rate equation fitted to the electron dynamics suggests a short lifetime of about 126 ps for the LUMO, and another one longer than 5 ns, which may originate from excitons with the same energy as the LUMO. The excitation probability of these states is measured as a function of photon energy, showing a maximum at 392 nm (3.16 eV). Using four-wave mixing in Xenon radiation at 150 nm (8.27 eV) is generated to investigate low-lying states. For measurement of long lifetimes a second laser is electronically delayed. The project is financially supported by the DFG in the SPP1093 "Dynamik von Elektronentransferprozessen an Grenzflächen"

O 43.4 Thu 18:15 WIL C207

Ultrafast interfacial electron transfer probed with two-photon photoemission — ●LARS GUNDLACH, RALPH ERNSTORFER, SILKE FELBER, RAINER EICHBERGER, and FRANK WILLIG — Hahn-Meitner-Institute, Department: Dynamics of Interfacial Reactions SE4, Glienickestrasse 100, 14109 Berlin

Two-photon photoemission (2PPE) is the method of choice for investigating ultrafast interfacial electron transfer because of its excellent sensitivity and time resolution. With this technique one can address adsorbates at coverages far below a monolayer. With the same chromophore perylene fixed with different anchor and bridge groups at the surface of rutile TiO₂(110) the corresponding 2PPE transients revealed the relevant parameters that characterize the contributing processes.

Instantaneous optical injection on one hand and slow injection over a long distance on the other hand were realized. Direct optical charge transfer was realized with the chromophore catechol that is known to form a charge transfer complex with Ti atoms on the surface of TiO₂. The slow

injection cases were realized by inserting rigid molecular bridges. The same experimental systems were investigated with fs-transient absorption. Comparing the different 2PPE transients and the corresponding transient absorption transients for the identical systems revealed the

physical processes and time scales that control the 2PPE transients. 2PPE measurements with different angle of incidents and polarizations of the pump pulse revealed the binding geometry of the different anchor groups on the surface.

O 44 Postdeadline session

Time: Thursday 20:00–21:00

Room: HSZ 02

O 45 Invited talk Föhlisch

Time: Friday 10:15–11:00

Room: TRE Phys

Invited Talk

O 45.1 Fri 10:15 TRE Phys

Surface electron dynamics on the atomic scale — ●ALEXANDER FÖHLISCH — Institut für Experimentalphysik, Universität Hamburg, Luruper Chaussee 149, 22761 Hamburg

Ultra fast electron dynamics play a decisive role in processes like photo- and electrochemistry as well as in molecular electronics and single electron devices. If we are interested in electron transfer processes in complex systems it is of equal importance to address the temporal evolution of the electron wave packet and the question at which atomic center an

electron resides before delocalization through charge transfer to neighboring atoms occurs. With element specific synchrotron based soft x-ray spectroscopy, called core hole clock spectroscopy, we can accomplish this. For adsorbates on surfaces we could show how the femtosecond electron transfer process depends in fine detail on the surface projected band structure of the substrate. Furthermore, we can directly observe on an attosecond timescale charge transfer dynamics originating from an atomically localized state by making use of extremely fast Coster Kronig decay processes of core-excited states.

O 46 Adsorption VI

Time: Friday 11:15–13:00

Room: TRE Phys

O 46.1 Fri 11:15 TRE Phys

The Structure of O-p(4x4)/Ag(111): results from surface sensitive x-ray techniques — ●A. STIERLE¹, A. REICHO¹, I. COSTINA¹, S. THIESS², J. ZEGENHAGEN², and H. DOSCH¹ — ¹MPI für Metallforschung, Heisenbergstraße 3, D-70569 Stuttgart — ²ESRF, B.P. 220, F-38043 Grenoble

Silver plays an important role as an oxidation catalyst and therefore many fundamental studies have been devoted to Ag surfaces. One important finding is that after oxidation of Ag(111) at 500 K either at O₂ pressures in the mbar regime, or using NO₂ at lower pressures a p(4x4) superstructure is formed, which was believed to be a prototype for a surface oxide O-Ag-O trilayer. The proposed models for this structure [1] are incompatible with the surface x-ray diffraction data obtained at the MPI-MF beamline at ANKA and the normal incidence x-ray standing wave results from ID32, ESRF. Instead, a model is favoured, that includes Ag adatoms on hcp and fcc sites and oxygen atoms filling the rows in between, which is also supported by recent scanning tunneling microscopy and core level spectroscopy results, combined with density functional theory calculations*.

*M. Schmid, et al., contribution at this conference

[1] A. Michaelides, K. Reuter, and M. Scheffler. *J. Vac. Sci. Technol.* A 23, 1487-1497 (2005).

O 46.2 Fri 11:30 TRE Phys

The p(4x4) structure of Ag(111): A soft O-induced reconstruction — ●MICHAEL SCHMID¹, GEORG KRESSE², JAN KLIKOVITS¹, OREST DUBAY², and PETER VARGA¹ — ¹Inst. f. Allgemeine Physik, TU Wien — ²Inst. f. Materialphysik and CMS, Universität Wien

Silver is a well-known catalyst for selective oxidation reactions, e.g., of ethylene (epoxidation). The phase on the (111) surface usually associated with this reaction is a p(4x4) superstructure, which has been studied since 1972 [1] and considered a surface oxide similar to a layer of the Ag₂O bulk structure since 1974. An X-ray diffraction study by A. Stierle et al. [2] has disproved essentially all Ag₂O-based models [3] so far. We have studied the mass transport during reduction of the p(4x4) structure by scanning tunneling microscopy (STM) to determine the number of Ag atoms per cell. Based on this input and the STM images, a structural model very different from Ag₂O emerges. The model is compatible with high-resolution core level spectroscopy data and was confirmed by surface x-ray diffraction [4]. The structure does not have the lowest energy of all possible models in density functional theory (DFT) calculations, a fact attributed an inherent problem of today's DFT calculations. Nevertheless, DFT is valuable for a detailed study of this structure and shows that it is very soft, exhibiting extremely high vibration amplitudes.

[1] G. Rovida et al., *J. Vac. Sci. Technol.* 9, 796 (1972).

[2] A. Stierle et al., contribution at DPG Frühjahrstagung 2004.

[3] A. Michaelides et al., *J. Vac. Sci. Technol.* A 23, 1487 (2005).

[4] A. Stierle et al., contribution at this conference.

O 46.3 Fri 11:45 TRE Phys

H-Induced Symmetry Break of the Hexagonal Surface Reconstruction of Ir(100) — ●D. LERCH¹, A. SCHMIDT¹, A. KLEIN¹, L. HAMMER¹, S. MÜLLER¹, K. HEINZ¹, H.-C. POON², and D. SALDIN² — ¹Festkörperphysik, Universität Erlangen-Nürnberg, Staudtstr. 7, D-91058 Erlangen — ²Univ. Wisconsin-Milwaukee

Upon H adsorption the (quasi-)hexagonal 5x1-reconstruction of clean Ir(100) is lifted. Yet, as this process is thermally activated the hexagonally close-packed surface Ir-layer persists as a metastable phase for sample temperatures below 200 K. We have investigated this 5x1-hex-H phase by the combined application of quantitative LEED and DFT. Using LEED spectra as a structural fingerprint we find that hydrogen considerably modifies the complex reconstruction pattern of the surface. Yet, though the clean surface structure could be reliably solved by quantitative LEED, the method fails to produce a satisfactory theory-experiment fit as long as all symmetry elements of the clean surface are enforced. Only by breaking the mirror symmetry of the 5x1 unit cell the reproduction of measured intensity data is possible. DFT calculations corroborate this symmetry break as well as the experimentally estimated H coverage of 0.6 ML. The calculations show that the symmetry break is due to only one of the three hydrogen atoms per unit cell which assumes an asymmetric hollow site near the centre of the troughs of the surface reconstruction. The resulting 33 (!) geometrical parameters describing the surface and sub-surface Ir structure are in quantitative agreement with those determined by the LEED analysis. The H-induced structure can be interpreted as a precursor phase for the reconstruction lifting transition.

O 46.4 Fri 12:00 TRE Phys

CO adsorption and CO and O coadsorption on Rh(111) — ●ROBERT SCHENNACH¹ and IMRE BAKO² — ¹Institute of Solid State Physics, Graz University of Technology, Graz, Austria — ²Chemical Research Institute of the Hungarian Academy of Sciences, Budapest, Hungary

The adsorption of CO and the coadsorption of CO and O on Rh(111) at 123 K was studied using reflection absorption infra red spectroscopy (RAIRS) and density functional theory (DFT). CO adsorption on Rh(111) proceeds via adsorption at on top sites at low coverages (less than 0,33 monolayer (ML)) and by on top and hollow site occupation at higher coverages (more than 0,33 ML). Evidence from the RAIRS

measurements shows that also some bridge sites are occupied from intermediate coverages up to a full monolayer. A new vibration in the on top region around 2085 cm^{-1} is found in the IR spectra at higher coverages, which has not been detected in high resolution electron energy loss spectroscopy (HREELS) studies. The origin of this new vibrational feature is discussed in detail using the results from DFT calculations. Experiments show that this new vibration vanishes during CO adsorption at elevated temperatures. Coadsorption of oxygen generally leads to a shift to higher wavenumbers of the CO vibrations. This is explained in terms of increased repulsive interactions between the adsorbed species. The adsorption sequence does not influence the vibrational spectra, however, the CO to O ratio and the surface temperature during adsorption show an influence. Thermal desorption from the coadsorbed layers shows some reaction between CO and O to form CO_2 .

O 46.5 Fri 12:15 TRE Phys

STRUCTURE AND PROPERTIES OF K-O COADSORBATE PHASES ON RH(110): CHEMICAL PATTERNS AND LOW PRESSURE PATHWAY TO SURFACE OXIDE FORMATION

— •SEBASTIAN GÜNTHER¹, FRIEDRICH ESCH², GIOVANNI COMELLI², and MAYA KISKINOVA³ — ¹Department Chemie, Ludwig-Maximilians Universität München, Butenandtstr. 11 E, 81377 München, Germany — ²Laboratorio TASC-INFN, Area Science Park, 34012 Trieste, Italy — ³Sincrotrone Trieste, Area Science Park, 34012 Trieste, Italy

The present study of K-O coadsorbate system on Rh(110) has been inspired by the peculiar chemical wave patterns observed during the $\text{H}_2 + \text{O}_2$ reaction on the K-covered Rh(110) surface. Using Low energy electron diffraction (LEED), Scanning tunneling microscopy (STM) and X-ray photoelectron spectroscopy (XPS) we found that coadsorption of O and K at $T > 450\text{ K}$ leads to a variety of ordered phases, all of them involving missing-row reconstructions of the substrate. The building blocks of these surface structures were determined. The massive restructuring of the surface at high K coverage is followed by growth of a surface oxide phase, which cannot be formed on a K-free surface under UHV conditions. The surface composition and activity of the coadsorbed phases were characterized by XPS, which revealed that although K adatoms promote the O_2 adsorption and oxidation of the substrate, they act as deactivators for the $\text{H}_2 + \text{O}_2$ reaction.

O 46.6 Fri 12:30 TRE Phys

An *ab initio* Study of Topographical Defects on NaCl(100) —

•BO LI, ANGELOS MICHAELIDES, and MATTHIAS SCHEFFLER — Fritz-Haber-Institut der Max-Planck-Gesellschaft Faradayweg 4-6, D-14195 Berlin, Germany

Ab initio calculations based on density-functional theory (DFT) within the plane-wave pseudopotential formalism have been performed for a wide variety of defects on NaCl surfaces. Specifically, Na and Cl vacancies and adatoms as well as neutral and polar steps have been examined.

These DFT calculations have yielded several interesting results, such as the first *ab initio* determinations of the surface energy of NaCl(100) and monatomic step formation energies. In addition, it is found that Cl adatoms exhibit a preference for adsorption on top of Cl substrate sites, rather than above Na substrate sites as might be anticipated. A series of second order Møller-Plesset perturbation theory (MP2) calculations for Cl adatoms on small NaCl clusters show the same binding site preference, thus lending support to this “non-textbook” result. The explanation for this unusual result is, however, perfectly textbook: a weak covalent bond that forms only when Cl adatoms reside above Cl substrate atoms.

O 46.7 Fri 12:45 TRE Phys

Tensor LEED and PIRS study of the monolayer C_2D_2 adsorbed on KCl(100) — •JOCHEN VOGT and HELMUT WEISS — Chemisches Institut der Universität Magdeburg, Universitätsplatz 2, 39106 Magdeburg, Germany

Growth and structure of the monolayer C_2D_2 adsorbed on KCl(100) single crystal surfaces were investigated by means of polarization infrared spectroscopy (PIRS) and low-energy electron diffraction (LEED). PIRS spectra in the region of the ν_3 fundamental mode show a sharp singlet absorption near 2396 cm^{-1} at 75 K . The ratio of the integrated intensities in s- and in p-polarization is consistent with a parallel orientation of the molecules with respect to the surface plane. LEED experiments indicate a $(\sqrt{2} \times \sqrt{2})\text{R}45^\circ$ lattice with two glide-planes under the same conditions. Integrated intensities of 5 beam orders were recorded as a function of electron energy and analyzed using the tensor LEED approach. Based on a structure model with two molecules in the surface unit cell the I(E) analysis supports an adsorption site 3.15 \AA above the K^+ cations. In the best-fit geometry the molecular axes of the two molecules enclose an angle near 60° . In contrast the appearance of the singlet absorption in the infrared spectra strongly support this angle to be 90° . These deviating results are discussed by taking into account the influence of frustrated rotations of the molecules on the LEED intensities within the model of ‘split positions’ [1].

[1] H. Over, M. Gierer, H. Bludau, G. Ertl, Phys. Rev. B 52, 16812 (1995)

O 47 Organic films IV

Time: Friday 11:15–13:00

Room: PHY C213

O 47.1 Fri 11:15 PHY C213

Comparison of the vertical bonding distances of PTCDA on Ag(111) and Au(111) — •S. K. M. JÖNSSON¹, O. BAUER¹, A. HAUSCHILD², T.-L. LEE³, M. SOKOLOWSKI², and F. S. TAUTZ¹ — ¹School of Engineering and Science, International University Bremen, P.O. Box 750561, 28725 Bremen, Germany — ²Institut für Physikalische und Theoretische Chemie, University of Bonn, 53115 Bonn, Germany — ³European Synchrotron Radiation Facility, Bote Postale 220, 38043 Grenoble Cedex, France

The model molecule PTCDA adsorbs on the Au(111) and Ag(111) surfaces in a planar configuration forming long range ordered superstructures. However, from different electron spectroscopies, STM and LEED data there is evidence that the bonding strength of PTCDA on Ag(111) is stronger than on Au(111). Hence the question arises, whether this also leads to a change of the vertical bonding distance of PTCDA with respect to the underlying surface. For this purpose we have measured the vertical distance of the carbon skeleton of PTCDA with respect to both surfaces using the normal incidence standing wave technique (NIXSW). Interestingly, we find that the bonding distance on Au(111) is by 0.4 \AA (or 15 %) larger than on Ag(111), in agreement with the expectation on the basis of a weaker bonding. This work was supported by the DFG and the ESRF.

O 47.2 Fri 11:30 PHY C213

LEED-IV for the structural investigation of the EC4T monolayer on Ag(111) — •JOHANNES ZIROFF¹, CHRISTIAN KUMPF¹, AZZEDINE BENDOUNAN¹, WOLFGANG MORITZ², and FRIEDRICH REINERT¹ — ¹Experimentelle Physik II, Physikalisches Institut, Univ. Würzburg — ²Sektion Kristallographie, Department für Geo- und Umweltwissenschaften, LMU München

The Low Energy Electron Diffraction-IV (LEED-IV) technique is a powerful tool for obtaining structural information on surfaces and is often used for the investigation of adsorbate systems or surface reconstructions. In the past this technique was frequently applied to inorganic systems. For organic adsorbates there is a severe demand for detailed structural information e.g., exact atomic coordinates. The unit cells of organic adsorbates are often very large and beam damage effects play an essential role. However, in some cases LEED-IV can be used to investigate organic adsorbate systems.

We report on a LEED-IV study of a well ordered monolayer of EC4T on Ag(111), the so called relaxed monolayer structure. Important geometric parameters like the position of the molecule (height above the surface and adsorption site) as well as possible bending and deformation of the molecule down to the variation of single atomic positions were investigated. The data are compared with results from other experimental methods (e.g., NIXSW, SXRD, NEXAFS), and the effect of radiation damage will be addressed. A structural model for EC4T on Ag(111) is presented.

O 47.3 Fri 11:45 PHY C213

Structural investigation of SnPc on Ag(111) using NIXSW — ●C. STADLER, F. POLLINGER, S. HANSEN, C. KUMPF, and E. UMBACH — Exp. Physik II, Univ. Würzburg

The investigation of the interaction of organic molecules with inorganic substrates is a key issue for understanding interface effects. We report on NIXSW measurements of two different superstructures of flat-lying tin-phthalocyanine (SnPc) molecules on Ag(111): an incommensurate monolayer at room temperature with one molecule per unit cell and a commensurate submonolayer (at 150K) with two molecules per unit cell. Precise information about the vertical bonding distance of different atomic species in the molecule with respect to the substrate is obtained. This results in a model for the RT structure with the Sn atom 0.75Å below the plane of carbon and nitrogen atoms, i.e., the molecules lie "tin-down" on the surface. The Sn-Ag distance is 2.44Å, which is very close to the Ag-Ag layer distance. In contrast, for the 150K phase a mixture of "tin-down" and "tin-up" orientations is formed. This is based on a strongly reduced coherent fraction of 0.42 for the Sn3d signal, which can be explained by two Sn-adsorption sites with a height of 2.37Å and 3.91Å respectively.

O 47.4 Fri 12:00 PHY C213

Adsorption behavior of the amino acid DOPA on single crystalline Au(110) surfaces — ●MIRKO WEINHOLD¹, RUSLAN TEMIROV², SERGUEI SOUBATCH², and STEFAN TAUTZ² — ¹Universität Bremen — ²International University Bremen

In investigations of proteins which are responsible for strong mussel adhesion, an unusually frequent appearance of the otherwise rare amino acid 3-(3,4-Dihydroxyphenyl)-L-alanine (DOPA) has been observed. This amino acid is thought to play a major role in the mechanism of mussel adhesion. Here we report an investigation of the molecule-substrate interaction between DOPA and the Au(110) surface. Several spectroscopic techniques (HREELS, LEED, XPS, IR) have been applied. Although DOPA decomposes close to the sublimation point, vapour deposition of the intact molecule without additional contamination turns out to be possible. DOPA molecules form a commensurate superlattice on Au(110). The chirality of the molecule leads to a one-domain chiral surface. Vibrational spectroscopy in conjunction with density functional calculations proves that DOPA adsorbs on Au(110) in its zwitter-ionic state. Annealing a DOPA/Au(110) monolayer to 550 K leads to partial desorption of the monolayer as well as catalyzed oxidation of DOPA to DOPAquinone.

O 47.5 Fri 12:15 PHY C213

Comparative UHV-STM study of adsorption structures formed from a family of oligo-(phenylene ethynyls) with systematic variation of geometry and functional groups — ●CHRISTIAN BOMBIS¹, CARSTEN BUSSE¹, SIEGRID WEIGELT¹, MARTIN NOERGAARD¹, MARTIN KNUDSEN², KURT V. GOTHELF², EVA RAULS¹, BJØERK HAMMER¹, FLEMMING BESENBACHER¹, and TROLLE R. LINDEROTH¹ — ¹Department of Physics and Astronomy, and iNANO, University of Aarhus, 8000 Aarhus C, Denmark — ²Department of Chemistry, and iNANO, University of Aarhus, 8000 Aarhus C, Denmark

Using scanning tunneling microscopy we have systematically explored the influence of the geometry of molecules and the chemical nature of their functional groups on formed adsorbate structures. For this purpose we utilized compounds from a family of organic molecules, oligo-(phenylene ethynyls), which have been deposited on the Au(111) surface under ultra high vacuum conditions. The elementary member of this family consists of a highly conjugated linear backbone functionalized with aldehyde, hydroxyl and bulky tert-butyl groups while compounds with

bent and three-spoke geometries represent geometrical variants. The study with systematic variation of the endgroup chemistry supports the hypothesis, that only in the case, where intermolecular hydrogen bonds can form, does a more open network phase form instead of a close packed structure held together by non-specific Van-der-Waals interactions. Theoretical modelling based on the DFT-B method is currently being performed to further illuminate this observation.

O 47.6 Fri 12:30 PHY C213

STM and LEED study on the Influence of Different Substituents on the Growth of Quaterylene Derivatives on Gold. — ●CHRISTIAN WAGNER¹, ROBERT FRANKE¹, SEBASTIAN FRANKE¹, THOMAS DIENEL¹, STEFAN MANNSFELD², and TORSTEN FRITZ¹ — ¹Institut für Angewandte Photophysik; TU-Dresden; George-Bähr-Straße 1; 01069 Dresden — ²Department of Chemical Engineering; Stanford University; 381 North South Mall; Stanford, CA 94305-5025

The possibility to tailor and control organic molecules for special purposes opens a new field of possible applications. There is a general interest in the question how even minor modifications e.g. different substituents change the behavior of a class of molecules. In highly ordered monolayers, the influence of the substituents can be studied in a well defined environment. As perylene derivatives [1] have already been studied intensively, we have now grown highly ordered monolayers of the larger IR absorbing quaterylene derivatives, quaterylene (QT) and quaterylenebisdicarboximide (QTCDI) on Au in UHV. The structure of QT has been studied by STM and LEED and fits nicely to state-of-the-art potential calculations [2] for the growth of large QT domains on gold. Due to the presence of imide groups the structure of QTCDI differs strongly from QT. Three different phases have been found which can be explained by the formation of hydrogen bonds. The capability of the potential calculations is demonstrated as all three phases are predicted.

[1] H. Proehl, T. Dienel, R. Nitsche und T. Fritz, PRL 93 (2004) 097403 [2] S.C.B. Mannsfeld and T. Fritz, PRB 93 (2004) 075416 & PRB 71 (2005) 235405

O 47.7 Fri 12:45 PHY C213

Aromatic selenolates as an attractive alternative to the respective thiolates — ●ANDREY SHAPORENKO¹, PIOTR CYGANIK², MANFRED BUCK², ANDREAS TERFORT³, and MICHAEL ZHARNIKOV¹ — ¹Angewandte Physikalische Chemie, Universität Heidelberg, Im Neuenheimer Feld 253, 69120 Heidelberg, Germany — ²School of Chemistry, St Andrews University, North Haugh, St Andrews, KY16 9ST, United Kingdom — ³Anorganische und Angewandte Chemie, Universität Hamburg, 20146 Hamburg, Germany

Self-assembled monolayers (SAMs) formed from bisbiphenyl-4-yl diselenide (BBPDSe) on Au(111) and Ag(111) substrates have been characterized by several complementary spectroscopic and microscopic techniques. BBPDSe was found to form contamination-free, densely-packed, and well-ordered biphenyl selenolate (BPSe) SAMs on both Au and Ag. Spectroscopic data suggest very similar packing density, orientational order, and molecular inclination in BPSe/Au and BPSe/Ag. STM data give a similar intermolecular spacing of 5.3 Å on both Au and Ag, but exhibit differences in the exact arrangement of the BPSe molecules on these two substrates. There is strong evidence for adsorbate-mediated substrate restructuring in the case of Au, whereas no clear statement on this issue can be made in the case of Ag. The film quality of the BPSe SAMs is superior to their thiolate analogues, which is presumably related to a better ability of the selenolates to adjust the surface lattice of the substrate to the most favorable 2D arrangement of the adsorbate molecules. This implies that aromatic selenolates represent an attractive alternative to the respective thiolates.

O 48 Nanostructures IV

Time: Friday 11:15–13:00

Room: WIL A317

O 48.1 Fri 11:15 WIL A317

Oxygen-Induced Faceting of Ir(210) — ●TIMO JACOB, PAYAM KAGHAZCHI, and MATTHIAS SCHEFFLER — Fritz-Haber-Institut der MPG, Faradayweg 4-6, 14195 Berlin

Although rough clean metal surfaces usually have higher surface free energies than their closed-packed analogs, adsorbates are able to modify this behavior and cause changes in surface morphology through reconstructions or facet formations. Using different surface sensitive techniques (e.g. STM or LEED) Madey *et al.* [1] found that Ir(210) shows

interesting surface faceting at high oxygen coverages ($\theta > 0.5$ ML). The facets were identified as three-sided nanoscale pyramids with two (311) and one (110) planes.

In order to understand this effect we used density functional theory in combination with the *ab initio* atomistic thermodynamics and studied the influence of an oxygen atmosphere on the structure of Ir(210). Assuming an oxygen partial pressure of 1 atm, it turned out that below $T < 1000$ K the oxygen-covered facets are thermodynamically more stable than non-faceted O/Ir(210). Further heating reverts the substrate structure to planar O/Ir(210).

While most nanoscale pyramids consist of smooth and unreconstructed planes, some (110) facets show a complex reconstructed superstructure. Thus, present studies aim on the stability and an atomistic understanding of those structures.

[1] I. Ermanoski *et al.*, *Surf. Sci.* **549**, 1 (2004).

O 48.2 Fri 11:30 WIL A317

Nickel Nanowire Formation on Ir(100) — ●ANDREAS KLEIN, LUTZ HAMMER, and KLAUS HEINZ — Lehrstuhl für Festkörperphysik, Universität Erlangen-Nürnberg, Staudtstr. 7, D-91058 Erlangen

On the H-induced 5x1 phase of Ir(100) [1], where extended monoatomic Ir chains reside on top of an unreconstructed substrate, the growth of nickel proceeds layerwise up to the sixth layer. Rather unusually, each new layer starts with the development of extended nanowires of several hundred Angstrom length instead of compact islands. Their number first increases, then they locally coalesce into islands until finally the layer is completed. The growth of new wires on a just completed nickel layer always proceeds within shallow troughs which come by the corrugation of the underlying Ni film. The width of the nanowires increases with film thickness, whereby on the xth layer they consist exclusively of (x-1)-atomic rows. This thickness-dependent size is due to the increasing width of the surface troughs which in turn is caused by local and layer dependent relaxations of the Ni layers above the Ir chains at the Ir-Ni interface. By Ni deposition on the clean reconstructed 5x1-hex phase of Ir(100) the hexagonal reconstruction is lifted ending up in the same local structure than on the 5x1-H phase, yet with considerably poorer long-range order. Consequently, the same nanowires are observed as before, however, with much shorter lengths and an earlier onset of coalescence leading to more compact island structures. [1] L. Hammer, W. Meier, A. Klein, P. Landfried, A. Schmidt, K. Heinz, *PRL* **91** (2003) 156101

O 48.3 Fri 11:45 WIL A317

Ordered cluster arrays on a graphite-Ir(111) moiré pattern — ●ALPHA NDIAYE, SEBASTIAN BLEIKAMP, and THOMAS MICHELY — I. Physikalisches Institut (IA) RWTH Aachen 52056 Aachen

Perfectly ordered Ir-cluster arrays can be formed on a functionalised Ir(111) surface. The clusters are bound in a hexagonal lattice with a lattice constant of 26 Å. Their size distribution is narrow and the size can be tuned from 6 to 150 atoms. The clusters possess a surprising thermal stability. Clusters with an average size of 5 atoms are stable up to 450 K. At low clustersizes, different types of clusters can be distinguished.

Functionalisation of the Ir(111) surface is achieved through preparation of monolayer graphite sheets, which can be formed by pyrolysis of hydrocarbons. The superposition of the graphite and Ir(111) surface gives rise to the emergence of a $\sqrt{91} \times \sqrt{91} R5.23^\circ$ moiré pattern. Ir clusters form, where threefold coordinated adsorption sites of the underlying Ir(111) lattice are in the center of the graphite honeycomb unit cells.

O 48.4 Fri 12:00 WIL A317

Scanning Tunneling Microscopy (STM) and Spectroscopy (STS) Investigations of Gold Nano-Particles in a Double-Tunneling-Junction Arrangement at Room-Temperature — ●ANNA TSCHETSCHETKIN, CHRISTOF DIETRICH, BERNDT KOSLOWSKI, and PAUL ZIEMANN — Abteilung Festkörperphysik, Universität Ulm, D-89069 Ulm

Au nano-particles were prepared on an epitaxial $Al_2O_3/Nb(110)/Sapphire$ layered system employing a micellar technique. This type of arrangement was analyzed by STM and STS at room temperature in ultra-high vacuum. For the as-prepared Au nanoparticles, STM shows an inhomogeneous surface of the particles while STS reveals Coulomb charging for about 60-70% of the particles if the tip is positioned at their apex. However, quantitatively the Coulomb gap is unexpectedly large and it depends sensitively on the tip position above the particle. By annealing the samples at temperatures up to 800°C, the surface of the particles becomes more homogeneous and is partly faceting, the Coulomb gap decreases, and its value becomes less sensitive to the tip position. The data then can be analyzed in terms of orthodox Coulomb blockade theory.

O 48.5 Fri 12:15 WIL A317

SERS substrates produced by tailor-made metal nanoparticles using laser irradiation — ●BLÁZQUEZ SÁNCHEZ D.¹, GALLASCH L.², SCHMIDT H.², KRONFELDT H.D.², HUBENTHAL F.¹, and TRÄGER F.¹ — ¹Institut für Physik and Center for Interdisciplinary Nanostructure Science and Technology-CINSA-T, Universität Kassel, Heinrich-Plett-Str. 40, 34132 Kassel, Germany — ²Institute of Optics, Technical University Berlin, Hardenbergstrasse 36, 10623 Berlin, Germany

New tailor-made SERS substrates are presented which are based on precise control of the shape of nanoparticles (NPs) prepared by self-assembly of atoms on dielectric substrates. By applying nanosecond light pulses of appropriate fluence and wavelength oblate Ag or Au particles with a fixed shape have been fabricated. The method relies on the pronounced shape dependence of the absorption coefficient of metal NPs dominated by the excitation of surface plasmon polaritons. These resonances lead to a field enhancement in the vicinity of the particle surface, an effect widely exploited in surface enhanced Raman spectroscopy. With our manufacturing method, SERS substrates with tunable plasmon resonances can be simply produced for specific excitation wavelengths and detection ranges. Ag substrates were prepared here with and without a protective coating having a plasmon resonance at about 2.4 eV. SERS spectra of pyrene were obtained with excitation at 514 nm for all substrates indicating a good reproducibility. The substrates did not show degradation during the measurements and those with protective coatings yielded still 60 % of the SERS intensity of uncoated substrates indicating their potential usefulness for the analytical detection of specific molecules.

O 48.6 Fri 12:30 WIL A317

Near- and Farfield Scattering Properties of Metal Nanoparticles Excited by Radially Polarized Light — ●PHILLIP OLK¹, T. HÄRTLING¹, J. RENGER¹, S. GRAFSTRÖM¹, L. M. ENG¹, B. GORZOLNIK², M. OTT², and M. MÖLLER² — ¹Institut für Angewandte Photo-physik, TU Dresden, 01062 Dresden — ²Deutsches Wollforschungsinstitut an der RWTH Aachen e.V., 52056 Aachen

We report on the optical investigation of gold nanoparticles (NPs) having a diameter between 8 and 100 nm. Single, optically isolated NPs as well as NPs in an ordered, quasi regular lattice obtained by a micellar technique [1] have been analyzed. Besides conventional linearly polarized illumination at several distinct wavelengths in the visible regime, we also consider radial polarization modes [2]. The latter polarization, if focused by a lens, causes the focal electric field vector to be perpendicular to the substrate surface. This allows us inducing an effective electrical dipole momentum \vec{p} in NPs which is parallel to the optical propagation direction \vec{k} . Field calculations by means of multiple multipole method [3] and intensity measurements using dielectric tips in our scanning near-field optical microscope (SNOM) are compared with respect to the fractional content of scattered light contributing to the signal detected by the optical near field probe. The aftermath for SNOM imaging of nanoscopic metal structures on transparent substrates is discussed.

[1] J. P. Spatz *et al.*, *Langmuir* **16**, 407 (2000).

[2] A. A. N. Mark *et al.*, *Opt.Lett.* **7**, 1929 (2002).

[3] Ch. Hafner, *The Generalized Multipole Technique for Computational Electromagnetics*; Artech House Books, Boston (1990).

O 48.7 Fri 12:45 WIL A317

Optical Properties of Gold Nanoparticles close to a Gold Surface — ●ADRIANA RUEDA, MARCO STEMMLER, NOELIA BOCCHIO, and MAX KREITER — Max-Planck Institute for Polymer Research, Ackermannweg 10, 55128 Mainz, Germany

Studies of the optical properties of spherical gold nanoparticles placed close to a gold flat surface will be discussed. According to electromagnetic theories [1] particles with localized electromagnetic resonances like gold nanoparticles can interact with a metal surface producing a special kind of resonance (called the gap mode) generating large enhancements of the near field in the gap between the particle and the surface. This effect was studied in some detail experimentally in an inorganic system by Okamoto *et al.* [2]. As a well-defined model system we use gold nanoparticles with diameters in the range of 20-250 nm linked to a thin gold film deposited onto a glass substrate by means of an organic self-assembled monolayer of linker molecules, allowing for a selective positioning of functionalities as fluorophores in the gap. The resulting multilayered system was studied with multiwavelength surface plasmon resonance measurements which are highly sensitive to effects taking place at the surface. If the gold nanoparticles are regarded as an effective layer [3], these measurements allow for the detection of resonances in the polarisability due to gap excitation.

[1] P.K. Aravind and H. Metiu, *Surface Science* **124**, 506 (1983)

[2] T. Okamoto and I. Yamaguchi, *J.Phys.Chem.* **107** (38), 10321 (2003)

[3] M.A.Plunkett *et al.*, *Langmuir* **19**, 6837 (2003)

O 49 Electronic structure IV

Time: Friday 11:15–13:00

Room: WIL B321

O 49.1 Fri 11:15 WIL B321

Self-energy and many-body effects in graphite — ●S. BENGIÒ¹, T. K. KIM¹, PH. HOFMANN¹, A. LEONARDO², and E. V. CHULKOV² — ¹Institute for Storage Ring Facilities and iNano Center, University of Aarhus, 8000 Aarhus C, Denmark — ²Donostia International Physics Center (DIPC), 20018 San Sebastián / Donostia, Basque Country, Spain

Graphite is a semimetal, a prototype of layered crystals and the parent compound for carbon nanotubes. Despite of its great importance, detailed studies of many body effects by angle-resolved photoemission (ARPES) are rare, mostly caused by the lack of high-quality samples. Here we present an ARPES study on high-quality graphite films grown on a SiC substrate. The temperature dependence of the self energy was determined by a systematic linewidth analysis for the Fermi surface states close to the \bar{K} point of the surface Brillouin zone. The Fermi surface crossing is sharp in momentum space (of the order of 0.07 \AA^{-1}) and its full width at half maximum is almost constant for temperatures between 70 and 600 K. The experimental results for the self-energy are compared to first principles calculations for one layer of graphene.

O 49.2 Fri 11:30 WIL B321

Fermi Surface of Be(0001) — ●IVANA VOBORNIK¹, JUN FUJII¹, MATTIA MULAZZI^{1,2}, GIANCARLO PANACCIONE¹, MICHAEL HOCHSTRASSER³, and GIORGIO ROSSI^{1,2} — ¹TASC National Laboratory, INFN-CNR, S.S. 14, km 163.5, I-34012 Trieste — ²Dipartimento di Fisica, Università di Modena e Reggio Emilia, Via Campi 213/A, I-41100 Modena — ³Laboratorium für Festkörperphysik, Wolfgang-Pauli-Str. 16, ETH Höggerberg, CH-8093 Zürich

We used angle-resolved photoemission (ARPES) to determine the Fermi surface of Be(0001). The Fermi surface cuts that were measured for more than twenty different photon energies enabled us to reconstruct the three-dimensional Fermi surface. We find that the Fermi surface obtained from the ARPES data differs significantly from the Fermi surface of bulk beryllium determined by de Haas - van Alphen oscillations. The so-called cigar features appear to be significantly shorter, while the cornet is enlarged. Furthermore, new states appear in the gap between the two subsequent cigars. This change of the Fermi surface topology is the consequence of the surface relaxation in Be(0001) and the ARPES surface sensitivity (mean free pass in the photon energy range used in our experiment is only 2-3 Å). Our data are relevant for any theory aiming to describe the considerable surface relaxation in Be(0001).

O 49.3 Fri 11:45 WIL B321

Surface electronic structure of Cr(001) — ●MICHAEL BUDKE¹, TOBIAS ALLMERS¹, MATTHIAS BODE², GEORGI RANGELOV¹, and MARKUS DONATH¹ — ¹Physikalisches Institut, Universität Münster, Wilhelm-Klemm-Str. 10, D-48159 Münster — ²Institute of Applied Physics and Microstructure Research Center, Jungiusstr. 11, D-20355 Hamburg

There is an ongoing controversy whether a sharp peak close to the Fermi level E_F which appears in scanning tunneling spectroscopy (STS) measurements on the Cr(001) surface is related to a d_{z^2} -like surface state [1] or to an orbital Kondo resonance [2]. A recent variable-temperature STS study was not able to bring about a decision which of the two interpretations is correct [3]. We have performed photoemission and inverse photoemission measurements on the Cr(001) surface to reveal the nature of the electronic states just below and above E_F . Surface- and bulk-like contributions are identified by their sensitivity to adsorbates. In agreement with previous STS data, we found a surface sensitive feature in our IPE measurements just above E_F . The results are discussed in terms of their compatibility to the surface state and Kondo resonance model.

[1] J. A. Stroscio *et al.*, Phys. Rev. Lett. **75**, 2960 (1995).[2] O. Y. Kolesnychenko *et al.*, Nature **415**, 507 (2002).[3] T. Hänke *et al.*, Phys. Rev. B **72**, 085453 (2005).

O 49.4 Fri 12:00 WIL B321

Electronic Structure of the (2×3) -N/Cu(110) Surface — ●PETER LENDECKE, TOBIAS ALLMERS, GEORGI RANGELOV, and MARKUS DONATH — Physikalisches Institut, Westfälische Wilhelms-Universität Münster, Wilhelm-Klemm-Str. 10, 48149 Münster

Sputtering a Cu(110) surface with nitrogen and subsequent annealing induces a (2×3) reconstruction. The copper atoms in the topmost layer are arranged in a nearly square array formed by additional $[1\bar{1}0]$ -rows. Nitrogen atoms are bonded in almost every second hollow site of this strongly corrugated pseudo-(100) layer [1].

We investigated the unoccupied electronic structure of this reconstructed surface by angle-resolved inverse photoemission. Preparation of the reconstruction was controlled by LEED and *in-situ* STM. Inverse photoemission spectra are dominated by Cu(110) bulk transitions. The reduced surface Brillouin zone along $[001]$ is reflected by surface *umklapp* processes. Unoccupied surface states of Cu(110) are already quenched at low nitrogen doses. The reappearance of a surface resonance along $[1\bar{1}0]$ in the high-dose regime is most probably due to improved long-range order of the surface.

[1] S. Moré *et al.*, Surf. Sci. **381**, L589 (1997)

O 49.5 Fri 12:15 WIL B321

Electronic structure of ZnO(11 $\bar{2}$ 0) single crystals and thin films — ●STEFAN ANDRES¹, CHRISTIAN PETTENKOFER¹, WOLFGANG BREMSTELLER¹, and LEONARD BROEKMAN² — ¹Hahn-Meitner-Institut, Glienicker Str. 100, D-14109 Berlin, Germany — ²Department of Physics, La Trobe University, VIC, 3086, Australia

Zinc oxide (ZnO) is a transparent semiconductor with a direct band gap of about 3.3eV. This makes ZnO an interesting candidate for future applications in transparent electronics and UV-light emission. In order to develop such devices a detailed understanding of the band structure of ZnO is necessary.

However, until now angle resolved photoemission spectroscopy (ARPES) studies on ZnO focussed only on the highly symmetric (0001), (000 $\bar{1}$) and (10 $\bar{1}$ 0) surfaces. We present comparative ARPES results from ZnO(11 $\bar{2}$ 0) single crystals and MOMBE grown thin films, recorded at the TGM7 beamline at BESSY II synchrotron light facility in Berlin. The spectra clearly show energy dispersions of the occupied valence states as a function of the wave vector both perpendicular and parallel to the surface. Our results are discussed along with band structure calculations.

O 49.6 Fri 12:30 WIL B321

Band structure of epitaxially grown CuInS₂ films — ●CARSTEN LEHMANN¹, RALF HUNGER², and CHRISTIAN PETTENKOFER¹ — ¹Hahn-Meitner Institut, SE6, Berlin, Germany — ²TU Darmstadt, Oberflächenforschung, Inst. f. Materialforschung

The ternary compound semiconductor CuInS₂ with a direct band gap of 1.53 eV seems to be very promising as absorber material for thin film solar cells. For a better understanding of the parameters determining the properties of a junction detailed information on the electronic structure is necessary. Besides a calculation of Zunger *et al* [1] no experimental data on the valence electronic structure of CuInS₂ are available.

We report on thin epitaxial CuInS₂ layers prepared on sulfur passivated GaAs (100). To have a better control on the deposition process we introduced a MOMBE type deposition with an organic sulfur precursor.

Clean and well defined surfaces were obtained despite a lattice mismatch of 2%. Samples were prepared in a dedicated UHV deposition and analysis system. Precharacterized samples were transferred by an UHV box within 15min to the TGM7 beamline at BESSY and investigated by ARUPS. We will discuss the obtained band structure with respect to available theoretical data and derive the effective mass from the valence band curvature. Implications of the observed reconstruction on the band structure will be discussed.

[1] E.J. Jaffe, A. Zunger, Phys. Rev. B **28**, 1983, 5822

O 49.7 Fri 12:45 WIL B321

Electronic bandstructure of the NiMnSb(001) surface below and above the Fermi energy — ●CHRISTIAN EIBL, JULIET SLAYTON CORREA, GEORGI RANGELOV, JÜRGEN BRAUN, and MARKUS DONATH — Physikalisches Institut, Westfälische Wilhelms-Universität Münster, 48149 Münster

For more than 20 years the Half-Heusler alloy NiMnSb has been investigated because of its predicted 100% spin polarization at the Fermi energy E_F [1]. Together with its high Curie temperature (750 K), this material is interesting for many technological applications.

We report on surface bandstructure measurements for the (001) surface of single crystal NiMnSb. The experimental techniques used are angle resolved ultraviolet photoemission spectroscopy (ARUPS) and inverse Photoemission spectroscopy (ARIPES) to probe the bandstructure both below and above E_F . ARUPS and ARIPES are used quasi-simultaneously in a multi-chamber UHV-system to ensure well defined and equal sample

preparation conditions.

We see both non-dispersive (ARIPES) and dispersive (ARUPS) structures in the spectra, which stem from d-like bulk states. Furthermore, by comparison with theoretical calculations, we have found a surface state candidate.

[1] R.A. deGroot et al., Phys. Rev. Lett. 50, 2024 (1983)

O 50 Time-resolved spectroscopy II

Time: Friday 11:15–13:00

Room: WIL C207

O 50.1 Fri 11:15 WIL C207

Time-resolved two-photon photoemission from the Si(557)Au surface — •TILMAN K. RÜGHEIMER¹, FRANZ J. HIMPSEL², and THOMAS FAUSTER¹ — ¹Lehrstuhl für Festkörperphysik, Institut für Physik der Kondensierten Materie, Universität Erlangen, Staudtstr. 7, D-91058 Erlangen — ²Department of Physics, University of Wisconsin-Madison, 1150 University Avenue, Madison, Wisconsin 53706, USA

Atomic chains of gold on silicon surfaces have attracted interest as model systems for one-dimensional conductors. For the Si(557)Au surface electronic states at the gold chains and the step edges are predicted by density functional theory [1]. Angle resolved photoemission [2] and scanning tunneling spectroscopy [3] assign the conduction to the gold chains and the step edges, respectively.

We have carried out two-photon photoemission experiments to clarify the electronic structure of the Si(557)Au surface. Pinning of the Fermi level and two strongly dispersing initial states below the Fermi energy have been found. A conduction band feature shows a complex population dynamics in time-resolved measurements. Finally, our results are compared to recent ab initio calculations [1].

[1] D. Sanchez-Portal et al., Phys. Rev. Lett. 93 (2004) 146803

[2] J. N. Crain et al., Phys. Rev. B 69 (2004) 125401

[3] H. W. Yeom et al., Phys. Rev. B 72 (2005) 035323

O 50.2 Fri 11:30 WIL C207

Electronic Structure of Si(100) at high excitation density: A Time-Resolved Photoemission Study with Combined Laser and Synchrotron Radiation. — •H. PRIMA GARCIA¹, T. GIESSEL¹, R. SCHMIDT¹, R. WEBER¹, W. WIDDRA², and M. WEINELT^{1,3} — ¹Max-Born-Institute, Berlin, Germany. — ²Martin Luther University, Halle, Germany. — ³Freie universität, Berlin, Germany.

We have studied the dynamics of laser-induced plasma-driven processes at the Si(100) surface. At the BESSY low- α hybrid mode we established an overall time-resolution of 10 ps. For 800 nm, 60 fs laser pulses induces an e-h plasma density of 10^{21} cm^{-3} and concomitant band gap narrowing in the bulk. Band gap renormalization occurs in 50 picoseconds and is distinguishable from photovoltage dynamics.

We observe in addition depopulation of the D_{up} surface state by more than 40%, which suggests a sizeable change of the surface electronic structure and a corresponding reduction of the dimer buckling. A recent time-dependent DFT study predicts this to occur on a subpicosecond time-scale [1].

Si 2p core level spectra show a transient increase of the linewidth, with the surface component broadening stronger than the bulk component. This is interpreted in terms of screening induced defect formation due to the high and long-lived transient carrier density at the surface upon IR laser excitation.

[1] Jan van Heys, Michael Lindenblatt, and Eckhard Pehlke, Phase transitions.in.press.00.May.2005)

O 50.3 Fri 11:45 WIL C207

Local Plasmon Excitations in Silver Nanodots: Spatio-temporal evolution and coupling dynamics probed by interferometric time-resolved PEEM — •JÖRG LANGE, CARSTEN WIEMANN, DANIELA BAYER, OKSANA GAIER, MARTIN ROHMER, CHRISTIAN SCHNEIDER, MICHAEL BAUER, and MARTIN AESCHLIMANN — University of Kaiserslautern, Department of Physics, Kaiserslautern, Germany

We have studied the temporal and spatial evolution of collective electronic excitations (Mie-plasmons) in silver nanostructures using phase resolved interferometric two-photon photoemission electron microscopy (PR-2PPEEM). The interference of a reference He:Ne laser beam was used to achieve a temporal resolution in the attosecond regime of the piezo driven scanning interferometer, which we used for the two-photon

photoemission pump-probe experiment. At the same time, the 2PPE-yield collected by the photoemission electron microscope allows a lateral resolution better than 40 nm. We demonstrate that this setup enables to monitor the temporal response of collective electronic excitations (Mie-plasmons) to an excited femtosecond laser pulse in silver nanodots. Regarding the plasmon induced inhomogeneous spatial distribution of the 2PPE-yield from single nanodots we observe a complex dependence on the temporal phase between the pump and the probe pulse. Furthermore, we were able to resolve spatio-temporal variations in the 2PPE-signal from pairs of close-lying nanodots, thus enabling insight into the dynamics of coupled plasmon excitations.

O 50.4 Fri 12:00 WIL C207

Ultrafast dynamics on the Gd(001) surface studied with time-resolved photoelectron spectroscopy — •PANAGIOTIS LOUKAKOS, MARTIN LISOWSKI, UWE BOVENSIEPEN, and MARTIN WOLF — Fachbereich Physik, Freie Universität Berlin

The Gd(001) surface is an interesting system to study the recently discovered coherent phonon-magnon mode as observed with magneto-optical experiments.¹ We use time-resolved photoelectron (TRPE) spectroscopy to analyze directly the dynamical evolution of the electron distribution, after excitation with 1.5 eV, 50 fs laser pulses. The dynamics of the excited system is probed by photoemission with a 6 eV, 80 fs laser pulse. Under normal emission we observe at T=30 K an exchange-split $5d_{z^2}$ surface state (SS) whose majority component lies 200 meV below the Fermi level. We present the ultrafast dynamics of the occupied SS and distinguish two different fluence and time regimes. At early times where the electron population is far from equilibrium and for low absorbed fluences ($<0.1 \text{ mJ/cm}^2$) the SS shifts away from the vacuum level. At later time delays, as the electron system thermalizes, the SS shifts towards the vacuum level with dynamics governed by electron-lattice energy transfer. At higher fluences ($\sim 1 \text{ mJ/cm}^2$) the SS shifts at all times towards the vacuum level. Also, an oscillatory behavior of the occupied SS with a period of 300 fs and an amplitude of only 1 meV is well resolved and observed for the first time in PE spectroscopy. This oscillation period is in excellent agreement with the one observed in optical experiments thereby corroborating the mechanism suggested in Ref. 1.

¹. Melnikov et al. Phys. Rev. Lett. 91, 227403 (2003)

O 50.5 Fri 12:15 WIL C207

Transition of Ar/Cu image-potential states from short-lived scattering resonances to long-lived quasi-bound interface states — •M. ROHLEDER, W. BERTHOLD, J. GÜDDE, and U. HÖFER — Fachbereich Physik, Philipps-Universität, D-35032

In the presence of thick Ar overlayers the image potential of Cu(100) gives rise to interface electronic states above the vacuum level. In previous experiments [1,2] we have shown that fundamental aspects of the dynamics of electronic decay at buried solid-solid interfaces and fast electron transfer processes through thin insulators can be investigated for this system by means of time-resolved two-photon photoemission (2PPE). Here, we demonstrate that these interface states may also be observed as final-state resonances in conventional one-photon photoemission (1PPE). Spectroscopically, this has advantages in terms of a higher accessible energy range above the vacuum level. With increasing layer thickness the hydrogen-like series shows a transition from broad resonances in the Ar conduction band into more narrow quasi-bound states confined to the Ar/Cu interface. We compare the experimental results with theoretical resonance positions and linewidths derived from a parametrized one-dimensional potential. For electrons with small momenta perpendicular to the surface we find excellent agreement between calculated and measured energies. The calculated widths of the lowest lying resonances agree well with the electron transfers times measured by 2PPE whereas the 1PPE spectra are apparently broadened by other contributions.

- [1] M. Rohleder *et al.*, Phys. Rev. Lett. **94**, 017401 (2005).
[2] M. Rohleder *et al.*, New. J. Phys. **7**, 103 (2005).

O 50.6 Fri 12:30 WIL C207

Ultrafast decay dynamics of a photoexcited adsorbate in interaction with a two-dimensional metallic substrate — •M. BAUER¹, M. WESSENDORF¹, S. MATTHIAS¹, J. LANGE¹, M. AESCHLI-MANN¹, V.M. SILKIN², A.G. BORISOV³, P.M. ECHENIQUE^{2,4}, J.P. GAUYACQ³, and E.V. CHULKOV^{2,4} — ¹Department of Physics, University of Kaiserslautern, 67663 Kaiserslautern — ²Donostia International Physics Center, San Sebastián, 20018, Spain — ³Laboratoire des Collisions Atomiques et Moléculaires, Université Paris-Sud, 91405 Orsay Cedex, France — ⁴Departamento de Física de Materiales and Centro Mixto, Facultad de Química, San Sebastián, Spain

The lifetime of adsorbate resonances is known to play a key role in the course of many photoinduced surface reactions. Control of the resonance lifetime would, therefore, be a means of manipulating surface chemical processes. In this paper we report on the tuning of a resonance lifetime by interaction of an adsorbate with epitaxially grown thin metal films at varying thickness. For the model system Cs/Ag/Cu(111) we observe that the lifetime of the cesium 6s resonance depends critically on silver film thickness and varies by a factor of three in the thickness regime between 1 and 7 ML. Our results are in qualitative good agreement with theoretical predictions. Quantitative discrepancies are related to structural (stress induced) modifications of the silver film and the copper substrate. Our result is a striking example for a fundamental property of adsorbate-surface interaction relevant for surface chemical processes modified by the dimensionality of the substrate.

O 50.7 Fri 12:45 WIL C207

Mapping the electron correlation at surfaces by two-electron photoemission — •FRANK O. SCHUMANN, CARSTEN WINKLER, GWILHERM KERHERVE, and JÜRGEN KIRSCHNER — Max-Planck-Institut für Mikrostrukturphysik, Weinberg 2, 06120 Halle

Established theoretical concepts show that the Coulomb and exchange interaction result in a tendency of two electrons to avoid each other leading to an exchange-correlation (xc) hole. We will report on double photoemission (DPE) experiments using a novel time-of-flight set-up consisting of a small central collector surrounded by a resistive anode. The first allows detection only within a narrow solid angle therefore fixing the momentum. The resistive anode covers a solid angle of ~ 1 sr, the determination of the impact position results in momentum resolution. As pulsed light source we used synchrotron radiation and studied a NaCl(100) surface upon excitation with 34 eV photons. The very existence of coincidences is already a manifestation of the correlation. The onset of pair emission occurs, when energy conservation allows the ejection of two electrons from the highest occupied level. We have made two key observations. If E_1 and E_2 are fixed such that pair emission from the top of the valence band is possible, a zone of reduced intensity with a diameter of $\sim 1.1 \text{ \AA}^{-1}$ is visible. Recent calculations on DPE from a Cu(100) surface display exactly such a feature due to the xc-hole. Hence we proof experimentally the very existence of the xc-hole in double photoemission. The zone of reduced intensity disappears, whenever emission below the top of the valence band becomes possible indicating the sensitivity of the xc-hole to inelastic scattering.