Section Surface Physics
Fachverband Oberflächenphysik (O)

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Overview of Invited Talks and Sessions

(lecture rooms H36, H38, H39, H41, and H42; Poster C)

Invited Talks

O 2.1	Mon	9:30–10:15	H36	**Broken symmetry states at surfaces: the ARPES view** — •Marco Grioni
O 3.1	Mon	10:15–11:00	H36	**Some aspects of chirality in molecules adsorbed at metal surfaces** — •Neville Richardson
O 20.1	Tue	9:30–10:15	H36	**Spin-Coupling in Engineered Atomic Structures** — •Cyrus Hirjibehedin, Christopher Lutz, Andreas Heinrich
O 21.1	Tue	10:15–11:00	H36	**Recent advances in simulating high-resolution scanning tunnelling microscopy and spectroscopy** — •Werner Hofer
O 29.1	Tue	14:45–15:30	H36	**Many-body interactions in clean and alkali-adsorbed graphene** — •E. Rotenberg, A. Bostwick, T. Ohta, J. McChesney, Th. Seyller, K. Horn
O 37.1	Wed	14:00–14:45	H36	**Gallium-Nitride-on-Silicon: Mission possible!** — •Armin Dadgar
O 38.1	Wed	14:45–15:30	H36	**Fluctuations of nanoscale structures** — •Ellen Williams, Chenggang Tao, William Cullen, Timothy Stasevich, Theodore Einstein, Alexander Bondarchuk, Timothy Bole, Philip Rous
O 47.1	Thu	9:30–10:15	H36	**Complex magnetic structures on the atomic scale revealed by spin-polarized STM** — •Kirsten von Bergmann
O 48.1	Thu	10:15–11:00	H36	**Semiconductor nanostructures: From self-assembly to self-ordering** — •Thomas Schmidt
O 54.1	Thu	14:00–14:45	H36	**Interplay between dimensionality and “exotic” properties: Model systems on surfaces** — •Alexander Menzel, Enrico Dona, Mariana Minca, Erminald Bertel
O 55.1	Thu	14:45–15:30	H36	**Real-time observation of organic layer growth: a spectro-microscopic study** — •Thomas Schmidt, Helder Marchetto, Ullrich Groh, Florian Maier, Pierre Lévesque, Rainer Fink, Hans-Joachim Freund, Eberhard Umbach

Sessions

O 1	Mon	8:30– 9:15	H1	**Plenary Talk Steven G. Louie: Understanding Nanostructures: Nanotubes, Nanowires, and Graphene Nanoribbons**
O 2	Mon	9:30–10:15	H36	**Invited Talk Marco Grioni: Broken Symmetry States at Surfaces: The ARPES View**
O 3	Mon	10:15–11:00	H36	**Invited Talk Neville R. Richardson (FV: DS+O): Some Aspects of Chirality in Molecules Adsorbed at Metal Surfaces**
O 4	Mon	9:30–13:00	H1	**Symposium: Spins in Semiconductors (FV: HL+MA+O+TT)**
O 5.1–5.6	Mon	11:15–12:45	H36	**Nanostructures at Surfaces I (Wires, Tubes)**
O 6.1–6.3	Mon	11:15–12:45	H38	**Symposium: Ultrafast Nanooptics I**
O 7.1–7.6	Mon	11:15–12:45	H39	**Metal Substrates: Adsorption I**
O 8.1–8.6	Mon	11:15–12:45	H41	**Methods: Scanning Probe Techniques I**
O 9.1–9.6	Mon	11:15–12:45	H42	**Oxides and Insulators: Adsorption I**
O 10	Mon	13:00–13:30	H1	**Special Talk Jorge E. Hirsch: The h-index: how useful is it as a measure of scientific achievement?**

O 11	Mon	13:30–14:00	H1	**Special Talk Philip Ball: Is it any good? Measuring scientific merit**
O 12.1–12.13	Mon	14:15–17:30	H36	**Nanostructures at Surfaces II (Wires, Tubes)**
O 13.1–13.10	Mon	14:15–18:00	H38	**Symposium: Ultrafast Nanooptics II**
O 14.1–14.14	Mon	14:15–17:45	H39	**Metal Substrates: Epitaxy and Growth**
O 15.1–15.14	Mon	14:15–17:45	H41	**Methods: Scanning Probe Techniques II**
O 16.1–16.13	Mon	14:15–17:30	H42	**Organic, Polymeric, and Biomolecular Films I**
O 17.1–17.87	Mon	17:30–20:30	Poster C	**Poster Session I (Nanostructures at Surfaces; Metal Substrates: Epitaxy and Growth; Methods: Scanning Probe Techniques; Phase Transitions)**
O 18	Mon	18:00–18:45	H1	**Plenary Talk Martin Pätzold: Venus Express**
O 19	Tue	8:30– 9:15	H1	**Plenary Talk Peter Lemke: Climate Change 2007: The Physical Science Basis**
O 20	Tue	9:30–10:15	H36	**Invited Talk Cyrus Hirjibehedin (FV: MA+O): Spin-Coupling in Engineered Atomic Structures**
O 21	Tue	10:15–11:00	H36	**Invited Talk Werner Hofer: Recent Advances in Simulating High-Resolution Scanning Tunnelling Microscopy and Spectroscopy**
O 22.1–22.4	Tue	11:15–12:15	H36	**Surface or Interface Magnetism**
O 23.1–23.6	Tue	11:15–12:45	H38	**Symposium: Ultrafast Nanooptics III**
O 24.1–24.6	Tue	11:15–12:45	H39	**Semiconductor Substrates: Epitaxy and Growth**
O 25.1–25.6	Tue	11:15–12:45	H41	**Phase Transitions**
O 26.1–26.4	Tue	11:15–12:15	H42	**Organic, Polymeric, and Biomolecular Films II**
O 27	Tue	13:00–13:45	H1	**Prize Talk Joel L. Lebowitz (Max Planck Medal): From Microscopic Dynamics to Macroscopic Behavior**
O 28	Tue	14:00–14:30	H10	**Invited Talk Patrick Bruno (FV: MA+O): Controlling Magnetism and Self-Organization of Adatoms on Surfaces by Using Quantum Interferences**
O 29	Tue	14:45–15:30	H36	**Invited Talk Eli Rotenberg: Many-Body Interactions in Clean and Alkali-Adsorbed Graphene**
O 30.1–30.8	Tue	15:45–17:45	H36	**Nanostructures at Surfaces III (Dots, Particles, Clusters)**
O 31.1–31.8	Tue	15:45–17:45	H38	**Surface Chemical Reactions and Heterogeneous Catalysis I**
O 32.1–32.7	Tue	15:45–17:30	H39	**Semiconductor Substrates**
O 33.1–33.8	Tue	15:45–17:45	H41	**Oxides and Insulators: Epitaxy and Growth**
O 34.1–34.8	Tue	15:45–17:45	H42	**Methods: Atomic and Electronic Structure I**
O 35	Wed	8:30– 9:15	H1	**Plenary Talk Atac Imamoglu: Quantum Dot Spin Manipulation**
O 36	Wed	9:15–10:00	H1	**Plenary Talk Hartmut Zabel: Magnetic Nanostructures in the Lateral and Perpendicular Direction**
O 37	Wed	14:00–14:45	H36	**Prize Talk Armin Dadgar (Gaede Prize): Gallium-Nitride-on-Silicon: Mission possible!**
O 38	Wed	14:45–15:30	H36	**Invited Talk Ellen D. Williams: Fluctuations of Nanoscale Structures**
O 39.1–39.8	Wed	15:45–17:45	H36	**Nanostructures at Surfaces IV (Dots, Particles, Clusters, Arrays)**
O 40.1–40.6	Wed	15:45–17:15	H38	**Particles and Clusters I**
O 41.1–41.7	Wed	15:45–17:30	H39	**Metal Substrates: Adsorption II**
O 42.1–42.3	Wed	15:45–16:30	H41	**Methods: Scanning Probe Techniques III**
O 43.1–43.4	Wed	15:45–16:45	H42	**Oxides and Insulators: Adsorption II**
O 44.1–44.81	Wed	17:00–19:30	Poster C	**Poster Session II (Semiconductors; Oxides and Insulators: Adsorption, Clean Surfaces, Epitaxy and Growth; Surface Chemical Reactions and Heterogeneous Catalysis; Surface or Interface Magnetism; Solid-Liquid Interfaces; Organic, Polymeric, Biomolecular Films; Particles and Clusters; Methods: Atomic and Electronic Structure; Time-resolved Spectroscopies)**
O 45	Wed	20:00–21:00	H1	**Evening Talk Eduard Arzt: Adhesion to Micro and Nano Structures: On Geckos, Minimushrooms and Smart Surfaces**

O 46	Thu	8:30– 9:15	H1	**Prize Talk Jonathan J. Finley (Walter Schottky Prize): Optically Probing Charge and Spin Interactions in Semiconductor Quantum Dots and Molecules**
O 47	Thu	9:30–10:15	H36	**Invited Talk Kirsten von Bergmann: Complex Magnetic Structures on the Atomic Scale Revealed by Spinpolarized STM**
O 48	Thu	10:15–11:00	H36	**Invited Talk Thomas Schmidt: Semiconductor Nanostructures: From Self-Assembly to Self-Ordering**
O 49.1–49.3	Thu	11:15–12:00	H36	**Nanostructures at Surfaces V (Self Organization of Molecules)**
O 50.1–50.6	Thu	11:15–12:45	H38	**Particles and Clusters II**
O 51.1–51.6	Thu	11:15–12:45	H39	**Metal Substrates: Adsorption III**
O 52.1–52.6	Thu	11:15–12:45	H42	**Methods: Atomic and Electronic Structure II**
O 53	Thu	13:00–13:45	H1	**Prize Talk Peter Grünberg (Stern Gerlach Medal): Spin Transfer Phenomena in Layered Magnetic Structures**
O 54	Thu	14:00–14:45	H36	**Invited Talk Alexander Menzel: Interplay between Dimensionality and “Exotic” Properties: Model Systems on Surfaces**
O 55	Thu	14:45–15:30	H36	**Invited Talk Thomas Schmidt: Real-Time Observation of Organic Layer Growth: A Spectro-Microscopic Study**
O 56.1–56.7	Thu	15:45–19:00	H36	**Symposium: The Solid-Liquid Interface: A Challenge for Theoreticians I**
O 57.1–57.11	Thu	15:45–18:30	H38	**Surface Chemical Reactions and Heterogeneous Catalysis II**
O 58.1–58.10	Thu	15:45–18:15	H39	**Metal Substrates: Adsorption IV**
O 59.1–59.12	Thu	15:45–18:45	H41	**Oxides and Insulators: Clean Surfaces**
O 60.1–60.11	Thu	15:45–18:30	H42	**Time-Resolved Spectroscopies**
O 61	Thu	19:30–20:00	H36	**General Meeting of the Surface Science Division**
O 62	Thu	20:00–21:00	H36	**Post Deadline Session**
O 63	Thu	21:00–24:00	H36 hallway	**Surface Science Symposion**
O 64	Fri	8:30– 9:15	H1	**Plenary Talk Jean-François Joanny: Active gels: toward a generic approach of cell mechanics**
O 65	Fri	9:15–10:00	H1	**Plenary Talk Jens K. Nørskov: Catalysis from First Principles**
O 66.1–66.7	Fri	10:15–12:00	H36	**Nanostructures at Surfaces VI (Surface Reconstructions)**
O 67.1–67.9	Fri	10:15–13:00	H38	**Symposium: The Solid-Liquid Interface: A Challenge for Theoreticians II**
O 68.1–68.6	Fri	10:15–11:45	H39	**Metal Substrates: Adsorption V**
O 69.1–69.6	Fri	10:15–11:45	H41	**Metal Substrates: Clean Surfaces**
O 70.1–70.7	Fri	10:15–12:00	H42	**Methods: Atomic and Electronic Structure III**

Annual General Meeting of the Section Surface Physics

Thursday 7:30 p.m. H36

- Report of the Chairman of the DPG section Surface Physics
- Miscellaneous

NOTES:

Poster Session O17 on Monday (5:30-8:30 p.m.) in Area C close to the lecture rooms H43-H45
Posters can be attached from Monday 8:30 a.m. and must be removed by Tuesday 5:00 p.m.

Poster Session O44 on Wednesday (5:00-7:30 p.m.) in Area C close to the lecture rooms H43-H45
Posters can be attached from Wednesday 8:00 a.m. and must be removed by Wednesday 9:30 p.m.

Post Deadline Session O63 on Thursday (8:00-9:00 p.m.) in H36, and (9:00 p.m.-12:00 a.m.) in the hallway in front of H36
Deadline for submission of abstracts is February 16, 2007; Notification on acceptance will be on March 3, 2007. The session will be sponsored by SPECS GmbH together with Bestec GmbH, Createc Fischer GmbH, and Surface Concept.

O 1: Plenary Talk Louie

Time: Monday 8:30–9:15 Location: H1

Understanding Nanostructures: Nanotubes, Nanowires, and Graphene Nanoribbons

O 2: Invited Talk Grioni

Time: Monday 9:30–10:15 Location: H36

Invited Talk O 2.1 Mon 9:30 H36

Broken symmetry states at surfaces: the ARPES view — •Marco Grioni — IPN-EPFL, Lausanne, Switzerland

The surface of a solid may exhibit electronic phases that break a symmetry present in the material's bulk. Photoelectron spectroscopy (ARPES) with high energy and momentum resolution can probe the properties of such electronic states with a rather unique sensitivity and selectivity. Here I will briefly discuss two such examples. Peculiar surface structures result from qualitatively different mechanisms: enhanced surface correlations in the former, and the genuine breaking of an underlying symmetry in the latter.

In the layered materials $1T$-$TaSe_2$ the interplay of temperature-dependent charge-density-waves (CDW) and electronic correlations yields a bandwidth-controlled metal-insulator surface transition on top of a metallic bulk. ARPES reveals the breakdown of the Fermi surface and the disappearance of the coherent quasiparticle weight.

In the epitaxial $PbAg_2$ alloy formed at the Ag(111) surface, the breaking of inversion symmetry in the presence of spin-orbit interaction lifts the Kramers' spin degeneracy, and states of opposite spin are separated in momentum. The giant splitting ($\Delta k = \pm\ 0.13\ \AA$) observed by ARPES cannot be explained by a standard free-electron (Rashba-Byckhov) model, and points to the crucial role played by the formation of the chemical bonds.

O 3: Invited Talk Richardson (FV: DS+O)

Time: Monday 10:15–11:00 Location: H36

Invited Talk O 3.1 Mon 10:15 H36

Some aspects of chirality in molecules adsorbed at metal surfaces — •Neville Richardson — School of Chemistry, North Haugh, Univeristy of St Andrews, St Andrews, KY16 9ST, UK

It is suprisingly common for achiral molecules, even those with a high degree of symmetry as isolated species to give rise to chiral adsorbates, chiral molecular clusters and chiral two dimensional arrays. The drivers for such behaviour arise from the subtle balances between adsorbate-adsorbate interactions and adsorbate-substrate interactions. Important contributors to the former may be relatively isotropic Van der Waals' interactions or more directional interactions such as H-bonding, while the latter depends on the extent to which there is a preferred adsorption site and substrate induced orientation of the adsorbate. Because of the delicate balance of the varying terms in these interactions relatively small changes in coverage, temperature or the nature of either adsorbate or substrate can induce, modify or remove the chirality of the system. It remains a challenge to the community of those working on the theory of larger molecular adsorbates to predict the outcome of the two dimensional assembly of chiral systems.

Scanning tunneling microscopy supported by spectroscopic methods and low energy electron diffraction is ideally suited to monitoring and characterising this behaviour in adsorbed systems. In this presentation, several examples of organic molecules on metal surfaces, both from our own work and that of others, will be described to illustrate these phenomena.

O 4: Symposium: Spins in Semiconductors (FV: HL+MA+O+TT)

Time: Monday 9:30–13:00 Location: H1

Invited talks and contributions

O 5: Nanostructures at Surfaces I (Wires, Tubes)

Time: Monday 11:15–12:45 Location: H36

O 5.1 Mon 11:15 H36

TiO_2 nanotubes, formation and properties — •Ghicov Andrei, Schmuki Patrik, Macak Jan, and Kunze Julia — WW4- LKO, University of Erlangen-Nuremberg, Martensstr.7, D-91058 Erlange

Electrochemically grown TiO_2 nanotubes represent a combination between a structure with a high effective surface area with numerous functional properties. The material has an adjustable crystalline structure (amorphous /anatase /rutile) which makes the ordered nanotube layers a candidate for even wider applications in different fields. The presentation will show how TiO_2 nanotubes can be grown on titanium substrates and how their geometry can be adjusted in desired ways by anodization parameters. The surface structure and - area are a key factors for wetting [1], biomedical [2], catalytic [3] and electronic [4] applications - some specific examples will be discussed.

References:

[1]. E. Balaur, J. M. Macak, L. Taveira, P. Schmuki, Electrochem. Commun, 7 (2005) 1066

[2]. H. Tsuchiya, M. Macak Jan, L. Muller, J. Kunze, F. Muller, P. Greil, S. Virtanen, P. Schmuki, J. Biomed. Mater. Res., Part A 77 (2006) 534

[3]. J. M. Macak, H. Tsuchiya, A. Ghicov, P. Schmuki, Electrochem. Commun, 7 (2005) 1133

[4]. R. Beranek, H. Tsuchiya, T. Sugishima, J. M. Macak, L. Taveira, S. Fujimoto, H. Kisch, P. Schmuki, Appl. Phys. Lett., 87 (2005) 243114

O 5.2 Mon 11:30 H36

Atomic-force microscopy investigations of semiconductor nanorods — Y. Hou[1], •C. Teichert[1], G. Brauer[2], A. Djurisic[3], V. Sivakov[4], R. Scholz[4], G. Andrä[5], and S. H. Christiansen[6] — [1]Institute of Physics, University of Leoben, Austria — [2]Institut f. Ionenstrahlphysik und Materialforschung, Forschungszentrum Rossendorf, Germany — [3]Department of Physics, University of Hong Kong, PR China — [4]Max Planck Institute of Microstructure Physics, Halle, Germany — [5]Institute of Physical High Technology (IPHT), Jena, Germany — [6]Physics Department, Martin-Luther-University Halle-Wittenberg, Germany

One-dimensional nanostructures, such as nanorods or nanotubes, exhibit technological potential for many device applications like electronic, photonic or sensing devices. However, achieving control on the growth of such nanostructures leading to proper dimensional confinement (nanorods diameter, length, density and orientation) is still a challenging task. So far, scanning electron microscopy and transmission electron microscopy are the methods of choice to characterize arrays of free standing semiconductor nanowires. Atomic force microscopy - at a first glance - might not be suited for such a task. Analyzing arrays of vertical ZnO nanorods grown on Si and ITO substrates and individual Si nanowhiskers grown by electron beam evaporation on Si(111), we demonstrate the capabilities of atomic-force microscopy to yield integral information for example on the height variation of the nanorod arrays as well as detailed information on the facet structure of the nanowhiskers.

O 5.3 Mon 11:45 H36

Topography and valencebandstructure of dysprosium-silicide on Si(557) — •Karolin Löser, Martina Wanke, Gerd Pruskil, and Mario Dähne — Institut für Festkörperphysik, Technische Universität Berlin, D-10623 Berlin

Rare Earth silicide structures on silicon are of special interest because of their extremely low Schottky barrier on Si(111) and the formation of nanowires on Si(001). Here we report on the self-assembled formation of dysprosium-silicide nanostructures on Si(557), which we investigated by high-resolution scanning tunneling microscopy and angle-resolved photoelectron spectroscopy. The formation of the different structures depends mainly on the dysprosium coverage less on the annealing temperature in the range of 600-750°C. Looking at the atomic structure we found three different types of nanostructures. Nanowires similar to those on Si(001) form for a coverage of 0.5 Å. At a coverage of 1,0 Å there is a 5×2-chain structure like that of Gd on vicinal Si(557). At higher coverages more than 3000 Å long and 50-100 Å wide structures form. These consist of $DySi_2$ with a 1×1 reconstruction for coverages around 2,0 Å, while they consist of $\sqrt{3} \times \sqrt{3}$ reconstructed $DySi_{1.7}$ for higher coverages. Both structures are known from the Si(111) surface. Our investigations by angle-resolved photoelectron spectroscopy verified these findings. The $DySi_2$ and $DySi_{1.7}$ structures are characterized by a two-dimensional electronic structure. In contrast, an anisotropic metallicity was found at low coverages for the nanowires and the 5×2-chain structure. This project was supported by DFG, project number DA 408/11.

O 5.4 Mon 12:00 H36

Plasmon dispersion in dysprosium silicide nanowires — •Eddy Patrick Rugeramigabo[1], Volkmar Zielasek[2], and Herbert Pfnür[1] — [1]Institut für Festkörperphysik, Leibniz-Universität Hannover — [2]Institut für Angewandte und Physikalische Chemie, Universität Bremen

By depositing Dy at around half monolayer coverage on single domain Si(001) surfaces miscut by 4° towards [110], we have grown $DySi_2$ nanowires in the submonolayer regime. Their plasmon spectrum has been studied by a combination of high resolution EELS and spot profile analysis of LEED in one instrument (ELS-LEED) which enables us to measure characteristic losses with high momentum resolution. Ultraclean conditions ($P \leq 1 \times 10^{-10}$ mbar during Dy deposition) allowed growth of high quality structures with minimal oxidation of Dy. Deposition of Dy at 500 °C results in the formation of single $DySi_2$ nanowires on each terrace, leaving the periodicity of the clean Si surface unchanged. In contrast, deposition at room temperature and subsequent annealing to 500°C reduces the average terrace width by up to 20%. Clearest results in EELS were obtained for a silicide layer with 0.4 ML of Dy deposited at 500°C. Broad loss features in the range between 0 and 1 eV with typical dipole characteristics were detected, their position being strongly dependent on momentum transfer. As expected these characteristic losses have no dispersion normal to the wires, while parallel to the wires the dispersion is non-linear and goes to zero at zero momentum transfer. Thus the typical behavior of one-dimensional surface plasmons is found.

O 5.5 Mon 12:15 H36

Two-dimensional Routing of Surface Plasmon Polaritons — •Liviu Chelaru and Frank Meyer zu Heringdorf — Universität Duisburg-Essen, Lotharstrasse 1, 47048 Duisburg

We investigated the excitation and propagation of Surface Plasmon Polaritons (SPPs) in single-crystalline Ag nanostructures of arbitrary shapes and sizes by photoelectron emission microscopy (PEEM). Here the photoelectrons are generated by femtosecond laser pulses through a nonlinear two-photon photoemission (2PPE) process. Under these conditions the SPP wave is visualized as a result of interference (beat pattern) between the primary laser pulse and the traveling SPP at the sample surface. We will show that the propagation length of the SPP wave depends on the size of the Ag nanostructures, and that it can extend for several micrometers along the surface. By comparing nanostructures of different geometry, we describe the guiding of the SPP wave, and the coupling of the light into and out of the nanostructures. Depending on the incidence angle of the propagating SPP wave on the nanostructure*s boundary, we observe either trapping of the SPP wave inside the metallic nanostructure or a photoemission yield enhancement in the vicinity of the nanostructure caused by the electric field of the SPP wave.

O 5.6 Mon 12:30 H36

In-situ preparation of contacts for metal nanostructures — •Svend Vagt, Tammo Block, Jan Rönspies, and Herbert Pfnür — Institut für Festkörperphysik, Leibniz Universität Hannover

For direct transport measurements on single ultrasmall structures leads are needed. We present different techniques for this purpose.

In a first attempt contact pads are prepared ex-situ via e-beam lithography and titanium evaporation, followed by annealing to about 1000K. This results in TiSi pads, that exhibit a good electrical conductance. However, to clean the Si areas between the pads, a flash temperature of 1400K is necessary, at which deep trenches are formed at the edges of the pad due to stress induced diffusion of Si into the TiSi pad. We present mulitilayer stacks of Ti and Si, that can be used to improve the situation.

Here we describe another method that completly avoids such step bunches by flashing the silicon prior to the evaporation of Ti. This whole process has to take place completely in UHV. A few microns thin tungsten wire acts as a simple "shadow mask"and is removed after metal deposition. This leads to ultrathin, but still well conducting TiSi pads, that are stable up to 1000K. The penumbra of the wire also forms a ramp-like shape at the border of the pad and avoids the formation of deeper trenches. Between such contact pads metallic nanostructures are prepared by electron-beam stimulated thermal desorption of oxygen (EBSTD) from a ultrathin SiO_2 layer on the remaining Si(111) area. Subsequent metal deposition and annealing leads to metallic structures in electric contact with the pads.

O 6: Symposium: Ultrafast Nanooptics I

Time: Monday 11:15–12:45 Location: H38

Invited Talk O 6.1 Mon 11:15 H38

A nanometer-sized femtosecond electron source — •Christoph Lienau[1,2], Claus Ropers[2], Daniel Solli[2], Claus Peter Schulz[2], and Thomas Elsaesser[2] — [1]Institut für Physik, Carl von Ossietzky Universität Oldenburg — [2]Max-Born-Institut, Berlin

Femtosecond electron and X-ray diffraction are currently among the most intriguing topics in ultrafast science, allowing for probing structural dynamics of molecular and solid state systems with previously unachievable temporal resolution. In electron diffraction, overcoming temporal smearing due to spatial propagation effects and to Coulomb repulsion of electron bunches produced at kHz repetition rates presents a considerable experimental challenge. Ultimately, therefore, a point-like source of single electrons with temporal resolution in the regime of few femtoseconds would be highly desirable.

In this paper, we describe and demonstrate a novel approach towards realizing such a point-like ultrafast electron source. By illuminating ultrasharp gold tips with 7-fs pulses from an 80 MHz Ti:sapphire oscillator, we induce emission of an intense flux of up to 10ˆ7 electrons per second. Due to the local field enhancement this emission is strongly localized at the apex of the metallic tip with a radius of curvature of only few tens of nanometers. We demonstrate the multiphoton character of the electron generation from a highly non-equilbrium electron distribution and report on quantitative measurements of the transient distribution function. The results of first imaging experiments using this novel electron source will be presented, demonstrating near-field imaging of local electric fields with sub-20 nm spatial resolution.

Invited Talk O 6.2 Mon 11:45 H38

Mastering optical near fields in nanostructured materials — •Javier Garcia de Abajo[1], Tobias Brixner[2], Walter Pfeiffer[3], and Christian Spindler[2] — [1]Instituto de Optica, CSIC, Serrano 121, 28006 Madrid, Spain — [2]2Physikalisches Institut, Universität Würzburg, Am Hubland, 97074 Würzburg, Germany — [3]Fakultät für Physik, Universität Bielefeld, Universitätsstr. 25, 33516 Bielefeld, Germany

The control of the flow of light at the nanoscale has attracted considerable interest over the past few years. Trully nanometer control is actually possible via localized states such as plasmons, which have given rise to the active field of plasmonics. Some basic properties of plasmons in nanoparticles and in nanopatterned surfaces will be reviewed in this talk. Phenomena such as plasmon hybridization, signal propagation, and extraordinary optical transmission will be discussed. Finally, energy transfer during interaction with ultrashort laser pulses will be considered and compared to the interaction of fast electrons with photonic nanostructures.

Invited Talk O 6.3 Mon 12:15 H38

Near-field second harmonic generation from single gold nanoparticles — •Giulio Cerullo, Michele Celebrano, Margherita Zavelani-Rossi, Paolo Biagioni, Marco Finazzi, and Lamberto Duò — Dipartimento di Fisica, Politecnico, Milano, Italy

Second-harmonic generation (SHG) from gold nanoparticles, both isolated and in high-density patterns, is investigated by a nonlinear scanning near-field optical microscope (SNOM). High peak power femtosecond polarized light pulses at the output of a hollow pyramid aperture allow efficient second-harmonic imaging, with sub-100-nm spatial resolution and high contrast. SHG on the nanoscale provides unique information on local field enhancement with respect to conventional linear SNOM and far-field microscopy. In particular, nanoscale SHG enhancement is shown to be very sensitive to localized surface plasmon resonances as well as to the morphology of the nanostructures. The combined analysis of linear and second harmonic SNOM images provides complementary information enabling to distinguish between near-field scattering, absorption and re-emission processes.

O 7: Metal Substrates: Adsorption I

Time: Monday 11:15–12:45 Location: H39

O 7.1 Mon 11:15 H39

Ground state search via cluster-expansion for a multi-site adsorption scenario: H in the Ir(100)-5×1-H phase — •Daniel Lerch, Ole Wieckhorst, Andreas Klein, Lutz Hammer, Stefan Müller, and Klaus Heinz — Festkörperphysik, Universität Erlangen-Nürnberg, Staudtstr. 7, D- 91058 Erlangen

Upon H adsorption the (quasi-)hexagonal 5×1-reconstruction of Ir(100) is lifted and a recently discovered hydrogen induced Ir(100)-5×1-H surface is formed [1]. Thereby, our density functional theory calculations have shown that there is a clear preference for H to adsorb on bridge sites. Within the 5×1 unit cell of the surface, six bridge sites can be found which are energetically relevant. Obviously this constitutes a very large configuration space when trying to determine the ground state configuration for the adsorption of more than one adsorbate per 5×1 unit-cell, or configurations with larger periodicities than the unit-cell. A sensible approach for the treatment of large configuration spaces is the cluster-expansion (CE). Its application to multisite adsorption systems has now been implemented successfully within our CE code UNCLE and used to determine the ground states for the adsorption of up to 1.2 ML H on Ir(100)-5×1-H. This is the first case where the CE formalism has been applied successfully to a problem with multiple adsorbate sites. The results from both DFT and CE will be presented along with experimental findings.

[1] L. Hammer et al. *PRL* **91** (2003) 156101

O 7.2 Mon 11:30 H39

Surface stress change during H-induced surface reconstruction on Ir(100) — •Zhen Tian[1], Wei Pan[2], Dirk Sander[1], and Jürgen Kirschner[1] — [1]Max-Planck-Institut für Mikrostrukturphysik, — [2]Department of Physics, National Chung Cheng University, Taiwan

Adsorption induced surface reconstructions are in some cases associated with a corresponding surface stress change [1]. In this work, we performed stress measurement during hydrogen exposure that induces structural reonstruction from Ir(100)-(5×1)hex to Ir(100)-(5×1)H surface[2]. We combine stress measurements by the crystal curvature technique with LEED experiments to investigate the correlation between the surface stress change and surface reconstruction. The change in surface stress is measured while introducing onto Ir(100)-(5×1)hex surface at room temperature. The surface stress starts to decrease once hydrogen is offered and gradually saturates when the amount of hydrogen reaches 4 langmuir. The total surface stress change is - 1.75 N/m. We find a linear relation between the surface stress change and the intensity ratio of LEED spots during the reconstruction, which suggests that the surface stress change is directly correlated with the structural transition.

[1] M. J. Harrison, D. P. Woodruff, and J. Robinson, D. Sander, W. Pan, and J. Kirschner, Phys. Rev. B 74, 165402 (2006).

[2] L. Hammer, W. Meier, A. Klein, P. Landfried, A. Schmidt and K. Heinz, Phys. Rev. Lett. 91, 156101 (2003).

O 7.3 Mon 11:45 H39

Surface phase transition in H/W(110) achieved by tuning the Fermi surface nesting vector by Hydrogen loading — Yoichi Yamada, •Wolfgang Theis, and Karl-Heinz Rieder — Freie Universität Berlin, Berlin, Germany

At a hydrogen coverage of one monolayer, W(110) is known to exhibit a Fermi nesting in its electronic surface states with an incommensurate nesting vector of 0.9 $Å^{-1}$ and a resulting phonon anomaly. Here we show that additional H-adsorption allows a controlled tuning of the nesting vector. As the nesting vector approaches the commensurate value of 1.0 $Å^{-1}$ the phonon anomaly becomes more pronounced, finally disappearing as the surface reconstructs from a clean surface c(2x2) to a p(8x2) superstructure. The gradual change in the nesting vector is attributed to an energetic shift of the surface state as the surface is loaded with additional hydrogen.

O 7.4 Mon 12:00 H39

Dispersion of the O(2x1) Cu(110) surface phonons — •Klaus Brüggemann and Harald Ibach — IBN-3 Forschungszentrum Jülich , Leo-Brandt-Str. , D-52428 Jülich

In the past the O(2x1) Cu(110) surface was investigated by serveral groups(1) with the main focus on the formation of the (2x1)superstructure built by the CuO-Chains. In this work we present the measurements of the dispersion of the CuO surface phonons. The surface of the Cu single crystal was oxidized with 6 Langmuir Oxygen so that it was fully covered with 1ML of CuO. After annealing to 660K the energy loss spectra of the ordered layer were measured by an HREELS Spectrometer (2) built in our Institute. The scattering plane of the electron beam laid along the [001] and [1-10] directions. In that way we were able to determine the dispersion of the suface phonons along Gamma to Y and Gamma to X of the Brillouin zone. It turned out that the phonon vibration could be tracked at an electron energy of ca. 50eV. In the Gamma to Y direction we measured a TO mode starting at a wavenumber of 750 1/cm in Gamma and ending with 690 1/cm in Y. In the Gamma to X direction was a LO mode starting at 400 1/cm in Gamma and ending with 370 1/cm in X.

(1)H.Ibach et al., Phys. Rev. B 72, 245408 (2005) ; K. Kern et al., Phys. Rev. Lett. 67, 855 (1991) ; O.Skibbe et al. Phys. Rev. B 66, 235418 (2002)

(2)H. Ibach, Electron Energy Loss Spectrometers, Springer Series in Optical Sciences Vol. 63 (Springer, Berlin 1991)

O 7.5 Mon 12:15 H39

Enhanced erosion rate by adsorbates in grazing incidence ion bombardment applications — •Alex Redinger[1] and Thomas Michely[2] — [1]I. Physikalisches Institut, RWTH Aachen University, 52056 Aachen, Germany — [2]II. Physikalisches Institut, Universität Köln, 50937 Köln, Germany

Noble gas ion bombardment not only causes erosion, but is also known to efficiently remove adsorbates from the retracting surface. However, little is known about the interaction between the impinging ions and the adsorbates and its consequences for the eroding surface. In order to gain more insight into the effects the surface morphology of Pt(111) was investigated by scanning tunneling microscopy after 5 keV Ar^+ ion bombardment at an angle of 83° to the surface normal. During the ion bombardment at 550 K the substrate has been exposed to different oxygen partial pressures. At 550 K oxygen adsorbs dissociatively on Pt(111) with a small sticking probability. The analysis shows that for small ion fluences the amount of removed material varies by an order of magnitude in dependence of the oxygen partial pressure. Subsequent annealing experiments were performed to take into account the subsurface damage. The origin of the dependence of the erosion rate on oxygen partial pressure is traced back to an adsorbate induced suppression of surface channeling.

O 7.6 Mon 12:30 H39

Adsorption of Molecules Studied by Collision-energy-resolved Electron Spectroscopy with He*(2^3S) Metastable Atoms: Benzenes, Acetonitrile, and Acetic Acid on the Ag(110) at 80K — •Andriy Borodin[1,2], Naoki Kishimoto[1], Koichi Ohno[1], and Michael Reichling[2] — [1]Department of Chemistry, Graduate School of Science, Tohoku University, Aramaki, Aoba-ku, Sendai 980-8578, Japan — [2]Department of Physics, University Osnabrueck, Barbarastr. 7, 49076 Osnabrueck, Germany

The interaction between metastable atoms and surfaces can be utilized for electron spectroscopy on surfaces (MIES). This technique is characterized by an extremely high surface sensitivity. Such a technique applied to the gas phase is also widely known as the 2D-PIES method, which provides information on the collision energy dependence of the ionization cross section for interaction between the He*(2^3S) atom and a target. In the presented work we show results of the 2D-method applied to acetonitrile, acetic acid, and benzenes adsorbed on Ag(110).

A strong collision-energy dependence of the band intensities was found for acetonitrile. The C-N group is attractive towards He*(2^3S), especially in a multilayer film, while He*(2^3S)-interaction with CH_3-group has a rather neutral character. The intermolecular interaction in adsorbed films was studied for the acetic acid. The acetic acid dimers were found to be formed even in a sub-monolayer film at 80 K. Moreover, the adsorption of C_6H_6, C_6H_5OH, and C_6H_5SH was investigated. Flat adsorption was detected by the collision-energy-resolved technique for films with thickness of about 0.5 ML and 2 ML.

O 8: Methods: Scanning Probe Techniques I

Time: Monday 11:15–12:45 Location: H41

O 8.1 Mon 11:15 H41

Tip-Sample Distance-Dependant Tunneling Spectroscopy of Ultra-Thin Layer of d8 Metal-Phthalocyanines — •Thiruvancheril Gopakumar, Jan Meiss, and Michael Hietschold — Chemnitz University of Technology, Institute of Physics, Solid Surfaces Analysis Group, D-09107 Chemnitz, Germany.

Tip-sample distance-dependant tunneling spectroscopy (TD-TS) on the thin layers of naphthalocyanine and tin-naphthalocyanine show a strong tip-sample distance-dependant HOMO-LUMO gap shrinking, which was assigned to the electronic nature of molecule-substrate interface.[a] For the clear understanding of this scenario and the factors which influence the HOMO-LUMO gap shrinking we have extended the TD-TS to ultra-thin film of d8 metal-phthalocyanine on HOPG (0001). A similar HOMO-LUMO gap shrinking is observed and the rate of change in HOMO-LUMO gap with respect to the distance is found to be decreasing/dependant on the molecular electronic nature, which is further understood in terms of molecular polarisabilty. Theoretical calculations were performed to correlate the molecular polarisability and the electronic nature (electron density) of frontier orbitals.

[a]. T. G. Gopakumar, F. Muller, M. Hietschold, J. Phys. Chem. B. 2006, 110(12), 6060-6065.

O 8.2 Mon 11:30 H41

Dispersion relation of field emission states — •Michael Fechner, Christian Heiliger, Peter Zahn, Ingrid Mertig, Stephan Grosser, Christian Hagendorf, and Wolf Widdra — Martin-Luther-Universität, Institut f. Physik D06099 Halle,Germany

Scanning tunneling microscopy (STM) and scanning tunneling spectroscopy (STS) have been applied to investigate field emission states on Ag(001) surfaces. The STS measurements have been performed in constant current mode where the distance z(V) between tip and sample as a function of the applied voltage is controlled by the tunneling current. Field emission states cause strong changes in z(V) which indicates their energetic position [1]. Combining STM and STS the dispersion relation of the field emission states have been measured as has been demonstrated earlier on Cu(001) [2]. The previous study on Cu(001) found a free electron dispersion with an effective electron mass smaller than the free electron mass. For Ag(001) we observe a free electron like dispersion with the band bottom shifted with respect to the energy of the field emission state. A theoretical model based on the finite-difference method has been developed to reproduce the z(V) characteristics and to simulate the combination of STS and STM experiments to obtain the dispersion relation. Our results emphasize that the effective mass found in previous studies is an artifact of the operation modus whereas the band offset is the consequence of the energy uncertainty of the field emission state.

[1] G. Binnig et al., Phys. Rev. Lett. 55, 991 (1985).
[2] P. Wahl et al., Phys. Rev. Lett. 91, 106802 (2003).

O 8.3 Mon 11:45 H41

Identification of vibrations in video-speed SPM scanners — •G.J.C. van Baarle[1,2], P. Schakel[1], L. Crama[1], T.H. Oosterkamp[1], J.W.M. Frenken[1], and M.J. Rost[1,2] — [1]Kamerlingh Onnes Laboratory, Leiden University, P.O. box 9504, 2300 RA Leiden, The Netherlands — [2]Leiden Probe Microscopy, 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.

In order to avoid crashes while scanning rough surfaces at high speeds, one has to be able to perform high speed feedback on the probe position. We will demonstrate that the excitation of vibrations in the microscope sets a limit to the resolution as well as the speed of the measurement. We will present a very sensitive method to measure the vibrations in an STM.

From the experimental data obtained with this method we can clearly identify the origin of vibrations. We will show that the obtained information can be used to tune the PI-regulator settings optimally, without having any 'a priori' knowledge of the closed loop transfer function of the entire system.

O 8.4 Mon 12:00 H41

A challenge in STM-technology: video-rate imaging during film growth — •Vincent Fokkema, Mark den Heijer, Arjen C. Geluk, and Marcel J. Rost — Kamerlingh Onnes Laboratory, Leiden University, P.O.Box 9504, 2300 RA Leiden, The Netherlands

We developed a scanning tunneling microscope (STM) that will be, for the first time, capable of monitoring film growth *during* the deposition of films with significant thicknesses. To capture the dynamics involved in film growth, both high spatial and temporal resolution are required. The wish to image a growing surface during physical vapor deposition (PVD) or during ion bombardment demands an open structure of the microscope, which contradicts the desired stability for high speed imaging. Bearing this in mind, we optimized the rigidity of the scanner to not be hampered by mechanical resonances, which would render the system incontrollable. To this end we modeled the complete STM with finite elements analysis (FEA), of which the results were compared with actual measurements. Finally we received new insights regarding the design rules for the ultimate STM.

O 8.5 Mon 12:15 H41

Quantitative probing of the thermal nearfield radiation on the nanometerscale — •Uli Wischnath, Joachim Welker, Andreas Knübel, and Achim Kittel — Energie- und Halbleiterforschung, Uni Oldenburg, Germany

Recent publications report experiments in the field of evanescent thermal radiation on the nanometer scale and the according theory. A description based on macroscopic stochastic Maxwell theory does not seem to hold on this length scales. We have developed an experimental tool to investigate this type of radiation. Our experimental setup consists of a Scanning Thermal Microscope based on a STM with a modified scanner and a thermocouple sensor. We measure tunneling current and temperature of the tip simultaneously and are able to retract the thermocouple sensor by a well defined distance from the surface. Thus we are able to take precise heat flux versus distance curves which are qualified to test the predictions made by the different theories. We have shown that the rise of the heat flux between a probe at room temperature and a cooled sample is far less steep for small distances than predicted from stochastic Maxwell theory. The predicted inverse power law behavior for the heat flux due to the contributions of evanescent modes can only be observed for distances ranging from about 50 nm to about 10 nm. For smaller distances deviations become evident which can be associated to correlations in the fluctuations of the electromagnetic radiation at length scales in the nanometer range[1]. This seems to be a fingerprint of the breakdown of a macroscopic theory.

[1] Kittel et al. (2005), Phys. Rev. Lett. 95, 224301 (2005)

O 8.6 Mon 12:30 H41

Eine neue Methode zur Berechnung von Zustandsdichten aus gemessenen Tunnelspektren — •Berndt Koslowski, Christof Dietrich, Anna Tschetschetkin und Paul Ziemann — Institut für Festkörperphysik, Universität Ulm, 89069 Ulm

Vorgestellt wird eine neue Methode zur Berechnung von elektronischen Zustandsdichten (DOS) aus I-V-Spektren, die mit dem Raster-Tunnel-Mikroskop gemessenen wurden. Ausgangspunkt ist die WKB-Näherung für 1-dimensionales Tunneln. Durch einfache Näherung lässt sich ein Ausdruck für die DOS ableiten, der im Gegensatz zu früheren Methoden nicht nur dI/dV, sondern neben bestimmbaren Parametern (Abstand, Austrittsarbeit) auch den Tunnelstrom I selbst enthält. Hiermit wird eine auf die Oberfläche zurückgerechnete DOS bestimmt. Ferner kann die DOS der Probe durch eine Volterra-Gleichung 2. Art ausgedrückt werden, so dass sich das Neumann*sche Näherungsverfahren anwenden lässt. Vergleich mit gerechneten Modellzustandsdichten zeigt, dass dieses Iterationsverfahren sehr schnell konvergiert und man bereits nach etwa drei Iterationsschritten die Modell-DOS aus dI/dV erhält. Analog lässt sich auch für die DOS der Tunnelspitze eine Volterra-Gleichung formulieren, so dass ein System von Integrodifferentialgleichungen entsteht. Falls sich zusätzliche experimentelle Informationen gewinnen lassen, z.B. die differentielle Barrierenhöhe d2I/(dVdz), so kann das Gleichungssystem selbstkonsistent gelöst werden. Damit erreicht man im Idealfall eine Entfaltung der beiden DOS von Probe und Spitze.

O 9: Oxides and Insulators: Adsorption I

Time: Monday 11:15–12:45 Location: H42

O 9.1 Mon 11:15 H42

Interrogating the strength of the bond between salt and water: a combined DFT and MP2 study — •Bo Li, Angelos Michaelides, and Matthias Scheffler — Fritz-Haber-Institut der Max-Planck-Gesellschaft Faradayweg 4-6, D-14195 Berlin, Germany

The interaction of water with salt (NaCl) is of widespread importance and of considerable general interest. Although numerous theoretical studies have been reported [1], none has provided a convincingly reliable estimate of the strength of the bond between water and a flat NaCl surface, such as NaCl(001). Moreover, the computed adsorption energies predicted by DFT vary from 0.2-0.7 eV/H_2O depending on the choice of exchange-correlation functional [2]. Here, we address this issue through an extensive series of periodic Hartree-Fock and post-Hartree Fock [Møller-Plesset perturbation (MP2) and coupled cluster (CCSD(T))] calculations. Periodic Hartree-Fock calculations have been performed for H_2O molecules adsorbed on NaCl slabs, and by evaluating the local dependence of the correlation contribution to the adsorption energy with respect to cluster size, we obtain accurate MP2 and CCSD(T) estimates of the H_2O adsorption energy on NaCl(001). Our computed adsorption energy, which is around 0.6 eV/H_2O, comes close to the experimental value [3] and is at the upper end of the range predicted by DFT.

[1] A. Verdaguer, G. M. Sacha, H. Bluhm, and M. Salmeron, Chem. Rev. 106, 1478 (2006). [2] B. Li, A. Michaelides, and M. Scheffler, in preparation. [3] L. W. Bruch, A. Glebov, J. P. Toennies, and H. Weiss, J. Chem. Phys. 103, 5109 (1995).

O 9.2 Mon 11:30 H42

Force controlled lateral manipulation of water adsorbed on CaF_2(111) — •Sabine Hirth, Frank Ostendorf, and Michael Reichling — Universität Osnabrück, Fachbereich Physik, Barbarastraße 7, 49076 Osnabrück

We demonstrate for the first time the force controlled manipulation of a molecular adsorbate on an insulating substrate. We show that physisorbed water can be manipulated along three principal symmetry directions of CaF_2(111). Imaging and manipulation of water molecules is accomplished by scanning the surface at different tip-surface-distances. During manipulation steps, the movement of the molecules results in characteristic chain-like features along the slow scanning direction having a periodicity of the CaF_2 surface lattice. The form of the profiles can be assigned to a pushing type interaction. The movement of the molecule from one position to another is instantaneous on the time scale of the measurement leading to a jump of the defect position within certain scan lines. Complicated scanning profile forms result from the manipulation of defect groups. We describe the manipulation protocol in detail, explain the manipulation mechanism and discuss possible improvements for the manipulation.

O 9.3 Mon 11:45 H42

High resolution imaging of stable and mobile water related defects on fluoride (111) surfaces — •Frank Ostendorf, Sabine Hirth, Lutz Tröger, and Michael Reichling — Fachbereich Physik, Barbarastrasse 7, 49076 Osnabrück

Fluoride (111) surfaces are chemically rather inert and surface degradation due to the interaction with the residual gas of a UHV system is a slow process. Atomic surface features occurring during this process and during a controlled exposure to water were investigated with highest resolution dynamic force microscopy and are analysed in detail. Two distinct types of defect features arise, namely stable defects that can be associated with specific ionic positions on the surface and mobile defects for which we have recently shown that they can be manipulated on the surface [1]. We discuss the kinetics of defect formation and phenomena of defect clustering on the basis of experiments involving a systematic variation of gas exposure parameters. From the experimental evidence we, furthermore, draw conclusions about the identity of the defects being either molecular water adsorbed onto the surface or dissociated water with hydroxyl groups embedded into the surface.

[1] Hirth S, Ostendorf F and Reichling M Nanotechnology 17 (2006) S148

O 9.4 Mon 12:00 H42

Hydrogen storage by adsorption on microporous materials — •Katja Hönes, Barbara Panella, and Michael Hirscher — Max Planck Institut für Metallforschung, Heisenbergstr. 3, 70569 Stuttgart

Different microporous materials have been investigated for their capability to store hydrogen by physisorption. The amount of adsorbed hydrogen for three metal organic frameworks (IRMOF 8, MIL 101 and MOF 74) and the zeolite NaX has been measured volumetrically by a Sieverts' apparatus at 77K and at room temperature. Additionally, thermal desorption spectroscopy measurements between 22K and 370K have been carried out in order to distinguish different adsorption sites. The highest hydrogen uptake at 77K was measured for MIL 101 (4.25 wt%), which posseses the highest specific surface area of all materials investigated. According to their lower specific surface area IRMOF 8 adsorbed 3.4wt%, MOF 74 2.3 wt% and NaX 1.3 wt% at 77K.

(We kindly acknowledge M. Hartmann, Universität Augsburg, U. Müller, BASF AG Ludwigshafen and D. Book, University of Brimingham for supplying the samples.)

O 9.5 Mon 12:15 H42

Ammonia adsorption on V$_2$O$_5$ - DFT custer model studies — •Malgorzata Witko and Pawel Hejduk — Institute of Catalysis and Surface Chemistry, PAS, ul. Niezapominajek 8, 30 239 Krakow, Poland

Catalysts based upon vanadia are used in many processes belonging to very different types of chemical reactions, among them to the selective catalytic reduction of NO$_x$ by NH$_3$. Although the last mentioned reaction is of a great technological importance its mechanism is still under debate. In order to understand the details of the process the adsorption on ammonia on hydoxyl groups existing on different low-indices (010), (100) and (001)V$_2$O$_5$ surfaces will be discussed based upon cluster model DFT calculations within GGA-RPBE functional. The results of the performed calculations indicate spontaneous stabilization of NH$_3$ at any surface hydroxyl groups with the adsorption energy in the range of 0.8 to 1.3 eV. Ammonia becomes adsorbed in various geometries and the reaction proceeds according to different mechanism depending on the type of oxygen forming OH group and on the type of surface. In all cases the significant role of hydrogen bonds of different strengths is found.

O 9.6 Mon 12:30 H42

Influence of Mo coordination on oxygen activation in hetero and homogeneous molybdena catalysts. DFT cluster model studies. — •Renata Tokarz-Sobieraj and Malgorzata Witko — Institute of Catalysis and Surface Chemistry, PAS, ul. Niezapominajek 8, 30 239 Krakow, Poland

Activation of the molecular oxygen may be caused by bonding it to the transition metal center in metal complex (homogeneous process) or to the metal center present at the solid surface (heterogeneous reaction). The electronic properties of the bonded molecular oxygen, and what follows, its reactivity depend on the character of bonding defined by the type of metal and its surrounding ligand(s) or surface atom(s). The aim of present studies is to examine O$_2$ activation process in molybdenum porphyrin (homogeneous systems) and molydbenum trioxide (heterogeneous catalysts) using quantum chemical DFT methods within GGA-RPBE functional. The preference to form superoxo or peroxo structure for each of the systems and their possible further transformed forms that are hydroperoxo or oxo species is considered. It is found that in any system the direct consequence of O$_2$ binding to the molybdenum ions is its activation expressed by the elongation and weakening of the O-O bond. The adsorption of the H atom on the O$_2$ species leads to the further weakening of the O-O bond. The second H atom undergoes adsorption and water species is formed. The later may desorb leading to the oxygen atom doubly bonded to the molybdenum ion. As the result the high valent oxo porphyrin complex or molybdenyl bond at the oxide surface is formed.

O 10: Special Talk Hirsch

Time: Monday 13:00–13:30 Location: H1

The h-index: how useful is it as a measure of scientific achievement?

O 11: Special Talk Ball

Time: Monday 13:30–14:00 Location: H1

Is it any good? Measuring scientific merit

O 12: Nanostructures at Surfaces II (Wires, Tubes)

Time: Monday 14:15–17:30 Location: H36

O 12.1 Mon 14:15 H36

Spin-Split Bands in a One-Dimensional Chain Structure — •Ingo Barke, Fan Zheng, Tilman Rügheimer, and Franz Himpsel — Dept. of Physics, University of Wisconsin Madison, 1150 University Ave, Madison, WI 53706, USA

Gold atom chains on vicinal Si(111) surfaces exhibit an unusual doublet of one-dimensional half-filled bands, whose origin has remained uncertain. The splitting is identified by angle-resolved photoemission as a spin splitting induced by the spin-orbit interaction (Rashba effect), in agreement with a theoretical prediction by Sánchez-Portal et al. [1]. This interaction leads to a characteristic pattern of avoided band crossings at a superlattice zone boundary [2]. Two out of four crossings are avoided, with a mini-gap $E_G = 85$ meV and a k-offset of 0.05 Å^{-1}. The finding solves a long-standing puzzle about the origin of split bands observed in a whole class of atomic chains and is essential for the analysis of their fractional electron count.

The work was supported by the NSF under Awards No. DMR-0240937 and DMR-0084402 (SRC). IB was supported by the German Academic Exchange Service (DAAD) and TKR by the Studienstiftung des Deutschen Volkes.

[1] D. Sánchez-Portal, S. Riikonen, and R. M. Martin, Phys. Rev. Lett. 93, 146803 (2004).

[2] I. Barke, Fan Zheng, T. K. Rügheimer, and F. J. Himpsel, Phys. Rev. Lett. 97, 226405 (2006).

O 12.2 Mon 14:30 H36

Switching between 1d and 2d by complete and incomplete Fermi nesting in Pb chains grown on Si(557) — •C. Tegenkamp[1], H. Pfnür[1], T. Ohta[2], J.L. McChesney[2], E. Rotenberg[2], and K. Horn[3] — [1]Institut für Festkörperphysik, Leibniz-Universität Hannover, 30167 Hannover, Germany — [2]ALS, Lawrence Berkley National Laboratory, Berkley, CA. 94720, USA — [3]FHI der Max-Planck Gesellschaft, 14195 Berlin, Germany

As shown recently by STM and LEED, the adsorption of 1ML Pb at low temperatures on Si(557) followed by annealing to 640K leads to the formation of Pb-chains with an interachain spacing of d=1.5nm. The closely packed Pb film on the micro-Si(111) facets forms locally a $\sqrt{3} \times \sqrt{3}$ structure, which shows in addition a 10-fold periodicity along the $[1\bar{1}0]$ direction. Conductivity measurements below 78K have shown that electronic transport occurs only along the chain direction, whereas insulating behavior is found in the perpendicular direction. Above 78K, the sytsem switches into a 2d-regime, i.e. activated transport is found in both directions. Using angle resolved photoemission (ARPES), we explored the origins of the quasi one-dimensional (1d) conductance found below 78K. The interchain distance is reflected directly by Umklapp structures in the $[11\bar{2}]$ direction close to E_F. As ARPES reveals further, ordering into the chain structure below 78K results in complete Fermi nesting in the $[11\bar{2}]$ direction and in energy reduction by band filling. The domain structure along the chains forms split-off valence bands with mesoscopic λ_F, responsible for the 1d conductance without further instabilities at low temperatures.

O 12.3 Mon 14:45 H36

Optical anisotropy of buried metallic nanowires — •Karsten Fleischer, Julie Jacob, Sandhya Chandola, and John F McGilp — Trinity College Dublin, School of Physics, Dublin 2, Ireland

Arrays of metallic nanowires frequently show strong optical anisotropies in the infrared due to conductance differences along and perpendicular to the main wire axis. We utilize reflectance anisotropy spectroscopy (RAS) and second harmonic generation (SHG) to investigate Ag nanowires on vicinal Si(111) surfaces and the influence of the offcut angle on the properties of the Ag wires. In a second step the

Ag structures are capped with amorphous Si in order to investigate the conductivity of buried nanowires which are stable under ambient conditions.

O 12.4 Mon 15:00 H36

Screening of electric field by a two-dimensional surface nanostructure — •Josef Mysliveček, Anna Stróżecka, Neelima Paul, and Bert Voigtländer — Institut für Bio- und Nanosysteme (IBN 3), and Center of Nanoelectronic Systems for Information Technology (CNI), Forschungszentrum Jülich, 52425 Jülich, Germany

A monolayer of Ge embedded in Bi-terminated Si(111) surface can form two-dimensional surface nanostructures like nanowires and nanorings [1]. We study the electronic properties of these nanostructures by scanning tunneling spectroscopy. Both the Bi-terminated Si(111) surface and the Ge areas feature a surface bandgap. On the Ge areas, however, the bandgap is smaller due to an electron state localized in the Ge-Si interface at an energy above the bulk valence band maximum [2]. We show that the electric field of the STM tip can depopulate this electron state creating a positive surface charge layer located on the Ge areas. Thus, the Ge areas screen the external electric field more efectively than the clean Bi-terminated Si(111) surface. This can be used e.g. to locally prevent the field-induced inversion of carriers in the subsurface region and to influence the surface conductivity on the nanoscale.

[1] M. Kawamura, N. Paul, V. Cherepanov, B. Voigtländer, *Phys. Rev. Lett.* **91**, 096102, 2003.

[2] R.H. Miwa, T.M. Schmidt, P. Venezuela, *Phys. Rev. B* **72**, 125403, 2005.

O 12.5 Mon 15:15 H36

Pt Nanowires on Ge(001): A Real- and K-Space Investigation — •Marc Wisniewski, Jörg Schäfer, Florian Sandrock, and Ralph Claessen — Universität, Würzburg, Germany

Electron confinement to one dimension is expected to reveal new phenomena due to the reduced electronic degrees of freedom. The possibility of charge density waves or a potential collapse of the Fermi liquid picture are key scenarios associated with such conditions. A highly one-dimensional model system is thus most desirable. In this respect, a number of quasi-one-dimensional metallic reconstructions on semiconductors, so-called nanowires, have been identified in the last years. A little explored class of noble metal nanowires are formed by self-organized platinum chains on the Ge(001) surface. These wires have a diameter of only one atom on their top, thereby representing single-atom chains. For clarifying their real space structure, scanning tunneling microscopy was performed at very low voltages and currents. In fact, the nanowires can be imaged in the millivolt regime, suggestive of a metallic behavior. A dimerization is seen at high tunneling bias. The various dimers are indicative of building blocks in the embankment, rather than a charge density wave. To obtain further evidence on the electronic properties near the Fermi level, angle-resolved photoemission studies are currently underway. A report on the key features of the electronic strucutre will be presented.

O 12.6 Mon 15:30 H36

Surface enhancend infrared absorption (SEIRA) on single gold nanowires — •Frank Neubrech[1], Gerhard Fahsold[1], Thomas Cornelius[2], Shafqat Karim[2], Javier Aizpurua[3], Reinhard Neumann[2], and Annemarie Pucci[1] — [1]Kirchhoff-Institut für Physik, Universität Heidelberg — [2]Gesellschaft für Schwerionenforschung, Darmstadt — [3]Donostia International Physics Center, San Sebastian

We perform surface enhanced infrared (IR) absorption of adsorbates on single gold nanowires using synchrotron light at the ANKA beamline (Forschungszentrum Karlsruhe). The examined nanowires with diameter of about 100nm are prepared by electrochemical deposition in polymeric etched ion track membranes and transferred onto infrared-transparent substrates (e.g. ZnS, CaF2). Performing spectroscopic IR-microscopy we observed antenna-like plasmon resonances for a few micrometer long nanowires. For a demonstration of SEIRA on single gold nanowires we used an octadecanthiol (ODT) monolayer as adsorbate. For wires with resonances in the 3 μm range we observe significant absorption bands at 2850 cm^{-1} and 2919 cm^{-1}, corresponding to the CH stretching vibrations of ODT. In the case of gold wires with antenna resonance at much higher resonance wavelength CH stretching vibrations could not be observed. The appearance of the absorptions bands is interpreted as an indication of local field enhancement due to the presence of the nanowire.

O 12.7 Mon 15:45 H36

Template-guided formation of cobalt chains on Au(110) — •Martin Ziegler, Jörg Kröger, Nicolas Néel, Patrick Schmidt, and Richard Berndt — Institut für Experimentelle und Angewandte Physik der Universität Kiel

We report on an ultra-high vacuum low temperature scanning tunnelling microscopy experiment which aimed at fabricating cobalt chains on a metal surface. To this end we employed the (1×2) reconstructed topmost layer of a Au(110) surface as a template to guide cobalt deposition. Scanning tunnelling microscopy reveals chain-like adsorbate assemblies which are oriented along the missing row direction of the surface reconstruction.

O 12.8 Mon 16:00 H36

Electronic properties of self-organized bi-atomic Fe chains on Ir(001) — •Matthias Menzel, André Kubetzka, Kirsten von Bergmann, Matthias Bode, and Roland Wiesendanger — Institut für Angewandte Physik, Universität Hamburg,

The clean Ir(001) surface layer rearranges in a quasi-hexagonal structure, thereby forming a (5×1) reconstruction. As previously shown by Hammer *et al.* [1], this Ir(001)-(5×1) surface is an ideal template for the self-organized formation of one-dimensional nanostructures, such as Fe chains, which may exhibit extraordinary electronic properties like endstates [2], i.e. the zero-dimensional analogon to surface states, or confinement states [3].

We have studied the structural and electronic properties of Fe/Ir(001) using scanning tunneling microscopy (STM) and spectroscopy (STS). At submonolayer coverage our growth studies confirm the results of Ref. [1]. In addition, we find a transition from anisotropic ($\leq$ 2 ML) to isotropic growth ($\geq$ 3 ML) at higher coverages. Low-temperature STS data obtained on bi-atomic Fe chains reveal the existance of pronounced endstates but give no evidence for confinement states.

[1] L. Hammer *et al.*, Phys. Rev. B, **67**, 125422 (2003)

[2] J. Crain *et al.*, Science, **307**, 703 (2005)

[3] S. Fölsch *et al.*, Phys. Rev. Lett., **92**, 056803 (2004)

O 12.9 Mon 16:15 H36

Tunable Quantum Wires: New Horizons in Plasmonics — •Dominic Zerulla[1], Stephanie Rehwald[2], Michael Berndt[1,2], Frank Katzenberg[3], Stephan Schwieger[4], Erich Runge[4], and Klaus Schierbaum[2] — [1]UCD Dublin, Physics, Dublin 4, Ireland — [2]Heinrich-Heine-Universität Düsseldorf, D-40225 Düsseldorf — [3]Universität Dortmund, FB Bio-und Chemieingenieurwesen, D-44227 Dortmund, — [4]Technische Universität Ilmenau, Theor. Physik I, D-98684 Ilmenau

Here we report on the excitation of surface plasmon polaritons (SPP's) on a periodical arrangement of quantum wires with tunable periodicity. The ability to vary its two-dimensional lattice constant results in an additional degree of freedom, permitting excitation of SPP's for any combination of wavelength and angle of incidence within the tuning range of the system. Moreover it allows crucial questions on a fundamental level to be answered by shedding light on the characteristic localization properties of SPP's. Planar waveguides and photonic crystal structures are being intensively investigated as primary solutions for integrated photonic devices. However, there is an alternative approach to the manufacturing of highly integrated optical devices with structural elements smaller than the wavelength, which nevertheless enables strong guidance and manipulation of light - the use of metallodielectric nanostructures in conjunction with SPP's. This approach is now branded as ”the next big step” in nanotechnology. Our novel design opens new vistas in the development of novel methodologies in spectroscopy including plasmonic sensors and chips.

O 12.10 Mon 16:30 H36

A Route to Generate Clean Nanostructures with Arbitrary Shapes on Silicon by Electron-Beam Induced Deposition (EBID) — •Michael Schirmer, Thomas Lukasczyk, Hubertus Marbach, and Hans-Peter Steinrück — Lehrstuhl für Physikalische Chemie II, Universität Erlangen-Nürnberg, Egerlandstraße 3, D-91058 Erlangen, Germany

EBID is a technique with a high potential for the fabrication of nanostructures on different surfaces. By utilizing a highly focussed electron beam, precursor molecules are locally cracked, resulting in the deposition of the non-volatile molecule fragments. A lithography package enables the fabrication of spatially well defined ultra-small deposit structures of arbitrary shapes. The distinct approach of this paper is to use a high resolution UHV electron column (resolution $<$ 3 nm), integrated in an ultra-high vacuum (UHV) apparatus, in order to avoid contaminations due to residual gases in the chamber. For the fabrication of metallic nanostructures on silicon substrates, various organometallic precursors, in particular transition metal carbonyls, were used. Iron pentacarbonyl, $Fe(CO)_5$, turned out to be a suitable precursor for clean EBID deposits. The resulting iron nanostructures exhibit a very high purity, which was determined by local Auger electron spectroscopy. On clean Si(111) and Si(100) surfaces, discontinuous iron structures are observed, which consist of small dots with a size of $<$ 10 nm. Auger measurements indicate that these EBID deposits grow on a composite layer, which homogeneously covers the silicon substrates.

O 12.11 Mon 16:45 H36

Local crystal structure of iron oxide nano particles synthesized form ferritin — •Michael Krispin, Marcus Preisinger, Peter Pfalzer, and Siegfried Horn — Lehrstuhl für Experimentalphysik II, Universität Augsburg, D-86135 Augsburg

We have investigated the size dependence of the local crystal structure of nanosized iron oxide by extended x-ray absorption fine structure (EXAFS) at the iron K-edge. Hematite (α-Fe_2O_3) nanoparticles of different diameters were produced by thermal treatment of horse spleen ferritin molecules and remineralized apo-ferritin molecules, respectively. The structure of these particles was compared to α-Fe_2O_3 and γ-Fe_2O_3 nanopowder references. The Fourier transformed EXAFS spectra of the nanoparticles differ significantly from hematite and maghemite reference spectra and change systematically as a function of particle diameter, signalling a corresponding evolution of the structure. We show that the Fe-O bond length decreases with decreasing diameter of the particles and with decreasing particle density. This is explained by a core-shell model, in which the fraction of a γ-Fe_2O_3 like particle shell increases while the α-Fe_2O_3 core decreases with decreasing particle size.

O 12.12 Mon 17:00 H36

Self-Organized growth of highly ordered metal-nanodots on C/W(110) — •Martin Gabl, Clemens Deisl, Norbert Memmel, and Erminald Bertel — Institute of Physical Chemistry, University of Innsbruck, Austria

The growth of Ag nanostructures on W(110) and C/W(110) is studied by LEED and STM. Whereas on clean W(110) and on the R(15x3) surface large Ag islands are formed, on the R(15x12)-C/W(110) surface the growth of Ag nanodots is observed. The R (15x12) carbon structure serves as a stable periodic template with a nanoscale unit mesh of 14Å x 31Å, which is replicated by the Ag nanodots. Most critical for the fabrication of a regular nanostructure array is the perfect preparation of the R(15x12)-C/W template. Interestingly, it forms more readily in the interior of large terraces, while small terraces tend to stay free of carbon. This implies a crucial role of steps in the C budget of the surface, most probably due to step-enhanced diffusion of carbon into the bulk. At optimum silver coverage (0.12 ML) the Ag nanodots show a narrow size distribution with most islands consisting of hexagonally shaped 7-atom clusters. However, clusters of this size are also observed at slightly higher silver coverages, if deposition temperatures around 500K are used. In this case excess silver agglomerates on terraces with a locally reduced carbon coverage. This implies that the 7-atom clusters are particularly stable, defining a *magic island size*. The present work was supported by the Austrian Science Fund (FWF) and the West-Austrian Initiative for Nano-Networking (WINN).

O 12.13 Mon 17:15 H36

Electron wave-vector quantization in nanostructures — •Sebastian Wedekind[1], Guillemin Rodary[1], Dirk Sander[1], Hui Liu[2], Hongwu Zhao[2], Larissa Niebergall[1], Valeri Stepanyuk[1], Patrick Bruno[1], and Jürgen Kirschner[1] — [1]Max-Planck-Institut für Mikrostrukturphysik, Weinberg 2, D-06120 Halle/Saale, Germany — [2]Institute of Physics, Chinese Academy of Science, Beijing, China

We use hexagonal vacancy islands on Cu(111) to study electron confinement in a nanostructure. Scanning tunneling microscopy shows that these monolayer deep depressions are often of almost perfect hexagonal shape and have a size of up to 24 nm. Low temperature scanning tunneling spectroscopy and ab initio based theory reveal electron wave-vector quantization due to electron confinement in the nanostructure. A Fourier transformation of the spatial modulation pattern of the local density of states (LDOS) indicates the quantization of the electron wave-vector within the nanostructure, which gives rise to a discontinuous, staircase-like dispersion relation. Our experimental and theoretical results show that each step of the dispersion relation corresponds to an extremum of the LDOS. The sequence of extrema identifies the complete eigenstate spectrum of the confined system.

O 13: Symposium: Ultrafast Nanooptics II

Time: Monday 14:15–18:00 Location: H38

Invited Talk O 13.1 Mon 14:15 H38

Nanoscale optical spectroscopy based on local field enhancement — •Achim Hartschuh[1], Huihong Qian[1], Tobias Gokus[1], Neil Anderson[2], and Lukas Novotny[2] — [1]Department Chemie und Biochemie and CeNS, LMU Muenchen, Germany — [2]The Institute of Optics, University of Rochester, USA

Spectroscopic techniques with nanoscale spatial resolution are essential for the detection and analysis of individual nanoobjects and nanostructured materials. We study and apply a near-field optical technique that is based on local field enhancement at the apex of a laser-illuminated metal tip. In this scheme, locally enhanced excitation and radiation fields in close proximity to the near-field probe are used to amplify the optical response of the sample. At present, using monochromatic cw-excitation, we achieve a spatial resolution of about 10 nm for both photoluminescence and Raman scattering of carbon nanotubes [1, 2]. Different contributions to the signal enhancement of photoluminescence and Raman scattering are evaluated based on experimental data achieved simultaneously for the same nanotube. The high-resolution capability of the technique is accompanied by an enhanced detection sensitivity making it ideally suited for nanoscale surface and subsurface imaging [3]. We discuss strategies for the advancement of the technique and its combination with ultrafast laser spectroscopy.

[1] A. Hartschuh et. al, Phys. Rev. Lett. 90, 095503 (2003). [2] A. Hartschuh et. al, Nano Lett. 5, 2310 (2005). [3] N. Anderson, Nano Lett. 6, 744 (2006).

Invited Talk O 13.2 Mon 14:45 H38

Coherent, Nonlinear, and Ultrafast Nanoplasmonics — •Mark Stockman — Department of Physics and Astronomy, Georgia State University, Atlanta, USA

This talk introduces and reviews recent new ideas and progress in coherent, nonlinear and ultrafast nanoplasmonics. It includes a brief Introduction to the topic and forefront, focus areas based partially on original contributions, including ultrafast, coherent, nonlinear, and stimulated phenomena. Spaser will be one of the focus points of the talk as an ultrafast generator of local optical field on nanoscale. We also consider dynamic, controllable, ultrafast localization of optical energy on the nanoscale and nonlinear photoelectron emission coherently controlled by the phases of the ultrashort excitation pulses. Finally, we consider a recent development based on the combination of the adiabatic concentration of optical energy on nanoscale and spatio-temporal modulation of surface plasmon polaritons.

Invited Talk O 13.3 Mon 15:15 H38

Attosecond resolved photoemission from metal surfaces — •Ulrich Heinzmann — University of Bielefeld, Faculty of Physics

The combination of the comb of high harmonics of a phase-stabilized ultrashort laser pulse focussed into a rare gas atomic beam[1] with an optimized multilayer mirror system as soft x-ray monochromator[2] yields isolated soft x-ray pulses of 250 and less attoseconds duration[3]. Thus photoelectron and Auger electron emission processes in atoms have been studied time resolved with a sub-fs time resolution[4]. The report discusses the efforts to apply these techniques in attosecond time resolved photoemission of condensed matter. It presents very first results of attosecond resolved photoelectron emission spectroscopy from a single crystal[5] and discusses what can be learned about the electronic dynamics in the bands of the surface and of the few atomic bulk layers the photoelectrons come from.

[1] R. Kienberger et al. Nature **427**, 817 (2004)
[2] A. Wonisch et al. Applied Optics **45**, 4147 (2006)
[3] E. Goulielmakis et al. Science **305**, 1267 (2004)
[4] M. Drescher et al. Nature **419**, 803 (2002)
[5] A. Cavalieri et al. to be published (2007)

30 min Break

O 13.4 Mon 16:15 H38

Ultrafast Spectroscopy of Single Gold Nanoparticles — •Markus Lippitz[1,2,3], Meindert van Dijk[1], and Michel Orrit[1] — [1]Huygens Laboratory, University of Leiden, The Netherlands — [2]4. Physics Institute, University of Stuttgart — [3]Max Planck Institute for Solid State Research, Stuttgart

Metal nanoparticles in the size of 1-100 nm have properties different from bulk metal. The particle size distribution present in even the best chemical preparation methods blurs the picture one can get. Optical spectroscopy of a single particle at a time removes the sample inhomogeneity and gives direct access to the individual particle's properties. We present nonlinear optical experiments on single gold nanoparticles.

We reported the first observation of third-harmonic signals from individual gold particles. Excited with short pulses (100 fs) at 1600 nm, the particles generate 533-nm light, close to the plasmon resonance. Contrary to our expectation, we found the third-harmonic intensity to vary as the fourth power of the diameter of the particles, which can be explained by the nonlinear optical response of the free electrons.

In another experiment we performed time-resolved absorption measurements of single gold nanoparticles, with a sensitive common-path interferometer. The variation of the plasmon resonance after absorption of a near-infrared pump pulse is probed in the visible wavelength range. At short times, the signal of the hot electrons dominates. At longer delay times, mechanical oscillations of the whole particle can be detected by periodic shifts of the plasmon frequency.

O 13.5 Mon 16:30 H38

Electronic properties of silver nanoclusters on oxide supports: Fluorescence microscopy and femtosecond two photon photoemission — Tobias Gleitsmann, Mihai E. Vaida, and •Thorsten M. Bernhardt — Institut für Oberflächenchemie und Katalyse, Universität Ulm, 89069 Ulm, Germany

In the quest for efficiently fluorescent nano-scale materials atomic silver clusters have attracted considerable interest in recent years. Possible applications are in all optical logic devices and in advanced optical data storage media. Unexpectedly, the observed optical properties of silver clusters in the size range with up to about 20 atoms per particle indicate that these clusters cannot yet be considered fully metallic. On the contrary, the observed fluorescence requires the presence of long-lived discrete electronic levels in the cluster-support system. Employing a laser scanning microscope and femtosecond radiation it is possible to write fluorescent silver cluster nano-structures in silver oxide thin films or silver oxide containing biopolymer matrices. The information is long-time stable and can be read out with conventional low intensity light sources. In order to furthermore identify the hitherto unknown electronic structure of atomic metal clusters at surfaces and thus to elucidate the origin of the observed luminescence properties time-resolved two photon photoemission spectroscopy is applied to mass-selected silver metal clusters which have been soft-landed onto a well-defined insulating substrate.

O 13.6 Mon 16:45 H38

Influence of the interband transition on the optical properties of gold nanoparticles — •Frank Hubenthal, Nils Borg, Christian Hendrich, and Frank Träger — Universität Kassel, Institut für Physik and Center for Interdisciplinary Nanostructure Science and Technology, Heinrich-Plett-Str. 40, 34132 Kassel, Germany

We present systematic measurements of the ultrafast dephasing time T_2 of surface plasmon resonances (SPRs) in gold nanoparticles (NPs) as a function of photon energy. The objective is to investigate the influence of the interband transition on the damping of the SPR, typically described by the damping parameter A. Gold NPs were prepared by deposition of thermal atoms followed by subsequent diffusion and nucleation, i.e. Volmer-Weber-growth. Thereafter, systematic measurements of T_2 were carried out by persistent spectral hole burning. The most essential among the numerous results is the observation of an increased damping of the SPR at the onset of the interband transition. While the damping parameter A amounts to 0.20 nm/fs for photon energies below the onset of the interband transition at 1.85 eV, the damping increases to $A = 0.32$ nm/fs at 1.85 eV. For higher photon energies the contribution of the interband transition becomes the dominant damping mechanism, resulting in a reduction of A to as little as 0.15 nm/fs. The high A-Factor at 1.85 eV cannot be explained semiclassically by taking only the surface scattering of the oscillating electrons into account. In fact, we observe an increased Landau damping in Au NPs at the onset of the interband transition, which has not been identified before for all other photon energies.

O 13.7 Mon 17:00 H38

Adaptive sub-wavelength control of nano-optical fields — Martin Aeschlimann[1], Michael Bauer[2], Daniela Bayer[1], •Tobias Brixner[3], F. Javier García de Abajo[4], Walter Pfeiffer[5], Martin Rohmer[1], Christian Spindler[3], and Felix Steeb[1] — [1]Fachbereich Physik, Technische Universität Kaiserslautern, Erwin-Schrödinger-Str. 46, 67663 Kaiserslautern, Germany — [2]Institut für Experimentelle und Angewandte Physik, Universität Kiel, Leibnizstr. 19, 24118 Kiel, Germany — [3]Physikalisches Institut, Universität Würzburg, Am Hubland, 97074 Würzburg, Germany — [4]Instituto de Optica, Serrano 121, 28006 Madrid, Spain — [5]Fakultät für Physik, Universität Bielefeld, Universitätsstr. 25, 33516 Bielefeld, Germany

We combine two previously separated research fields, adaptive quantum control and nano-optics, to achieve dynamic localization of electromagnetic intensity at sub-wavelength nanoscopic spatial resolution. This is demonstrated experimentally with femtosecond polarization shaping and photoemission electron microscopy (PEEM). The electric near field in the vicinity of Ag nanostructures is controlled by employing femtosecond laser pulses with specifically modulated vectorial properties. Two-photon PEEM probes the lateral intensity distribution, and a learning algorithm optimizes the external field such that photoemission is localized in the desired places. Thus pulse shaping and quantum-control concepts are now also available with nanoscale resolution.

O 13.8 Mon 17:15 H38

Ultrafast polariton dynamics in metallic photonic crystal superlattices — •Tobias Utikal[1], Thomas Zentgraf[1,2], Jürgen Kuhl[2], Sergei Tikhodeev[3], and Harald Giessen[1] — [1]4. Physikalisches Institut, Universität Stuttgart, Germany — [2]MPI für Festkörperforschung, Stuttgart, Germany — [3]General Physics Institute, Moscow, Russia

We present time- and frequency-resolved nonlinear autocorrelation measurements of gold nanowire photonic crystal superlattices on a dielectric waveguide layer. In these structures an external light field can excite electronic and photonic modes at the same time. A strong coupling of the two resonances leads to the formation of a polaritonic state which can further be modified by introducing a periodically structured unit-cell into the lattice. The frequency resolved measurements show a rather complex behaviour of the third harmonic signal. It consists of several spectral components, which differ in intensity and time dynamics. To describe the nonlinear processes we use a simple model, in which each resonance in the fundamental extinction spectrum is considered as an eigenmode of the polaritonic system and can be described as a Lorentzian oscillator with a certain amplitude and lifetime. The resonance frequencies of these eigenmodes can mix in the nonlinear regime, leading to third harmonic and sum frequency generation. Within this model it is possible to relate the spectral components in the higher harmonic signal to the different third harmonic and sum frequency processes. We find dephasing times of the different polariton modes which range from 10 up to 60 fs.

O 13.9 Mon 17:30 H38

Plasmon Enhanced Photoemission Microscopy — •Frank Meyer zu Heringdorf and Liviu Chelaru — Universität Duisburg-Essen, Lotharstrasse 1, 47048 Duisburg

Excitation and propagation of light in metallic nanostructures by means of plasmons is one of the most promising techniques for scaling down photonic devices to their ultimate limit. This perspective has created a tremendous interest in the interaction of light with metallic particles. Two Photon Photoemission Microscopy with femtosecond laser pulses is particularly well suited to study plasmons in small metallic nanostructures, as the existence of a plasmon enhances the nonlinear photoemission yield and provides for direct visualization of the plasmon. We use the self-organization of Ag islands and wires on various Si surfaces to form structures that act as waveguides for surface plasmon polariton waves. Such waves travel along the surface of the wires and form an interference pattern with the exciting light. Pump-Probe Microscopy allows observation of the time-dependent beating pattern of the plasmon wave that is excited by a first laser pulse and probed by a second laser pulse.

O 13.10 Mon 17:45 H38

Quasi Particles as Quantum Phenomena at Surfaces — •Dominic Zerulla, Brian Ashall, and Michael Berndt — UCD Dublin, School of Physics, Dublin 4, Ireland

Surface Plasmon Polaritons (SPP's) are mixed states between photons and electron density waves propagating along the surface of a conductor. While the principle excitation of such phenomena is well understood the focus of this talk is on the detailed properties of these quasi-particles, such as localization, lifetime, causality and re-emission characteristics. The localization of surface plasmons can be used to tailor the accompanying near- and far-fields to exhibit, for example, a strongly focused character. Furthermore we will show that SPP's are ultra fast phenomena which range typically from ps to fs time scales, while the propagation lengths in the visible are of the order of 80 micrometers. Finally, we will demonstrate the stunning coherence of the phenomenon via discussing the re-emission characteristics of SPP's which nicely underline the mixed state nature of the phenomenon.

[1] G. Isfort, K.-D. Schierbaum, D. Zerulla; Causality of Surface Plasmon Polariton Emission Processes, Phys. Rev. B, 73, 033408 (2006)

[2] G. Isfort, K. Schierbaum, D. Zerulla; Polarization Dependence of Surface Plasmon Polariton Emissions, Phys Rev. B, 74, 033404 (2006)

O 14: Metal Substrates: Epitaxy and Growth

Time: Monday 14:15–17:45 Location: H39

O 14.1 Mon 14:15 H39

Determination of the <110> and <100> step edge Ehrlich Schwoebel barriers on Cu(001) — •Frank Everts, Frits Rabbering, Herbert Wormeester, and Bene Poelsema — Solid State Physics, MESA+ Institute for Nanotechnology, University of Twente, Enschede, The Netherlands

Paths available for interlayer mass transport determine the morphology evolution in multilayer growth. On Cu(001) the paths over the closed packed and open step edge compete. Their availability for interlayer diffusion is expressed by the so-called Ehrlich-Schwoebel barrier. Their height determines the layer distribution already in the early stages of growth as measured from the specular reflection of a thermal energy He atom beam. The value of the barriers for the two pathways is obtained from comparing the experimental roughness evolution with a Monte Carlo simulation incorporating both intra- and interlayer diffusions. A triangulation of experimental and simulated results at different temperatures and coverage enables an accurate determination of the two very different Ehrlich Schwoebel barriers.

O 14.2 Mon 14:30 H39

Shape anisotropy of adatom islands as a probe for long range dipolar forces — •Herbert Wormeester, Frits Rabbering, Teun Warnaar, and Bene Poelsema — Solid State Physics, MESA+ Institute for Nanotechnology, University of Twente, Enschede, The Netherlands

The observation of shape anisotropy of adatom, islands obtained after grazing incidence growth of Cu on Cu(001) was explained with the steering effect. This effect describes the local variation of incident flux due to attractive interaction between the incoming atoms and the surface. High-Resolution Low Energy Electron Diffraction was used to measure the shape anisotropy as a function of coverage from 0.3 to 0.6 ML. Simulations of the growth process including an evaluation of the steering effect also show the evolution of anisotropy. The strength of the long range attractive potential as a result of dipolar interactions is in the simulation varied between absent and stronger than expected on the basis of an analysis of the optical properties of both the atom and the half infinite substrate. We found counter-intuively that a stronger long range interaction decreases the shape anisotropy. This can be explained by its influence on the flux distribution on adatom islands. Diffraction profiles evaluated for the simulated morphologies are used for comparison with experimental observations. This indicates that long range forces play a dominant role in the observed anisotropy and that their strength seems to be stronger than derived from optical properties.

O 14.3 Mon 14:45 H39

Surface state mediated atomic-string and superlattice — •Haifeng Ding[1,2], Chunlei Gao[1], Marta Waśniowska[1], Nikolay Negulyaev[1], Larissa Niebergall[1], Valeriy Stepanyuk[1], Patrick Bruno[1], and Jürgen Kirschner[1] — [1]Max-Planck-Institut für Mikrostrukturphysik, Weinberg 2, Halle, 06120, Germany — [2]National Laboratory of Solid State Microstructures and Department of Physics, Nanjing University, Nanjing, 210093, China

We present a joint experimental and theoretical study of Fe atoms alignment on a flat and a vicinal Cu(111) surface. A few percent monolayer of Fe atoms are deposited at around 5 K on a clean Cu(111)surface. Upon deposition, the Fe atoms are randomly distributed on the sample surface without apparent ordering. With annealing to 13 K, the Fe atoms form ordered structures on both flat and vicinal surfaces. On the flat surfaces, hexagonal superlattice with nearest neighbor distance of 1.2±0.1 nm is found. On the vicinal surfaces, we find the Fe atoms form a string like structure along the step edges. The Fe atoms also have the same nearest neighbor distance as the superlattice and they have a fixed separation of 0.8±0.1 nm away from the step edges. Together with the first principle calculation and Monte-Carlo simulations, our findings evidence that the surface state can mediate atom diffusion, resulting the formation of atomic string and superlattice.

O 14.4 Mon 15:00 H39

Initial growth of Co on Cu(100) by pulsed laser deposition — •Carsten Tröppner, Andreas Dobler, and Thomas Fauster — Lehrstuhl für Festkörperphysik, Universität Erlangen-Nürnberg, Staudtstr. 7, 91058 Erlangen

Pulsed laser deposition (PLD) provides an increase of the instantaneous particle flux by more than 4 orders of magnitude compared to thermal deposition (TD) and particle energies up to 100 eV. In order to better understand the improved layer-by-layer growth in epitaxy of thin metal films by PLD, we investigated the system Co/Cu(001) in the submonolayer regime by scanning tunneling microscopy. For this system, Co atoms may be incorporated into the top layer of the substrate by thermally activated exchange.

After deposition at 303 K, we recorded the resulting island and defect densities as well as island-size distributions as function of coverage and particle flux for PLD and TD. Defect nucleation at incorporated Co atoms dominates the initial growth so that identical defect densities measured for both methods lead to identical island densities for a wide range of parameters. Differences in the island-size distributions and in the island densities below 0.1 monolayers are found which can be assigned to the high flux at PLD. The high particle energies enhance the adatom mobility, which suppresses the second-layer growth, and cause some sputtering.

O 14.5 Mon 15:15 H39

Growth of Co nanoislands on Cu(111): theoretical and experimental study — •Nikolay Negulyaev[1], Valeriy Stepanyuk[2], Patrick Bruno[2], Lars Diekhöner[3], Peter Wahl[4], and Klaus Kern[4] — [1]Fachbereich Physik, Martin-Luther-Universität, Halle (Saale), Germany — [2]Max-Planck-Institut für Mikrostrukturphysik, Halle (Saale), Germany — [3]Institut for Fysik og Nanoteknologi, Aalborg Universitet, Denmark — [4]Max-Planck-Institut für Festkörperforschung, Stuttgart, Germany

We report on the theoretical and experimental study of the growth of Co nanoislands on Cu(111) at 80-300 K. The detailed molecular dynamics and kinetic Monte Carlo simulations are performed. Atomistic processes at edges, kinks, corners of islands and interlayer mass transport are studied. We reveal the effect of the strain in the substrate and nanoislands on the growth process. The temperature dependence of shape and structure of nanoislands is investigated. We report on the blocking effect: novel kinetic mechanism related to the interlayer mass transport and responsible for the growth of Co nanoislands of two monolayers height at room temperature. Results of the theoretical studies are compared with STM observations.

O 14.6 Mon 15:30 H39

Strain relief within thin films of Co and Ni on unreconstructed Ir(100)

— •Wolfgang Meyer, Andreas Klein, Lutz Hammer, Stefan Müller, and Klaus Heinz — Lehrstuhl für Festkörperphysik, Universität Erlangen-Nürnberg, Staudtstr. 7, D-91058 Erlangen

As reported earlier, Co and Ni grows layerwise and pseudomorphically on the unreconstructed Ir(100) surface up to a thickness of at least five monolayers despite the large lattice misfit of about 8 % between Co/Ni and Ir. However, STM shows that the films are atomically flat only up to two monolayers, while thicker films show surface corrugations in the range 0.1 - 0.3 Å increasing in amplitude and frequency with film thickness. Moreover, LEED intensity analyses reveal large atomic displacements within the whole volume of the films much beyond usual thermal vibrations. Consistently, film layer spacings derived from LEED are somewhat larger than predicted from DFT calculations for ideal films. We interpret these displacements as the onset of a strain relief mechanism, a picture, which is also corroborated by surface stress measurements performed elsewhere [1]. The nature of this mechanism is discussed in detail on the basis of both the available experimental data as well as DFT model calculations.
[1] C. Tian, D. Sander, J. Kirschner, MPI Halle, unpublished.

O 14.7 Mon 15:45 H39

The growth of Co on Cr/W(110) investigated by STM and STS

— •Torsten Methfessel and Hans Joachim Elmers — Johannes Gutenberg-Universität Mainz, Institut für Physik, Staudingerweg 7, D-55099 Mainz

Highly spinpolarised metals are of great interest e.g. for the application in spin-valves. Recently observed large tunneling magnetoresistance effects indicate that the metastable bcc phase of Co provides a high spin-polarisation at the Fermi edge. Previous investigations of Co on Cr(110) with high-resolution low-energy electron diffraction (LEED) indicated pseudomorphic growth of bcc-Co on Cr(110) [1]. In order to prepare a Cr(110) substrate, we deposited a 8 ML Cr film on W(110) that was annealed to 500 K. The annealing results in high islands with a perfect Cr(110) surface, that serves as a substrate for Co. Using STM and STS we investigated local structural and electronic properties of the Co films. While the Co monolayer is pseudomorphic to the Cr(110) surface we oberserve significant variations of the local conductivity on thicker Co coverages indicating different electronic structures. The variation of the electronic structure results from different crystallographic structures of the Co. Comparing the tunneling spectra with previously measured spectra of pure Co films on W(110) [2] we conclude that the Co grows in a hcp and fcc structure. Areas with different stacking sequences are separated by dislocation lines similar to the growth of Co on W(110).

[1] S. Fölsch et al., Phys.Rev.B **57**, R4293 (1998).

[2] M. Pratzer et al Phys.Rev.B **72**, 035460 (2005).

O 14.8 Mon 16:00 H39

The initial growth of silver on Pt(111) revisited

— •Esther van Vroonhoven and Bene Poelsema — Solid State Physics, MESA+ Institute for Nanotechnology, University of Twente, Enschede, The Netherlands

Ultrathin films of silver on Pt(111) are quite commonly considered as a model system for surface confined alloying: If deposited (or heated) at, or above, 550 K the first monolayer has been reported to initially form an alloy, followed by de-alloying towards monolayer completion [1].

New mesoscopic measurements, performed with LEEM, reveal evidence for yet unanticipated and highly complex behaviour. Various unanticipated and complex process, governed by different aspects of stress and strain, determine the evolution of the growing film. They include alloying, de-alloying, segregation, re-entrant partial alloying and gradual de-alloying.

As will be shown and discussed, the concept of a neatly behaving, simple model system for surface confined alloying need substantial revison.

[1] H. Roeder, R. Schuster, H. Brune and K. Kern, Phys. Rev. Lett. 71, 2086 (1994)

O 14.9 Mon 16:15 H39

Quantum-Well Wave-Function Localization and the Electron-Phonon Interaction in Thin Ag Nanofilms

— •Stefan Mathias[1], Martin Wiesenmayer[1], Martin Aeschlimann[1], and Michael Bauer[2] — [1]Department of Physics, University of Kaiserslautern, 67663 Kaiserslautern, Germany — [2]Institut für Experimentelle und Angewandte Physik, Universität Kiel, 24098 Kiel, Germany

The electron-phonon interaction in thin Ag nanofilms epitaxially grown on Cu(111) is investigated by temperature-dependent and angle-resolved photoemission from silver quantum-well states. Clear oscillations in the electron-phonon coupling parameter as a function of the silver film thickness are observed [1]. Different from other thin film systems where quantum oscillations are related to the Fermi-level crossing of quantum-well states, we can identify a new mechanism behind these oscillations, based on the wavefunction localization of the quantum-well states in the film.

[1] S.Mathias, M. Wiesenmayer, M. Aeschlimann, M.Bauer, Phys. Rev. Lett. 97, 236809 (2006)

O 14.10 Mon 16:30 H39

Alloying and dealloying in pulsed laser deposited Pd on Cu(001)

— •Holger Meyerheim, Elena Soyka, and Jürgen Kirschner — Max-Planck-Institut f. Mikrostrukturphysik, Weinberg 2, 06120 Halle

Using surface x-ray diffraction we have studied the geometric structure of ultra thin Pd films grown at room temperature on Cu(001) by pulsed laser deposition (PLD) in the coverage regime between 0.4 and 4 monolayers (ML). We find a complicated growth mechanism characterized by alloying, dealloying and Pd-agglomeration above an alloyed structure. The growth sequence is governed by the balance of the free surface energy, the strain energy and the activation energy for interlayer exchange. Up to about 2 ML, the interface formation is characterized by an alloying-dealloying mechanism, where Pd is incorporated into the Cu substrate for less than half filled layers, but expelled if the Pd coverage is close to a complete layer. In this case the top layer is composed of Pd. Above 2 ML, Pd agglomeration sets in characterized by Pd-rich alloy layers covered by Pd-layers. Interlayer spacings linearly depend on the Pd-concentration (x) in the Pd(x) Cu(1-x) alloy layers. Our study shows that the film structure is inhomogeneous with respect to both, layer composition and interlayer spacings. It thus provides new structure informations for the strain relief mechanism developed for PLD grown Pd/Cu(001). So far, layer-by-layer growth of a homogeneous non-alloyed Pd-film was assumed as concluded by reflection high electron diffraction and scanning tunneling microscopy [1]. [1] Y. Lu et al., PRL 94, 146105 (2005).

O 14.11 Mon 16:45 H39

Atomic distribution in 2D surface alloys - linking STM results with DFT studies via effective cluster interactions

— •Andreas Bergbreiter[1], Harry E. Hoster[1], Yoshihiro Gohda[2], Axel Gross[2], and R. Jürgen Behm[1] — [1]Institut für Oberflächenchemie und Katalyse, Universität Ulm, 89069 Ulm — [2]Institut für Theoretische Chemie, Universität Ulm, 89069 Ulm

Surface alloys such as $\mathrm{Pt}_x\mathrm{Ru}_{1-x}$/Ru(0001), $\mathrm{Pd}_x\mathrm{Ru}_{1-x}$/Ru(0001), $\mathrm{Cu}_x\mathrm{Pd}_{1-x}$/Ru(0001), or $\mathrm{Au}_x\mathrm{Pt}_{1-x}$/Pt(111) are governed by a local equilibrium [1,2], i.e., intermixing is confined to the outermost layer, and the lateral atomic distributions depend on the intermetallic interactions. These can be described by an Ising type Hamiltonian based on effective cluster interactions (ECIs). From atomically resolved STM images of the distinct surface alloys we have derived ECIs by an Inverse Monte Carlo approach. Complementary, the respective parameters can also be derived from energies attained for ordered surface alloys of varying unit cell compositions and geometries via Density Functional Theory (DFT). This allows us to compare theoretically predicted with experimentally found atomic distributions of systems without long-range order.

[1] A.V. Ruban et al., in *Surface Alloys and Alloy Surfaces*, *Vol. 10*, (ed.: D. P. Woodruff), Elsevier; Amsterdam **2002**, pp. 1-29.

[2] H.E. Hoster, E. Filonenko, B. Richter, R.J. Behm, Phys. Rev. B 73 (2006) 165413.

O 14.12 Mon 17:00 H39

Adsorption geometry and electronic properties of Ag(111)-Cs

studied by scanning tunnelling microscopy and spectroscopy — •Martin Ziegler, Jörg Kröger, and Richard Berndt — Institut für Experimentelle und Angewandte Physik der Universität Kiel

A scanning tunnelling microscope operated in ultra-high vacuum and at low temperatures is used to study superstructures of ultrathin Cs films on Ag(111) at various coverages. Hexagonally ordered adsorption domains which are rotated with respect to each other are observed. Mutual Cs atom distances are discussed in terms of surface state-mediated interactions. Electronic properties of the different Cs adsorption layers are investigated by tunnelling spectroscopy. Quantum well states as well as a modified Ag(111) surface state are present.

O 14.13 Mon 17:15 H39

Vanadium Oxide Superstructures and their Transitions on W(110) — •Benjamin Borkenhagen, Gerhard Lilienkamp, and Winfried Daum — Institut für Physik und Physikalische Technologien, TU Clausthal, Leibnizstr. 4, D-38678 Clausthal-Zellerfeld

Epitaxially grown ultrathin vanadium oxide films on a W(110) single crystal surface exhibit a wealth of superstructures, depending on growth conditions such as temperature and oxygen partial pressure. The thickness of the deposited vanadium oxide films was in the range from submonolayer to a few monolayers as determined by a quartz microbalance. The structure of the films and their composition was analysed by LEED and AES, respectively. The oxidation state of vanadium in the films was determined by AES. For atomically smooth films, low energy electron microscopy (LEEM) reveals flat terraces with widths up to 6 μm separated by monoatomic steps. Using dark-field imaging the domain structure of the films is resolved with high contrast. Depending on the preparation conditions (oxygen partial pressure, heating rate), a more granular or a more homogeneous domain structure is obtained. Structural transitions of the thin oxide films under oxidising or reducing conditions have been monitored by LEEM.

O 14.14 Mon 17:30 H39

Wachstum und Manipulation von Ferrocene Molekülen auf der Au(111) Oberfläche — •Kai-Felix Braun[1], Violeta Iancu[1], Natalya Pertaya[1], K.-H. Rieder[2] und S.-W. Hla[1] — [1]Department of Physics and Astronomy, Ohio University, Athens OH, USA — [2]Institut für Experimentalphysik, Freie Universität Berlin, Arnimallee 14, D-14195 Berlin, Germany

Mit Hilfe von Rastertunnelmikroskopie wurde das Wachstum von Ferrocene Molekülen bei tiefen Temperaturen untersucht. Die Ferrocene Moleküle wachsen in einer inkommensuraten Struktur bestehend aus zwei Schichten. Laterale Manipulation ermöglicht die genaue Bestimmung der Höhen einzelner Fragmente. Zur Bestimmung der Fragmente wurden Rechnungen im Rahmen der Dichtefunktionaltheorie durchgeführt. Dabei ergeben sich in der ersten Schicht Eisen-Cyclopentadyenyl Einheiten mit einer dreizähligen Symmetrie und in der obersten Lage Cyclopentadienyl Einheiten mit einer vierzähligen Symmetrie. Die verschiedenen molekularen Wechselwirkungen, die zu dieser Struktur führen, werden diskutiert.

O 15: Methods: Scanning Probe Techniques II

Time: Monday 14:15–17:45 Location: H41

O 15.1 Mon 14:15 H41

Advances in High Resolution 3-Dimensional Force Field Spectroscopy — •Alexander Schwarz, Uwe Kaiser, and Roland Wiesendanger — Institut für Angewandte Physik, Department Physik, Universität Hamburg, Jungiusstr. 11, 20355 Hamburg

Atomic force microscopy using the frequency modulation technique (FM-AFM) can be employed to image surfaces with atomic resolution. Force spectroscopy allows determining the distance dependence of the tip-sample interaction force. Recently, both methods have been combined by recording spectroscopy curves at every x, y image point. This 3-dimensional force field spectroscopy technique (3D-FFS) [1,2] can be used to evaluate details of the tip-sample interaction with high resolution.

In our presentation, we will discuss the requirements to acquire high-resolution 3D-force-fields together with the dissipation signal due to non-conservative tip-sample interactions. As sample we will show data obtained on NiO(001). At close tip-sample separations, the force field $F(x, y, z)$ and the dissipation $E_{\mathrm{Diss}}(x, y, z)$ is analysed with respect to reconfigurations of atoms at the tip apex. Such reconfigurations influence the atomic scale contrast and are therefore very important to understand the relevant effects and mechanisms during atomic resolution imaging.

[1] H. Hölscher et al. Appl. Phys. Lett. **81**, 4428 (2002).

[2] S. M. Langkat et al. Surf. Sci. **521**, 12 (2003).

O 15.2 Mon 14:30 H41

Measuring energy dissipation in torsional resonance mode AFM using frequency modulation — •Ayhan Yurtsever, Alexander M. Gigler, and Robert W. Stark — Ludwig-Maximilians-Universität München, Germany

The atomic force microscope (AFM) may be used as a tool to probe hardness, elastic and viscous properties of the surface at the nanoscale. In-plane properties such as friction or shear stiffness of the sample can be measured with a lateral force modulation microscopy or by analyzing torsional vibrations. The torsional resonance mode (TR mode) allows shear force microscopy with standard cantilevers [1]. The torsion about the cantilevers long axis actuates a pendulum-like oscillation of the tip apex parallel to the sample surface with typical amplitudes of 0.2 nm to 2.0 nm. In this study, the dynamics of the torsionally vibrated cantilever are analysed by the transfer function method and finite element analysis (FEA). The results explain the fundamental mechanism for the topography feedback in TR-mode. Experimentally, we measure the energy dissipation and the frequency shift in torsional resonance mode AFM using frequency-modulation on a PMMA surface. To regulate the FM detection scheme, we utilized a Nanosurf (Liestal, Switzerland) Phase-Loop-Lock controller/detector (PLL). By monitoring the changes in the resonance frequency and excitation amplitude required to keep the oscillation amplitude constant, we were able to measure both frequency shift and dissipation caused by the tip-sample interaction.

[1] L. Huang, C. Su, Ultramicroscopy 100 (2004) 277-285

O 15.3 Mon 14:45 H41

Frequency Modulation Dynamic Force Microscopy applying amplitudes in the low nm range: Questions, findings — •Georg Hermann 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

Atomically resolved images of various surfaces of semiconductors [1], insulators [2] and metals [3] are given in the literature. Most of them being the result of large amplitude measurements with soft cantilevers while some have been obtained with stiff quartz tuning forks [4, 5] and small amplitudes (few nm or less). Such high resolution with small amplitudes, despite the success, raises questions concerning sensitivity, measured forces and signal to noise ratio.

Here, we have started a detailed analysis of frequency shift-distance curves obtained by our low temperature dynamic force microscope operated with a quartz tuning fork sensor in the small amplitude regime. The experimental data is compared to a simple theoretical model and results from literature. From the findings further conclusions for sensor improvement can be drawn.

[1] F. J. Giessibl, Science 267, 68 (1995)

[2] M. Reichling, C. Barth, Phys. Rev. Lett. 83, 768 (1999)

[3] K. Yokoyama, T. Ochi, Y. Sugawara, S. Morita, Phys. Rev. Lett. 83, 5023(1999)

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

[5] M. Heyde, M. Sterrer, H.-P. Rust, H.-J. Freund, Appl. Phys. Lett. 87, 083104 (2005)

O 15.4 Mon 15:00 H41

Optimum excitation and detection of cantilever oscillations in vacuum — •Jannis Lübbe[1], Stefan Torbrügge[1], Sebastian Gritschneder[1], Lutz Tröger[1], Holger Schnieder[1], Toyoaki Eguchi[2], Yukio Hasegawa[2], and Michael Reichling[1] — [1]Fachbereich Physik, Universität Osnabrück, 49076 Osnabrück, Barbarastraße 7, Germany — [2]Institute for Solid State Physics, Tokyo

University, 5-1-5, Kashiwa, Chiba 277-8581, Japan

The atomic resolution imaging performance of a dynamic scanning force microscope in the ultra-high vacuum critically depends on several technical parameters related to the excitation and detection of the cantilever oscillation. We designed a testing stage allowing the easy insertion and removal of a set of twelve commercial standard cantilevers for quality control prior to measurements. Resonance curves are taken by excitation of a piezo stage with a variable frequency oscillator and detection with a Lock-In amplifier. The Detection of the cantilever motion is based on a deflected laser beam coupled into the vacuum by an optical fibre and focused by an in-vacuo lens. As a laser source we use a current and temperature stabilised low noise laser diode. For low noise detection of the cantilever deflection signal, an in-vacuum quadrant detector connected to a home-built pre-amplifier was used. The detection sensitivity of this set-up and commercially available SFM setups used in our group are measured by analysing the thermally excited vibration of the cantilever and noise in the vicinity of the cantilever with a Fourier analyser.

O 15.5 Mon 15:15 H41

Increasing the Q-factor in the constant-excitation mode of frequency-modulation atomic force microscopy in liquid — •Daniel Ebeling[1,2], Hendrik Hölscher[1,2], Jan-Erik Schmutz[1,2], and Boris Anczykowski[3] — [1]Center for Nanotechnology (CeNTech), Heisenbergstr. 11, 48149 Münster — [2]Physikalisches Institut, Wilhelm-Klemm-Str. 10, 48149 Münster — [3]nanoAnalytics GmbH, Heisenbergstr. 11, 48149 Münster

The application of dynamic force spectroscopy in vacuum allows the mapping of tip-sample forces down to the atomic-scale. It has been shown that dynamic force spectroscopy works also in ambient conditions [1] and liquids [2] enabling the precise measurement of tip-sample forces.

By adding a Q-Control electronics to the set-up of the constant-excitation mode of the frequency-modulation atomic force microscope we are able to increase the effective Q-factor of a self-oscillated cantilever in liquid to values comparable to ambient conditions. During imaging of soft biological samples adsorbed on a mica substrate we observed an increased corrugation of the topography with increased Q-factors. This effect is caused by the reduction of tip-sample indentation forces as demonstrated by numerical simulations and an analytical approach [3].

[1] H. Hölscher and B. Anczykowski. Surf. Sci. **579**, 21 (2005).
[2] T. Uchihashi et al., Appl. Phys. Lett. **85**, 3575 (2004).
[3] D. Ebeling, H. Hölscher, B. Anczykowski, Appl. Phys. Lett. **89**, 203511 (2006).

O 15.6 Mon 15:30 H41

Influence of the Local Adsorption Environment on the Intra-Molecular Contrast of Organic Molecules in Non-Contact Atomic Force Microscopy — •Andre Schirmeisen[1], Bartosz Such[2], Domenique Weiner[1], and Harald Fuchs[1] — [1]Center for Nanotechnology (CeNTech), University of Münster, Heisenbergstr.11, 48149 Münster, Germany — [2]Marian Smoluchowski Institute of Physics, Jagiellonian University, Reymonta 4, 30-059 Krakow, Poland

Organic molecules have fascinating electrical and optical properties making them promising candidates as fundamental building blocks for miniaturized and high-capacity electronic devices. In the effort to exploit the opportunities offered by organic molecules, however, one has to take into account that the local chemical environment of the molecule may strongly influence its properties. Thin epitaxial layers of the organic molecule 3,4,9,10-perylenetetracarboxylic dianhydride (PTCDA) on a Cu(111) surface were imaged using non-contact atomic force microscopy in ultrahigh vacuum [1]. The second layer molecules show a distinct intra-molecular structure, which is compared to the internal charge distribution of the molecule. The molecules in the first layer, though, exhibit no detectable intra-molecular features. This effect is discussed with respect to the presence of the metallic substrate for the first layer molecules, which demonstrates the strong influence of the local adsorption environment on the internal electronic properties of organic molecules. [1] Such et al., Appl. Phys. Lett. 89, 093104 (2006)

O 15.7 Mon 15:45 H41

Kelvin Probe Force Microscopy on Electrically Inhomogeneous Fe/W(001) Films — •Ung Hwan Pi, Rene Schmidt, Alexander Schwarz, and Roland Wiesendanger — Institute of Applied Physics, University of Hamburg, Jungiusstrasse 11, 20355 Hamburg

Noncontact scanning force microscopy can give information about the real topography of the sample. However, this is valid only when the dominant tip-sample interaction is due to the van der Waals force. If the sample is electrically inhomogeneous, e.g., the sample has an inhomogeneous electric charge distribution, it causes additional electrostatic forces between tip and sample, which prevent real topography measurement. To nullify the electrostatic effect, the tip bias can be regulated with a special feedback scheme called Kelvin probe force microscopy. Here we applied Kelvin probe force microscopy to the pseudomorphic Fe thin film grown on W(001). In this highly strained film, the electric properties depend on the number of layers, yielding different contact potentials in each layer. The samples were prepared and measured in-situ under ultra high vacuum condition without exposing them to the atmospheric environment. When the tip bias was not regulated, the apparent step height of the film changed depending on the tip-sample bias, and a reliable measurement of topography was impossible. With Kelvin probe force microscopy, the contact potentials different in each layer could be compensated, and the real topography image could be obtained.

O 15.8 Mon 16:00 H41

Contact area dependence of friction on the nanoscale — •Dirk Dietzel[1,2], Tristan Mönninghoff[2], Andre Schirmeisen[2], Harald Fuchs[1,2], and Udo Schwarz[3] — [1]Forschungszentrum Karlsruhe (FZK), Karlsruhe, Germany — [2]Institute of Physics, University of Münster, Münster, Germany — [3]Department of Mechanical Engineering, Yale University, New Haven, CT, USA

A promising approach to analyze the fundamentals of friction on the nanometer scale is the lateral manipulation of small adsorbed islands by atomic force microscopy. In our case, the samples under investigation were metallic islands with diameters between 50-500 nm grown by thermal evaporation of antimony on highly oriented pyrolytic graphite (HOPG). With a newly developed manipulation procedure, which relies on contact-mode AFM operation, we have a simple and straightforward technique to manipulate the islands. Thereby, the lateral force signal of the AFM cantilever gives direct and quantitative information about the additional friction forces induced by the island pushing process. Using this technique, we focused on the contact area dependence of friction forces on the nanometer scale. By pushing a large variety of islands of different sizes, we found that the system shows a very clear behaviour with a linear dependence between the friction force and the contact area, thus reinforcing Amonton's law on the nanometer scale.

O 15.9 Mon 16:15 H41

Design of a High-Frequency Electric-Force Scanning Force Microscope for Vibration Spectroscopy at Single Macromolecules — Patrick Steffen, Ivo Knittel, and •Uwe Hartmann — Fachbereich Experimentalphysik, Im Stadtwald, Geb. C6.3, 66041 Saarbrücken

Mechanical properties of single macromolecules on timescales down to sub-nanoseconds are relvant to the understanding of the biological function of cell components. For an effective mechanical spectrocsopy at single macromolecules, a local excitation, with high amplitude and narrow bandwidth is necessary. In addition, detection should as well be local, and with narrow bandwidth. A complete microscope design is discussed in this contribution. A mechanical resonance of a sample macromolecule is excited by a charged AFM-tip. The oscillating sample molecule leads to an additional static force because of nonlineal tip-sample interaction. The size of this force is estimated by analytic and numerical methods. For the force modulation, signal-tonoise ratios and stabiltiy are investigated for several variants. The optimized design is suggested, incuding a suitable waveguide, and a suitable modulation of the exciting microwave.

O 15.10 Mon 16:30 H41

Optimum Excitation Conditions for SNOM-based Particle-enhanced Fluorescence Microscopy — •Thomas Härtling, Phillip Reichenbach, Marc-Tobias Wenzel, Phillip Olk, and Lukas Eng — Institut für Angewandte Photophysik, TU Dresden

Tip-enhanced microscopy, carried out for example by using a scattering near-field optical microscope (s-SNOM), is a powerful tool for nano-optical investigations. In this context, the manipulation of the fluorescent behavior of molecules with the help of single metal nanoparticles attached to the apex of a dielectric SNOM tip has been followed in the last years. This technique not only offers the advantages of high signal intensities confined to small spatial volumes. It equally provides deeper insight into processes involved in fluorescence emission stemming from molecular dipole transitions in the vicinity of metallic structures. It is known that the distance between the emitting molecular dipole and the metallic nanoparticle in such a configuration plays a key role in the competition between radiative and non-radiative decay processes of the excited dipolar state. Consequently, the fluorescence signal is strongly distance-dependent. We will discuss this dependence quantitatively both in theory and experiment taking into account parameters such as the excitation and emission wavelength of the dipole, the resonance wavelength of the particle, and the effect of the dielectric constant of the surrounding medium. Consequences concerning the optimum excitation conditions for particle-enhanced fluorescence microscopy are lined out.

O 15.11 Mon 16:45 H41

Second-harmonic near-field optical microscope in illumination mode — •Georgios Ctistis[1] and Paul Fumagalli[2] — [1]Center of Advanced European Studies and Research (caesar), Ludwig-Erhard-Allee 2, 53175 Bonn, Germany — [2]Institut für Experimentalphysik, Freie Universität Berlin, Arnimallee 14, 14195 Berlin, Germany

Until now, studying non-linear properties of nanostructures or thin films in the near field was limited to apertureless near-field microscopy. However, the separation of the signal resulting from the sample from that resulting from the tip has proven to be difficult. Here, we present our studies for a scanning near-field optical microscope working in illumination mode with a metal-coated fiber tip as aperture. For such a set-up, some difficulties have to be overcome before the method can be used: propagation of short pulses through the fiber, choice of metal-coating material, and maximum intensity usable. As a result, we were able to clearly assign the generated second-harmonic signal to the surface of the silver and cobalt films measured.

O 15.12 Mon 17:00 H41

Infrared Mapping of Material and Doping Contrasts in Microelectronic Devices at Nanoscale Spatial Resolution — •A. Huber[1], J. Wittborn[2], F. Keilmann[1], and R. Hillenbrand[1] — [1]MPI für Biochemie, Nano-Photonics Group, 82152 Martinsried, Germany — [2]Infineon Technologies AG, 81726 München, Germany

We demonstrate that infrared scattering-type scanning near-field optical microscopy (s-SNOM) allows mapping of different materials and electron concentrations in cross-sectional samples of industrial integrated circuit device structures at nanoscale spatial resolution.

Our s-SNOM is based on an atomic force microscope (AFM) where the metallized probing tip is illuminated by infrared light from a tuneable CO2-laser (λ=9-12μm). The tip functions as an optical antenna, concentrating light at its apex to nanoscale dimensions independent of the wavelength. The scattering originating from the optical tip-sample near-field interaction is measured interferometrically yielding nanoscale resolved infrared amplitude and phase images along with the topography.

The optical near-field interaction depends on the sample's local optical properties determined by the dielectric function $\epsilon(\omega)$. As $\epsilon(\omega)$ is highly material specific the near-field interaction enables the non-destructive characterization of nanostructures. Here we present how s-SNOM can be applied for material specific mapping of cross-sectional samples of state-of-the-art microelectronic devices. The doped areas in Si exhibit distict infrared contrasts arising from the near-field interaction between the probe tip and free carriers (plasmons) in Si.

O 15.13 Mon 17:15 H41

A 30-nm-wide slit as a waveguide for light to the aperture of a near-field optical probe — •Daniela Diessel[1], Nicole Neuberth[1], Fabián Pérez-Willard[2], and Andreas Naber[1] — [1]Institut für Angewandte Physik, Universität Karlsruhe (TH) — [2]CFN Service Laboratory, Universität Karlsruhe (TH)

Recently we have introduced a triangular aperture probe (TA probe) for scanning near-field optical microscopy (SNOM) that combines a high optical resolution capability with a high transmission of light [1]. The near-field pattern is highly confined to only one side of the triangular aperture so that the resolving power is almost doubled as compared to a circular aperture of equal size. We could demonstrate that the TA probe is particularly suited for imaging of single molecules at a resolution down to 30 nm [2]. So far, we created the aperture by controlled squeezing of the entirely aluminum-coated tip against a smooth surface. Now we applied focused ion beam (FIB) milling for aperture formation which allowed us to routinely fabricate triangular apertures with a side length even below 20 nm. To further increase the transmission of the TA probes we used a FIB to produce a 30-nm-wide slit into the metal surface as a waveguide for light to the aperture. As a result of the slit-waveguide we observed a considerable enhancement of the near-field optical intensity at the aperture.

[1] G. Colas des Francs et al., Phys Rev B 72, 165111 (2005).
[2] D. Molenda et al., Optics Expr. 13, 10688 (2005).

O 15.14 Mon 17:30 H41

Electrical Characterization of individual nanowires with the LEEPS microscope — •Dirk Henning Weber[1], André Beyer[1], Berthold Völkel[1], Armin Gölzhäuser[1], Bianca Postels[2], Andreas Waag[2], Martin Gräser[3], Andreas Greiner[3], and Joachim Wendorff[3] — [1]Physik supramolekularer Systeme, Universität Bielefeld — [2]Institute of Semiconductor Technology, Technische Universität Braunschweig — [3]Makromolekulare Chemie, Philipps-Universität Marburg

We introduce the Low Energy Electron Point Source (LEEPS) microscope as a tool for the electrical characterization of individual free-standing nanowires. We contacted single nanowires in the LEEPS electrically and measured the specific conductivity. In addition we analysed the LEEPS image itself to extract electrical properties.

The LEEPS microscope is a projection electron microscope with electron energies from 20eV to 200eV. These electrons are emitted by a field emission tip with a radius in the atomic range. Due to the very low energy of the electrons the LEEPS image includes information about weak electrostatic fields near the object. The interference pattern of conductive nanowires appears much brighter than the interference pattern of nonconductive nanowires. With a sharp manipulation tip as a movable electrode individual nanowires were contacted electrically and the I/U curves were measured. Contacting and measurement can be observed with the LEEPS microscope subsequently. We will present I/U curves of single nanowires (i.e. ZnO, CdS, Co) as well as a comparison of LEEPS images of conductive and nonconductive wires.

O 16: Organic, Polymeric, and Biomolecular Films I

Time: Monday 14:15–17:30 Location: H42

O 16.1 Mon 14:15 H42

Molecular Chirality uncovered - Circular Dichroism of Adsorbed Chiral Molecules — •Thorsten Kampen[1], Philipp Martin Schmidt[1], Jeong Won Kim[2], Hugo Dil[1], and Karsten Horn[1] — [1]1 Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, Germany — [2]Nano-Surface Group, Korea Research Institute of Standards and Science, Daejon, Korea

The chirality of molecules is an intrinsic structural property that has a huge impact upon biological and chemical reactions. However, the identification of the chiral nature of molecules in the adsorbed phase has been proven difficult. Here, we report on the characterization of adsorbed chiral molecules with respect to handedness and chemical composition using photoemission spectroscopy with circular polarized light. The emission from the carbon atoms in tartaric acid adsorbed on Cu(110) surfaces shows circular dichroism, and the asymmetry changes sign as a function of the emission angle. Changing the handedness of the molecule reverses the sign in the measured asymmetry. No asymmetry in the angular distribution is observed for the achiral meso-tartaric acid. Alanine and cysteine are two amino acids with the same next-neighbor environment of the chiral center, with cysteine containing an additional sulfur atom in the end group. This difference leads to different adsorption behavior and opposite optical activity. However, the circular dichroism in core-level photoemission is identical for both molecules.

The above mentioned results show that the angular dependent asymmetry is an absolute representation of the molecular chirality.

O 16.2 Mon 14:30 H42

Surface and Interface Properties of Chrysene on inert Substrates — •Bengt Jaeckel and Bruce Parkinson — Colorado State University; Department of Chemistry; 200 West Lake Street; Fort Collins, CO-80523/USA

The growth and electronic structure of chrysene thin films was studied on four different inert substrates (Au(111), Ag(111), HOPG and SnS$_2$) under ultra high vacuum (UHV) conditions. These substrates have hexagonal symmetry and lattice constants much smaller than the growing chrysene overlayer. A flat-lying chrysene molecule has a 2D or pseudo chirality and ordered surface structures can form ordered chiral domains, racemic 2D unit cells or disordered structures. Variable temperature scanning tunneling microscopy (VT-STM) was used to study the surface structure and ordering of the molecules while X-Ray photoelectron spectroscopy (XPS) and ultraviolet photoelectron spectroscopy (UPS) were used to study the electronic properties of the interfaces.

O 16.3 Mon 14:45 H42

Electronic and geometric structure of F4TCNQ on Cu(111): A joint experimental and theoretical study — Lorenz Romaner[1], Alexander Gerlach[2], Frank Schreiber[2], Steffen Duhm[3], Norbert Koch[3], Gerold Rangger[4], Georg Heimel[4], Jean-Luc Brédas[1], and •Egbert Zojer[1] — [1]Institut für Festkörperphysik, Technische Universität Graz, A-8010 Graz, Austria — [2]Institut für Angewandte Physik, Universität Tübingen, 72076 Tübingen, Germany — [3]Institut für Physik, Humboldt-Universität zu Berlin, D-12389 Berlin, Germany — [4]School of Chemistry and Biochemistry and Center for Organic Photonics and Electronics, Georgia Institute of Technology, Atlanta, Georgia 30332-0400, USA

The physical and chemical properties of organic/metal interfaces are of high interest for organic and molecular electronics. We present results of ultraviolet photoelectron spectroscopy (UPS) and X-ray standing wave (XSW) measurements for F4TCNQ adsorbed onto the copper (111) surface.

To gain insight into the nature of the interaction between the metal and the molecules, the interface was modeled by means of density functional theory band-structure calculations using the VASP code. The results provide an accurate description of charge donation from the -CN lone pairs to the metal and the back donation from the metal into the molecular LUMO. The molecules are strongly bent and display a transition from a quinoidal to a benzoidic structure. From a real space analysis of the charge redistribution and the electrostatic properties of the layer the overall workfunction increase can be explained.

O 16.4 Mon 15:00 H42

Polymorphism of Porphyrin Molecules on Ag(111): and how to weave a rigid monolayer — •Hubertus Marbach, Florian Buchner, Karmen Comanici, and Hans-Peter Steinrück — Universität Erlangen-Nürnberg, Lehrstuhl für Physikalische Chemie II, Egerlandstraße 3, D-91058 Erlangen, Germany

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. In the present paper we focus on studying the molecular arrangements of Cobalt-5,10,15,20-Tetraphenylporphyrin (CoTPP) and Cobalt-5,10,15,20-Tetrakis-(3,5-di-tert-butyl)-phenyl*porphyrin (CoTTBPP) on an Ag(111) surface by means of scanning tunneling microscopy (STM) in ultra high vacuum. In the monolayer regime, ordered domains were found for both investigated porphyrins. Whereas the smaller CoTPP exhibits only one molecular arrangement (square order), for the larger CoTTBPP four clearly distinguishable phases (two hexagonal, one square and one herringbone) were observed. Submolecularly resolved STM images reveal that the different molecular arrangments go together with different conformations of the individual molecules. The herringbone structure was solely observed after a thermal treatment and consists of interwoven molecules, which makes this phase especially rigid.

This work has been funded by Sonderforschungsbereich 583

O 16.5 Mon 15:15 H42

Microscopic Identification of Different Porphyrin Species in Composite Layers — •Florian Buchner, Veronika Schwald, Karmen Comanici, Ken Flechtner, Sven Schöffel, Thomas Lukasczyk, Michael Gottfried, Hubertus Marbach, and Hans-Peter Steinrück — Lehrstuhl für Physikalische Chemie II, Universität Erlangen-Nürnberg, Egerlandstraße. 3,

The self-assembly of organic molecules on single crystal surfaces is an approach towards the creation of novel materials with outstanding properties. Porphyrins represent a group of molecules, which are of great interest for various applications and also for basic science. In this study, composite films of different mixtures of the free-base 2H-5,10,15,20-Tetraphenylporphyrin (2HTPP) and Metallo-TPPs (namely FeTPP and CoTPP) were prepared on Ag (111), and imaged in UHV using scanning tunnelling microscopy (STM). A novel preparation method was applied by in-situ deposition of iron atoms onto the 2H-TPP monolayer. Microscopic evidence for the successful complexation of 2HTPP with Fe will be given [1]. This method is now also exploited to fabricate composite layers with 2HTPP, CoTPP and FeTPP. Depending on the bias voltage, the different molecules appear as protrusions or depressions, with changing shapes. Considering the different electronic configurations and additional UPS measurements, the different porphyrins can be identified.

[1] Buchner et al., ChemPhysChem (in press) This work has been funded by Sonderforschungsbereich 583

O 16.6 Mon 15:30 H42

Dynamics in ordered networks of adsorbed oligopyridine molecules — •Harry Hoster, Michael Roos, Matthias Roos, Achim Breitruck, and Jürgen Behm — Institute of Surface Chemistry and Catalysis, Ulm University, Germany

Using time resolved scanning tunneling microscopy we have studied selected dynamic phenomena in adlayers of bis(terpyridine)derivatives BTP on HOPG, Au(111), and Ag(111) at around room temperature. While the mobility of single molecules is too high for a direct observation in this temperature region, it is possible to evaluate the mobility of island edges and domain boundaries of ordered two dimensional networks. This reveals important information about typical process rates in self assembly processes. The roles of molecule-molecule and molecule-substrate interactions, with a particular focus on anisotropy effects due to the shape of the molecules, are discussed.

O 16.7 Mon 15:45 H42

A structural and electronic phase transition at a metal-organic interface: The role of intermolecular interactions — •S. Soubatch[1], L. Kilian[2], A. Hauschild[3], R. Temirov[1], A. Schöll[2], A. Bendounan[2], F. Reinert[2], F. S. Tautz[1], M. Sokolowski[3], and E. Umbach[2] — [1]International University Bremen (Jacobs University Bremen as of spring 2007), Bremen, Germany — [2]Universität Würzburg, Würzburg, Germany — [3]Universität Bonn, Bonn, Germany

For the organic semiconductor 3,4,9,10-perylene-tetracarboxylic-dianhydride (PTCDA) adsorbed on the Ag(111) surface, it is found experimentally that molecules in the diluted and disordered phase, prepared at low temperatures, and the ordered commensurate monolayer phase are in significantly different adsorption states. This is deduced from comparison of their structural organization (LEED and STM), vertical bonding distances and intermolecular distortions (NIXSW), and the electronic properties (STS and UPS). The experimental data prove that the observed difference in properties of these two states is primarily caused by strong intermolecular interactions.

O 16.8 Mon 16:00 H42

A photooptical switch - azobenzene carrying alkanethiols on gold — Daniel Brete[1,2], Wolfgang Freyer[1], Cornelius Gahl[1], Sanja Korica[1,2], •Roland Schmidt[1,2], and Martin Weinelt[1,2] — [1]Max-Born-Institut, Max-Born-Str. 2A, 12489 Berlin — [2]Freie Univerität Berlin, Fachberecih Physik, Arnimallee 14, 14195 Berlin

The photoisomeric switch azobenzene can be linked to gold surfaces by alkanethiols forming self-assembled monolayers (SAMs, Au-S-(CH$_2$)$_n$-O-C$_6$H$_4$-N-N-C$_6$H$_5$). Sufficient decoupling of the azobenzene group from the surface is thereby necessary to maintain its ability to photoisomerize. Using the core-hole-clock technique and Resonant-Raman-Auger Spectroscopy we prove that the decay of the N1s-LUMO excitation is independent of chain lengths down to n=3. The resonance lifetime of $\geq$ 20 fs falls in the timescale of trans-cis conformational photo-isomerization. Functionalizing the azobenzene entity with an electronegative CF$_3$ endgroup leads to a shift of the HOMO and HOMO-1 orbitals and modifies the oscillator strength of the corresponding transitions. This may be relevant for the switching process. All SAMs are well oriented with the azobenzene entity adopting the trans-isomerization. Admixture of alkanes to the layer does not affect the molecular orientation. NEXAFS spectra show clear indication for optical switching of the molecules upon optical excitation at 350 nm.

O 16.9 Mon 16:15 H42

DFT applied to functionalized Azobenzene: Towards a description of molecular switches on alkanethiol SAMs

— •Erik McNellis, Volker Blum, Patrick Rinke, and Karsten Reuter — Fritz-Haber-Institut, Faradayweg 4-6, D-14195, Berlin

Molecules with a reversible and controllable binary property are a research topic of increasing relevance. Azobenzene (C_6H_5-N_2-C_6H_5) and its derivatives represent one class of such 'molecular switches', with a known cis-trans isomerization in solution. In surface mounted geometries, ligands may be used to decouple the switch from the solid surface. The ligand may itself be chosen with a particular functionality in mind: e.g., an alkanethiol chain adds self-assembly capability to the molecular switch.

We employ density-functional theory (DFT) and linear response time-dependent DFT to study the effect of such ligands and different non-polar or polar head groups (e.g. CF_3, CH_3) on the molecular geometry and the resonant excitation energies, discussing the results in the context of self-assembled monolayers (SAMs). Depending on the nature of the linker group (e.g. O, NH, CH_2) used to bind the alkane, as well as the employed head group, the excitation energies may be tuned by approximately 0.5 eV. The computed structural properties provide conceptual insights into steric effects and a possible orientational order of the molecular switches.

O 16.10 Mon 16:30 H42

Photothermal patterning of organic monolayers: Monolayers from fluorinated silanes and alkynes

— •Benjamin Klingebiel, Steffen Franzka, Nils Hartmann, and Eckart Hasselbrink — Fachbereich Chemie, Universität Duisburg-Essen, Universitätsstraße 5, 45141 Essen

Organic monolayers offer great opportunities to modify the surface properties of solid substrates. Many advanced applications require patterned organic monolayers. Recently, we reported a simple photothermal procedure for patterning of alkylsiloxane monolayers grown on native silicon substrates [1]. A focused beam of an argon ion laser at a wavelength of 514 nm is used for rapid large-area patterning. Despite a laser spot diameter of about 2.5 microns line widths down to 200 nm are reached [1,2]. Here we present new results which focus on patterning of monolayers which are formed i) via coating of native silicon substrates in millimolar solutions of fluorinated silanes and ii) via hydrosilylation of H-terminated silicon substrates with long-chain alkynes. Similar to alkylsiloxane monolayers, these monolayers exhibit a high thermal and chemical stability. Hence, photothermal patterning, yields narrow lines with widths down to 300 nm and 400 nm, respectively. In order to determine the effective activation energies of the overall patterning process, the experimental data is analyzed considering a simple photothermal model.

[1] T. Balgar, S. Franzka, N. Hartmann, E. Hasselbrink, Langmuir 2004, 20, 3525 [2] D. Dahlhaus, S. Franzka, E. Hasselbrink, N. Hartmann, Nano Lett. 2006, 6, 2358

O 16.11 Mon 16:45 H42

Laser-assisted fabrication of nanostructured organic templates for the selective adsorption of gold nanoparticles into confined domains

— •Nils Hartmann, Daniel Dahlhaus, Steffen Franzka, and Eckart Hasselbrink — Fachbereich Chemie, Universitätsstr. 5, Universität Duisburg-Essen

A new laser-assisted procedure for the fabrication of nanostructured organic templates is reported. Octadecylsiloxane monolayers are grown on native Si(100) substrates. Subsequently these coatings are patterned using a focused beam of an argon ion laser. Local irradiation results in photothermal decomposition of the monolayers and provides a means for rapid large-area patterning with a lateral resolution significantly below the laser spot diameter [1]. In particular, at a spot diameter of about 2.5 microns, structures with a width below 100 nm are prepared. The patterned monolayers then are chemically functionalized via amination of the remaining hydrocarbon tails. The final chemical patterns represent functional templates which are suitable to direct the adsorption and self-assembly of nanoscopic components into micro- and nanostructured arrays [2]. In particular, citrate-coated gold nanoparticles with an average diameter of 16 nm are shown to self-assemble into one-dimensional arrangements, such as single chains.

1. T. Balgar, S. Franzka and N. Hartmann, Appl. Phys. A 82 (2006) 689.
2. D. Dahlhaus, S. Franzka, E. Hasselbrink and N. Hartmann, Nano Letters 6 (2006) 2358.

O 16.12 Mon 17:00 H42

Electrospray Ion Beam Vacuum Deposition of Organic Molecules and Inorganic Clusters

— •Stephan Rauschenbach, Nicha Thontasen, Nicola Malinowski, and Klaus Kern — Max-Planck-Institut for Solid State Research, Nanoscale Science Department, Heisenbergstr. 1, 70569 Stuttgart

Electrospray Ionization (ESI) is widely used as ionization technique for mass spectrometric applications in biology and organic chemistry, because of the unique destruction free ionization of even large biological molecules from solution.

In our experiment ESI is used to bring nonvolatile compounds into gas phase. An apparatus employing differential pumping, ion optical devices and time-of-flight mass analysis (TOF-MS) was constructed in order to deposit ions created by ESI under very controlled conditions on solid surface in ultra-high-vacuum (UHV). The samples can be analyzed ex-situ or in-situ by a variable temperature UHV-STM/AFM.

The technique is demonstrated by two examples: the deposition of clusters and the creation of monolayer films of organic salts. Various types of large inorganic clusters could be ionized and deposited. The layers of organic salts on the other hand were formed from small cluster ions of the type $A^+(AB)_n$. AFM images show single or double molecular layers depending on the substrate. On the surface the molecules can diffuse and align along substrate features like step edges.

S. Rauschenbach, F. Stadler, E. Lunedei, N. Malinowski, S. Koltsov, G. Costantini, K. Kern, *Electrospray Ion Beam Depostion of Clusters and Biomolecules*, Small **4** (2006)

O 16.13 Mon 17:15 H42

Abnormal pinning of the Fermi and vacuum levels in monomolecular self-assembled films

— Heejoon Ahn[1], James Whitten[1], and •Michael Zharnikov[2] — [1]Department of Chemistry, The University of Massachusetts Lowell, Lowell, MA 01854, USA — [2]Angewandte Physikalische Chemie, Universität Heidelberg, D-69120 Heidelberg, Germany

Ultrathin organic monomolecular films, while electric insulators, are generally believed to be in electrical contact with a photoelectron spectrometer when adsorbed on metal substrates due to electron tunnelling that results in alignment of the Fermi levels of the film and the spectrometer. We show, however, that this generally applicable model is incorrect for these systems and that energy level alignment in photoemission experiments occurs in a complex fashion, involving both vacuum and Fermi levels of the monomolecular film, conductive substrate, and the spectrometer. While the Fermi levels of the substrate and spectrometer are aligned, vacuum level instead of Fermi level alignment occurs between the substrate and the SAM. As a result, the binding position of the photoemission peaks related to the monomolecular film is not only determined by its chemical identity, but also by changes in the work function of the substrate and film itself. This effect should certainly be taken into account in drawing conclusions from photoemission spectra of self-assembled organic films and adsorbate systems.

O 17: Poster Session I (Nanostructures at Surfaces; Metal Substrates: Epitaxy and Growth; Methods: Scanning Probe Techniques; Phase Transitions)

Time: Monday 17:30–20:30 Location: Poster C

O 17.1 Mon 17:30 Poster C

Growth and characterization of carbon nanotubes on silicon carbide — •Reinhard Volkmer, Alexander Hartung, and Bernd Schröter — FSU Jena, IFK, Max-Wien-Platz 1, 07743 Jena

Due to their remarkable mechanical and electronical properties, carbon nanotubes (CNTs) have acquired a significant position in the field of nano research since the discovery in 1991. The defined growth of these tubes is an essential requirement for their utilization in nanoelectronics and nanooptics. Though CNTs with various parameters such as diameter, length, chirality or number of walls can already be produced in great quantities by standard practices like arc discharge, chemical vapor deposition (CVD) and laser ablation, the task of placing single tubes with the desired properties like chirality at defined positions is a not yet solved problem.

We used an alternative fabrication technique by growing carbon nanotubes on SiC(0001) surfaces in ultra high vacuum (UHV) [1]. The UHV environment allows the diversified characterization of the substrate surfaces and CNTs by means of microscopy (STM, AFM, SEM), spectroscopy (XPS) and electron diffraction (LEED) and pulls together the parameters of growth conditions and properties of the CNTs. We succeeded in growing single wall and Y-junction nanotubes at temperatures of about 1500°C whose position, alignment and characteristics depend on the substrate geometry and which feature a high purity because of the omission of catalysts in this technique.

[1] V. Derycke, R. Martel, M. Radosavljevic, F. M. Ross and Ph. Avouris, Nano Lett., Vol. 2, No. 10, 1043 (2002)

O 17.2 Mon 17:30 Poster C

Untersuchung chemisch funktionalisierter Kohlenstoffnanoröhen mittels Rastertunnelmikroskopie — •Peter Lauffer[1], Adrian Jung[2], Ralf Graupner[1], Andreas Hirsch[2] und Lothar Ley[1] — [1]Technische Physik, 91058 Erlangen — [2]Institut für Organische Chemie, 91054 Erlangen

Einwandige Kohlenstoffnanoröhren, die man sich aus dem nahtlosen Aufrollen von Graphen entstanden denken kann, besitzen eine Vielzahl faszinierender Eigenschaften. Besonders vielversprechend für zukünftige Anwendungen erscheint die Möglichkeit, Nanoröhren mit definierten chemischen Gruppen zu versehen, sie zu funktionalisieren, um zum Beispiel deren Löslichkeit zu beeinflussen. Die Funktionalisierung mit aromatischen Molekülen mittels der π-π-Stapelwechselwirkung bietet dabei den Vorteil, die Struktur der Nanoröhre intakt erhalten zu können. Gegenstand unserer Arbeit ist die Untersuchung dieser so funktionalisierten Nanoröhren mittels Rastertunnelmikroskopie. Damit konnte der Nachweis einzelner Funktionalmoleküle auf der Seitenwand erbracht werden und deren elektronische Eigenschaften durch Abbildung ihrer differentiellen Tunnelleitfähigkeit lokal dargestellt werden. Diese Ergebnisse sind in guter Übereinstimmung sowohl mit auf Au (111) adsorbierten Funktionalmolekülen als auch mit quantenchemisch berechneten Molekülorbitalen.

O 17.3 Mon 17:30 Poster C

Structural and electronic properties of SiC and BN nanotubes — •Björn Baumeier, Peter Krüger, and Johannes Pollmann — Institut für Festkörpertheorie, Universität Münster, Wilhelm-Klemm-Str. 10, 48149 Münster

The initial discovery of carbon nanotubes (NTs) in 1991 has sparked considerable interest in this kind of nanosized one-dimensional structures due to their unique physical properties and the associated potential for applications.

We present the results of a comparative *ab initio* study of composite single-walled SiC and BN nanotubes in zigzag and armchair configurations. Using pseudopotentials that incorporate self-interaction-corrections in density functional theory calculations, we arrive at reliable quantitative results for both structural and electronic properties of the respective bulk crystals, as compared to available experimental data. Within this approach, we investigate the dependence of the strain energy, Young modulus, atomic relaxation and electronic structure on NT diameter. Qualitatively, both wide-band-gap materials show similar behavior with respect to the formation of a radially buckled geometry upon atomic relaxation or the saturation of the Young modulus and band-gap energies for large NT diameters. The calculated fundamental gap of zigzag NTs varies more strongly for small and medium tube diameters than that of their armchair counterparts, which is due to a more pronounced curvature-induced rehybridization effect on conduction band states.

O 17.4 Mon 17:30 Poster C

Optical properties of self-assembled Pb nanowires on Si(335)/Au — •M. Klevenz, M. Möller, F. Neubrech, R. Lovrincic, and A. Pucci — Kirchhoff-Institut für Physik, Heidelberg

A macroscopic array of aligned lead nanowires was produced by molecular beam epitaxy on a vicinal Si(335)/Au surface under UHV conditions. The optical properties of this system were studied by infrared spectroscopy and reflection of light in the visible range. We were able to observe a phase transition and to characterize the nanostructure during the whole growth process. This was possible due to the observation of excited resonances in the wires which provide an insight into their size. The measurements were performed at different temperatures. Temperature dependent diffusion properties of the lead atoms lead to differences in the wire shape and size.

O 17.5 Mon 17:30 Poster C

Metallic nanostructures on silicon — •Jan Rönspies, Tammo Block, Svend Vagt, and Herbert Pfnür — Institut für Festkörperphysik, Abteilung Oberflächen, Leibniz Universität Hannover, Appelstr.2, 30167 Hannover, Germany

In our experiment we produced nanowires by a lithographic process with electron-beam stimulated thermal desorption of oxygen (EBSTD) in UHV from an ultrathin SiO_2 layer deposited on Si(557) substrates. Recently the Pb/Si(557) system was shown to exhibit a quasi one-dimensional conductance along the Si(557) step direction on a macroscopic scale, associated with a metal-semiconductor phase transition.

The electronic properties of low–dimensional systems are intimately related to their geometric structure. In ideal one dimensional systems the electron confinement is important. Particularly in one-dimensional systems the enhanced interaction is accompanied by instabilities, which can be seen by metal-insulator transitions measurements.

We apply EBSTD to bare windows of clean silicon with lateral dimensions down to $10nm$ in the oxide layer. Subsequent metal epitaxy leads to the formation of continuous thin metal nanowires in the window areas. We formed nanowires with a length of several hundred nanometers by using this lithographical method to perform measurements on only a few of these wires selected out of the "wire array"of the Pb/Si(557) system. We present first results of conductivity of such wires.

O 17.6 Mon 17:30 Poster C

Fermi-nesting in ordered Pb-chains grown on vicinal Si(557) — C. Tegenkamp[1], •T. Block[1], H. Pfnür[1], T. Ohta[2], J.L. McChesney[2], and K. Horn[3] — [1]Institut für Festkörperphysik, Leibniz-Universität Hannover, 30167 Hannover, Germany — [2]ALS, Lawrence Berkley National Laboratory, Berkley, CA. 94720, USA — [3]FHI der Max-Planck Gesellschaft, 14195 Berlin, Germany

The adsorption of 1ML Pb at low temperatures on Si(557) followed by annealing to 640K leads to the formation of Pb-chains with an interachain spacing of d=1.5nm as seen by LEED and STM. The closely packed Pb film on the micro-Si(111) facets forms locally a $\sqrt{3} \times \sqrt{3}$ structure, which shows in addition a 10-fold periodicity along the $[1\bar{1}0]$ direction. Conductivity measurements below 78K have shown that electronic transport occurs only along the chain direction, whereas insulating behavior is found in the perpendicular direction. Above 78K, the sytsem switches into a 2d-regime, i.e. activated transport is found in both directions. Using angle resolved photoemission (ARPES), we explored the origins of the quasi one-dimensional (1d) conductance found below 78K. The interchain distance is reflected directly by Umklapp structures in the $[11\bar{2}]$ direction close to E_F. As ARPES reveals further, ordering into the chain structure below 78K results in complete Fermi nesting in the $[11\bar{2}]$ direction and in energy reduction by band filling. The domain structure along the chains forms split-off valence bands with mesoscopic λ_F, responsible for the 1d conductance.

O 17.7 Mon 17:30 Poster C

Ab initio study of electronic confinement on stepped Cu(111) surfaces — •Pavel Ignatiev[1], Valeriy Stepanyuk[1], Andriy Klavsyuk[1], Wolfram Hergert[2], and Patrick Bruno[1] — [1]Max-Planck-Institut für Mikrostrukturphysik, Weinberg 2, D-06120 Halle, Germany — [2]Fachbereich Physik, Martin-Luther-Universität, Halle-Wittenberg, Friedemann-Bach-Platz 6, D-06099 Halle, Germany

We report on study of surface states on clean and decorated Cu(111) stepped surfaces by means of ab initio Korringa-Kohn-Rostoker (KKR) Green's function method [1]. Surfaces with the terrace width ranging from 12 to 21 A are considered. Confined electronic states are revealed close to the Fermi energy. This finding is in agreement with experiments of M. Hansmann et al. [2]. Our calculations confirmed that the position of such states strongly depends on the terrace width. The strength of the potential barrier at the step edges calculated using the Kronig-Penney model and our ab initio results is found to be in a good agreement with experimentally determined values. It is shown that the strength of the confining barriers on Cu(111) vicinals can be significantly affected by decoration of step edges with monoatomic Fe wires, similar to recent experimental finding of S. Shiraki et al. [3]. Due to spin-dependent scattering of surface-states electrons at Fe wires surface states become spin-polarized. The majority states remain unaffected, but the confinement picture of the minority states is suppressed by a strong scattering of surface-states electrons at the minority states on Fe wires. [1] P.A. Ignatiev et al., submitted to PRB [2] M. Hansmann et al. PRB 67, 121409 (2003) [3] S. Shiraki et al. PRL 92, 096102 (2004)

O 17.8 Mon 17:30 Poster C

The metal-insulator transition of Rb:TaS2 observed with PEEM — Jens Buck[1], •Ole Mühlfeld[1], Kai Rossnagel[1], Florian Kronast[2], Ruslan Ovsyannikov[2], Hermann Dürr[2], and Lutz Kipp[1] — [1]Christian-Albrechts-Universität zu Kiel — [2]BESSY, Berlin

The transition metal dichalcogenide TaS2 exhibits a change from metallic to insulating behavior upon deposition of rubidium. We present first results of this system studied by PEEM. Measurements with a spatial resolution of about 100 nm reveal the transition from metal to insulator in the presence of rubidium. Among other layered crystals, TaS2 shows the well-known formation of nanowire networks when rubidium is deposited. Here, evaporation-induced surface features with a mesh-like structure and a size distribution between some microns and the resolution limit were observed. They appear to be independent of local changes in rubidium concentration. The experiments were carried out at BESSY, beamline UE49-PGMa. This work was supported by the Deutsche Forschungsgemeinschaft, Forschergruppe 353.

O 17.9 Mon 17:30 Poster C

Stepped Si(111) surfaces as template for the growth of nanostructures — •Vasily Cherepanov, Konstantin Romanyuk, and Bert Voigtländer — Institute of Bio and Nanosystems (IBN 3), and cni - Center of Nanoelectronic Systems for Information Technology, Research Centre Jülich, 52425 Jülich, Germany

The preparation of template surfaces is a crucial step for the growth of nanostructures by self organization. A template surface with a desired arrangement of monoatomic steps can be used subsequently for deposition of materials which preferentially incorporate at the step edges. In this study we optimized the conditions to produce regular array of the slip steps on various inclined Si wafers. Applied external stress to a Si wafer forms an array of $(\bar{1}\bar{1}2)$ slip steps at Si(111) surface. New steps form by gliding crystal planes in the bulk during plastic relaxation of the wafer. Those new steps intersect with the surface steps which originate from the miscut of the wafer. Thus a network of "crossing"steps is formed at Si(111) surface. Subsequent step-flow growth of Ge can be used to produce a network of crossing Ge wires attached to the stepped template. Ge deposition on Bi terminated stepped Si surface was used to produce a network of crossing Ge nanowires on the atomic scale.

O 17.10 Mon 17:30 Poster C

Si-nanowires and 1D-electron confinement on SiC($1\bar{1}02$) — •Chariya Virojanadara, Martin Hetzel, and Ulrich Starke — Max-Planck-Institut für Festkörperforschung, Heisenbergstr. 1, D-70569 Stuttgart

SiC surfaces oriented perpendicular or diagonal to the basal plane should expose the complicated polytype stacking sequence along the c-axis and thus provide large unit cell surface periodicities. In combination with the typical electronic correlation effects between dangling bonds found on the basal plane surfaces this opens a route for intrinsic nanostructures with low-dimensional electronic states. On the 4H-SiC ($1\bar{1}02$) surface, i.e. an orientation cut diagonally within the bulk unit cell, surface phases of according periodicities can indeed be observed. After Si deposition and annealing to 800-900°C a Si-rich surface develops which shows a well-ordered (2×1) superstructure in low-energy electron diffraction (LEED). Scanning tunneling microscopy (STM) reveals the presence of adatoms that form atomic nanowires with a separation of the (2×1) unit cell size. These adatoms are positioned on top of a Si adlayer. From core level photoemission data the Si thickness can be calculated to be about 3 Å. A prominent surface state can be observed in the valence band spectra of this phase. Applying angle resolved ultra-violet photoelectron spectroscopy (UPS) to this state we can identify a one-dimensional electron confinement. Dispersion is only observed along the direction of the nanowires, not between the wires. The band width of about 0.2 eV corresponds well to the dangling bond bands observed for several basal plane surface phases.

O 17.11 Mon 17:30 Poster C

Chemical bonding identification in metal-organic chains of trimesic acid on Cu(110) — Rishav Chopra, •Chariya Virojanadara, Thomas Classen, Giovanni Costantini, Ulrich Starke, and Klaus Kern — Max-Planck-Institut für Festkörperforschung, Heisenbergstr. 1, D-70569 Stuttgart

Functional groups of hydrocarbon molecules provide chemical selectivity, e.g. for sensing or biological interactions, or can serve as linking key for the development of molecular networks on surfaces. In this context, trimesic acid (TMA) with its carboxylic groups can interact in different ways with surfaces. In the present work the adsorption of TMA is investigated on Cu(110). Scanning tunneling microscopy (STM) and low-energy electron diffraction (LEED) experiments show that molecular linking to Cu adatoms leads to ordered metal-organic chains. The detailed bond configuration of the molecule on the surface can be determined using X-ray photoelectron spectroscopy (XPS). Analysis of chemical shifts reveals that the link is provided by a dehydrogenation of the acid groups, i.e. carboxylate groups are connected via the oxygen atoms to the Cu substrate. At low coverage this takes place already at room temperature. A denser phase at higher coverage still contains carboxylic groups at room temperature. Dehydrogenation is only observed when the chain is fully developed after 220°C annealing. The oxygen-Cu coordination is different for the two phases and depends on the density of the molecular adsorbate.

O 17.12 Mon 17:30 Poster C

Investigation of plasmon resonances and Bragg diffraction properties of metallic nanostructures — •André Siegel, Manuel Rodrigues Gonçalves, Ralf Ameling, and Othmar Marti — University of Ulm, Institute of Experimental Physics, Albert-Einstein-Allee 11, D-89069 Ulm, Germany

The excitation of surface plasmon polaritons (SPP) at metallic nanoparticles using total internal illumination and the associated local field enhancement are of special importance for surface enhanced Raman scattering. In order to understand the coupling of light with SPPs in nanoparticles of complex shape, it is important to investigate the scattering of light by these particles.

Therefore, we have built a setup to measure the scattering of light of arrays of identical nanoparticles. We found, that the diffraction patterns – besides their dependency on size, lattice constant and material – are very sensitive to the shape of the particles. The results are compared to models of Bragg diffraction using different form factors.

Moreover, by varying the angle of illumination, it is possible to measure the dispersion relation and plasmon resonances of the SPPs for these arrays of nanoparticles.

O 17.13 Mon 17:30 Poster C

Fabrication of Clean Nanostructures on Metal Surfaces via Electron-Beam Induced Deposition — •Thomas Lukasczyk, Michael Schirmer, Hubertus Marbach, and Hans-Peter Steinrück — Lehrstuhl für Physikalische Chemie II, Universität Erlangen-Nürnberg, Egerlandstr. 3, D-91058, Erlangen

Electron-beam induced deposition (EBID) is a versatile method to produce well defined deposit structures in a controlled manner. Precursor molecules are decomposed via a sharp highly focussed electron beam, resulting in the deposition of the non-volatile fragments. In order to study EBID in an environment free of residual gases and to investigate its potential as a tool to generate pure nanostructured deposits, an ultra-high vacuum system is used. The integrated high resolution electron-column in combination with a lithographic package enables the controlled fabrication of nanostructures with lateral dimensions below 20 nm, which can be characterized via scanning electron microscopy, scanning tunneling microscopy and Auger electron spectroscopy. Iron pentacarbonyl, $Fe(CO)_5$, proved to be an effective precursor to generate iron structures of arbitrary shape on metal surfaces like rhodium or gold. Auger spectroscopy demonstrates a high purity of the deposits. The contamination level can be lowered even further by moderate heating. Exposure of the iron nanostructures to oxygen at elevated temperature leads to the formation of iron oxide, while the substrate surface remains almost unchanged. This demonstrates the capability to generate specific catalyst surfaces via EBID, which can be tuned to the requirements of certain reactions.

O 17.14 Mon 17:30 Poster C

Influence of pulsed laser light on gold triangles: Experiment vs. theory — •Andreas Kolloch[1], Juliane König-Birk[1], Kevin Shuford[2], George Schatz[2], Paul Leiderer[1], and Johannes Boneberg[1] — [1]Fachbereich Physik, Universität Konstanz, Fach M676, 78457 Konstanz — [2]Chemistry Department, Northwestern University

The optical properties of nanostructures are a topic of considerable current interest. In analogy to the near-fields around a Hertz dipole one expects in the optical range similar near-fields in the surrounding of nanostructures when they are illuminated with light. 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 laser pulses. The intensity is adjusted such that no influence of the illumination is detectable on the bare substrate. In the vicinity of the nanostructures, however, local ablation of the substrate is observed due to the intensity enhancement in the optical near-field. The resulting field distribution patterns depend on both the polarization of the laser light and the size of the triangles, as well as the arrangement of the nanostructures in the case of periodic arrays. A comparison with simulations shows qualitative agreement, but also some discrepancies with the experiments.

O 17.15 Mon 17:30 Poster C

AFM-Manipulation und optische Spektroskopie von Nanopartikeln — •Reiner Jansen, Alpan Bek, Thomas Klar und Jochen Feldmann — Ludwig-Maximilians-Universität München, Photonics and Optoelectronics Group, Amalienstraße 54, D-80799 München

Das AFM gekoppelt mit einem inversen Mikroskop ermöglicht die Beobachtung der Wechselwirkungen zwischen Nanopartikeln bei gleichzeitiger Variation ihrer Anordnung auf der Nanometerskala. So können die starke Abstandsabhängigkeit des Förster-Energietransfers (FRET) sowie Feldverstärkungseffekte gemessen werden. Die verwendeten Objekte mit einigen Nanometern im Durchmesser sind zum einen Gold-Kolloide, zum anderen fluoreszierende Nanopartikel. Mit der AFM-Spitze ist es möglich, je ein Goldpartikel und ein fluoreszierendes Partikel einander langsam und kontrolliert anzunähern. Nach jedem Manipulationsschritt wird die Veränderung im Fluoreszenzverhalten des Farbstoffes beobachtet. Ziel unseres Projektes ist es, eine graduelle Abstandsvariation zwischen Gold und Farbstoff zu erreichen um ein möglichst genaues Bild der Abhängigkeit des Energietransfers vom Abstand zu erhalten.

O 17.16 Mon 17:30 Poster C

Investigation of hafnium silicide nano structures on a Si(100) surface by means of photoelectron diffraction — •C.R. Flüchter[1,2], D. Weier[1,2], A. de Siervo[3], M. Schürmann[1], A. Beimborn[1], F. Schönbohm[1], S. Dreiner[1], M.F. Carazzolle[4], R. Landers[3,4], G.G. Kleiman[4], and C. Westphal[1,2] — [1]Experimentelle Physik 1 - Universität Dortmund, — [2]DELTA - Universität Dortmund, Maria-Goeppert-Mayer-Str. 2, D 44227 — [3]Laboratório Nacional de Luz Síncrotron, C.P. 6192, — [4]Inst. de Fisica - Universidade Estadual de Campinas,

Ultrathin films of hafnium were deposited on a silicon sample and annealed at 750°C forming rectangular shaped hafnium silicide islands on the surface. This silicidation process causes the thermal instability of HfO_2 films on silicon substrates. The latter system is under investigation in the field of high-k dielectrics to replace the system SiO_2/Si(100) in MOSFET devices [1]. We investigated the structure of the $HfSi_2$ island for different initial film thicknesses of hafnium by means of atomic force microscopy, photoelectron spectroscopy and photoelectron diffraction. Synchrotron light in the soft X-ray regime ($h\nu$=180 eV) was used for excitation. The resulting diffraction patterns were compared to calculated patterns of model structures by an R-factor analysis. As a result, we propose a modified zirconium silicide model to describe the structure of the system.

[1] C. J. Först, C.R. Ashman, K. Schwarz, and P.E. Blöchl, Nature **427**, 53 (2004)

O 17.17 Mon 17:30 Poster C

Spatially resolved eletronic and vibronic characteristics of a single higher diamondoid molecule — Yayu Wang[1], •Daniel Wegner[1], Xinghua Lu[1], Ryan Yamachika[1], Andre Wachowiak[1], Emmanouil Kioupakis[1], Steven Louie[1], Mike Crommie[1], Jeremy Dahl[2], Shenggao Liu[2], and Robert Carlson[2] — [1]Department of Physics, University of California at Berkeley, and Materials Science Division, Lawrence Berkeley National Laboratory, Berkeley, California, USA. — [2]MolecularDiamond Technologies, Chevron Technology Ventures, Richmond, CA, USA

Diamondoids are hydrocarbon molecules with diamond-like cage structures. Their structural complexity and chemical bond tunability make them ideal building blocks for creating novel nanostructures. We have investigated the recently discovered higher diamandoids at the single-molecule level using cryogenic scanning tunneling microscopy (STM) and spectroscopy (STS). STM images of individual 121-tetramantane molecules display pronounced nodal features across the molecular surface. Despite a large energy gap auround the Fermi level, STS and IETS reveal strong interactions between tunneling electrons and the diamondoid C-H stretch mode. The strength of the vibronic coupling has a distinct spatial distribution and peaks strongly at the topographic line nodes. Density-functional theory calculations have been used to reproduce the basic electronic structure and the peculiar geometric features of the higher diamondoids.

O 17.18 Mon 17:30 Poster C

Atomic Structure and Electronic Properties of Pt/Si(111)-$\sqrt{3}\times\sqrt{3}$ — •Florian Sandrock, Marc Wisniewski, Jörg Schäfer, and Ralph Claessen — Universität, Würzburg, Germany

Atomic Structure and Electronic Properties of Pt/Si(111)-$\sqrt{3}\times\sqrt{3}$

An increase of the electronic interaction is expected by decreasing the dimensionality of a system. In conjuction with suitably localized electrons, a metal-insulator transition can occur. While this is known from bulk structures, it is intriguing to look for such indications in surface systems. Metal adsorbates on semiconductor surfaces show a variety of two-dimensional superstructures which provide a playground to study such correlation phenomena. Among the quasi-two-dimensional reconstructions formed on the (111) surface of silicon and germanium, there are the $\sqrt{3}\times\sqrt{3}$ phases formed by e.g. Sn or Pb and other metals. In principle, such $\sqrt{3}\times\sqrt{3}$ systems can be instable against a two-dimensional charge density wave at low temperature. Moreover, the triangular lattice of this system is reminiscent of a crystal with a frustrated spin lattice, and it may be a candidate for a Mott transition at low temperature. A fascinating and yet sparsely examined system is the Pt/Si(111) $\sqrt{3}\times\sqrt{3}$ reconstruction, bringing a d-electron transition metal into play. Images obtained by scanning tunneling microscopy show a large area reconstruction. Dislocation defects lead to domains with threefold symmetry. Furthermore, ARPES measurements are underway which can serve to identify the metallicity of the system. Studies as a function of temperature will then explore possible phase transitions in this two-dimensional noble metal surface phase.

O 17.19 Mon 17:30 Poster C

Homogeneous preparation of ultrathin graphitic layers on hexagonal SiC surfaces — •Christian Riedl[1], Ulrich Starke[1], Jens Bernhardt[2], and Klaus Heinz[2] — [1]Max-Planck-Institut für Festkörperforschung, Heisenbergstr. 1, D-70569 Stuttgart — [2]Lehrstuhl für Festkörperphysik, Universität Erlangen-Nürnberg, Staudtstr. 7, D-91058 Erlangen

During the last years the peculiar properties of single and few-layer graphite (graphene) have attracted much interest. One method of choice to produce graphene with a high quality is the graphitization of SiC(0001)-surfaces by high temperature annealing in vacuum. The initial stage of graphitization is the $(6\sqrt{3}\times 6\sqrt{3})$R30°-reconstruction whose nature is discussed controversially. Whereas this structure is often entitled as "(6×6)" we explicitly show by means of Low Energy Electron Diffraction (LEED) and Scanning Tunneling Microscopy (STM) that the true periodicity of this inherent surface reconstruction is indeed $(6\sqrt{3}\times 6\sqrt{3})$R30°. The characteristic properties of graphene develop with the first layer of graphite on top of the $(6\sqrt{3}\times 6\sqrt{3})$R30°-structure. We analyze the growth of graphite layers by Auger Electron Spectroscopy (AES), LEED and STM. A different number of graphite layers results in a different corrugation in the STM-topography.

O 17.20 Mon 17:30 Poster C

Optical anisotropy in a self-assembled molecular film — •Thorsten Kampen[1], Simona Silaghi[2], Philipp Martin Schmidt[1], Rocio Cortes[3], Arantzazu Mascaraque[3], Norbert Esser[2], and Karsten Horn[1] — [1]Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, Germany — [2]Institute for Analytical Sciences, Berlin, Germany — [3]Depto. Física de Materiales, Universidad Complutense de Madrid, Madrid, Spain

Among the class of molecules which may be used as molecular switches, stilbene and its derivatives are promising candidates. Here, we present a study on the optical properties of self-assembled 4,4'-stilbene dicarboxylic acid (DCSB) layers on Cu(110). Photoemission spectra show the deprotonation of both carboxylic end-groups upon adsorption resulting in a chemical bonding of the molecule to surface. Scanning tunnelling microscopy images reveal that nucleation of the first molecular layer starts on top of the Cu step edges. The molecular growth proceeds from the stabilized steps into the terraces and two different chiral phases are observed: a metastable enantiomorphically pure phase and a thermodynamically preferred "racemic mixture". The derived surface dielectric anisotropy from the RAS spectra show features assigned to the Cu surface state which vanish for coverages above 1ML. Even for submonolayer coverages spectral features above 3eV are observed and are assigned to optical transitions in DCSB. Specifically, the HOMO-LUMO transition dipole moment which is oriented along the long symmetry axis of the molecule is almost oriented parallel to the $[1\bar{1}0]$ substrate direction. This is supported by STM.

O 17.21 Mon 17:30 Poster C

Towards Substrate-Independent Self-Assembling Monolayers: Investigation of Short Nylon Oligomers — •Manuela Pluntke[1], Sabine Letsche[2], Dirk Volkmer[2], and Othmar Marti[1] — [1]Institute of Experimental Physics, Ulm University, D-89069 Ulm, Germany — [2]Institute of Inorganic Chemistry II, Ulm University, D-89068 Ulm, Germany

Self-assembled monolayers provide a convenient and simple route to tailor the surface properties of a material. Our current efforts are focussed on the design of molecules which form stable two-dimensional monolayers on a broad variety of substrate surfaces. This requires a robust and close packing of molecules in a two-dimensional layer in which the supramolecular entities are stabilized by hydrogen bonds. For that purpose we have synthesized short nylon oligomers with different functional groups (e.g. N,N'-Bis(isonicotinyl)-1,6-hexamethylendiamin) and we have investigated their self-assembly on mica by means of atomic force microscopy and STM.

O 17.22 Mon 17:30 Poster C

Metal deposition into ordered molecular precursor layers - an STM study — •Achim Breitruck[1], Christoph Meier[2], Matthias Roos[1], Michael Roos[1], Harry E. Hoster[1], Ulrich Ziener[2], and Rolf J. Behm[1] — [1]Institut für Oberflächenchemie und Katalyse, Universität Ulm, 89069 Ulm — [2]Institut für Organsiche Chemie III, Universität Ulm, 89069 Ulm

Oligopyridine molecules vapor deposited onto single crystalline surfaces (HOPG, Au(111), Ag(111)) form highly ordered 2D networks, with a geometry depending on coverage, preparation temperature and substrate, which mainly result from C-H***N type hydrogen bridges between neighboring molecules. They can be imaged by UHV-STM with high resolution even at room temperature. Using these adlayers as precursors, we investigate the effect of metals subsequently vapor deposited onto these networks, which in many cases leads to the formation of new ordered metal organic structures. The influence of metal-molecule, metal-substrate, molecule-substrate and molecule-molecule interactions on the structure formation is discussed.

O 17.23 Mon 17:30 Poster C

Controlled fabrication of nanopit-patterns on a graphite surface using focused ion beams and oxidation — •Farhad Ghaleh[1], Robert Köster[1], Heinz Hövel[1], Lars Bruchhaus[2], Sven Bauerdick[2], Jürgen Thiel[2], and Ralf Jede[2] — [1]Universität Dortmund, Experimentelle Physik I, 44221 Dortmund — [2]Raith GmbH, Hauert 18, Technologiepark, 44227 Dortmund

We produced nanopits on a highly oriented pyrolytic graphite (HOPG) substrate arranged in a given pattern with a combination of Focused Ion Beam (FIB) irradiation and an oxidation process. The FIB irradiation was carried out using a newly developed dedicated FIB nano fabrication tool [J. Gierak et al., Appl. Phys. A 80, 187 (2005)]. After oxidation of the sample surface defects produced by single ions were imaged as one monolayer deep nanopits with scanning tunneling microscopy. The penetration depth of the ions could be measured by oxidation of the defective volume produced on points irradiated with high ion doses. An array of well separated nanopits with a periodicity of 50 nm could be produced.

O 17.24 Mon 17:30 Poster C

Modification of a HOPG and DLC/Si surface after radiation with the Free elektron LAser in Hamburg (FLASH) — •Björn Siemer[1], Carsten Thewes[1], Tim Hoger[1], Marco Rutkowski[1], Helmut Zacharias[1], Rolf Treusch[2], and Stefan Düsterer[2] — [1]Physikalisches Institut, Westfälische Wilhelms-Universität Münster, 48149 Münster — [2]HASYLAB, DESY, 22603 Hamburg

The new free electron laser (FEL) at FLASH combines high photon energy with high pulse energy. A diamond like carbon (DLC) and HOPG surface were illuminated with photon energies of 58 eV and 38 eV. The pulse energy averaged around $30\,\mu J/pulse$ and the intensity around $10^{12} W/cm^2$. DLC is commonly used for the construction of XUV mirrors. We use HOPG for chemical reactions on surfaces activated by XUV radiation. The action of these light pulses on DLC/Si and graphite under focussed radiation of 58 eV for DLC/Si and 38 eV for HOPG is analysed. A change in reflectivity is visible under a light microscope. But an AFM profile and measurements with a profilometer yield no topology changes for both surfaces. We further present recent results of STM measurements of the modified surface.

O 17.25 Mon 17:30 Poster C

Ion-induced surface ripples in silicon — •Andreas Biermanns[1], Joerg Grenzer[2], Stefan Facsko[2], Souren Grigorian[1], and Ullrich Pietsch[1] — [1]Institute of Physics, University of Siegen,Walter Flex 3, 57078 Siegen, Germany — [2]Institute of Ion Beam Physics and Materials Research,Bautzner Landstrasse 128,D-01328 Dresden, Germany

The morphological evolution of surfaces during ion-beam irradiation has attracted a significant interest due to possibility of the development and the controlling of selforganization in nanostructures. Pattering and texture on nanometer length scale at metal and semiconductor surfaces has become a topic of intense research. In particular the surface and subsurface ripple formation under 40Ar+ ion-beam irradiation of Si (100) crystal has been studied recently. Strong ripple formation has been found for an irradiation energy of 60keV and incident angles around 60°. During implantation a corrugated surface layer is formed, consisting of a strongly damaged, amorphous near-surface layer followed by a nearly sinusoidal shaped interface towards the crystalline material. In the present work, we investigate the onset and evolution of ripple-formation as function of implantation energy and incidence angle of the ion beam.

O 17.26 Mon 17:30 Poster C

Nanostructures on insects eyes—-Grasshopper — •Fengzhen Zhang[1], Alexander Schmatulla[1], Othmar Marti[1], and Harald Wolf[2] — [1]Institute of Experimental Physics — [2]Institute of Neurobiology

Abstract: Insects use compound eyes to see the world, a totally different way from us. They are excellent at detecting motions and have good ultraviolet vision. The optical system of the insects is the apposition of the ommatidia, each of which is an optical unit, composed of layers (around 100) and crystalline cones. The image formation of grasshopper eye is similar to telescopes, both of which are angle magnification. The aim of our research on insects' eyes is to get information about how the compound eyes look like both on the surface and inside. We will explain how the compound eyes function. AFM, a powerful tool for nanoscale measurement, is mainly used to get shapes and lengths of structures of the compound eyes. In general, single eyes are analyzed perfect hexagons in the center of the facets while they are squeezed on the edges. A statistics of the area of the hexagons shows differences among different parts of the eye. The images of the cross section of the grasshopper eyes are measured with AFM.

O 17.27 Mon 17:30 Poster C

CO ADSORPTION ON METAL SURFACES: A HYBRID DENSITY FUNCTIONAL STUDY WITH PLANE WAVE BASIS SET — •ALESSANDRO STROPPA, KONSTANTINOS TERMENTZIDIS, JOACHIM PAIER, and GEORG KRESSE — Institut für Materialphysik, Universität Wien, Sensengasse 8/12, 1090 Wien, Austria

We present a detailed study of the adsorption of CO on Cu, Rh, and Pt (111) surfaces in top and hollow sites. The study has been performed with a gradient corrected functional (PBE) and PBE0 and HSE03 hybrid Hartree-Fock density functionals within the framework of generalized Kohn-Sham density functional theory using a plane-wave basis set. As expected, the gradient corrected functional shows the tendency to favor the hollow sites, at variance with experimental findings that give the top site as the most stable adsorption site. The PBE0 and HSE03 functionals reduce this tendency. Indeed, they predict the correct adsorption site for Cu and Rh but fail for Pt. But even in this case, the hybrid functional destabilizes the hollow site by 50 meV compared to the GGA description. This suggests that hybrid functionals give an overall better description of the chemisorption of CO molecules on metal surfaces, but, in general, they still do not predict the correct adsorption site. The results of the total energy calculations are presented along with an analysis of the projected density of states and Loewdin charges

O 17.28 Mon 17:30 Poster C

STM study of the adsorption of Au on Mo(110) — •Wojciech Linhart[1], Adam Paruszewski[1], Izabela Cebula[1], Zbigniew Jankowski[1], Tomasz Kobiela[2], and Aleksander Krupski[1] — [1]Institute of Experimental Physics, University of Wrocław, Poland — [2]Institute of Physical and Theoretical Chemistry, University of Bonn,Germany

Scanning tunneling microscopy (STM) has been used for the first time to investigate the growth of ultrathin Au films on the Mo(110) surface.The measurements were carried out in a metal ultrahigh-vacuum. The Mo(110) crystal was cleaned by repetitive flashing at 1200 K in oxygen atmosphere to remove the residual carbon contamination. The oxygen was removed by flashing the sample at 2400 K. Gold was evaporated onto the crystal surface from a tantalum crucible surrounded by a tungsten resistive heater. The clean Mo(110) surface exhibits smooth single-step terraces ranging in width from 10 to 40 nm. These terraces are long and narrow and terminate in straight step-edges.

O 17.29 Mon 17:30 Poster C

STM study of the adsorption of Pb on Mo(110) — •Izabela Cebula, Wojciech Linhart, Zbigniew Jankowski, Dominika Grodzinska, Miroslaw Karpicki, Jakub Cichos, and Aleksander Krupski — Institute of Experimental Physics, University of Wrocław, Poland

Scanning tunneling microscopy (STM) has been used for the first time to investigate the growth of ultrathin Pb films on the Mo(110) surface.The measurements were carried out in a metal ultrahigh-vacuum. The Mo(110) crystal was cleaned by repetitive flashing at 1200 K in oxygen atmosphere to remove the residual carbon contamination. The oxygen was removed by flashing the sample at 2400 K. Lead was evaporated onto the crystal surface from a tantalum crucible surrounded by a tungsten resistive heater. The clean Mo(110) surface exhibits smooth single-step terraces ranging in width from 10 to 40 nm. These terraces are long and narrow and terminate in straight step-edges.

O 17.30 Mon 17:30 Poster C

UPS investigations of ultrathin Au films deposited on Pt(111) — •Tomasz Kobiela[1], Marco Moors[1], Wojciech Linhart[2], Iza Cebula[2], Aleksander Krupski[2], Conrad Becker[1], and Klaus Wandelt[1] — [1]Institute of Physical and Theoretical Chemistry, University of Bonn, Wegelerstr. 12, 53115 Bonn, Germany — [2]Institute of Experimental Physics, University of Wroclaw, pl. Maxa Borna 9, 50-204 Wroclaw, Poland

The structure and the local electronic properties of ultrathin Au films deposited on Pt(111) under UHV conditions have been studied by UPS and LEED. Investigations of bimetallic systems concerning morphology and adsorption properties are of great interest for the development of new catalysts with higher efficiency and durability. LEED measurements indicated an initial pseudomorphic growth of the Au films. UPS and PAX experiments showed a strong temperature dependence of the surface morphology. The Au-Pt surface prepared at 150 K is quite rough and smoothens significantly only above RT. At a temperature of 900 K gold starts to diffuse into the bulk forming a surface alloy with platinum and gold sites. The electronic properties of the resulting Au-Pt surface alloy seem to be nearly independent from the deposited Au amount in the investigated range of 1 - 10 monolayers. The removal of Au from the surface regions has been verified by STM. Adsorption experiments with various probe molecules showed a significant lower affinity of the Au-Pt surface alloy towards e.g. CO, but similar adsorption properties concerning butadiene in comparison to the clean Pt surface.

O 17.31 Mon 17:30 Poster C

Interaction of nitric oxide with the clean and oxygen-covered *Re*(10-10) surface — •Viktor Scherf, Christian Pauls, and Klaus Christmann — Institut für Chemie und Biochemie, FU Berlin, Germany

The molecular and dissociative adsorption of nitric oxide (NO) on the Re(10-10) surface was studied in UHV between 120 and $1200K$ by means of LEED, HREELS, TDS, and work function change ($\Delta\Phi$) measurements. On the initially oxygen-free Re surface and at $120K$, a minor fraction of NO spontaneously dissociates into O_{ad} and N_{ad}, while the majority of NO adsorbs in two molecular α states. Exposing NO at about $490K$, however, leads exclusively to the dissociation products. TDS exhibits both associative (first-order kinetics) and dissociative (second-order kinetics) desorption states, the work function increases (at $120K$) by $750meV$, and the N=O stretching vibrations ν_{NO} appear at $1706cm^{-1}$ (α_1 state) and at $1468cm^{-1}$ (shoulder, α_2 state) and are associated with NO held in the terminal and the bridge position, respectively. Pre-adsorption of oxygen ((1x5)-O-phase) facilitates molecular NO adsorption and causes a decrease of $\Delta\Phi$, thus reflecting a strong influence of co-adsorbed O on the *NO-Re* bonding chemistry. Our data are discussed and compared with similar investigations reported in the literature for Ru and Pt surfaces.

O 17.32 Mon 17:30 Poster C

Interaction of propene with the clean and oxygen-covered Au(110)*(1x2) surface — •Inga Spreine and Klaus Christmann — Institut für Chemie und Biochemie, FU Berlin, Germany

The adsorption and reaction of propene (C_3H_6) on the (1x2) reconstructed Au(110) surface has been studied in the temperature range from 30 K to 500 K by means of low energy electron diffraction (LEED), UV photoemission (UPS), temperature-programmed thermal desorption (TPD) and work function change ($\Delta\Phi$) measurements. On the clean Au surface increasing exposures $(0,06 \cdots 9,0$ L) lead to molecular adsorption in monolayers and multilayers; six different adsorption states can be attributed to chemisorbed and weakly held (physisorbed and condensed) propene, respectively. Upon heating, associative desorption sets in at 85 K and ends at 260 K. In the accessible temperature and coverage range, no ordered LEED phases can be observed indicating the absence of phases with long-range order. According to a recipe by Gottfried et al. [1] we used electron irradiation of physisorbed O_2 layers to accumulate reactive oxygen atoms at the surface and studied both the adsorption and reaction of propene with the O-covered Au(110). Our results are discussed and compared with similar investigations reported recently for the Au(100) and Au(111) surfaces [2,3].

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

O 17.33 Mon 17:30 Poster C

Phthalocyanines on Surfaces — •Stefan Kuck, Jens Brede, Francois Vonau, Germar Hoffmann, and Roland Wiesendanger — Institute of Applied Physics, University of Hamburg

Phthalocyanines are aromatic metallo-organic complexes with a single metal atom (M) in its central position and used, e.g., as dye molecules in industrial applications. Phthalocyanines have a planar geometry and are volatile and therefore ideally suited for experiments in ultra high vacuum with local probes. We prepared different Phthalocyanines (M = Cu, Co, Fe) on various substrates from bare metallic surfaces to sandwiched structures with insulating interface layers in an ultra high vacuum environment at a coverage below a monolayer. These molecular systems were then investigated by scanning tunneling microscopy and spectroscopy. The experiments were performed in an home-built variable-temperature scanning tunnling microscope working at temperatures down to 17 K. We will discuss the preparation and the role of the substrates on the orientation and on the electronic molecular states of studied Phthalocyanines.

O 17.34 Mon 17:30 Poster C

Interface molecular dipoles on metal surfaces — •Fernández-Torrente Isabel[1], Sergio Monturet[2], Katharina Jennifer Franke[1], Nils Henningsen[1], Nicolás Lorente[2], and José Pascual[1] — [1]Institut für Experimentalphysik, Freie Universität Berlin, Germany — [2]Université Paul Sabatier, Toulouse, France

Association of molecules with donor and acceptor character forms the so called molecular charge transfer complexes. Tetrathiafulvalene 7,7,8,8-tetracyanoquinodimethane (TTF-TCNQ) is a well-known example of a compound with a metal conducting behaviour governed by charge transfer interactions between the TTF (donor) and the TCNQ (acceptor). Here we report on the submonolayer growth of TTF on a Au(111) surface studied by Low Temperature Scanning Tunneling Microscopy. We find that TTF lies tilted on the surface and two S atoms dominate the adsorption. As a function of coverage we resolve several phases of the growth with different dimensionalities. In combination with DFT calculations we show that the growth is mediated by the balance between a repulsive and an attractive interaction. The repulsive force is associated to the creation of a dipole between TTF and the metallic surface while the attractive interaction is related to the formation of intermolecular H-bonds. At low coverage, molecules show primarily repulsion and they adsorb as monomers. As the coverage increases the attractive interaction gains importance and the molecules self-assemble in one and two dimensional structures.

O 17.35 Mon 17:30 Poster C

Adsorption and diffusion of CH$_3$S–Au(111) — •Andreas Franke and Eckhard Pehlke — Institut für Theoretische Physik und Astrophysik, Christian-Albrechts-Universität zu Kiel

Alkanethiols have adopted the role of model systems for the bonding of organic molecules on metal surfaces via sulfur anchors and the formation of self-assembled monolayers. So far, however, little is known about the detailed diffusion mechanism of such molecules on the surface. As a starting point, we present a DFT-study of the adsorption and diffusion of CH$_3$S–radicals on the Au(111)(1×1) surface in the low coverage regime using *ab initio* methods as implemented in the VASP code [1]. Unreconstructed Au(111) surfaces can be prepared under certain conditions at electrochemical interfaces [2]. In accordance with other DFT-studies (see e.g. [3] and references therein) we find that the most stable adsorption position is a tilted fcc-bridge geometry for all analysed coverages (Θ=1, 1/3, 3/16 molecules per $(\sqrt{3}\times\sqrt{3})$ Au(111) surface unit cell) with a S-Au bond strenght of 1.86 eV ($\Theta = 1$) to 1.99 eV ($\Theta = 3/16$) and a tilt angles of 51° and 50° to the surface normal. Using the nudged elastic band (NEB) and the dimer-method, local transition states along the minimum energy path with diffusion barriers of 130 meV, 240 meV and 270 meV are identified. Calculations for CH$_3$S adsorbed ontop of Au adatoms are underway.

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[3] C. Masens, M.J. Ford, M.B. Cortie, Surf. Sci. **580**, 19 (2005).

O 17.36 Mon 17:30 Poster C

Towards real surfaces: adsorption of ferrocene dithiolate between defective Ag(111) surfaces — •Thomas Bredow[1], Herbert Pfnür[2], Christoph Tegenkamp[2], and Jörg Meyer[3] — [1]Universität Bonn, Institut für Physikalische und Theoretische Chemie, Wegelerstr. 12, 53115 Bonn, Germany — [2]Leibniz-Universität Hannover, Institut für Festkörperphysik, Appelstr. 2, 30167 Hannover, Germany — [3]Fritz-Haber-Institut, Faradayweg 4-6, 10033 Berlin, Germany

In recent experiments ferrocene-1,1'-dithiol (FDT) has been successfully tested as a molecular contact between silver electrodes. A large conductance without activation thresholds was observed and confirmed by theoretical studies. Our earlier model calculations considered FDT adsorption at perfect Ag(111) surfaces. As real electrode surfaces are expected to contain defects such as adatoms, steps and vacancies, the adsorption of FDT at defective Ag(111) surfaces has been studied. Periodic slab calculations are performed at DFT level with the plane-wave code VASP employing the projector-augmented wave method. Based on our previous experience FDT is adsorbed dissociatively as thiolate via the sulfur atoms. Various adsorption sites above or near single point defects or small 2x2 terraces are considered. We found that FDT-surface interaction is substantially enhanced by the presence of defects. The molecule is slightly deformed for optimal bond formation with the surface atoms. The projected density of states near the Fermi level is compared to previous results for the perfect surfaces and related to the measured conductivity.

O 17.37 Mon 17:30 Poster C

Photoelectron microscopy on inhomogeneously alkali adsorbed transition-metal dichalcogenides — •Dirk Rahn[1], Hans Starnberg[2], Jens Buck[1], Sönke Harm[1], Kai Rossnagel[1], and Lutz Kipp[1] — [1]Institut für Experimentelle und Angewandte Physik, Universität Kiel, D-24098 Kiel, Germany — [2]Department of Physics, Göteborg University and Chalmers University of Technology, SE-41296 Göteborg, Sweden

The behavior of alkali metals deposited on transition-metal dichalcogenides (TMDC) is of great interest in basic research and in applications, for example in battery development.

The question in which way the alkali metal adsorbs on the TMDC is not finally answered. On the one hand, a certain amount of alkali atoms intercalates into the van der Waals gaps of the TMDC, while a small amount remains at the surface. On the other hand, the formation of nano-structures in the uppermost layer is observed. To get better insight into the differences between the two scenarios and to determine in particular the diffusion length of the alkali atoms on the TMDC surface, we have prepared samples with two different concentration domains. We have investigated such a sample with the photoelectron microscope at BL 31 at the Max-lab in Lund (Sweden) with a spacial resolution of 4 μm. Photoelectron images of the sample surface at constant kinetic energies and photoelectron spectra with different alkali metal concentrations for TaS$_2$ and TaSe$_2$ will be presented.

This work is supported by the DFG Forschergruppe FOR 353.

O 17.38 Mon 17:30 Poster C

Development of a fast SPM controller — •Christopher Zaum and Karina Morgenstern — Institut für Festkörperphysik, Gottfried Wilhelm Leibniz Universität , Appelstr. 2, D-30167 Hannover, Germany

Results in scanning probe microscopy depend heavily on the quality and stability of the utilized microscope controller. Therefore commercial SPM controllers make up roughly half the price of a microscope assembly. We developed a low-cost SPM controller based on National Instrument's CompactRIO real-time system. The controller features a low noise level, scan speeds up to one image per second, and full remote access over Ethernet at only tenth of the price of a commercial electronics. Furthermore, our system can control different piezo scanners, supplies two HV-channels for external approach mechanism, and controls the approach-process over a build-in RS-232 interface. The SPM controller is accessed via a menu-driven software based on LabVIEW. It offers a full range of microscope control options as well as advanced image processing and analyzing functions in a multi-monitor environment. Due to its compact and lightweight design, our SPM controller is part of the SONOS-project of the European Space Agency.

O 17.39 Mon 17:30 Poster C

Measurement of stress in AFM cantilevers by Raman spectroscopy — •Michael Bauer, Alexander M. Gigler, and Robert W. Stark — Crystallography, Dep. Earth and Environmental Sci., Ludwig-Maximilians-Universität München, 80333 München, Germany

The most prominent Raman peak of silicon at 523 wave numbers (1/cm) is known to shift upon stress. The peak shift is caused by a change in the crystal structure of the silicon and, hence, a change in the phonon bands under stress. This shift can be used to measure and visualize the spatial distribution of surface stresses in bent AFM cantilevers. The measurements were done using a confocal Raman microscope with diffraction limited lateral resolution. With a estimated resolution of 0.02 1/cm, the system has a nominal resolution of 9 MPa (shifts up to -12 1/cm were observed). The measured stresses can be compared qualitatively to results from finite elements methods (FEM). In this contribution, the Raman shift observed in the cantilever will be discussed in comparison to the shift introduced by the strain of a Vickers indent. The algebraic sign of the shift depends on the type of strain compressive or tensile. Together with the shift, a broadening of the peak and a lower maximum at the centre occurs. The procedure helps to tailor the cantilever properties such as resonant frequencies or bending shape to desired values.

O 17.40 Mon 17:30 Poster C

Material contrast measurement with a multifrequency AFM — •Maximilian Baumann, Alexander M. Gigler, and Robert W. Stark — CeNS and Crystallography, Dep. Earth and Environmental Sci., Ludwig-Maximilians-Universität München, 80333 München, Germany

Mapping topography and material contrast of a surface simultaneously with a scanning probe microscope is influenced by the crosstalk between the two. To avoid this, we present a new measurement technique, the so called multifrequency approach, as proposed by Rodriguez et al.[1]. In this mode of operation, a conventional AFM in non-contact tapping mode is operated with two different mechanical excitation frequencies, the first and second eigenmode of the cantilever. The first eigenmode is used to map the topography and to maintain close contact with the surface. The second eigenmode allows to determine the phase and amplitude signal with minimal topographical crosstalk. A lock-in amplifier is used to demodulate the signal with respect to the second eigenmode.

[1] T.Rodriguez et al.: Compositional mapping by excitation of the second cantilever mode, Appl.Phys.Letters 84 (3), pp.449-451 (2004).

O 17.41 Mon 17:30 Poster C

Measuring the Anisotropy of Atomic-Scale-Friction by Friction Force Microscopy — •Peter Köchling[1,2], Markus Schäfer[1,2], Jan-Erik Schmutz[1,2], and Hendrik Hölscher[1,2] — [1]Physikalisches Institut, Westfälische Wilhelms Universität Münster, Wilhelm-Klemm-Str.10, 48149 Münster, Germany — [2]CeNTech (Center for Nanotechnology), Heisenbergstr. 11, 48149 Münster, Germany

Friction anisotropy is defined as the dependence of friction on the relative orientation of two sliding surfaces. This fundamental tribological phenomenon is of high interest for the analysis of the origin of atomic scale friction [1-3].

In order to investigate the friction anisotropy between a Si-tip and different sample surfaces we included a rotation stage into a commercial Friction Force Microscope (FFM). In this way we are able to control the orientations between tip and sample without the limitation to specific samples [1,3] or sensors [2].

Using this experimental set-up we measured frictional properties like adhesion and friction coefficients in dependence of the sample orientation. We will compare these results with theoretical predictions and published experiments.

[1] Liley et al. Science 280, 273 (1998)

[2] Dienwiebel et al. Phys. Rev. Lett. 92, 126101 (2004)

[3] Park et al. Science 309, 1354 (2005)

O 17.42 Mon 17:30 Poster C

Force Interactions in Atomically Defined Tip-Sample Contacts — •D. Braun[1], J. Falter[1], A. Schirmeisen[1,3], H. Hölscher[3], U. D. Schwarz[2], and H. Fuchs[1,3] — [1]Institute of Physics, University of Münster, Münster, Germany — [2]Department of Mechanical Engineering, Yale University, New Haven, CT, USA — [3]Center for Nanotechnology (CeNTech), University of Münster, Münster, Germany

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. Meaningful comparisons with theoretical simulations would require knowledge of the exact position and identity of all atoms at the tip apex. A determination of the position of the last atoms of the tip is possible using field ion microscopy (FIM). We build an AFM for operation at low temperatures and under ultrahigh vacuum (UHV) conditions using a tuning fork (TF) as force sensor, allowing us to choose an appropriate material such as tungsten as tip material while maintaining atomic-scale resolution capabilities in AFM mode. The combination of an AFM operated in static contact mode with a FIM allows the correlation of interatomic forces with the atomic-scale tip configuration [1]. However, the dynamic mode of operation using the TF technique is expected to greatly enhance the force sensitivity of such measurements. First results obtained with both microscopy methods are presented. Tip radii obtained with the FIM are correlated to the force distance curves measured with the same tips.

[1]G. Cross et al., Phys. Rev. Lett. 80, 4685 (1998)

O 17.43 Mon 17:30 Poster C

The influence of temperature on stick-slip friction — •Lars Jansen[1,2], André Schirmeisen[1,2], Mykhaylo Evstigneev[3], Peter Reimann[3], and Harald Fuchs[1,2] — [1]Physikalisches Institut, Universität Münster, Wilhelm-Klemm-Straße 10, 4819 Münster — [2]CeNTech, Center for NanoTechnology, Heisenbergstraße 11, 48149 Münster — [3]Fakultät für Physik, Universität Bielefeld, 33615 Bielefeld

The stick-slip phenomenon, where the sliding body performs a sawtooth like motion over a surface, is believed to be a fundamental process in atomic friction.

We measured atomic scale stick-slip friction on a HOPG surface with an atomic force microscope under ultrahigh vacuum conditions in a temperature range from 100 K to 300 K. In this work, we present our investigations of the temperature dependence of atomic friction.

On the one hand we show a direct analysis of the influence of temperature by measuring friction vs. scan-speed curves for different temperatures and compare our results with the thermally activated Thomlinson model as described by Sang et al. [1].

On the other hand we present a direct verification of our measurements with results predicted by rate-theory, where the thermal transitions are described by Kramer's rate and show that this theory only holds for fast sliding velocities [2]. We hypothesize that the failure of rate theory in the slow velocity regime is related to multiple contact formation at the tip sample contact.

[1] Sang et al., Phys. Rev. Lett. 84, 174301 (2001)

[2] Evstigneev et al., Phys. Rev. Lett. 97, 240601 (2006)

O 17.44 Mon 17:30 Poster C

Scanning mass spectrometer setup for spatially resolved reactivity studies on model catalysts — •Matthias Roos, Christian Schirling, Stefan Kielbassa, Joachim Bansmann, and Jürgen Behm — Institut für Oberflächenchemie und Katalyse, Universität Ulm, D-89069 Ulm

A scanning mass spectrometer with micrometer-scale resolution was developed for investigations on the catalytic activity of microstructured planar model catalysts. Products of local surface reactions can be detected via a fine capillary orifice in a differentially pumped quadrupole mass spectrometer. The position of the sample with respect to the capillary is controlled by three piezo-driven translators. The surface reactivity of a resistive heated sample can be depicted in a spatially resolved topogram, taking into account the influence of the distance between sample and capillary on the magnitude of the QMS signal and the lateral resolution.

Photolithographic structured reactive patterns on top of an inactive substrate enable investigations of mesoscopic transport effects such as coupling between catalytically active areas and of (reverse) spillover phenomena on one sample by varying the size and the distances of the active areas.

O 17.45 Mon 17:30 Poster C

A scanning tunneling microscope for application at 300 mK and 14 T. — •Viktor Geringer, Stefan Becker, Torge Mashoff, Marcus Liebmann, and Markus Morgenstern — II. Physikalisches Institut B, RWTH Aachen, Otto-Blumenthal-Straße, 52074 Aachen

We present a scanning tunneling microscope (STM) for operation at 300 mK in ultra high vacuum (UHV) and at magnetic fields of up to 14 T. The STM features two linear piezo drives with slip-stick mechanism: a z-approach motor for the piezo scanner and a x-y-positioning drive for the sample stage. Furthermore an in situ tip exchange is implemented in the system. The microscope exhibits a very compact and symmetric design to increase stability and resonance frequencies. We discuss the design concept and present first measurements at room temperature.

O 17.46 Mon 17:30 Poster C

Strategies for manipulation of nanometer-scale metallic islands in ultrahigh vacuum by atomic force microscopy techniques — •T. Mönninhoff[1], D. Dietzel[1,2], A. Schirmeisen[1], H. Fuchs[1,2], and U. D. Schwarz[3] — [1]Inst. of Physics, University of Münster, Germany — [2]Forschungszentrum Karlsruhe, Germany — [3]Dept. of Mechanical Engineering, Yale University, New Haven, USA

The fundamentals of friction are still insufficiently understood, in particular the relation between friction force and contact area. Conventional friction force microscopy is unsuitable in this regard due to the ill-defined tip-sample-contact. This limitation can be circumvented by investigating evaporated metal islands with a well-defined and clean contact to the substrate. Using appropriate scanning parameters for AFM contact mode operation, it is possible to move the metallic islands on the substrate. Simultaneously, the friction can be measured by the torsion of the cantilever. In this work, we have focused on the manipulation of antimony islands on graphite samples. Two different strategies have been applied. In the 1st approach, a predefined sample area has been scanned with a normal force close to the threshold of lateral manipulation. In this case, multiple manipulations of islands orthogonal to the fast scan direction make the interpretation difficult. Therefore a 2nd strategy has been developed, where high load was applied only at a few lines, yielding well-defined displacement events. Before and after the contact-mode manipulation the area was imaged using non-contact techniques, avoiding unwanted manipulation of small islands.

O 17.47 Mon 17:30 Poster C

Tunnelmikroskopie und -Spektroskopie von Terthiophen/Au(111) bei tiefen Temperaturen — •Anna Tschetschetkin[1], Berndt Koslowski[1], Christof Dietrich[1], Elena Mena-Osteritz[2], Peter Bäuerle[2] und Paul Ziemann[1] — [1]Institut für Festkörperphysik — [2]Institut für Organische ChemieII, Universität Ulm, 89069 Ulm

Wir berichten über erste Ergebnisse zur Untersuchung der elektronischen und vibronischen Eigenschaften von adsorbierten Oligothiophenen mittels Rastertunnelmikroskopie bei tiefen Temperaturen. Hierzu wurde in situ Terthiophen im Submonolagen-Bereich auf Au(111) aufgedampft. Die Moleküle adsorbieren zuerst statistisch verteilt auf der Metalloberfläche und gehen im Laufe der Zeit oder induziert durch den Tunnelstrom in eine geordnete Phase über. Die Moleküle richten sich hier an der Herringbone-Rekonstruktion der Goldoberfläche aus indem sie sich senkrecht zu den Solitonenwänden und bevorzugt in die fcc-Bereiche legen, ohne die Herringbone-Rekonstruktion erkennbar zu stören. Dies drückt sich in der elektronischen Struktur aus, indem auf den Molekülen immer noch der Shockley-artige Oberflächenzustand der Au(111)-Oberfläche gemessen werden kann. Während sich die im L-Gap des Goldes liegenden Molekülzustände bei ca. +2 eV (LUMO) einwandfrei von der Unterlage abheben, scheinen die Molekülzustände bei -2 eV (HOMO) so mit den d-Zuständen der Unterlage zu hybridisieren, dass sie mittels STS nicht von der Unterlage unterschieden werden können.

O 17.48 Mon 17:30 Poster C

Preparation and Characterization of Silicon Carbide Surfaces for Scanning Probe Microscopy Studies — •Kai Ruschmeier[1], Domenique Weiner[1], André Schirmeisen[1], Harald Fuchs[1], Nabi Aghdassi[2], Ralf Ostendorf[2], and Helmut Zacharias[2] — [1]CeNTech, Center for NanoTechnology, Heisenbergstraße 11, 48149 Münster — [2]Physikalisches Institut, Universität Münster, Wilhelm-Klemm-Straße 10, 48149 Münster

Silicon carbide (SiC) is a semiconductor that due to its unique properties is particularly well suited for electronic devices under extreme conditions, such as high temperature, high voltage and high frequency. However, the fabrication of adequate substrate surfaces, which is an important step in the production technology of high performance devices, is difficult because of its mechanical hardness and chemical inertness. We applied hydrogen etching at high temperatures to epilayer SiC substrates to reduce scratches of the polishing process and prepared different surface configurations by simultaneous annealing and evaporation of Si at different sample temperatures. We used LEED to verify several reconstructions such as (1×1), (3×3) and $(\sqrt{3}\times\sqrt{3})$. Additionally, the surface was analyzed with Auger electron spectroscopy (AES) and inverse photoemission spectroscopy (IPES). We applied scanning tunnelling microscopy (STM) in ultrahigh vacuum to analyse the surface topology at different stages of the preparation process. Our aim is to study different surface configurations with noncontact atomic force microscopy (NC-AFM) at the atomic scale.

O 17.49 Mon 17:30 Poster C

Phase-controlled Homodyne Interferometric Detection for s-SNOM — •Marcus Cebula, Susanne Schneider, and Lukas Eng — Institute of Applied Photophysics, TU Dresden, D-01062 Dresden

Apertureless or scattering-type scanning near-field optical microscopy (s-SNOM) is a versatile technique for high-resolution optical investigations of various materials. Common systems contain homodyne or heterodyne interferometric detection with lock-in demodulation to analyse the optical near-field signal. These methods are restricted in there application especially concerning their wavelengths range.

To eliminate these restrictions, a phase-controlled homodyne interferometric setup was designed. This setup can be used in the entire near-UV to far-IR spectral range. It consists of an enhanced homodyne interferometer containing a phase-modulated reference beam. By using additional lock-in demodulation and controlling techniques, a wavelength independent phase-regulation and therewith the possibility to measure both the optical amplitude and phase of the near-field signal, becomes available. The two signals can be measured simultaneously and also up to higher harmonic modes.

Our setup is designed to allow interferometric near-field measurements by the use of a free-electron laser, available at the Forschungszentrum Rossendorf. This precisely tunable light source covers the wavelength regime from 4 to 100 micrometer, and was used up to now for near-field optical investigations of organic thin films and ferroelectric single crystals by means of a direct intensity analysis.

O 17.50 Mon 17:30 Poster C

Conductivity measurements using a beetle-type double-tip STM — Philipp Jaschinsky, Josef Mysliveček, Peter Coenen, Helmut Stollwerk, Gerhard Pirug, and •Bert Voigtländer — Institut für Bio- und Nanosysteme (IBN 3) und Center for Nanoelectronic Systems for Information Technology (CNI), Forschungszentrum Jülich, 52425 Jülich, Germany

We demonstrate applications of a double-tip scanning tunnelling microscope (STM) with a scanning electron microscope (SEM) in ultrahigh vacuum (UHV) environment [P. Jaschinsky et al., Rev. Sci. Instrum. 77 (2006), 093701]. This new instruments consists of two beetle type STM's stacked into each other. The ability of this apparatus to work at the nanoscale will be shown. Since the positioning of the two tips can be controlled down to 50nm by an add-on electron column, it was possible to provide direct mechanical contact of the STM tip to nanosized GaAs/AlGaAs resonant tunnelling diodes and measure I/V curves of these diodes. Furthermore, due to the compact design, both STM's exhibit a high stability which facilitates atomically resolved imaging with each tip. The stability allows also non-destructive electrical contacts to surfaces via the tunnelling gaps. Two-point electrical measurements via tunnelling contacts on the Si(111)-7×7 surface will be presented as function of the distance of the probe tips and compared to a model for the charge transport on this surface.

O 17.51 Mon 17:30 Poster C

Automatisierte Bildanalyse von Rasterkraftmikroskopieaufnahmen — •Christian Franke[1,2], Marcus Böhme[2], Enrico Kienel[1], Sabine Scherdel[2], Nicolaus Rehse[2] und Robert Magerle[2] — [1]Graphische Datenverarbeitung und Visualisierung, TU Chemnitz, D-09107 Chemnitz — [2]Chemische Physik, TU Chemnitz, D-09107 Chemnitz

Mit Hilfe der Rasterkraftmikroskopie lässt sich die Strukturbildung von dünnen Blockcopolymerfilmen in situ beobachten. Für die Auswertung dieser Experimente ist eine umfassende Bildverarbeitung nötig, die eine quantitative Erfassung von Strukturen im Realraum erlaubt. Dabei kommen Algorithmen zur Filterung, Binarisierung und Skelettierung zur Anwendung. Da diese Art der Auswertung oft Wochen oder Monate in Anspruch nimmt, haben wir begonnen die Bildverarbeitung echtzeitfähig zu realisieren. Dazu wurden von uns einige effiziente Algorithmen implementiert, so dass schon während des Experiments charakteristische Defektstrukturen erkannt werden können. Das Ziel ist bereits während des Experiments auf Änderungen zu reagieren und so gezielt Parameter zu verändern, die die Strukturbildung beeinflussen. Weiterhin ist geplant, diese Algorithmen auch in der Nanotomographie einzusetzen, bei der ebenfalls große Mengen an Rasterkraftmikroskopiebildern anfallen.

O 17.52 Mon 17:30 Poster C

Nanotomography of polystyrene-*block*-polybutadiene block copolymer — •Christian Dietz, Eike-Christian Spitzner, Sabine Scherdel, Nicolaus Rehse, and Robert Magerle — Chemische Physik, TU Chemnitz, D-09107 Chemnitz

Thin films of polystyrene-*block*-polybutadiene block copolymer (SB) form self organized structures during solvent annealing. At the given composition of the copolymer the polystyrene phase can form different morphologies. We find cylinders lying perpendicular or parallel to the surface or perforated lamellae depending on the film thickness and the solvent concentration. Using Nanotomography, a layer by layer volume imaging technique based on scanning probe microscopy (SPM), we are able to study the volume structure of layers beneath the surface of such films. An improved in-situ etching technique is introduced, where the etching is directly executed in an SPM liquid cell connected to reservoirs of water and an etchant. Here we use a solution of potassium permanganate in sulfuric acid for stepwise eroding the surface of the polymer. The water is used for flushing the liquid cell after each etching step and for imaging the surface in water. The liquid flow is controlled with solenoid valves, which allow for an automated etching/flushing/imaging protocol which is integrated into the SPM software. We present our latest results achieved with this new method on defects of SB films.

O 17.53 Mon 17:30 Poster C

Experimental setup of a combined scanning tunnelling microscope and atomic force microscope at ultrahigh vacuum conditions and low temperature — •Thomas König, Georg Hermann 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

Scanning tunnelling microscopy (STM) is sensitive to the electronic structure of conducting and semiconducting samples. A different technique which has been improved over the last years is the atomic force microscope (AFM). This technique gained atomic resolution on metals [1], semi conductors [2] and insulators [3] and has still not reached its limit in scientific work. Here we present the experimental setup and challenges of our combined STM and AFM in an ultrahigh vacuum chamber at low temperatures. Our setup is similar to the one developed by P.S. Weiss et al. [4]. An insight into the sensor setup of the microscope will be given as well as description of our amplifier arrangement [5]. Moreover we point out the next challenges we are facing on the way to enhanced the sensitivity of our combined STM and AFM.

[1] Ch. Loppacher, M. Bammerlin, M. Guggisberg, S. Schär, R. Bennewitz, A. Baratoff, E. Meyer, H.J. Güntherrodt, Phys. Rev. B, 62, 16944 (2000). [2] Y. Sugawara, M. Ohta, H. Ueyama, S. Morita, Science, 270, 1646 (1995). [3] C. Barth and M. Reichling, Nature, 414, 54 (2001). [4] P.S. Weiss, D.M. Eigler, NATO ASI Series E, 235, 213 (1993). [5] H.-P. Rust, M. Heyde, H.-J. Freund, Rev. Sci. Instr., 77, 043710 (2006).

O 17.54 Mon 17:30 Poster C

Miniaturised Columnar Sensors for Ultrasensitive Mass Detection — •Jenny Kehrbusch[1,2], Matthias Hullin[1], and Egbert Oesterschulze[1,2] — [1]Physics and Technology of Nanostructures, University of Kaiserslautern, D-67663 Kaiserslautern, Germany — [2]Nano+Bio Center, University of Kaiserslautern, Germany

Cantilever based microsensors are commonly used as ultrasensitive mechanical balances operating in gases and liquids. They are sensitive to changes of the viscosity of the surrounding fluid, chemically induced surface effects, and mass loading of their surface. So far their sensitivity with respect to mass loading in fluidic media is limited due to the strong viscous damping of the vibrating cantilever. The quality factor in liquids is by orders of magnitude smaller compared to gases even with active stimulation. Furthermore, the huge dimension of conventional cantilevers hinders to achieve high quality factors.

To overcome this limitation an improved concept of a columnar strongly miniaturized sensor is introduced. This sensor is oscillating in air where only the top surface is immersed in the liquid analyte. Thus both the quality factor and the signal-to-noise-ratio are improved. The new design combines additional advantages. Instead of an intricate double-sided fabrication process, simple single sided few steps manufacturing applying high aspect ratio deep plasma etching offers the possibility of further miniaturisation. Reduction of the geometrical dimensions implies higher resonance frequencies and thus an improved sensitivity per area. This is an important issue for the application of miniaturized balances, e.g. single-cell detection in liquid media.

O 17.55 Mon 17:30 Poster C

A UHV-STM system for measurements at 4 K with 3D-rotatable magnetic field — Torge Mashoff, Marco Pratzer, and •Markus Morgenstern — 2. Physikalisches Institut B, RWTH Aachen, Otto-Blumenthal-Straße, 52074 Aachen

We designed and built a 3-chamber ultra high vacuum system with a 4.2 K cryostat containing three superconducting magnets which allow us to apply fields of 7 T, 3 T and 0.5 T in different directions and a full rotatable field of 0.5 T. The system will be equipped with a homebuilt scanning tunnelling microscope providing a tip exchange mechanism and a sample positioning stage. The STM features a very compact design to increase its stability and resonance frequencies. The satellite chambers contain several devices for sample and tip preparation including heating up to 2300 K, sputtering and material evaporation. The whole system is placed on damping legs inside an acoustically insulating room. First test measurements will be presented.

O 17.56 Mon 17:30 Poster C

Higher harmonics and frequency mixing in electrical force microscopy (EFM) — •Benjamin Graffel[1], Falk Müller[2], Anne-Dorothea Müller[2], and Michael Hietschold[1] — [1]Chemnitz University of Technology, Institute of Physics, 09107 Chemnitz, Germany — [2]Anfatec Instruments AG, 08606 Oelsnitz (V), Germany

Electrical force microscopy (EFM) in the dynamic non-contact mode is a suitable technique to measure local distributions of surface potentials on electronic devices as well as to detect different doping concentrations in semiconductors. The electrical force between tip and sample is proportional to the derivative of the capacitance of the tip-sample arrangement with respect to the tip-sample distance z and proportional to the potential difference U squared. In our experiments this voltage consists of a direct voltage and an additional alternating voltage with the frequency f_{el}. While the capacitance of a completely metallic tip-sample arrangement only depends on z, it also depends on U in the case of a semiconductive sample.

In this work we show that these nonlinear effects lead to further signals at higher harmonics of f_{el} and at frequencies that arise from mixing with the mechanical excitation frequency of the oscillating cantilever. The frequency spectrum of the cantilever was measured for different parameters such as various set points and different values of U. Detailed studies of the distance dependencies in connection with imaging indicate that the lateral resolution can be improved by detecting signals at mixed frequencies.

O 17.57 Mon 17:30 Poster C

Dynamic Force Spectroscopy on Gadolinium Islands epitaxially grown on W(110) — •Rene Schmidt, Alexander Schwarz, and Roland Wiesendanger — Institut für Angewandte Physik, Universität Hamburg,

Gd/W(110) is prepared in UHV by evaporating gadolinium onto a clean tungsten substrate. Additional annealing leads to the growth of Gd islands on a base Gd-wetting layer. Atomic force microscopy in the dynamic mode using the frequency modulation technique (FM-AFM) and a Gd coated tip is employed for imaging these islands. Some parts of the Gd-islands are covered by hydrogen, which is the main compound present in the residual gas of the UHV-system. Hydrogen locally alters the work function of the Gd islands[1] and can therefore be distinguished by bias spectroscopy. Moreover, the application of dynamic force spectroscopy enables to quantify the complex interaction of the different surface species on a local scale. With the focus on the distance dependence of the forces between tip and surface, we perform single $\Delta f(z)$-curves while retracting into the long-range regime and single curves and spectroscopy fields whilst approaching the surface. As all the curves are taken with varying amplitudes due to the feedback regulation, the force-calculation uses a formalism given by Schirmeisen *et al*[2]. A model of the tip-surface interaction potential allows to fit the force-distance-curves and to determine the influence of the hydrogen on the tip-sample force.

[1] M. Getzlaff *et al.*, Phys. Rev. B **59**, 8195 (1999)

[2] A. Schirmeisen *et al.*, Nanotechnology **16**, S13 (2005)

O 17.58 Mon 17:30 Poster C

Scanning tunneling spectroscopy on the chalcopyrite solar cell absorber material Cu(In,Ga)Se$_2$ — •Harry Mönig[1], Sascha Sadewasser[2], Ahmed Ennaoui[2], Christian Kaufmann[2], Timo Kropp[2], Iver Lauermann[2], Tim Münchenberg[2], Rodrigo Saez-Araoz[1], Hans-Werner Schock[2], Ferdinand Streicher[2], and Martha Lux-Steiner[1,2] — [1]Freie Universität Berlin — [2]Hahn-Meitner-Institut Berlin

Cu(In,Ga)Se$_2$-based thin film solar cells have reached efficiencies close to 20 % [1]. Nevertheless, little is known about electronic transport and carrier recombination in this material on a microscopic scale. Especially grain boundaries in these polycrystalline materials are considered to play an important role in the performance of these solar cells [2]. We applied scanning tunneling microscopy and spectroscopy to gain more insight in the electronic microstructure of the material. Our results point to lateral electronic inhomogeneities on the absorber surface and to an enhanced density of states at grain boundaries. The influence of charging effects is discussed.

[1] M.A. Contreras et al. Prog. Photovoltaics Res. Appl. 13, 209 (2005)

[2] S. Siebentritt et al., Phys. Rev. Lett. 97, 146601 (2006)

O 17.59 Mon 17:30 Poster C

Towards the ultimate STM: design, modeling and characterization — •Mark den Heijer, Vincent Fokkema, Arjen C. Geluk, and Marcel J. Rost — Kamerlingh Onnes Laboratory, Leiden University, P.O.Box 9504, 2300 RA Leiden, The Netherlands

We developed a video-rate scanning tunneling microscope (STM) for *in-situ* and *real-time* observation of film growth. The key element in achieving high frame rates is a rigid mechanical structure, but the objective of imaging the surface during deposition poses severe restrictions on the geometry of the STM.

To achieve an optimal design we used finite element analysis (FEA) to model the complete STM. By including damping and piezoelectric properties, we obtained not only the eigenfrequencies and eigenmodes but also the real amplitudes of the vibrations. Finally we compare our calculated predictions with the measured characteristics of the microscope.

O 17.60 Mon 17:30 Poster C

Erste Experimente mit einem EBIT-basierten Edelgas-FIB — Falk Ullmann[1], •Frank Grossmann[1], Vladimir Ovsyannikov[1], Jacques Gierak[2], Erik Bourhis[2] und Günter Zschornack[3] — [1]DREEBIT GmbH, Dresden — [2]Technische Universität Dresden, Dresden — [3]LPN/CNRS Marcoussis, Frankreich

In FIB formierte hochfokussierte Ionenstrahlen sind von speziellen Interesse für Anwendungen in der Materialforschung, der Halbleiterindustrie und anderen Applikationsfeldern. Beschrieben wird hier die Formierung von Edelgasionenstrahlen in einer am LPN/CNRS Marcoussis entwickelten Nano-FIB-Säule, wobei als Quelle für die verwendeten Edelgasionen eine Dresden EBIT diente.

Die Dresden EBIT zeichnet sich durch eine gute Strahlemittanz, ihre Kompaktheit und ihre robuste Betriebsweise aus. In ersten Experimenten wurde das Funktionsprinzip eines Edelgas-FIB mit einem He^{1+}-Ionenstrahl demonstriert. Dabei wurde gezeigt, dass die Ionenstrahlen bis in den Submikrometerbereich fokussiert werden können.

An verschiedenen Beispielen wird vermittels von Sekundärelektronenspektroskopie die Leistungsfähigkeit der Anlage als Ionenmikroskop demonstriert und über den Einsatz von Helium- Argon- und Xenonstrahlen wird berichtet.

Prinzipiell können mit der Kopplung einer FIB-Säule mit einer Dresden EBIT auch Strahlen hochgeladener Ionen erzeugt werden. Mögliche Parameter einer solchen Anlage werden diskutiert.

O 17.61 Mon 17:30 Poster C

Design of a UHV/300 mK/9 T scanning tunneling microscope (STM) system — •Torben Hänke, Grzegorz Urbanik, Christian Hess, Marko Kaiser, Steffen Lessny, Ralf Voigtländer, Dirk Lindackers, and Bernd Büchner — IFW Dresden, Institute for Solid State Research, P.O. Box 270116, D-01171 Dresden, Germany

To study electronic and spin structures of high temperature superconductor (HTS) and related transition metal oxide materials (TMO) with high resolution scanning tunneling spectroscopy (STS) we are designing an ultra high vacuum (UHV) low temperature STM for temperatures down to 300 mK and magnetic fields up to 9 T. The microscope will be placed inside a UHV compatible ^{3}He cryostat which is integrated into a three-chamber UHV system for *in situ* tip and sample preparation including LEED/Auger analysis and molecular beam epitaxy (MBE). The STM is equipped with a tip-exchange mechanism, x, y-sample positioner and five additional leads to the sample to combine STM with transport measurements. For vibration isolation the entire system is mounted on a rigid supporting frame on air damping stages.

O 17.62 Mon 17:30 Poster C

Calibration of a thermal profiler in a scanning tunneling microscope in terms of measuring the near-field heat transfer — •Andreas Knübel, Uli Wischnath, and Achim Kittel — University of Oldenburg, Institute of Physics, Department of Energy and Semiconductor Research, 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 ultrahigh 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 resistance 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. We developed a specially designed set-up to evaluate the thermal resistance of the thermocouple tip under ultra-high vacuum conditions. Current experimental results are presented.

O 17.63 Mon 17:30 Poster C

Conductivity of Thin Films and Nanostructures Analysed by EFM — •Thomas Koch[1,2], Patrick Dupeyrat[1,2], Roland Gröger[1,2], Sheng Zhong[1,2], Norman Mechau[2], Gabi Schierning[2], Roland Schmechel[2], and Thomas Schimmel[1,2] — [1]Institute of Applied Physics, University of Karlsruhe, D-76128 Karlsruhe, Germany — [2]Institute of Nanotechnology (INT), Forschungszentrum Karlsruhe, D-76021 Karlsruhe, Germany

ITO (Indium Tin Oxide), Si or Ge nano-particles and small micron and submicron metal structures, mixed together with polymers and other carrier systems, are promising materials in the field of micro electronics and especially printable electronics to build thin conducting or dielectric films. Independently pure nano-particle systems or metals are also of interest for these applications.[1] For the exploration of these topics AFM is a powerful tool which can give information to identify the electric properties of materials at surfaces with local contrast on the nanometer scale. In this work we demonstrate the use of Electrostatic Atomic Force Microscopy (EFM) to map the conductive properties of nano-particle based sintered thin ITO films, of ITO/Baytron composite systems and of metal based ribbon cable nano structures. References 1. J. R. Sheats, J. Mater Res. 19 (7), 1974, (2004)

O 17.64 Mon 17:30 Poster C

Homoepitaxy under the influence of step edge barriers in the presence of screw dislocations — •Oliver Ricken[1], Alex Redinger[1], Joachim Krug[2], and Thomas Michely[1] — [1]II. Physikalisches Institut, Universität zu Köln — [2]Institut für Theoretische Physik, Universität zu Köln

The presence of screw dislocations solves the nucleation problem in crystal growth and allows growth even for supersaturation too small for nucleation. Growth spirals are also frequently observed in thin film deposition. In classical models for spiral growth a fixed slope of the resulting cone is predicted. Motivated by the observation of growth spirals in organic thin film growth with shapes similar to those of mounds in homoepitaxy with step edge barriers, we performed a set of model experiments. The growth of Pt on Pt(111) is studied by STM after creation of screw dislocations on the surface in a temperature range from 250 K to 450 K. The screw dislocations are produced by the mechanism of "dislocation loop punching" through He^+ bombardment. Growth spirals and normal mounds are observed after deposition and can be directly compared in the STM images. Both mound types show the typical 3D-growth mound forms with a plateau on top and deep crevices between them. However, growth spirals show much smaller plateaus and average base areas than normal mounds, but are, on average, taller. The smaller plateaus of growth spirals compared to mounds result, because the dislocation obviates the nucleation problem on the top terrace, which is analogous to an increase in the effective step edge barrier energy.

O 17.65 Mon 17:30 Poster C

Preparation of two-dimensional Fe-Cr-Fe multistripes on W(110) — •Torsten Methfessel and Hans Joachim Elmers — Johannes Gutenberg-Universität Mainz, Institut für Physik, Staudingerweg 7, D-55099 Mainz

Multilayers consisting of alternating layers of Fe an Cr are interesting because of the discovery of the giant magnetoresistance effect (GMR). In analogy to these multilayersystems we were interested in the possibility to prepare two dimensional multistripes on W(110) by sequential epitaxy and self organized growth of pseudomorphic Fe and Cr. These multistripes have been investigated using scanning tunneling microscopy (STM) and scanning tunneling spectroscopy (STS). With these methods we were able to distinguish between different materials along the edges of the W-substrate. Comparing the STS spectra of the multistripes with those of pseudomorphic pure element monolayers we could show that multistripes of alternating pure Fe and Cr stripes grow at appropriate substrate temperatures. Interdiffusion occurs for temperatures larger than 500 K, while deposition at room temperature leads to island growth.

O 17.66 Mon 17:30 Poster C

Effective interaction energies for the description of two dimensional alloys: calculation from experimental and density functional theory data — •Andreas Bergbreiter[1], Harry E. Hoster[1], Yoshihiro Gohda[2], Axel Gross[2], and R. Jürgen Behm[1] — [1]Institut für Oberflächenchemie und Katalyse, Universität Ulm, 89069 Ulm — [2]Institut für Theoretische Chemie, Universität Ulm, 89069 Ulm

The atomic distribution in two-dimensional, surface confined alloys can be approximately described by an Ising Hamiltonian based on pairwise and trio interactions. We show, how the effective interaction energies can be derived from atomic resolution STM images in an inverse Monte Carlo (IMC) approach. In addition, the total energy of ordered surface alloys can be calculated via density functional theory (DFT). Based on the energies for a number of unit cells with varied composition and internal geometry it is possible to derive a second set of ECIs in a least-squares approach, i.e., by simple matrix inversion, which can be compared to the one generated by IMC.

O 17.67 Mon 17:30 Poster C

Laser-assisted Carbon Burning (LACB) - Removal of Organic Impurities at Room Temperature — •Jonas Bock, Andreas Assmuth, Ulrich Abelein, Torsten Sulima, and Ignaz Eisele — Universität der Bundeswehr München, Institut für Physik, 85579 Neubiberg, Germany

The cleaning of silicon surfaces is one of the most important issues for the fabrication of novel semiconductor devices. Taking into account out-diffusion of dopants or mechanical stress of SiGe hetero structures, high temperatures have to be avoided. Therefore a maximum processing temperature of $T = 700\,^\circ\mathrm{C}$ must not be exceeded by any processing step, which applies accordingly to the removal of the two main contaminants of Si wafers - organic impurities and the native oxide. One possible approach is using gaseous precursors excited by plasma or laser. Because high energy ions caused by plasma excitation roughen the surface and laser beam radiation perpendicular to the substrate may lead to high temperatures, the investigations have been carried out using an excimer laser combined with an UHV system where the laser beam is guided parallel to the wafer. An in-situ cleaning step based on laser excitation of oxygen will be presented. The influence of temperature, oxygen partial pressure and laser energy have been studied, the effectiveness will be shown by SIMS analysis and I-V-measurements of devices, that were built on LACB cleaned substrates.

O 17.68 Mon 17:30 Poster C

Time-resolved two-photon photoemission study of C_{60} — Benjamin Göhler, •Arne Rosenfeldt, and Helmut Zacharias — Physikalisches Institut, Westfälische Wilhelms-Universität, 48149 Münster, Deutschland

Ordered films of C_{60} with different thicknesses between 10 and 200 ML are evaporated onto Cu(111) and cooled down to 130 K. Using four-wave mixing in Xenon photons with 8.27 eV (150 nm) are generated. They have sufficient energy to probe low lying and occupied states and are used to check the preparation. Photons with 5.88 eV have sufficient energy to probe the excitons. Photons with 4.71 eV have sufficient energy to probe half of the LUMO, the LUMO+1, and the LUMO+2.

Two-photon photoemission is employed to populate intermediate states and probe their dynamics. The excitation probability of these states is measured as a function of photon energy. Time-resolved measurements are performed with both a Q-switched laser delivering 2.33 eV pulses with 150 ns duration and 3.50 eV pulses with 100 ns duration, and a mode-locked laser tunable between 2.35 and 5.88 eV with 75 ps pulse duration. A rate equation fitted to the electron dynamics suggests a lifetime of about 126 ps for the LUMO, 1 ns for the singlet exciton, $(21 \pm 3)\,\mu s$ for the triplet exciton, and shorter lifetimes for LUMO+1 and LUMO+2. Pumping with 2.3 eV the result depends on pulse energy and pulse length.

The project is financially supported by the DFG in the SPP1093 “Dynamik von Elektronentransferprozessen an Grenzflächen”.

O 17.69 Mon 17:30 Poster C

Nanoparticle removal by laser induced acoustic waves — •Tobias Geldhauser, Florian Merkt, Florian Ziese, Johannes Boneberg, and Paul Leiderer — Fachbereich Physik, Universität Konstanz, Fach M676, 78457 Konstanz

Different approaches can be used for particle removal from surfaces like Ultra-/Megasonic 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 opposing 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. In order to develop a model for the removal process of the particles we measure in addition the detachment velocity of the particles by a light-scattering technique.

O 17.70 Mon 17:30 Poster C

Ablation dynamics of solid carbon dioxide after ns laser illumination — •Johannes Graf, Laura Hennemann, Johannes Boneberg, and Paul Leiderer — Fachbereich Physik, Universität Konstanz, Fach M676, 78457 Konstanz

In recent publications we already introduced a new laser based cleaning technique called Matrix Laser Cleaning. In this technique a matrix of an cryogenic solid , e.g. carbon dioxide, is condensed onto the substrate prior to the laser pulse. After ns laser irradiation the subsequent vaporization of the matrix molecules constitutes the dominant cleaning mechanism. By a careful adjustment of the process parameters cleaning down to at least 50 nm sized particles can be achieved with an efficiency close to 100%. In contrast to Steam Laser Cleaning this technique does not face wetting problems or the formation of watermarks.

In this presentation we want to focus on first experiments on the underlying mechanism, the ablation of the cryogenic matrix. Therefore we built a reflectometry and scattering light setup with sub-ns time resolution to investigate the ablation dynamics with a vertical resolution of a few nanometers. By careful analysis of these signals conclusions on the underlying mechanisms can be drawn. The results of ns- and fs-illumination will be compared.

O 17.71 Mon 17:30 Poster C

Steam laser cleaning with infrared pulses — •Pascal Frank, Florian Lang, Paul Leiderer, and Johannes Boneberg — Fachbereich Physik, Universität Konstanz, Fach M676, 78457 Konstanz

Steam Laser Cleaning is a powerful technique for removing very small contaminating particles from sensitive surfaces like Si wafers. The traditional concept of this method is to adsorb a thin liquid film (e.g. water or isopropanol) on the sample surface and then heat the sample with a short laser pulse. Heat transfer from the substrate to the liquid leads to explosive evaporation of the adsorbed film, connected with a removal of the particles. We have investigated here an alternative route by not heating the substrate, but rather the liquid layer directly with an appropriate laser pulse. For this purpose we use an optical parametric oscillator which generates light at 2.94 um, right at the maximum of the OH stretching mode in water and isopropanol. The absorption depth is around 1 micron. First experiments with model contaminants (PS colloid spheres between 200 and 1000nm diameter) show that cleaning of Si as well as glass surfaces is possible, both by irradiation from the front or the back side of the sample. This holds a number of advantages compared to the commonly used technique.

O 17.72 Mon 17:30 Poster C

Combined ab initio quantum-mechanical/molecular-mechanical molecular-dynamic simulations for Si(001) — Jan van Heys and •Eckhard Pehlke — Institut für Theoretische Physik und Astrophysik, Christian-Albrechts-Universität Kiel, 24098 Kiel

There is an ongoing interest in how fast and due to which mechanism surface atomic vibrations decay after an initial excitation by a fs laser-pulse. When such vibrational processes are to be simulated directly by ab initio molecular dynamics, slabs with a thickness of more than 1000 layers become inevitable in order to exclude artefacts due to unwanted back-reflections of phonons from the bottom surface of the slab. In order to carry through such simulations we have implemented a combined quantum-mechanical (for the surface atoms) and molecular-mechanical (for the atomic vibrations sufficiently far away from the surface) molecular-dynamics scheme. One should be extremely cautious, however, when choosing standard empirical potentials for the molecular-dynamics part of the simulation, because slight deficiencies of the empirical potentials to correctly describe the bulk-phonon dispersion may considerably flaw the calculated surface vibrational lifetimes. To circumvent this problem, we suggest to use a simulation with truly ab initio quality by using ab initio force constants up to 8th-nearest neighbors for the molecular-mechanical part of the simulations. Results for Si(001) using slabs with 6400 atoms and simulation times up to 10 ps will be presented.

O 17.73 Mon 17:30 Poster C

Adsorption of molecular hydrogen on SiC(001), Si(001) and C(001) surfaces: An ab-initio investigation — •Xiangyang

Peng, Peter Krüger, and Johannes Pollmann — Institut für Festkörpertheorie, Wilhelm-Klemm-Str. 10, 48149 Münster

In experiment, the exciting observation has been made that H_2 molecules readily adsorb dissociatively on the c(4×2) but not on the 3×2 surface of SiC(001) at room temperature. To unravel this spectacular reactivity difference, we have investigated a variety of H_2 reaction scenarios within density functional theory using the generalized gradient approximation. It turns out that *intradimer* adsorption is unlikely at both surfaces while *interdimer* adsorption depends crucially on the distinct spatial arrangement and dangling-bond topology of the Si dimers at the surfaces. The results clearly reveal barrierless reaction pathways for dissociative H_2 adsorption on the c(4×2) surface as opposed to pathways with significant energy barriers on the 3×2 surface. The latter finding also allows us to explain the inertness of self-organized Si addimer nanolines on the c(4×2) surface to H_2 uptake. To better understand the influence of the surface atomic structure and the dangling-bond topology on H_2 adsorption at group IV semiconductor surfaces, we have investigated the adsorption of H_2 molecules on Si(001) and C(001), as well.

O 17.74 Mon 17:30 Poster C

Adsorption of ethylene and acetylene on the SiC(001)-(3×2) surface — •Jürgen Wieferink, Peter Krüger, and Johannes Pollmann — Institut für Festkörpertheorie, Universität Münster

Most studies on the adsorption of small hydrocarbons on semiconductor surfaces have been focused on Si(001). Here, we present a complementary investigation of the adsorption on the silicon rich SiC(001)-(3×2) surface. This surface is characterized by two partial Si adlayers and a buckled Si dimer in the top adlayer which is remarkably similar to the Si(001) surface dimer.

Ethylene (C_2H_4) only adsorbs in an *on top* position above this dimer. Due to the saturation of the Si dangling bonds the buckling of the Si dimer is removed. Our calculations reveal that a twist in the C-C axis with respect to the Si dimer is energetically slightly favorable. This behavior is well known from C_2H_4 on Si(001) at saturation coverage and has been explained by intermolecular hydrogen Pauli repulsion. The existence of a twist on the more isolated dimers on SiC(001)-(3×2) strongly indicates that also *intra*molecular Pauli repulsion may play a vital role.

Acetylene (C_2H_2), on the other hand, may additionally adsorb on lower adlayers, though also in this case the *on top* structure is energetically favored. We show that *on top* acetylene impedes adsorption of acetylene on other layers due to a shift of the Fermi level. Thus, our studies suggest that the *on top* sites will rapidly become occupied while very high exposures would be needed for further acetylene adsorption.

O 17.75 Mon 17:30 Poster C

UV laser induced desorption of NO from C_{60}/Cu(111) — •Tim Hoger, Daniel Grimmer, and Helmut Zacharias — Universität Münster, Physikalisches Institut, Wilhelm-Klemm-Str. 10, 48149 Münster

The laser induced desorption of NO from an epitaxially grown C_{60}/Cu(111) surface is reported. The pump-probe experiment detects desorbing NO molecules with respect to their rovibrational population and their kinetic energy. Two channels are observed of which the first channel yields highly excited molecules with a rotational temperature of $T_{rot} = 800\,\mathrm{K}$, a kinetic temperature of $T_{kin}/(2k) = 1000\,\mathrm{K}$ and a comparatively low vibrational excitation below $T_{vib} = 600\,\mathrm{K}$. A strong translational-rotational coupling is observed. The second channel yields less excited molecules with a rotational temperature of $T_{rot} = 260\,\mathrm{K}$ and an arrival time spectrum of slow molecules far below the thermal desorption temperature. This desorption is probably caused by a long-lived electronic excitation in the substrate for which a lifetime of $\tau = 155\,\mu\mathrm{s}$ is derived.

O 17.76 Mon 17:30 Poster C

Adsorbate Induced Modifications of SiC Surfaces studied by High Resolution Electron Energy Loss Spectroscopy — Maxim Eremtchenko, Rolf Öttking, Jens Uhlig, Anita Neumann, •Syed Imad-Uddin Ahmed, and Juergen A. Schaefer — Institut für Physik und Institut für Mikro- und Nanotechnologien, Technische Universität Ilmenau, P.O. Box 100565, 98684 Ilmenau, Germany

Silicon carbide (SiC) is a wide band gap semiconductor that is suited for high power, high temperature and high frequency applications in which surface and interface chemical reactivity need to be thoroughly understood. For this material, we are able to monitor changes in carrier concentration profiles and band bendings owing to the C- and Si-terminated cubic and hexagonal SiC as well as vibrational properties of atmospheric adsorbates like, for e.g, oxygen, by comparing HREELS-data with simulations based on dielectric theory. The surface state density is directly related to the type of reconstruction and surface composition and plays an important role in correlation with the substrate temperature. In particular, on 6H-SiC (0001), we observed for the first time new vibrational modes, which can be identified with distinct Si-O-Si vibrations, namely its asymmetric- and symmetric stretching vibrations and its wagging motion. In particular, the energy and intensity of the asymmetric stretching frequency is strongly dependent upon oxygen coverage and substrate temperature, analogous to the situation of initial stage oxidation of Si surfaces.

We acknowledge financial support by the Deutsche Forschungsgemeinschaft - DFG under grant Scha 435/17-1.

O 17.77 Mon 17:30 Poster C

Oxidation of lateral polarity heterostructure GaN — •Pierre Lorenz, Vadim Lebedev, Richard Gutt, Juergen A. Schaefer, Oliver Ambacher, and Stefan Krischok — Institut für Mikro- und Nanotechnologien, TU Ilmenau, P.O. Box 100565, 98684 Ilmenau, Germany

We study GaN-based lateral polarity heterostructures (LPH) for nonlinear optics using surface sensitive techniques. The GaN was grown on Al_2O_3 substrates by molecular beam epitaxy (MBE). The N-face was directly grown on Al_2O_3 whereas the Ga-face was grown on a 20 nm thick AlN nucleation layer structured by photolithography. The examined LPH GaN samples consist of a stripe pattern with a periodicity of 1-100 μm of the N-face and Ga-face domains. The GaN surface properties were studied using atomic force microscopy (AFM), X-ray and ultraviolet photoelectron spectroscopy (XPS, UPS). The samples exhibit smooth Ga-face regions and lower quality N-face areas, separated by sharp and well defined inversion domain boundaries. The changes in the work function and the valence band structure are investigated upon adsorption of oxygen at room temperature. Special attention has been drawn to the interaction of O_2 with the inversion domain boundary region by employing photoelectron emission microscopy (PEEM).

O 17.78 Mon 17:30 Poster C

Au induced faceting of Si (112) surfaces and their relevance for vapour-liquid-solid epitaxy — •Christian Wiethoff, Frank Meyer zu Heringdorf, and Michael Horn-von Hoegen — Universität Duisburg-Essen

Silicon nanowires formed during vapour-liquid-solid (VLS) epitaxy, with Au as a catalyst [1] show sidewalls with [112]-orientations. These sidewalls are faceted and it was suggested that Au is the driving force for the faceting [2]. In order to investigate the influence of the catalyst in more detail, we studied Au induced faceting of [112] surfaces at 750°C with spot-profile-analysing-LEED (SPALEED). After quenching to room temperature the structure and step morphology was determined by reciprocal space mapping [3]. After some different phases of faceting a hill and valley structure with giant facets of [111] and [113] orientation form. They reach height modulations of more than 20nm at a periodic length of about 200nm. We suggest that the facets found on the nanowires consist of these orientations. With further Au adsorption, the [113] facets level off and the surface reaches a stable and reasonably smooth faceting configuration.

[1] J. B. Hannon, S. Kodambaka, F. M. Ross and R.M. Tromp, Nature 440, 04574 (2006)

[2] F. M. Ross, J. Tersoff and M. C. Reuter, Phys. Rev. Lett. 95, 146104 (2005)

[3] Frank-J. Meyer zu Heringdorf and Michael Horn-von Hoegen, Rev. Sci. Instrum. 76, 085102, (2005)

O 17.79 Mon 17:30 Poster C

GIXRD and XRR Studies on Thin Bi(111) Films on Si(001) — •Carsten Deiter[1], Giriraj Jnawali[2], Boris Krenzer[2], Michael Horn-von Hoegen[2], Thomas Weisemoeller[1], Lars Boewer[1], and Joachim Wollschläger[1] — [1]Fachbereich Physik, Universität Osnabrück, Barbarastr. 7, 49076 Osnabrück, Germany — [2]Fachbereich Physik, Universität Duisburg-Essen, Lotharstr. 1, 47057 Duisburg, Germany

Investigating the phenomena of quantum transport and finite-size effects, bismuth has been extensively studied due to its large Fermi wavelength and long carrier mean free path. Its material properties are advantageous for the realization of spin based electronic devices, and result also in large magnetoresistance effects. Here we report on bismuth films with a thickness of 6nm investigated by grazing incident x-ray diffraction (GIXRD) and x-ray reflectivity (XRR) measurements.

MBE fabricated samples were examined by AFM and spot profile analysis low energy electron diffraction (SPA-LEED) directly after the growth process. Thereafter the x-ray experiments were performed at the beamlines BW2 and W1 at HASYLAB. Sample A was fabricated at 150K with additional annealing at 450K for 30min (solid phase epitaxy, SPE). Contrary to this two step method the substrate of sample B was kept at a temperature of 300K during the coating and no additional annealing step was performed.

The experimental results show that the deposition method of SPE with its two step process leads to flat films with less roughness than the conventional technique.

O 17.80 Mon 17:30 Poster C

Initial stages of Pt nanowire formation on Ge(001) — •Daan Kockmann, Marinus Fischer, Arie van Houselt, Bene Poelsema, and Harold Zandvliet — Physical Aspects of NanoElectronics & Solid State Physics, MESA+ Institute for Nanotechnology, University of Twente, P.O. Box 217, 7500 AE Enschede, The Netherlands

Recently, the formation of defect- and kink-free Pt nanowires with a cross section of only one atom and lengths up to 500 nm on Ge(001) surfaces was reported. Here we present scanning tunneling microscopy data that reveal the initial stages of the Pt nanowire formation process. Upon room temperature deposition the Pt atoms first dive into the Ge(001) substrate. However, annealing at temperatures of 1000 K or higher causes the Pt atoms to pop up again. The Pt atoms form dimers and are positioned within the troughs between the substrate dimer rows. The Pt-Pt dimer bond is aligned along the substrate dimer bonds. Most of the Pt dimers are found in isolation or units of two dimers. Amazingly the Pt dimers in the trough seem to push both neighboring substrate dimer rows apart, leading to a zipper like structure. In case the concentration of Pt dimers within a trough is sufficiently high, they rotate by 90 degrees and line-up in virtually perfect Pt chains.

O 17.81 Mon 17:30 Poster C

Heteroepitaxial Praseodymium sesquioxide films on Si(111): A future model catalyst system for praseodymium oxide based catalysts — •Andreas Schaefer[1], Thomas Schröder[2], Gregorz Lupina[2], Yulia Borchert[1], Jarek Dabrowski[2], Christian Wenger[2], and Marcus Bäumer[1] — [1]Universität Bremen, Institut für Angewandte und Physikalische Chemie, Leobener Str. 2, 28359 Bremen — [2]IHP-Microelectronics, Im Technologiepark 25, 15236 Frankfurt (Oder)

Rare Earth Oxides (REO) are promising candidates for applications in catalysis based on their high oxygen storage capability and oxygen mobility. In order to look into the atomic details of oxygen transport and transfer of such materials interacting with adsorbed molecules, a simplified two dimensional model system of the generally three dimensional catalyst may be prepared and studied under controlled conditions in an UHV environment. The structure, growth and stoichiometry of heteroepitaxial Pr_2O_3 films on Si(111) were characterized by a combined RHEED, XRD, XPS and UPS study as a prerequisite for any future model catalytic investigations. RHEED and XRD confirm the growth of a (0001) oriented hexagonal Pr_2O_3 phase on Si(111). After an initial nucleation stage RHEED growth oscillation studies point to a Frank-van der Merwe growth mode up to a thickness of approximately 12 nm. XPS and UPS prove that the initial growth of the Pr_2O_3 layer on Si up to 1 nm thickness is characterized by an interface reaction with Si. Nevertheless stoichiometric Pr_2O_3 films of high crystalline quality form on top of these Pr-silicate containing interlayers.

O 17.82 Mon 17:30 Poster C

Electronic Structure of Mn_{12} Derivatives on the Clean and Functionalized Au(111) Surface — •Sönke Voss[1], Mikhail Fonin[1], Michael Burgert[2], Yuriy S. Dedkov[3], Ulrich Groth[2], and Ulrich Rüdiger[1] — [1]Fachbereich Physik, Universität Konstanz, 78457 Konstanz — [2]Fachbereich Chemie, Universität Konstanz, 78457 Konstanz — [3]Institut für Festkörperphysik, Technische Universität Dresden, 01062 Dresden

Single-molecule magnets (SMMs) like Mn_{12}-acetate and its derivatives have attracted much attention due to their unique magnetic properties such as quantum tunneling of magnetization. Up to date, most experiments on Mn_{12} have been performed on bulk material while there are only a few reports on transport properties and electronic structure of individual molecules. Here, we present a study on the electronic structure of monolayers of Mn_{12} SMMs grafted on clean as well as on functionalized Au(111) surfaces. X-ray absorption spectroscopy indicates the fragmentation of the Mn_{12}-core after deposition on clean Au(111). However, resonant photoemission spectroscopy was employed to show that the structural integrity of Mn_{12} clusters can be retained by using an appropriate pre-functionalization of the Au(111) surface. The obtained spectra are in good agreement with previous LDA+U calculations [1]. Scanning tunneling microscopy and spectroscopy measurements confirm the ResPES results for the valence band structure near E_F.

[1] Boukhvalov *et al.*, J. Electron Spectrosc. Relat. Phenom. 137-140, 735 (2004).

O 17.83 Mon 17:30 Poster C

Ab initio calculation of image potential states — •Alexander Hanuschkin, Daniel Wortmann, and Stefan Blügel — Institut für Festkörperforschung, Forschungszentrum Jülich, Germany

Recently image-potential states were investigated using spin-polarized STM. A potential well between metal surfaces with a band gap at the vacuum energy and the image potential creates hydrogenlike states above the surface. Additionally this states exhibit a small spin splitting if the surface is ferromagnetic. DFT calculations with the Greenfunction embedding technique allow to treat surfaces with a semi-infinite substrate. To capture the image potential states the DFT potential has to be modified to include the correct 1/z like asymptotic behavior towards the vacuum. In our scheme this is efficiently done by calculating and adding the correspondent embedding potential for the vacuum. We will present details of the computational scheme as well as results for image potential states of transition metal surfaces.

O 17.84 Mon 17:30 Poster C

Dynamics of laser induced phase transitions of liquids at surfaces — •Sebastian Fischer, Florian Lang, Johannes Boneberg, and Paul Leiderer — Fachbereich Physik, Universität Konstanz, Fach M676, 78457 Konstanz

The phase-transition dynamics of isopropanol films with thicknesses on the order of 100 nm deposited on silicon wafers are investigated. A nanosecond laser pulse is used to heat the substrate. 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 nanometrescale 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 insight into the nature of the very early stages of the phase transition.

O 17.85 Mon 17:30 Poster C

Transmission increase upon switching of VO2 films on microstructured surfaces — •Stephen Riedel[1], Ismael Karakurt[2], Johannes Boneberg[1], Paul Leiderer[1], and Richard Haglund[3] — [1]Fachbereich Physik, Universität Konstanz, Fach M676, 78457 Konstanz — [2]Department of Physics, Isik University, Maslak, Istanbul , Turkey — [3]Department of Physics and Astronomy, Vanderbilt University , 6301 Stevenson Center Lane, Nashville TN 37235-1807, USA

Vanadium dioxide is one of the most-studied transition metal oxides due to its reversible thermochromism. It shows a semiconductor-metal phase transition occurring at a critical temperature Tc of 68 oC. The material is a semiconductor below the critical temperature while above Tc it is a metal. The Optical properties of the oxide, as well as the electrical properties, change upon the phase transition. The transmission through VO2 films decreases dramatically in the metallic state in the infrared region. We prepare VO2 films on different substrates (smooth glass substrates and on spherical SiO2 colloidal monolayers) and compare their switching behaviour upon heating with a ns-pulsed Nd:YAG-laser at 532nm. The observed behavior of the films on the two substrates is qualitatively different: while the smooth layers show the expected transmission decrease, the film on the micro-structured surfaces exhibit an increase in transmission when heated. We show that this at first glance unexpected behaviour can be explained by the additional contribution of diffraction which also changes at the phase transitions.

O 17.86 Mon 17:30 Poster C

Dynamics of nanobubble formation around absorbing nanoparticles in liquid — •Stefan Weber, Sebastian Fischer, Paul Leiderer, Anton Plech, and Johannes Boneberg — 1.Fachbereich Physik, Universität Konstanz, Fach M676, 78457 Konstanz

Nanosecond laserpulses (wavelength of 532nm) are used to illuminate Au nanoparticles of different sizes in aqueous solution. At sufficient high intensities bubbles form around the nanoparticles, expand and collapse again on a time scale of nanoseconds. Time-resolved optical transmission and scattering measurements simultaneously performed at different wavelengths - and especially on both sides of the plasmon resonance of the particles - allow to follow these processes in detail.

O 17.87 Mon 17:30 Poster C

On the freezing and melting of water confined in mesoporous silica thin films investigated by X-ray Reflectivity — •Sandrine Dourdain[1], Heiko Schroeder[1], Markus Mezger[1], Sebastian Schoeder[2], Harald Reichert[1], and Helmut Dosch[1] — [1]Max-Planck-Institute for Metallforschung, Heisenbergstr.3, D-70569 Stuttgart — [2]ESRF, 6 rue Jules Horowitz, F-38000 Grenoble

Since water in nano-scaled pores is involved in many biological systems, it is of paramount interest to probe its behavior in such conditions. We study the solid-liquid phase transition of water when it is confined in mesoporous silica thin films. Templates of mesopores organized in a thin film give the possibility to resolve the electron density profile by X-ray reflectivity on the nanometer scale. Changing the temperature or the size of the mesopores, the density of the confined water, as well as the mechanical deformations of the mesostructure, can be followed during the freezing and the melting transitions. In addition, owing to the possibility to chemically modify the walls of the mesopores, the effect of a varying hydrophilicity is accessible.

O 18: Plenary Talk Pätzold

Time: Monday 18:00–18:45 Location: H1

Venus Express

O 19: Plenary Talk Lemke

Time: Tuesday 8:30–9:15 Location: H1

Climate Change 2007: The Physical Science Basis

O 20: Invited Talk Hirjibehedin (FV: MA+O)

Time: Tuesday 9:30–10:15 Location: H36

Invited Talk O 20.1 Tue 9:30 H36

Spin-Coupling in Engineered Atomic Structures — •Cyrus Hirjibehedin, Christopher Lutz, and Andreas Heinrich — IBM Research Division, Almaden Research Center, San Jose, CA 95120 USA

Magnetic nanostructures are increasing data storage capacities and are promising candidates for implementations of novel spin-based computation techniques. The relative simplicity and reduced dimensionality of nanoscale magnetic structures also make them attractive model systems for studying the interactions between small numbers of quantum spins. Using a high-field low-temperature scanning tunneling microscope, we assemble linear chains of Mn atoms one atom at a time on thin, insulating layers of copper nitride. We probe the excitation spectra of the individual magnetically-coupled chains with inelastic electron tunneling spectroscopy and observe excitations of the coupled atomic spins that can change both the total spin and its orientation. Comparison with a model spin-interaction Hamiltonian yielded the collective spin configuration and the strength of the coupling between the atomic spins.

O 21: Invited Talk Hofer

Time: Tuesday 10:15–11:00 Location: H36

Invited Talk O 21.1 Tue 10:15 H36

Recent advances in simulating high-resolution scanning tunnelling microscopy and spectroscopy — •Werner Hofer — Liverpool Institute of Nanoscale Science, Engineering and Technology, Liverpool, UK

Since its invention scanning tunnelling microscopes have rapidly become the key instrument not only for the atomic scale analysis of surfaces, interfaces, and molecular structures, the instrument*s resolution has made it increasingly possible to detect electronic processes which before remained elusive. Driven by experimental advances sophisticated theoretical techniques have been developed, which make direct comparisons with quantitative results a close to routine procedure. The key ingredient in these techniques is the inclusion the STM tip in the simulations, and the use of highly accurate electronic structure methods. We provide several examples of the present state of theory, ranging from traditional problems of adsorption and catalysis[1], single adatom properties[2], to new magnetic structures, organic interfaces, and semiconductors[3]. Particular emphasis shall be placed on functionalising interfaces and molecular structures, which can be analyzed in great detail by STM[4-6].

[1] F Calleja et al. Phys. Rev. Lett. 92, 206101 (2004) [2] L. Limot et al. Phys. Rev. Lett. 94, 126102 (2005) [3] L. Zotti, W. A. Hofer and F. Giessibl, Chem. Phys. Lett. 420, 177 (2006) [4] P. Piva et al., Nature 435, 658 (2005) [5] S. Dobrin et al., Surf. Sci. Lett. 600, L43 (2006) [6] Z. T. Deng et al., Phys. Rev. Lett. 96, 156102 (2006)

O 22: Surface or Interface Magnetism

Time: Tuesday 11:15–12:15 Location: H36

O 22.1 Tue 11:15 H36

Image potential states: a sensor for magnetization? — Martin Pickel[1], •Markus Donath[1], Anke Schmidt[2], Ilja Panzer[2], Fabian Giesen[2], and Martin Weinelt[2,3] — [1]Physikalisches Institut, Universität Münster, 48149 Münster — [2]Max-Born-Institut, 12489 Berlin — [3]Freie Universität Berlin, Fachbereich Physik, 14195 Berlin

Image-potential surface states (IPS) at ferromagnetic surfaces exhibit exchange splittings which are explained by the exchange-split boundaries of the projected bulk band gap [1]. So far, no experimental study is available that deals with the response of this splitting to changes of the magnetization as a consequence of, e.g., temperature variation. Spin-resolved two-photon photoemission spectroscopy on the first IPS on 7 ML Fe/Cu(100) has been employed to study the influence of temperature, especially close to T_C, on the spin dependence of its binding energy, spin polarization and linewidth. The evolution of the linewidths as a function of the temperature contradicts the temperature behavior of the exchange splitting and the spin polarization, both suggesting a much lower T_C. This is manifested by measurements with different light polarization, which can be used to deduce the exchange splitting from spin-integrated measurements. The discrepancy is explained by domain formation below T_C leading to an apparent loss of spin polarization and exchange splitting significantly below T_C in the spin-resolved measurements. This experiment demonstrates the strength of using specific electronic states as sensors for magnetization, however, it shows also the danger of misinterpretation.

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

O 22.2 Tue 11:30 H36

Electronic structure and magnetic properties of two-dimensional metal-organic coordination structures at a metal surface — •Sebastian Stepanow[1,2], Alexandre Dmitriev[2], Subhra Sen Gupta[3], Jan Honolka[2], Sylvain Clair[4], Stephane Pons[4], Magali Lingenfelder[2], Peter Bencock[5], Dipankar Das Sarma[3], Nian Lin[2], Harald Brune[4], Johannes Valentin Barth[6], Klaus Kern[2,4], and Pietro Gambardella[1,7] — [1]ICN, Barcelona — [2]MPI-FKF, Stuttgart — [3]IIoS, Bangalore — [4]EPFL, Lausanne — [5]ESRF, Grenoble — [6]UBC, Vancouver — [7]ICREA, Barcelona

Recently various 2D metal-coordination structures at a Cu(100) surface have been synthesized. The arrays contain mono- and dinuclear Fe ions embedded in defined ligand-field environments tunable by the employed organic ligand molecules and further manipulated by adsorbed gas molecules. Polarized x-ray absorption spectroscopy was used to investigate the electronic structure and magnetic properties of the metal ions. The results demonstrate that the properties of the Fe centers are mainly determined by the strong coordination bonds to the ligands which drive the effective dehybridization of the Fe atoms from the surface. In-plane and out-of-plane magnetic anisotropy orientations as well as isotropic compounds can be obtained. The temperature dependence of the magnetic anisotropy and related orbital magnetization indicate the thermally excited molecular states present different magnetic properties compared to the ground state. XMCD spectra are discussed in the framework of a simple atomic multiplet theory considering the influence of the crystal-field and spin-orbit coupling on the Fe ^{5}D term.

O 22.3 Tue 11:45 H36

Magnon-enhanced intraband scattering on a d-band ferromagnet — •Anke Schmidt[1,2], Fabian Giesen[1], Martin Weinelt[1,2], Martin Pickel[1,3], and Markus Donath[3] — [1]Max-Born-Institut, Max-Born-Straße 2A, 12489 Berlin, Germany — [2]Freie Universität Berlin, Fachbereich Physik, Arnimallee 14, 14195 Berlin, Germany — [3]Physikalisches Institut, Universität Münster, Wilhelm-Klemm-Straße 10, 48149 Münster, Germany

Experimental access to the spin-dependent decay processes of low-energy electrons in d-band ferromagnets remains a challenge despite advanced techniques such as spin-polarised electron energy loss spectroscopy [1] or spin-resolved two-photon photoemission of image-potential states (IPS). In a spin- and time-dependent photoemission study of thin iron and cobalt films, we have combined the advantages of both methods. The dispersing IPS electron is employed as observer or primary electron, thus effectively separating low-energy losses from direct decay into d-holes. We found that intraband decay on iron is not only much stronger than on cobalt, but also highly spin-dependent. We interpret this in terms of magnon-enhanced exchange scattering between opposite spin-bands, consistent with theoretical predictions [2] that spin-flip processes contribute significantly to the decay of minority electrons in iron.

[1] J. Kirschner, Phys. Rev. Lett. **55**, 973 (1985)

[2] M. Plihal and D.L. Mills, Phys. Rev. B **58**, 14407 (1998), V.P. Zhukov, E.V. Chulkov, and P.M. Echenique, Phys. Rev. Lett. **93**, 096401 (2004).

O 22.4 Tue 12:00 H36

Magnetic linear dichroism in time-resolved two-photon photoemission — Martin Pickel[1], Anke Schmidt[2], Andreas Goris[2], •Fabian Giesen[2], Martin Weinelt[2,3], and Markus Donath[1] — [1]Physikalisches Institut, Universität Münster, Wilhelm-Klemm-Str. 10, 48149 Münster — [2]Max-Born-Institut, Max-Born-Str. 2A, 12489 Berlin — [3]Freie Universität Berlin, Fachbereich Physik, Arnimallee 14, 14195 Berlin

Magnetic linear dichroism in photoemission spectroscopy, i.e. a magnetization-direction dependence of the intensity, has so far only been observed in direct excitation processes [1].

We will present a two-photon photoemission (2PPE) study on ultrathin cobalt films on Cu(100), where the image-potential states (IPS) show a strong dichroism. Varying the photon energy, however, reveals that its origin is caused by initial-states of the 2PPE process. What is more, a spin-dependent lifetime of the IPS in combination with a magnetization direction dependent spin polarization leads to a ”dichroic”lifetime in time-resolved 2PPE. This enables a determination of the initial state quantum number without any spin-resolution. The corresponding direct spin-resolved measurements substantiate this possibility and demonstrate that spin-resolved 2PPE can be used as a probe for the electronic structure of occupied states close to the Fermi-level with respect to the spin polarization and the symmetry quantum number.

[1] W. Kuch and C. M. Schneider, Rep. Prog. Phys. **64**, 147 (2001)

O 23: Symposium: Ultrafast Nanooptics III

Time: Tuesday 11:15–12:45 Location: H38

O 23.1 Tue 11:15 H38

Mapping the Plasmon Dynamics in Silver Nano-particles using Phase-Resolved PEEM — Jörg Lange[1], Martin Rohmer[1], Daniela Bayer[1], Christian Schneider[1], Carsten Wiemann[1], Martin Aeschlimann[1], and •MIchael Bauer[2] — [1]Fachbereich Physik, TU Kaiserslautern, 67663 Kaiserslautern — [2]Institut für Experimentelle und Angewandte Physik, CAU Kiel, 24098 Kiel

Phase-resolved Two-Photon Photoemission (PR-2PPE) in combination with Photoemission Electron Microscopy (PEEM) is used to locally address the femtosecond dynamics associated with localized surface plasmon excitations (LSP) in well-defined silver nano-particles. At a lateral resolution in the sub-50 nm regime we are able to map the phase evolution of the particle-internal field as governed by the plasmon resonance energy and resonance width with sub-femtosecond accuracy. An illustrative example that will be presented is the observation of the dephasing process of the local field response between two neighbouring particles exhibiting differing plasmon energies. Furthermore we find particle-internal lateral inhomogenities in the dynamical response to the external laser-field, which we assign to the phase propagation of the excited plasmon mode through the particle.

O 23.2 Tue 11:30 H38

Efficient modelling of nonlinear wave propagation and radiation dynamics in nano-photonic systems — •Kurt Busch, Michael König, Jens Niegemann, Martin Pototschnig, and Lasha Tkeshelashvili — Institut für Theoretische Festkörperphysik, Universität Karlsruhe, 76128 Karlsruhe, Germany

Time-domain simulations play a very prominent role in the investigation and design of three-dimensional micro- and nano-photonic structures. In many cases, these strongly scattering systems need to be modeled on long time-scales with high precision. Such high accuracy, combined with unconditional stability and efficient performance, can be achieved via an operator-exponential method based on Krylov-subspace techniques[1].This approach is capable of handling optically anisotropic, lossy and dispersive materials as well as CFS-PML boundary conditions. Therefore, it is very well suited to study most experimentally relevant photonic nano-structures. Furthermore, it is straightforward to extend the scheme to handle nonlinear wave propagation, wave mixing phenomena and coupled systems, where similar accuracy and performance characteristics are achieved.

[1] J. Niegemann, L. Tkeshelashvili, and K. Busch, "Higher-order time-domain simulations of Maxwell's equations using Krylov-subspace methods", J. Comput. Theor. Nanosci., in press

O 23.3 Tue 11:45 H38

Light confinement via grating coupling of surface plasmons onto nanoscopic metal tips — •Claus Ropers[1], Catalin Neacsu[1], Thomas Elsässer[1], Martin Albrecht[2], Markus Raschke[1,3], and Christoph Lienau[1,4] — [1]Max-Born-Institut, D-12489 Berlin — [2]Institut für Kristallzüchtung, D-12489 Berlin — [3]Department of Chemistry, University of Washington, Seattle, WA 98195-1700 — [4]Institut für Physik, Carl von Ossietzky Universität Oldenburg, D-26129 Oldenburg

Localized and delocalized surface plasmon polaritons (SPPs) promise an unprecedented amount of microscopic light control and confinement. Structuring the surface of metals with nanometer precision allows for a tailoring of the SPP excitation and propagation. This may lead to new forms of nano-focusing, as proposed theoretically for tapered SPP waveguides. In this context, the achievement of highly localized light at the apex of a metal nano-tip is particularly desirable, as currently most apertureless near-field optical techniques are affected by considerable far-field background light.

Here, we realize a local femtosecond light source by focusing SPPs on nano-fabricated metallic tips with with radii down to 10 nm. By the use of focused ion beam milling, one-dimensional gratings are written onto the tip shaft, several micrometers away from the apex. Illumination of the grating with a broadband 7-fs Ti-sapphire oscillator leads to resonant excitation of SPPs, which travel to the tip apex and are reradiated. The clear spatial separation of the excitation from the tip end carries great potential as a novel light source in near-field microscopy.

O 23.4 Tue 12:00 H38

Multiphoton-Photoemission Microspectroscopy of Polystyrene Microspheres — •Gerhard Lilienkamp, Florian Lindla, Christoph Senft, and Winfried Daum — Instuitut für Physik und Physikalische Technologien, TU Clausthal, Leibnizstraße 4, 38678 Clausthal-Zellerfeld

Previous multiphoton-photoemission microscopy (PEEM) studies have focused on metallic and magnetic nanostructures. We have extended the application of multiphoton-PEEM to a dielectric system. Polystyrene (PS) microspheres with diameters between 300 nm and 1000 nm deposited on an oxidized Pt substrate have been imaged using a photoelectron microscope with 400 nm (3.1 eV) femtosecond laser excitation. Despite of a minimum energy of 7.6 eV required to excite electrons from the HOMO of PS to the vacuum level [1], strong photoemission from the microspheres is observed upon illumination with 3.1 eV laser photons. Analysis of the dependence of the photoemission on the power density of the laser pulses yields a nearly pure quadratic dependence for the Pt substrate consistent with two-photon photoemission while the emission from PS contains both linear and quadratic contributions. This finding can be rationalized in terms of a population of an unoccupied state in PS by two-photon excitation with a lifetime that is large compared to the time between two consecutive laser pulses (12.5 ns). Using energy-resolved PEEM, we observed laser-induced photoconductivity of PS which is consistent with a highly filled intermediate state.

[1] C.B. Duke et al. Phys. Rev. B 187 (1978) 571

O 23.5 Tue 12:15 H38

Nanoscale force manipulation in the vicinity of a metal nanostructure — C. Spindler[1], T. Brixner[1], J. Carcía de Abajo[2], and •W. Pfeiffer[3] — [1]Physikalisches Institut, Universität Würzburg, Am Hubland, 97074 Würzburg, Germany — [2]Instituto de Optica, Serrano 121, 28006 Madrid, Spain — [3]Fakultät für Physik, Universität Bielefeld, Universitätsstr. 25, 33516 Bielefeld, Germany

The tight focus of Gaussian beams is commonly used to trap dielectric particles in optical tweezers. The corresponding field distribution generates a well-defined trapping potential that is only marginally controllable on a nanometer scale. Here we investigate the influence of a metal nanostructure that is located in the vicinity of the trapping focus on the trapping potential by calculating the corresponding field and force distributions. Even for an excitation wavelength that is tuned far from the plasmonic resonance of the nanostructure the trapping potential is significantly altered by the presence of the nanostructure. For the given nanostructure, i.e. a ring of spheres that is illuminated in axial direction, a stronger localization of the focus in all directions is observed. The superposition of this non-resonant Gaussian field with a planar wave illumination that is tuned on the plasmonic resonance gives a handle to modify the trapping potential. Polarization and intensity of the resonant illumination allows modifying the equilibrium position of the trapping potential providing thereby means to steer dielectric particles with nanometer precision.

O 23.6 Tue 12:30 H38

Dephasing time and damping mechanisms of surface plasmon polaritons in gold nanoparticles — •Nils Borg, David Blazquez Sanchez, Christian Hendrich, Frank Hubenthal, and Frank Träger — Institut für Physik und Center for Interdisciplinary Nanostructure Science and Technology - CINSaT, Universität Kassel, Heinrich-Plett-Straße 40, D-34132 Kassel

The ultrafast electron dynamics in gold nanoparticles (NPs) was studied by measuring the dephasing time T_2 of the surface plasmon polariton by means of persistent spectral hole burning. The dephasing time of gold grown on sapphire and TiO_2 substrates was measured as a function of photon energy and the particle size. Dephasing times ranging from 5 to 17 fs were extracted. Furthermore, an explicit influence of the reduced dimension of the NPs has been determind, which plays a role for NPs with radii below 12 nm already. Most importantly, a dependence of T_2 on the decreasing particle dimensions which fulfilled a $1/R$-dependence was found and we could obtain a damping parameter for gold on sapphire of $A = (0.32 \pm 0.06)$ nm/fs. Comparison with other measurements as well as with theoretical predictions could identify surface scattering and Landau-damping as the most important mechanisms. Recent further experiments on gold NPs supported on TiO_2 showed a further reduction of the dephasing time. For example, for NPs with a radius of approximately 13 nm we observed a decrease from $T_2 \approx 15$ fs for NPs grown on sapphire to $T_2 \approx 12$ fs for NPs grown on TiO_2 at a photon energy of 1.65 eV. This indicates an additional damping mechanism, i.e. chemical interface damping.

O 24: Semiconductor Substrates: Epitaxy and Growth

Time: Tuesday 11:15–12:45 Location: H39

O 24.1 Tue 11:15 H39

Ultrafast Electron Diffraction of epitaxial Bi(111) films on Si(001) — •Anja Hanisch, Boris Krenzer, and Michael Horn-von Hoegen — Universität Duisburg-Essen, Experimentalphysik, 47057 Duisburg

Ultrafast time resolved electron diffraction experiments in a RHEED geometry allow the observation of the surface temperature evolution after laser excitation. Diffraction patterns of epitaxially Bi(111)-films grown on Si(001) taken at different delays between pumping laser pulses and probing electron pulses are converted to the transient surface temperature using the Debye-Waller effect. A rapid increase of the surface temperature from 80 K up to 190 K is followed by a slow exponential decay with a decay constant of 640 ps for 5,5 nm thin film [1], which is determined by the thermal boundary resistance at the interface between Bi and Si. While the decay constant is almost independent of the pump energy (fluence ramping from 0,33 mJ/cm2 to 3 mJ/cm2) we observe a linear dependence of the decay constant with the filmthickness for filmthicknesses between 6 nm and 12 nm. A detailed analysis shows that this linear behaviour cannot be explained in terms of existing models describing the thermal boundary resistance. In order to explain the observed behaviour the existing models have to be expanded which will be presented in this talk.

[1] A.Janzen et al., Surface Science 600, 4094 (2006).

O 24.2 Tue 11:30 H39

Lattice accommodation by a periodic array of interfacial misfit dislocations in Bi(111)/Si(001) heteroepitaxy — •Giriraj Jnawali, Hichen Hattab, Frank M. zu Heringdorf, Boris Krenzer, and Michael Horn von Hoegen — Fachbereich Physik, Universität Duisburg-Essen, Lotharstr. 1, 47048 Duisburg, Germany

Ultra-smooth Bi(111) films with very low defect density could be grown on Si(001) following a recipe published by Jnawali et al.[1]. Surprisingly the hexagonal Bi(111) lattice fits quite well with the rectangular Si(001) lattice with a low misfit in both the [110] and $[1\bar{1}0]$ directions. A remaining lattice mismatch of 2.3 % is accommodated by the formation of a periodic array of misfit dislocations at the interface. The dislocations are generated during annealing of a 6 nm thick Bi(111) film from 150 K to 450 K while the film relaxes. The periodic one dimensional dislocation array is observed via its strain fields and the accompanied surface undulation by spot splitting in high resolution LEED (SPA-LEED). From the satellite spot intensity at different scattering phases, the amplitude Δh = 0.66 Å and the average length Γ = 200 Å of the wave-like periodic surface undulation is determined. Comparing these results with a continuum theory for elastic distortion by Springholz et al.[2] we conclude that the misfit dislocation at the interface is a full-dislocation with Burgers vector of $b = \frac{1}{2}[1\bar{1}0]$ defined by the surface lattice constant of the Si(001) surface.

[1] G. Jnawali, H. Hattab, B. Krenzer, and M. Horn von Hoegen, Phys. Rev. B, 74, 195340 (2006).

[2] G. Springholz, Appl. Surf. Sci. 112, 12 (1997).

O 24.3 Tue 11:45 H39

Symmetry breaking in the growth of 2D Ge islands on Bi/Si(111) — •Konstantin Romanyuk and Bert Voigtländer — Institute of Bio and Nanosystems (IBN 3), and cni - Center of Nanoelectronic Systems for Information Technology, Research Centre Jülich, 52425 Jülich, Germany

The threefold rotational symmetry of the Si(111) surface usually leads to the formation of threefold symmetric islands (triangular or hexagonal) in the initial stages of epitaxial growth. However, for Ge growth on the Bi$(\sqrt{3}\times\sqrt{3})R30°$ terminated Si(111) surface we find islands with a reduced symmetry. The Ge islands have a rhomb shape with only one mirror plane and are terminated by $<1\bar{1}0>$ steps. We demonstrate that not only the bulk lattice symmetry but the symmetry of the combined substrate/island system is important to define the shape of the islands. It will be shown that the symmetry of the two level system is reduced due to the surface reconstruction to only one σ mirror reflection symmetry. The mirror plane run along small diagonal of the rhomb islands. The triangular symmetry of the Si(111) surface which includes 3 mirror planes leads to three different orientations of the rhomb shaped islands on the surface, as observed in the experiments.

O 24.4 Tue 12:00 H39

Epitaxial growth of Aluminium on Silicon (111) studied by SPA-LEED and STM — •Thomas Payer, Christian Wiethoff, and Michael Horn-von Hoegen — Universität Duisburg-Essen, FB Physik, AG Horn-von Hoegen, Lotharstraße 1 47057 Duisburg

We studied the epitaxial growth of Aluminium on Si (111) on Al-induced reconstructions as well as on the plain Si (111) (7x7) reconstruction. The film and surface morphology was studied in-situ by scanning tunnelling microscopy (STM). During deposition, the growth kinetics was observed by spot profile analyzing LEED (SPA-LEED). The deposition temperature varied between room temperature and 700K. On Si(111) Al grows in (111)-orientation. Both lattice constants of Al (111) and Si (111) fit in a 4 to 3 ratio with a small remaining mismatch of only 2%. Growth on top of the Al-induced $(\sqrt{3}\times\sqrt{3})$ reconstruction in a temperature regime of 500 - 550 K yields the smoothest films. Compared to films directly deposited on top of the Si (111) (7x7), the film roughness is reduced by a factor of five to 2nm rms roughness for a 20nm thick film. Growth on top of other Al-induced reconstructions do not provide any advantages in comparison to deposition on top of the clean Si (111) (7x7) surface. Instead, islands are formed and the films show an enhanced surface roughness. Growth at temperatures above 600K results in a Stransky-Krastanov mode with large Al islands on the Al-induced γ-reconstruction.

O 24.5 Tue 12:15 H39

Self-organized thickness engineering of Al thin films by alternation of dense and diluted atomic layers — •Ying Jiang[1,2], Kehui Wu[1], Zhe Tang[1], Philipp Ebert[2], and Enge Wang[1] — [1]Institute of Physics, Chinese Academy of Sciences, Beijing 100080, China — [2]Institut für Festkörperforschung, Forschungszentrum Jülich GmbH, 52425 Jülich, Germany

We studied the growth of Al on Si(111)-$\sqrt{3}$x$\sqrt{3}$ -Al substrates by scanning tunneling microscopy and low energy electron diffraction. We found that the Al film grown on an atomically sharp Al/Si interface exhibits of a superlattice structure of alternating densely-packed (1x1) and loosely-packed (likely $\sqrt{3}$x$\sqrt{3}$) atomic layers, at film thicknesses ¡ 0.9 nm. Above 0.9 nm Al starts to grow in the normal stacking of Al(111) layers. The phenomenon is explained within the theory of the quantum size effects in a jellium metal combined with strain effects.

O 24.6 Tue 12:30 H39

Untersuchung der Homoepitaxie auf GaAs(001) mit Molekularstrahlepitaxie und in-situ-STM — •Sylvia Hagedorn, Jan Grabowski, Holger Eisele und Mario Dähne — Technische Universität Berlin, Institut für Festkörperphysik, PN4-1, Hardenbergstraße 36, D-10623 Berlin

Mit einer UHV-Anlage zur Molekularstrahlepitaxie (MBE) mit den Komponenten Indium, Gallium und Arsen, die mit einem Rastertunnelmikroskop (STM) gekoppelt ist, wurde die Homoepitaxie von GaAs auf GaAs(001) untersucht. Ziel ist es, den Einfluss verschiedener Substratrekonstruktionen auf das Wachstum von InAs-Quantenpunkten zu studieren. Nach der Reinigung von GaAs(001)-Wafern durch Ionenbeschuss und Ausheilen (IBA-Zyklus) wurden grundlegende Wachstumsparameter wie Probentemperatur, Teilchenfluss und Wachstumsrate variiert, um verschiedene Oberflächenrekonstruktionen zu erzielen. Hierbei wurde die Homoepitaxie von GaAs auf GaAs(001) erfolgreich durchgeführt. Bei verschiedenen Präparationsbedingungen konnte die Präparation der GaAs(001) beta2(2x4)-Rekonstruktion sowie der GaAs(001) c(4x4)-Rekonstruktion durchgeführt und mit Reflektion hochenergetischer Elektronen (RHEED) kontrolliert werden. In STM-Untersuchungen mit atomarer Auflösung konnten weite defektarme Oberflächenbereiche beobachtet werden. STM-Untersuchungen des Wachstums von InAs-Quantenpunkten auf diesen GaAs(001)-Oberflächen stehen kurz bevor.

O 25: Phase Transitions

Time: Tuesday 11:15–12:45 Location: H41

O 25.1 Tue 11:15 H41

Order-disorder phase transitions: a DFT - (Wang-Landau) MC study — •Mira Todorova[1], Mikael Borg[2], Catherine Stampfl[3], and Matthias Scheffler[4] — [1]Max-Planck Institut für Eisenforschung, Max-Planck-Str. 1, 40237 Düsseldorf — [2]University of Toronto, Toronto, Canada — [3]School of Physics, The University of Sydney, Australia — [4]Fritz-Haber-Institut der MPG, Faradayweg 4-6, 14195 Berlin

Using a hybrid statistical mechanics method comprising the use of a Lattice-gas Hamiltonian (LGH) determined from density-functional theory and subsequent Monte Carlo (MC) calculations, we obtain a phase diagram for Na-Al surface alloys from first-principles and compare it to experimental results [1].

A safe approach towards parametrizing a LGH from the self-consistent evaluation of the electronic structure starts with an analytic form for the long-range pair-interactions. This expression is corrected in the short and medium range using DFT derived data, also including near-sighted many-body terms. An ensuing cross-validation is of utmost importance to ensure that the corrections (to the long-range part) are assessed with an optimum accuracy. The thus extracted LGH is used to perform MC calculations, also using the new Wang-Landau MC algorithm [2], which allows us to reliably determine the transition temperature.

[1] M. Borg, *et al.*, Chem. Phys.Chem. **6**, 1923 (2005).

[2] F. Wang and D.P. Landau, Phys. Rev. Lett. **86**, 2050 (2001).

O 25.2 Tue 11:30 H41

Phase diagram of oxygen adsorbed on Ni(111) and thermodynamic properties from first-principles — •Cesar Lazo[1] and Frerich Keil[2] — [1]Inst. of Applied Physics, Hamburg University, Jungiusstr. 9a, 20355 Hamburg. — [2]Inst. of Chemical Reactions, Hamburg University of Technology, Eissendorfer Str. 38, 21073, Hamburg.

Thermodynamic properties and the surface phase diagram of O/Ni(111) have been calculated from Metropolis and Wang-Landau Monte Carlo simulations based on lateral interactions derived from density functional theory (DFT) calculations. The DFT energies were mapped onto an Ising-like Hamiltonian according to the cluster expansion technique formalism[1]. Both, fcc and hcp adsorption sites were included in the Hamiltonian. Different criteria were used to evaluate competing parameter sets: cross-validation score CV, Mallow's C_p statistics and adjusted R^2 statistics. The parameter space was searched using genetic algorithms in order to find optimum sets. Excellent agreement is found when comparing the shape and stability regions of the theoretical and experimental (from the literature[2]) phase diagrams. Additionally, we were able to elucidate the nature of the $p(2\times2)$ phase transition at 1/4 ML oxygen coverage (experimental results in the literature disagree about the nature of this transition). Differences arise when comparing the values of the calculated and experimental transition temperatures owing to imprecision in present-day DFT calculations.

[1] van de Walle *et al.*, J. Phase Equilib. **23**, 348 (2002).

[2] Schwennicke *et al.*, Phys. Rev. B **56**, 224207 (1997).

O 25.3 Tue 11:45 H41

Repulsive interaction between organic molecules upon adsorption: the case of Sn-phthalocyanine/Ag(111) — •Christoph Stadler, Sören Hansen, Christian Kumpf, and Eberhard Umbach — University of Würzburg, Experimental Physics II, 97074 Würzburg, Germany

The properties of organic thin films largely depend on the balance between molecule-molecule and molecule-substrate interactions and often can be tuned by changing the preparation conditions like temperature or coverage. This is also the case for the family of phthalocyanines (Pc), which are frequently studied as adsorbates on various surfaces. Here we present results on SnPc/Ag(111), a non-planar representative of this family. We used high resolution (SPA-)LEED to investigate the phase diagram of the monolayer regime.

At room temperature the adsorbed SnPc molecules show no long-range order in SPA-LEED up to a coverage of about 0.9. Above this coverage, the film forms incommensurate superstructures, the unit cell parameters of which change *continuously* with increasing coverage. This behavior can be explained by a repulsive intermolecular interaction of the SnPc molecules on the Ag surface. Interestingly, upon cooling below 230 K the film forms a commensurate superstructure between a coverage of 0.6 and 0.9 monolayer.

O 25.4 Tue 12:00 H41

Structural implications of the 1d-2d-transition in Pb wires on Si(557) — •Marcin Czubanowski, Shima Akbari, Christoph Tegenkamp, and Herbert Pfnür — Instittut für Festkörperphisik Leibniz Universität Hannover

The adsorption of Pb on Si(557) substrates leads to the formation of anisotropic metallic structures as revealed by conductivity measurements, STM and ARPES. The annealing of at least 1ML Pb to 640K forms atomic chain structures, which show below T_c=78K a metallic conductance along the wires $(\bar{1}10)$, whereas in the $(\bar{1}\bar{1}2)$ direction an insulating behavior is found. This quasi one-dimensional conductance below T_c is originated by complete Fermi nesting in the direction normal to the structure and split-off valence bands with mesoscopic Fermi-wavelengths along the Pb-chains. These observations are coupled with structural changes that were investigated systematically close to T_c by SPA-LEED experiments described here. The Pb-chains reorganize the structure of Si(557) substrate into [223] facets with $4\frac{2}{3}$ Si unit cells in the $[11\bar{2}]$ direction, as seen by a spot-splitting of 21,3%. This terrace structure undergoes a reversible incommensurate-incommensurate phase transition at T_c, which increases the average interchain distance d and destroys the perfect nesting condition. Simultaneously, the Pb-induced regularly spaced domain wall network, as evident from a 10-fold splitting of the $\sqrt{3}$ structure, disappears. These findings explain qualitatively the observed transport properties, as will be shown.

O 25.5 Tue 12:15 H41

Reversible martensitic phase transition in 4 ML Fe films on Cu(100): A variable temperature STM study — •Albert Biedermann — Institute of Materials Physics, University of Vienna, 1090 Vienna, Austria

In recent years it has been established that 3–4 ML Fe films grown on Cu(100) show a bcc-like structure in terms of crystallography ("nano-martensite")[1] and electronic structure [2]. This work addresses the question whether there also exists a reversible martensitic phase transition between this bcc-like and the fcc phase. Temperature dependent LEED and SMOKE data by Zharnikov et al. [3] suggest a transformation from the ferromagnetic phase to the fcc phase in 4 ML films between 250 and 330 K and a slow reverse transformation after cooling to below 180 K. Indeed, variable temperature STM images obtained in the present experiments show a transition from the bcc-like to the fcc phase between 280 and 330 K in 4 ML films. The reverse transition occurs around 200–250 K on the slow time scale of the VT-STM experiment. This reversible martensitic transition confirms the rather strict correlation between bcc-like structure and ferromagnetic ordering in 4 ML films. The temperature dependent growth of the 2D martensitic "grains" and their characteristic length scales will be discussed.

[1] A. Biedermann, R. Tscheliessnig, M. Schmid, P. Varga, Phys. Rev. Lett. 87 (2001) 086103

[2] D. Spisak, J. Hafner, Phys. Rev. Lett. 88 (2002) 056101

[3] M. Zharnikov, A. Dittschar, W. Kuch, C. M. Schneider, and J. Kirschner, Phys. Rev. Lett. 76 (1996) 4620

O 25.6 Tue 12:30 H41

Temperature Dependent Phase Transitions in 3d-Metal Intercalated Titanium Dichalcogenides — •Eike F Schwier[1], Andreas Nuber[1], Svetlana Titova[2], Alexander Titov[3], and Friedrich Reinert[1] — [1]Universität Würzburg, Experimentelle Physik II, 97094 Würzburg, Germany — [2]Institute of Metallurgy, Urals Division of RAS, Russia — [3]Institute of Metal Physics, Urals Division of RAS, Russia

To this day, it is not fully understood why certain titanium dichalcogenides show the presence of superstructures and others do not. By systematically intercalating these layered solids with electrons from 3d-metal atoms, we want to gain a deeper understanding of the electronical and structural processes within these compounds, that lead tonthe formation of superstructures and their supression.

Previous conductance measurements suggest a second order phase transition at 420 K for Ag_xTiTe_2 (x = 0.65 - 0.74) and at 120 K for $Mn_{0.145}TiSe_2$. By angle-resolved UPS (He I and He II) and XPS (Al K_α) we investigated the influence of the phase transition to the electronic structure along the high-symmetry directions M'-Γ-M and Γ-K of the two materials and relate it to the band structure calculations, the conductance behavior of electronic structure and structural changes.

O 26: Organic, Polymeric, and Biomolecular Films II

Time: Tuesday 11:15–12:15 Location: H42

O 26.1 Tue 11:15 H42

High-resolution ARUPS study of thin NTCDA films on Ag(111) — •Simon Hame, Johannes Ziroff, Azzedine Bendounan, and Friedrich Reinert — University of Würzburg, Experimental Physics II, 97074 Würzburg, Germany

We present high-resolution photoemission data of the valence band structure of organic thin films on noble metal surfaces, in particular on the epitaxial system of a 1,4,5,8-naphtalene-tetracarboxylic acid dianhydide (NTCDA) monolayer on a Ag(111) surface in the relaxed configuration. The electronic structure close to the Fermi edge shows two features: the HOMO peak and a peak assigned to the former LUMO which is partially filled because of charge transfer from the substrate. There appears an additional sharp feature with a pronounced temperature dependence right at the Fermi energy. In high-resolution ARUPS the backfolding of Ag 5s states can be seen as well. We also present data of the order-disorder transition upon cooling beneath 155 K and discuss the relation of quasi-2D and localized molecular properties.

O 26.2 Tue 11:30 H42

Cooling rate dependence of the glass transition of poly(propylene glycol) — •Simone Streit[1], Christian Gutt[2], and Metin Tolan[1] — [1]Fachbereich Physik, Universität Dortmund, Otto-Hahn-Str. 4, 44221 Dortmund, Germany — [2]Deutsches Elektronen Synchrotron (HASYLAB), Notkestr. 85, 22607 Hamburg, Germany

We performed in-situ x-ray reflectivity measurements to determine the cooling rate dependent freezing of capillary waves on the polymer melt poly(propylene glycol) (PPG). Only above the glass transition temperature T_G the surface roughness σ can be described by the capillary wave model for simple liquids, whereas the surface fluctuations are frozen in at lower temperatures. As the state of a glass forming liquid strongly depends on its thermal history, this effect occurs for fast cooling rates already at higher T than for slow cooling. For the fastest cooling rates an astonishingly high shift of T_G up to around 240 K compared to the bulk value of 196 K could be observed.

O 26.3 Tue 11:45 H42

Surface-confined coordination chemistry with metalloporphyrins: *In-situ* metalation and axial coordination — •Ken Flechtner, Yun Bai, Sven Schöffel, Marie-Madeleine Walz, Liam Bradshaw, J. Michael Gottfried, and Hans-Peter Steinrück — Universität Erlangen-Nürnberg, Lehrstuhl für Physikalische Chemie II, Egerlandstr. 3, 91058 Erlangen, Germany

Metalloporphyrins represent the reactive centers in various biological and chemical systems, in which axial coordination of molecules on the central metal ion is essential for their specific functionalities as an enzyme, catalyst, or sensor. Here, we applied and extended concepts of solution-based coordination chemistry to surface reactions of metalloporphyrins adsorbed on an Ag(111) surface. Employing photoelectron spectroscopy and complementary techniques, we focused on: (A) Synthesis of adsorbed metalloporphyrins by direct metalation of porphyrin monolayers with iron, cobalt, and zinc. Also, we demonstrated that adsorbed porphyrins "pick up"pre-deposited Zn atoms from the Ag surface [1]. (B) The electronic interaction between porphyrin-coordinated metal ions and a metal surface in well-defined distances, which were adjusted with different spacer substituents. (C) Axial coordination of small molecules such as NO on the metal centers of the adsorbed porphyrins, resulting in competition between the newly formed coordinate bond and the bond between ion and surface (trans effect). Supported by the Deutsche Forschungsgemeinschaft through SFB 583.

[1] A. Kretschmann *et al.*, Chem. Commun. 2007, DOI: 10.1039/b614427f.

O 26.4 Tue 12:00 H42

Functional immobilization of proteins on solid substrates: An approach to protein chip nanotechnologies — •Andrey Turchanin[1], Ali Tinazli[2], Mohamed El-Desawy[1], Robert Tampé[2], and Armin Gölzhäuser[1] — [1]Physics of Supramolecular Systems, Department of Physics, University of Bielefeld, D-33615 Bielefeld — [2]Institute of Biochemistry, Johann Wolfgang Goethe-University, D-60438 Frankfurt am Main

To study protein function and interaction, there is a high demand for specific, stable, locally immobilized, and functional protein arrays on solid substrates. To implement this, we propose a protein chip approach based on the combination of electron induced chemical nanolithography [1] with aromatic self-assembled monolayers (SAMs) and multivalent chelators [2] for high-affinity capturing of His6-tagged proteins. Templates for functional and switchable His-tagged protein architectures were created by electron beam induced changes in 4*-nitro-1,1*-biphenyl-4-thiol SAMs on gold placed in a protein repellent matrix. As a model system carboxy derivative EG3-tris-NTA and His6-tagged proteasome were studied. Different steps of the biochip templates fabrication were characterized by X-ray photoelectron spectroscopy. Their functionality was tested via in situ atomic force and fluorescence microscopy. We will present first results of functional protein arrays with about one micrometer lateral dimensions. [1] A. Gölzhäuser, W. Eck, W. Geyer, V. Stadler, T.Weimann, P. Hinze, M. Grunze, Adv. Mat. 13 (2001) 806. [2] A. Tinazli, J. Tang, R.Valiokas, S. Picuric, S. Lata, J. Piehler, B. Liedberg, R. Tampé, Chemistry 11 (2005) 5249.

O 27: Prize Talk Lebowitz (Max Planck Medal)

Time: Tuesday 13:00–13:45 Location: H1

From Microscopic Dynamics to Macroscopic Behavior

O 28: Invited Talk Bruno (FV: MA+O)

Time: Tuesday 14:00–14:30 Location: H10

Invited Talk O 28.1 Tue 14:00 H10

Controlling magnetism and self-organization of adatoms on surfaces by using quantum interferences — •Patrick Bruno, Valeri Stepanyuk, Nikolay Negulyaev, and Larissa Niebergall — Max Planck Institute of Microstructure Physics, Halle, Germany

Due to the presence of a surface state, a quasi-free two-dimensional electron gas (2DEG) floats on the (111) surface of noble metals. This 2DEG mediates long-range oscillatory interactions among adatoms, and therefore controls to a large extent the formation of magnetic nanostructures on such surfaces. The competition between this long-range inter-adatom interaction and the adatom-surface interaction gives rise to a wide variety of structures, depending on the nature of adatoms, on their density, on temperature, on the presence of atomic steps, etc. These processes have been studied theoretically by using a combination of first-principles and kinetic Monte-Carlo methods. We have also investigated the spin-polarization and the exchange interaction among adatoms mediated by the 2DEG, as well as how they can be influenced by using quantum confinement and quantum interferences.

V. S. Stepanyuk et al., Phys. Rev. Lett. 94, 187201 (2005)
N.N. Negulyaev et al., Phys. Rev. B 74, 035421 (2006)
L. Niebergall et al., Phys. Rev. Lett. 96, 127204 (2006)
V.S. Stepanyuk et al., Phys. rev.. Lett. 97, 186403 (2006)
P. Wahl et al., Phys. Rev. Lett (in press, 2007)

O 29: Invited Talk Rotenberg

Time: Tuesday 14:45–15:30 Location: H36

Invited Talk O 29.1 Tue 14:45 H36

Many-body interactions in clean and alkali-adsorbed graphene — •E. Rotenberg[1], A. Bostwick[1], T. Ohta[1,2], J. McChesney[1], Th. Seyller[3], and K. Horn[2] — [1]E. O. Lawrence Berkeley Natl. Lab. 6-2100, Berkeley, CA 94720 USA — [2]Fritz-Haber-Institut der MPG, Faradayweg 4-6, 14195 Berlin, Germany — [3]Lehrstuhl für Techn. Physik, U. Erlangen-Nürnberg, Erwin-Rommel-Straße 1, D-91058 Erlangen, Germany

Graphene, a single layer of carbon atoms arranged in a simple honeycomb lattice, is the building block of graphite, fullerenes, and carbon nanotubes and has fascinating electronic properties deriving from the effectively massless, relativistic behavior of its charge carriers. The study of many-body interactions among these carriers is of interest owing to their contribution to superconductivity in these systems.

I will report the characterization of graphene thin films grown on SiC using angle-resolved photoemission spectroscopy (ARPES). We determined the spectral function for monolayer graphene, which encodes the many-body interactions in the system–namely the charge and vibrational excitations. The bands around the Dirac crossing point E_D are heavily renormalized by electron-electron, electron-plasmon, and electron-phonon couplings, which must be considered on an equal footing to understand the quasiparticle dynamics in graphene and related systems. At alkali coverages comparable to graphite intercalation compounds (GICs), renormalization of the carrier mass near E_F becomes significant, supporting the importance of electron-phonon coupling in superconductivity in GICs.

O 30: Nanostructures at Surfaces III (Dots, Particles, Clusters)

Time: Tuesday 15:45–17:45 Location: H36

O 30.1 Tue 15:45 H36

Co on Pt(111): from monolayer islands to single atoms — •Focko Meier, Kirsten von Bergmann, Paolo Ferriani, Jens Wiebe, Matthias Bode, Katsushi Hashimoto, Stefan Heinze, and Roland Wiesendanger — Institute of Applied Physics, Hamburg University, D-20355 Hamburg, Germany

We used spin-resolved scanning tunneling spectroscopy (STS) to study the electronic and magnetic properties of Co monolayer islands and single atoms on the Pt(111) surface.

Within the Co monolayer islands the local stacking changes at the scale of only a few Å. This results in a highly inhomogeneous electronic structure due to the strong stacking dependence of the d-like surface resonance with respect to the Pt(111) substrate.[1] A similar stacking dependence of the electronic structure has been found on the single atoms where spectroscopic differences are related to the two possible adsorption sites of the Co atoms on the Pt(111) substrate.

Despite the electronic inhomogeneity, the magnetic domains and domain walls are clearly observed by spin-resolved STS. New insights into the anisotropy K of the Co were found by analyzing the width of the domain walls. Based on our analysis we propose an out-of-plane anisotropy of +0.08 meV/atom – +0.17 meV/atom for atoms within the islands which are out-of-plane magnetized, independently of their size.

[1] F. Meier et al. Phys. Rev. B 74, 195411 (2006)

O 30.2 Tue 16:00 H36

Single-atom contact and spectroscopy — •J. Kröger[1], N. Néel[1], L. Limot[1], H. Jensen[1], R. Berndt[1], K. Palotas[2], and W.H. Hofer[2] — [1]Christian-Albrechts-Universität zu Kiel, D-24098 Kiel, Germany — [2]University of Liverpool, Liverpool L69 3BX, United Kingdom

The tip of a scanning tunnelling microscope is controllably brought into contact with a flat surface of Au(111), with individual gold atoms on Au(111) and with a single Co atom adsorbed on Cu(100). Contact between the tip and the sample as well as between the tip and single atoms is established at roughly a conductance quantum. Conductance measurements performed on the face-centered cubic and hexagonal close-packed stacking domains of the Au(111) surface reconstruction lead to similar results. While for Cu(100)-Co the Kondo effect-induced resonance is retained in contact it becomes broader than in the tunnelling regime. Calculations indicate that the proximity of the tip shifts the cobalt d-band and thus affects the Kondo temperature.

O 30.3 Tue 16:15 H36

Quantum Confinement of Surface-State Electrons in Atomic-Scale Nanostructures — •L. Niebergall, V. S. Stepanyuk, and P. Bruno — Max-Planck-Institut für Mikrostrukturphysik, Weinberg 2, 06120, Germany

Surface-state electrons on (111) noble metal surfaces form a two-dimensional (2D) nearly free electron gas. Particularly fascinating phenomena occur if the surface electrons are confined to closed structures (quantum corrals, nanoislands, vacancy holes). Such structures can be considered as quantum resonators for surface-state electrons. We present the state of the art ab initio studies of quantum mirages and magnetic interactions in atomic-scale nanostructures [1]. We show that the spin-polarization of surface-state electrons can be projected to a remote location by quantum states of resonators. We find that the spin-polarization of surface-state electrons on transition metal surfaces can be manipulated by exploiting the quantum confinement of electrons [2]. Adatom self-organization induced by quantum confinement of surface electrons is demonstrated [3].

1. V.S. Stepanyuk, L. Niebergall, W. Hergert, P. Bruno, Phys. Rev.

Lett. **94**, 187201 (2005).

2. L. Niebergall, V. S. Stepanyuk, J. Berakdar, P. Bruno, Phys. Rev. Lett. **96**, 127204 (2006).
3. V.S. Stepanyuk, N.N. Negulyaev, L. Niebergall, R. Longo, P. Bruno, Phys. Rev. Lett. **97**, 186403 (2006).

O 30.4 Tue 16:30 H36

Evolution of spin-polarized surface states on magnetic nanostructures: from a single adatom to monolayers — •Pavel Ignatiev, Valeriy Stepanyuk, Larissa Niebergall, and Patrick Bruno — Max-Planck-Institut für Mikrostrukturphysik, Weinberg 2, D-06120 Halle, Germany

Co nanoislands on metallic substrates have been investigated recently both theoretically and experimentally [1-3]. Surface states on Co nanoislands are spin-polarized. A pronounced peak of minority-spin character originating from strong hybridization of Co d-states with s-p states has been found below the Fermi energy. Here, we present the state-of-the-art ab initio calculations of electronic surface states on magnetic cobalt nanostructures placed on metallic substrates (Cu(111), Ag(111) and Au(111)). The evolution of spin-polarized surface states from a single adatom to monolayers is demonstrated. Interplay between structure of cobalt nanoislands and spin-polarized surface states is discussed.

[1] L. Diekhöner, M. A. Schneider, A. N. Baranov, V. S. Stepanyuk, P. Bruno, and K. Kern, PRL 90, 236801 (2003)

[2] O. Pietzsch, A. Kubetzka, M. Mode, and R. Wiesendanger, PRL 92, 057202 (2004)

[3] M. V. Rastei, J.P. Bucher, P.A. Ignatiev, V.S. Stepanyuk, and P. Bruno, submitted to PRB

O 30.5 Tue 16:45 H36

Selfassembled growth and magnetism of ordered arrays of nanometer size Co clusters — •Axel Enders, Jian Zhang, Violetta Sessi, Jan Honolka, and Klaus Kern — MPI für Festkörperforschung, Heisenbergstraße 1, D-70569 Stuttgart

In this talk we will show how spherical clusters of less than 3 nm diameter can be fabricated on substrates by buffer layer assisted growth, without the implications usually associated with epitaxy. The resulting clusters are randomly distributed over the bare substrate surface. However, the application of such clusters as individually addressable magnetic units requires their controlled arrangement into well-defined ordered arrays. We are therefore guiding the clusters with the morphology of periodic network structures prefabricated on the substrate. We use mechanically extremely stable boron nitride nanomeshes as template surfaces. We will demonstrate that ordered cluster layers with a filling factor of more than 75% are achieved by repeated cluster deposition cycles onto the nanomesh. We will discuss the magnetic properties of the cluster ensemble as well as the application of the mesh as reactor for the fabrication of ordered, binary alloy clusters.

O 30.6 Tue 17:00 H36

Co clusters on the boron nitride nanomesh — •Thomas Brugger, Martina Corso, Simon Berner, Thomas Greber, and Jürg Osterwalder — Physik-Institut, Universität Zürich, Winterthurerstrasse 190, 8057 Zürich

Recently a new boron nitride nanostructure was discovered. Exposing a Rh(111) surface to borazine $(HBNH)_3$ at high temperature leads to a very regular 13-by-13 superstructure of hexagonal boron nitride (*h*-BN). This self-assembled nanostructure called nanomesh exhibits pores of the size of about 2 nm and a periodicity of 3.2 nm [1]. The nanomesh is thermally very stable and even resistant against air and water exposure.

We study the use of the nanomesh as a template for metal cluster growth. Scanning tunneling microscopy was used to examine the size distribution and the location of the clusters. Former studies of Co on *h*-BN/Ni(111) show 3D clusters with a linear height to apparent width relation and 2D clusters of constant height for several apparent widths [2]. On the nanomesh we find quite monodisperse 3D clusters of Co that preferably stick in the nanomesh pores. They have an apparent diameter comparable to the mesh pore diameter. This demonstrates that the nanomesh works as a template. The magnetic properties of the clusters are under investigation.

[1] M. Corso et al., Science 303 (2004) 217

[2] W. Auwärter et al., Surface Science 511 (2002) 379

O 30.7 Tue 17:15 H36

interaction of scanning tunneling microscopy tip with adatoms, mesoscopic islands and molecules on metal surfaces — •kun tao[1], ren z huang[1], volodymyr v maslyuk[2], mads brandbyge[3], ingrid mertig[2], valeri stepanyuk[1], patrick bruno[1], and jurgen kirschner[1] — [1]Max-Planck-Institute of Microstructure Physics, Weinberg 2, 06120 Halle, Germany — [2]Martin-Luther-University Halle-Wittenberg, Fachbereich Physics , 06099, Halle,Germany — [3]Condensed Matter Theory Group, Department of Physics, Uppsala University, SE-751, Sweden

We perform a realistic atomistic modeling and ab initio calculations for the tip interaction with magnetic adatoms, nanoislands and single molecules on metal surfaces. The electronic states and the magnetic moment of adatoms are found to depend strongly on the distance between the tip and the adatom[1]. Our results reveal tip-induced shape transitions in nanoislands as the tip approaches the surface[2]. Atomic relaxations in the tip, nanoislands and a substrate are discussed. The interaction between 3d adatoms and a single benzene molecule on Cu(001) is studied. Our results show that magnetic and transport properties of such magnetic systems can be significantly affected by the STM tip.

1.R.Z. Huang, V.S. Stepanyuk, A.L.Klavsyuk, W. Hergert, P.Bruno, and J. Kirschner,Phys. Rev. B 73 153404 (2006).

2.R.Z. Huang, V.S. Stepanyuk, and J. Kirschner, J. Phys. Cond. Matter 18, L217(2006).

O 30.8 Tue 17:30 H36

Mechanical properties of Au_{55} clusters investigated by NC-AFM — •Georgeta Radu, Dirk Mautes, and Uwe Hartmann — Institute of Experimental Physics, Saarland University, D-66041 Saarbrücken, Germany

In recent years, non-contact atomic force microscopy (NC-AFM) became a powerful tool for imaging at high resolution as well as for probing specific surface properties. In order to investigate the mechanical properties of individual clusters, thin films of ligand-stabilized Au_{55} clusters have been deposited on Au(111) and highly oriented pyrolytic graphite (HOPG) substrates. The NC-AFM images show locally ordered monolayer islands on the Au(111) substrate and disordered ones on the HOPG substrate. Frequency shift- and damping-versus-distance measurements on individual clusters as well as on the bare substrate were performed. The interaction force and dissipated energy were deduced from the experimental curves. Combining the experimental results with theoretical models, the strength and the distance dependence of the interaction force between tip and an individual Au_{55} cluster has been analyzed quantitatively. Furthermore, the individual contributions of the gold core and the ligand shell could be identified in the interaction between tip and an individual Au_{55} cluster. The measured energy dissipation is of the same order as the energy of vibrational modes due to bondstretching in the ligands and between the gold atoms and the ligands. Therefore, the energy is most likely dissipated into vibrations of the ligands through a stochastic dissipation mechanism.

O 31: Surface Chemical Reactions and Heterogeneous Catalysis I

Time: Tuesday 15:45–17:45 Location: H38

O 31.1 Tue 15:45 H38

Theoretical insight into the oxidation of nanoporous carbon materials — •Johan M. Carlsson and Matthias Scheffler — Fritz-Haber-Institut der Max-Planck-Gesellschaft, Faradayweg 4-6, D-14195 Berlin

Nanoporous carbon(NPC) may be visualized as crumpled graphene sheets with a significant amount of voids. Oxygen can be used to modify its properties and STM indicates that O_2 etches edges and vacancies in graphitic materials[1]. TPD shows desorption of CO and CO_2 indicating the presence of C-O-groups on the surface[2]. However, the characterization of the actual surface structure of oxidized NPC is unsatisfactory and the individual reaction steps for the oxidation are still not well known. We have therefore carried out an extensive study of NPC using ab-initio thermodynamics. Our density-functional theory (DFT) calculations show that O_2 dissociation is endothermal on defect free graphene surfaces, but exothermal at vacancies. The O-atoms attach to the undercoordinated C-atoms at vacancies forming C-O-groups. C-O-C (Ether) groups dominate and C=O (Carbonyl) groups may also appear. The C=O groups are precursors for CO-desorption, but two C-C bonds needs to be broken to desorb the CO-molecule. Our thermodynamic treatment shows that CO therefore only desorbs above 700 K from these sites in agreement with the TPD experiment[2]. Based on these results we propose that the oxidative etching of NPC materials proceeds via a sequence of dissociative O2 adsorption and CO desorption. [1] J. J. Paredes *et al.* , Carbon **38**, 1183, (2000). [2] M. J. Nowakowski *et al.*, J. Am. Ceram. Soc. **76**, 279 (1993).

O 31.2 Tue 16:00 H38

Initial kinetic-energy and isotope dependence of electronic energy dissipation during chemisorption of H/Al(111) — Michael Lindenblatt and •Eckhard Pehlke — Institut für Theoretische Physik und Astrophysik, Christian-Albrechts-Universität Kiel, 24098 Kiel

The amount of energy dissipated into electron-hole pairs during chemisorption or scattering of H-atoms at the Al(111) surface has been investigated as a function of the mass of the incoming hydrogen atom and its initial kinetic energy. The energy dissipation into electronic degrees of freedom, which occurs parallel to the energy dissipation into substrate vibrations, is evoked by electronic friction effects as well as strongly non-adiabatic effects during transfer of the local electronic spin polarization at the incoming H-atom to the substrate upon adsorption [1]. We report results from *ab initio* molecular dynamic simulations based on time dependent spin-density-functional theory combined with Ehrenfest dynamics for the motion of the nuclei. Essentially, the results for the energy dissipated electronically during one passage of the H-atom through the spin transition break down onto a single curve, if plotted versus the velocity of the H-atom at the spin-transition point. The respective Kohn-Sham electronic excitation spectra exhibit an asymmetry between spin-up and spin-down electrons [2], as to be expected for a delayed non-adiabatic transfer of spin polarization from the H-atom to the reservoir of substrate electrons.

[1] M.S. Mizielinski *et al.*, J. Chem. Phys. **122**, 084710 (2005).

[2] M. Lindenblatt, E. Pehlke, Phys. Rev. Lett. 97, 216101 (2006).

O 31.3 Tue 16:15 H38

Water formation studies on vanadium oxide thin film covered Pd(111) — •Markus Kratzer, Johanna Stettner, and Adolf Winkler — Institute of Solid State Physics, University of Technology Graz, Petersgasse 16, A-8010 Graz

The formation of D_2O on vanadium oxide (VO_x) thin film nano structures on Pd(111) has been investigated. Quadrupole mass spectrometry has been used to determine the flux of the reaction products desorbing from the surface. Low energy electron diffraction (LEED) and Auger electron spectroscopy (AES) were applied to monitor possible changes in the surface composition during reaction. The experiments were carried out at sample temperatures of 523 K and 700 K, respectively. The water reaction was fed with atomic deuterium via bulk permeation and simultaneous dosing of molecular oxygen. It turned out that the VO_x coverage as well as the sample temperature have significant influence on the reaction. The D_2O formation rate drops with increasing VO_x coverage and increases with rising sample temperature. Additionally, we found evidence that the VO_x structures change during water formation, especially at 700 K.

O 31.4 Tue 16:30 H38

Local investigation of femtosecond laser induced processes: CO on Cu(111) — •Michael Mehlhorn, Heiko Gawronski, and Karina Morgenstern — Institut für Festkörperphysik, Leibniz Universität Hannover, Appelstr. 2, D-30167 Hannover, Germany

A combination of femtosecond laser excitation with a low temperature scanning tunneling microscope is used to study two key processes, diffusion and close approach of reactants, of a non-adiabatic surface reaction for adsorbed CO molecules on a Cu(111) surface in real space. For the first process we obtain two different electron mediated excitation pathes by analyzing the dependence of the hopping rate of individual molecules on laser fluence. The first one involves inelastic scattering of one photo-excited substrate electron on the CO molecule whereas for the second process thermalized substrate electrons play the major role. For the second key process we investigate the generation of CO dimers. Femtosecond laser excitation leads to a transient attraction of usually repelling CO molecules. We model both processes quantitatively and extract a diffusion barrier of 87 meV and a CO-attraction energy of 30 meV.

O 31.5 Tue 16:45 H38

Interaction of O_2, CO, and Methanol with Bimetallic Model Catalysts — T. Nowitzki[1], B. Jürgens[1], H. Borchert[1], •V. Zielasek[1], T. Risse[2], H.-J. Freund[2], S. Giorgio[3], C.R. Henry[3], and M. Bäumer[1] — [1]Institut für Angewandte und Physikalische Chemie, Universität Bremen — [2]Fritz-Haber-Institut der Max-Plack-Gesellschaft, Berlin — [3]CRMCN-CNRS, Campus de Luminy, Marseille

Bimetallic particles may exhibit catalytic activities which reach far beyond those of the monometallic components. For the Co/Pd combination which is, e.g., of technological relevance for the hydrogenation of CO on the route from natural gas to liquid fuel, we have studied the interaction of model catalysts with CO, O_2, and methanol on the molecular scale. Experiments were performed in UHV by TPD, FTIR, and ferromagnetic resonance, as well as in ambient conditions by DRIFTS and gas phase analysis. In UHV, mono- and bimetallic nanoparticles were prepared by physical vapour deposition on thin epitaxial alumina films on NiAl(110). Upon exposure to O_2 and annealing, a complex oxidation-reduction scheme of the particles is observed which involves the substrate and depends on the particle composition. After exposure to methanol, we find a CO-desorption-limited route of decomposition via C-H bond scission which is universal for monometallic and bimetallic particles. We will show close correlations between the results obtained in UHV and turn-over experiments for CO oxidation and methanol decomposition at Pd and CoPd nanoparticles on MgO in ambient conditions.

O 31.6 Tue 17:00 H38

Electronic energy dissipation of deuterium and hydrogen atoms on gold and platinum surfaces — Beate Mildner, Eckart Hasselbrink, and •Detlef Diesing — Fachbereich Chemie and Centre for Nanointegration (CeNIDE), Universität Duisburg-Essen, D-45117 Essen, Germany

Chemical surface reaction as adsorption and **L**angmuir **H**inshelwood (LH) reaction may dissipate their excess energy to substrate and adsorbate vibrations or to electronic degrees of freedom. The latter ones can only be detected externally by light emission or when the dissipated energy exceeds the electronic work function Φ of the metal. Electronic surface excitations $E < \Phi$ can be monitored on the surface of thin film tunnel devices. We use tantalum–tantalum oxide–top metal tunnel junctions. As top metal 5 nm thick Pt films or 12 nm thick Au films were used. Both enable a ballistic transport of excited electrons (holes) with excess energies up to 1 eV from the surface to the oxide interface. The excited carriers are then detected in the tantalum backelectrode as a tunnel current. Bunches of H and D atoms ($5 \cdot 10^{15}$ atoms in 20 seconds) were emitted to the top metal. On Au surfaces the tunnel current trace can be assigned predominantly to LH reactions. H atoms cause a 4.5 times higher tunnel signal than D atoms. On Pt surfaces the tunnel current trace is dominated by the adsorption process which is reasonable due the higher binding energy. On Pt surfaces the tunnel current signals of hydrogen and deuterium are comparable. The results are compared to recent DFT calculations.

O 31.7 Tue 17:15 H38

(4x4)O structure on Ag(111): LEED-I/V analysis and high-pressure STM — •Robert Reichelt, Sebastian Günther, Joost Wintterlin, and Wolfgang Moritz — Ludwig-Maximilians-Universität, München, Germany

The (4x4)O structure on Ag(111) plays a central role in the Ag/O system, and it is assumed that structurally similar oxygen species contribute to the ethylene epoxidation on Ag surfaces. Several models of the (4x4)O structure on Ag(111) have been discussed in the past. We have performed a LEED-I/V (low-energy electron-diffraction) analysis using two different experimental setups. One was a conventional LEED system mounted into a laboratory UHV system, the second was a LEEM (low-energy electron microscope). The (4x4)O structure was prepared by exposure to NO2. The two data sets agree very well with each other, demonstrating that I/V structure analyses can be performed either with LEED or with LEEM. The structure obtained in the analysis confirms a recently proposed model that involves a reconstruction of the Ag(111) surface. Previous models based on a thin layer of Ag2O are disproved. The (4x4)O structure was also investigated by high-pressure STM in an attempt to study its role in the partial oxidation of ethylene. The formation of the (4x4)O structure could be monitored in situ, under oxygen pressures in the mbar regime and at elevated temperatures. When ethylene was added massive structure changes occurred, indicating that the (4x4)O structure is most likely not the active phase under reaction conditions.

O 31.8 Tue 17:30 H38

Photothermal patterning of H-terminated Si(100) substrates: Experiments in an ultrahigh vacuum environment — •Mareike Mathieu, Rafael Bautista, Nils Hartmann, and Eckart Hasselbrink — Fachbereich Chemie, Universität Duisburg-Essen, Universitätstr. 5, 45117 Essen

Silicon substrates are widely used as platforms in many micro- and nanofabrication schemes, e.g. in order to build up organic templates [1,2]. For this purpose suitable patterning techniques are needed. In a previous study, we reported a simple laser-assisted technique for patterning of H-terminated Si(100) substrates under ambient conditions [1]. A focused beam of an argon ion laser at a wavelength of 514 nm is used to create well-confined, ultra-thin oxide structures. Despite a laser spot diameter of about 2.5 microns line widths down to 300 nm are reached. In order to investigate the underlying mechanism, recent experiments were carried out at well-defined conditions in an ultrahigh vacuum environment. HF etched Si(100) substrates, Si(100)-(1x1)-dihydride and Si(100)-(2x1)-monohydride adsorbate phases were prepared for patterning. On the basis of the results, the nonlinear dependence of the patterning process on the laser intensity is traced back to the interplay between the laser-induced temperature rise and the thermally activated hydrogen desorption.

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

[2] D. Dahlhaus, S. Franzka, E. Hasselbrink, N. Hartmann, Nano Letters 6 (2006) 2358

O 32: Semiconductor Substrates

Time: Tuesday 15:45–17:30 Location: H39

O 32.1 Tue 15:45 H39

Dynamics and energetics of Ge(001) dimers — •Harold Zandvliet, Arie van Houselt, Raoul van Gastel, and Bene Poelsema — Physical Aspects of NanoElectronics & Solid State Physics, MESA+ Institute for Nanotechnology, University of Twente, P.O. Box 217, 7500 AE Enschede, The Netherlands

The dynamic behavior of surface dimers on Ge(001) has been studied by positioning the tip of a scanning tunneling microscope over single flip-flopping dimers and measuring the tunneling current as a function of time. We observe that not just symmetric, but also asymmetric appearing dimers exhibit flip-flop motion. The dynamics of flip-flopping dimers can be used to sensitively gauge the local potential landscape of the surface. Through a spatial and time-resolved measurement of the flip-flop frequency of the dimers, local strain fields near surface defects can be accurately probed.

O 32.2 Tue 16:00 H39

Interlayer interaction and electronic screening in multilayer graphene — •Karsten Horn[1], Taisuke Ohta[2], Aaron Bostwick[2], Jessica McChesney[3], Thomas Seyller[4], and Eli Rotenberg[2] — [1]Fritz-Haber-Institut der MPG, Berlin — [2]Advanced Light Source, LBL Berkeley — [3]Montana State Universtiy, Bozeman, Montana — [4]Inst. F.Physik der Kondens. Materie, Universität Erlangen-Nürnberg

Much recent attention has been given to the electronic structure of multilayer films of graphene, the honeycomb carbon sheet which is the building block of graphite, carbon nanotubes, C60 , and other mesoscopic forms of carbon. Recent progress in synthesizing or isolating multilayer graphene films has enabled access to their physical properties, and revealed many interesting transport phenomena, including an anomalous quantum Hall effect, ballistic electron transport at room temperature, micron-scale coherence length, and novel many-body couplings. The unusual transport properties of graphene originate from the effectively massless Dirac Fermion character of the carriers derived from graphene's valence bands, which exhibit a linear dispersion degenerate near the so-called Dirac point. We determine the shape of the π bands and their characteristic splitting, and the transition from a pure 2D to quasi-2D behavior for 1 to 4 layers of graphene by angle-resolved photoemission. By exploiting the sensitivity of the π bands to the electronic potential, we derive the layer-dependent carrier concentration, screening length and strength of interlayer interaction by comparison with tight binding calculations, yielding a comprehensive description of multilayer graphene's electronic structure.

O 32.3 Tue 16:15 H39

High energy femtosecond UV photo desorption dynamics of NO from HOPG at FLASH — •Tim Hoger[1], Björn Siemer[1], Carsten Thewes[1], Marco Rutkowski[1], Helmut Zacharias[1], Stefan Düsterer[2], and Rolf Treusch[2] — [1]Universität Münster, Physikalisches Institut, Wilhelm-Klemm-Str. 10, 48149 Münster — [2]DESY, Hasylab, Notkestr. 85, 22603 Hamburg

The interaction of nitric oxide under high energy irradiation is an important issue in understanding the heating of the atmosphere and the formation of acid rain. At low temperatures NO adsorbs on dust grains or Mi particles. We present recent results of the interaction of NO adsorbed on graphite with high energy radiation. The desorption is achieved by the free electron laser at Hamburg (FLASH) supplying femtosecond pulses of up to $100\,\mu$J with a photon energy of $57\,$eV. All internal energies of NO molecules desorbing from a highly oriented pyrolytic graphite (HOPG) sample are resolved in a pump-probe experiment. Highly excited molecules with a vibrational temperature around $T_{vib} \approx 2500\,$K and a high rotational excitation up to $T_{rot} \approx 1200\,$K are detected. Possible excitation and desorption mechanisms in this high energy regime are discussed.

O 32.4 Tue 16:30 H39

Photoisomerization of Stilbene on Si(100): Gaining further insight by combined theoretical and experimental C 1s NEXAFS spectra — •Christine Kolczewski[1], Klaus Hermann[1], Ralph Püttner[2], Philipp Martin Schmidt[1], Thorsten Kampen[1], and Karsten Horn[1] — [1]Fritz-Haber-Institut der Max-Planck-Gesellschaft, Faradayweg 4-6, 14195 Berlin, Deutschland — [2]Freie Universität Berlin, Institut für Experimentalphysik, Arnimallee 14, 14195 Berlin, Deutschland

Stilbene is a prototype molecule for studying photoinduced cis-trans isomerization. To gain further insight into the isomerization of stilbene at the Si(100) surface the system was investigated by several spectroscopic methods such as UPS and NEXAFS.

In this work, we present density-functional theory (DFT) calculations of both stilbene isomers on $Si_{14}H_{28}$ clusters simulating the reconstructed Si(100) surface. Both isomers bind to Si with their central C=C double bond but differ in the arrangement of their phenyl rings with the overall binding being quite strong (binding energy of

3-4 eV). The obtained geometries have been used to calculate theoretical polarization-resolved C 1s NEXAFS spectra which are compared with recent experimental data and yield excellent agreement. This confirms the identification of both isomers for a further investigation of the isomerization process.

In addition, theoretical and experimental C 1s NEXAFS spectra of the free stilbene molecules are used to study adsorption induced changes in geometry and electronic structure.

O 32.5 Tue 16:45 H39

Identifying isomerization - combined experimental and theoretical NEXAFS studies — •Philipp Martin Schmidt[1], Ralph Püttner[2], Christine Kolczewski[1], Klaus Hermann[1], Karsten Horn[1], and Thorsten Kampen[1] — [1]1 Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, Germany — [2]Freie Universität Berlin, Institut für Experimentalphysik, Berlin, Germany

When studying the isomerization of molecules, identification and distinction of the different isomers is a critical issue. Here cis- and trans-Stilbene are a model system for ”molecular switches”. We have investigated their adsorption on Si(100) and Au(111) surfaces, and for comparison, in gas-phase. In this work we demonstrate the use of NEXAFS-spectroscopy as a versatile tool to investigate the interaction of the molecules with the surface and the arising consequences for isomerization. NEXAFS-spectra of the molecules in gas-phase show spectral features in the π^*-resonance that allow for a clear distinction of the isomers. Upon adsorption on surfaces these spectral features remain unchanged - thus clearly identifying the isomers - while the σ^*-resonances and the higher π^*-resonances undergo changes. In combination with theoretical calculations these changes can be used to identify the interaction of the molecules with the substrates and to reveal the adsorption geometry. Furthermore the implication of adsorption on the photoinduced isomerization, especially the inhibition of the isomerization-pathways known for gas-phase and solution, is explained.

O 32.6 Tue 17:00 H39

Individual molecules of hexaphenyl on Si(100)-2x1 — •Marion Cranney, Marta Martin, Andrew Mayne, Damien Riedel, and Gérald Dujardin — Laboratoire de PhotoPhysique Moléculaire, Orsay, France

Hexaphenyl molecules are very attractive for applications in molecular opto-electronics since they have quite interesting electrical and optical properties.

We have worked with a LT-STM at 5 K in order to study the structural properties of individual hexaphenyl molecules on Si(100)-(2x1). We observed that this molecule is weakly chemisorbed on Si(100) when deposited at 5 K. We analysed carefully STM pictures of each conformation in order to understand how the molecule of hexaphenyl interact with silicon dimers.

Moreover we have investigated the electronic and dynamical properties of these molecules with the LT-STM by exciting each phenyl ring of different conformations of the molecule with voltage pulses. The molecule change its conformation reversibly without diffusing across the surface. The location of the pulses on the molecule determines the molecular dynamics. This is due to different interactions of each phenyl with the silicon atoms, an effect that is shown by measurements of scanning tunneling spectroscopy.

O 32.7 Tue 17:15 H39

Investigations of Ga adsorption on Si(113) with scanning tunneling microscopy — •Moritz Speckmann, Thomas Schmidt, Subhashis Gangopadhyay, David Krueger, Torben Clausen, and Jens Falta — Institute of Solid State Physics, University of Bremen,

High index surfaces are of strong interest in today‘s research because they are supposed to be a candidate for self-assembling systems, for example nano wires.

In this work the adsorption of Ga on Si(113) has been investigated in dependence on the growth temperature. After Ga adsorption one discovers two kinds of facets on the surface. We used scanning tunneling microscopy (STM) and low energy electron diffraction (LEED) to characterise the facets regarding their properties like length, heigth, width, and their tilt to the (113) surface as well as surface reconstructions.

The facets grow in $[\bar{1}10]$-direction. Depending on temperature a very regular arrangement of facets can be achieved. Due to their tilt towards the (113) surface and their surface reconstructions they are identified as (112) and (115) facets. We observed mainly (6×1) and (4×1) reconstructions on the (112) facets and on the (115) facets, respectively. Regarding their dimensions both facets are found to be strongly influenced by the growth temperature, whereat the (112) facets seem to be thermally more stable than the (115) facets. The STM images and the corresponding LEED images give hints that the (115) facets merge into (114) or (227) facets at temperatures of 600°C and higher.

O 33: Oxides and Insulators: Epitaxy and Growth

Time: Tuesday 15:45–17:45 Location: H41

O 33.1 Tue 15:45 H41

Ab-initio study of the epitaxial growth of germanium on SrHfO3(001) using strontium as surfactant — •Andrei Reyes Huamantinco and Peter Blöchl — Clausthal University of Technology, Institute for Theoretical Physics, Leibnizstr. 10, D-38678 Clausthal-Zellerfeld, Germany

The channel in a MOSFET must consist of layers with smooth morphology and low defect density. When germanium (high mobility channel) is deposited on SrHfO3 (high-k oxide) it clusters. Nevertheless, we find that depositing a full monolayer of strontium on SrHfO3(001) and using it as template for germanium overgrowth, inhibits clustering. Formation of the first two epitaxial germanium monolayers occurs via consolidation of so-called germanium zig-zag chains which are pieces of the first and second Ge(001) monolayers, and an structural element of the diamond crystal structure. During consolidation of the zig-zag chains, some atoms from the strontium monolayer diffuse to the surface in order to saturate the germanium dangling bonds. After deposition of two germanium monolayers, the resulting configuration consists of strontium half monolayer at the surface, two epitaxial germanium monolayers, the other half monolayer of strontium that remained at the interface, and SrHfO3(001). Further deposition of germanium results in a surfactant-mediated epitaxial layer-by-layer growth because half monolayer of strontium stabilizes the germanium surface and strontium is not incorporated into bulk germanium. The interfacial half monolayer of strontium stabilizes the interface, and provides adequate valence and conduction band offsets for transistor applications.

O 33.2 Tue 16:00 H41

Oxidation on the nanoscale - the tungsten-water reaction in high electric fields — •Carsten Nowak[1], Guido Schmitz[2], Reiner Kirchheim[1], and Christian Oberdorfer[2] — [1]Institut für Materialphysik, Universität Göttingen, D-37077 Göttingen — [2]Institut für Materialphysik, Universität Münster, D-48149 Münster

The oxidation of nanoscale needle-shaped tungsten tips in water vapor at room temperature is strongly depending on the electric field around the nanotip. Above a critical field strength of the order of 10^9 V/m the natural oxidation process is extended by a field-induced oxidation reaction. Investigation of the oxidation kinetics reveals that the oxidation reaction virtually terminates after some seconds. The morphology of the formed oxide layer shows a distinct pressure dependence in the range of 10^{-4} to 10^1 mbar H_2O, with a characteristic size of the formed oxide layer of up to some 100 nm. Using pulsed laser atom probe tomography, the stoichiometry of the formed oxide is determined to be WO_3.

Calculation of the electric field distribution around the tip with the finite element method allows conclusions about the field-influence on oxide growth and the appearance of different morphologies in dependence of the water pressure. Special attention will be paid to the aspect of charge compensation, and it will be discussed to which degree the enhanced oxidation reaction under the influence of the electric field is material independent.

O 33.3 Tue 16:15 H41

Structural and vibrational properties of ultrathin MnO films

on Pt(111): An HREELS, STM and LEED study — S. Sachert[1], B. Bochmann[1], Ch. Hagendorf[1], K. Kostov[2], and •W. Widdra[1] — [1]Martin-Luther-Universität Halle-Wittenberg, Institute of Physics , Halle — [2]Bulgarian Academy of Science, Sofia, Bulgaria

The atomic structure and the vibrational properties of ultrathin MnO films on Pt(111) have been studied using high-resolution electron energy loss spectroscopy (HREELS), scanning tunneling microscopy (STM), and low-energy electron diffraction (LEED). The formation of several Mn oxide structures during Mn deposition in an O_2 atmosphere has been investigated as a function of film thickness up to 6 ML, substrate temperature and subsequent annealing cycles up to 1200 K. Within the monolayer, three different Mn_xO_y structures with Mn/O ratios between 1 and 2 have characterized by HREELS, STM, LEED, and thermal oxygen desorption : The MnO monolayer grown in an oxygen atmosphere of about 8x10^{-8} mbar is characterized by a strong optical phonon at 364 cm^{-1}, a (19x1) superstructure which is stable up to 1100 K. Annealing in p_{O2}=1x10^{-6} mbar converts this phase to a hexagonal structure with a lattice constant of 0.42 nm and MnO_2 stoichiometry. It shows two characteristic vibrations at 580 and 716 cm^{-1}, is stable up to 840 K and identified as single O-Mn-O layer of MnO(111). Reduction of this phase in CO or annealing above 840 K in UHV results in a third oxide structure with two strong phonons at 332 and 391 cm^{-1}. This oxide is stable up to 1000K.

O 33.4 Tue 16:30 H41

Preparation and Investigation of well ordered thick Silica films on Mo(112) — •Martin Baron, Dario Stacchiola, Sarp Kaya, Shamil Shaikhutdinov, and Hajo Freund — Fritz-Haber-Institut der Max-Planck-Gesellschaft, Faradayweg 4-6, 14195 Berlin, Germany

Recently our group has demonstrated the preparation of well ordered thin silica films on Mo(112) substrate [1]. The structure of the film has been determined employing varies experimental techniques and theoretical calculations [2]. In this work we use a similar approach for growth of thicker silica films which resemble the structure and properties of bulk silica. The experimental results of XPS, IRAS, STM and LEED will be presented.

[1] Schroeder T, Adelt M, Richter B, et al., SURFACE REVIEW AND LETTERS 7 (1-2): 7-14 FEB-APR 2000

[2] Todorova TK, Sierka M, Sauer J, et al., PHYSICAL REVIEW B 73 (16): Art. No. 165414 APR 2006

O 33.5 Tue 16:45 H41

Layer-resolved study of the local electronic structure of ultrathin NiO(001) films on Ag(001): A STS and DFT study — •S. Grosser[1], Chr. Hagendorf[1], M. Däne[1], A. Ernst[2], M. Lüders[3], Z. Szotek[3], W. M. Temmerman[3], W. Hergert[1], and W. Widdra[1] — [1]Martin-Luther-Universität Halle-Wittenberg, Institute of Physics, Halle — [2]MPI for Microstructure Physics, Halle — [3]Daresbury Laboratory, Warrington, U.K.

Scanning tunneling microscopy (STM), scanning tunneling spectroscopy (STS), and density functional theory (DFT) have been applied to study the local electronic and atomic structure of thin NiO films on Ag(001). Differential conductance spectra (dI/dV) for precursor phases, oxide bilayer and thin oxide films up to 5 ML exhibit distinct differences in the electronic structure. The region of the unoccupied states up to 4 eV above E_F is dominated by the local density of states within the oxide film. Especially for 2 ML islands and thicker films strong and well-resolved unoccupied Ni 3d-states are found. At energies above 4.5 eV, the experimental spectra exhibit strong field emission resonances which are characteristically modified by the thickness-dependent oxide band structure. The experimental determined electronic structure will be compared with DFT calculations considering also different magnetic ordering within the NiO film. The strong electron correlation effects in the oxide are taken into account via self-interaction corrections. The calculated layer-dependent evolution of the NiO electronic structure and the appearance of a Ni 3d-derived surface state compare well with the experimental results.

O 33.6 Tue 17:00 H41

Electronic structure and quasiparticle calculations of molecules on thin epitaxial films - a DFT and GW study — •Christoph Freysoldt, Patrick Rinke, and Matthias Scheffler — Fritz-Haber-Institut der MPG, Berlin, Germany

To study insulator surfaces with surface-science techniques that require conducting samples such as photoelectron spectroscopy or STM epitaxial films are often employed. However, the difference in the dielectric properties between the film and the substrate intrduces additional polarization effects that modify the electronic states of the film and of molecules adsorbed on it. Here, we present G_0W_0 quasiparticle calculations that incorporate these effects in a natural way, for the electronic structure of molecule/film/substrate system, using NaCl/Ge(001) as a prototypical insulator/semiconductor interface and CO as a model adsorbate. The atomic structure of the NaCl/Ge(001) in interface – so far unknown from experiment – is determined using density-functional theory. We observe that the quasiparticle gap of CO adsorbed on the NaCl film varies as a function of the film thickness. The dielectric response of the substrate also introduces a z-dependence of the quasiparticle corrections within the NaCl film, which then differ by up to 0.6 eV between the Ge-interface and the surface. In experiments either metallic substrates are used or the semiconducting substrates are strongly doped to increase their conductivity. We expect that the effects reported here will be even more pronounced for these substrates due to their larger polarizability.

O 33.7 Tue 17:15 H41

Growth of One-dimensional Pd Nanowires on the Reduced SnO_2(101) Surface — Alexander Urban[1], •Bernd Meyer[1], Khabibulakh Katsiev[2], Matthias Batzill[2], and Ulrike Diebold[2] — [1]Lehrstuhl für Theoretische Chemie, Ruhr-Universität Bochum — [2]Department of Physics, Tulane University, New Orleans, USA

The adhesion of metals on insulating surfaces is usually much weaker than the cohesion within the metal itself. Therefore, in vapor deposition experiments metals do not ‘wet’ most surfaces of insulators, but 3D cluster formation is observed even at very low metal coverage. In a recent STM experiment [1] however, it was observed that Pd, vapor-deposited on the fully reduced SnO_2(101) surface, forms one-dimensional islands with a uniform width of one substrate unit cell and a height of one atomic layer. Neighboring islands do not merge, and the length of the nanowires is only limited by the size of the substrate terraces. DFT calculations have been performed to investigate the atomic processes which lead to this, for metal oxide substrates unusual, overlayer growth [1] It is found that the one-dimensional wires are not the thermodynamically most stable structure, but their formation is dominated by kinetic effects. A pronounced one-dimensional diffusion, combined with a strong interaction of Pd with the surface Sn atoms and the lack of stable binding sites at the sides of the nanowires are responsible for the formation of the one-dimensional islands.
[1] K. Katsiev, M. Batzill, U. Diebold, A. Urban, B. Meyer, submitted to Phys. Rev. Lett.

O 33.8 Tue 17:30 H41

The initial stages of Chromium growth on Titaniumdioxide-Investigations using synchrotron radiation — •Sebastian Müller and Dieter Schmeisser — Brandenburgische Technische Universität Cottbus, Lehrstuhl Angewandte Physik-Sensorik, Postfach 10 13 43, 03013 Cottbus

We investigate the interface of Cr-TiO_2 during the initial stages of Cr deposition. Experiments are carried out at BESSY II (BL U49/2-PGM2). Using XPS, XAS and ResPES we obtain information about electronic structure at the interface. We confirm the results of growth studies by Christian Winde obtained by TEM-EELS. In addition, we find that Cr deposition induces two gap states which appear about 1 eV and 3 eV below E_F. Using ResPES, these states can be identified as being Cr-like and Ti-like respectively. Core-level-XPS and CIS-spectra of the lower gap state indicate the existence of mainly Cr^{4+} at low coverage (< 1 ML).

At higher coverage ($\approx$ 2.5 ML) metallic Cr is observed as well as metallic Ti. Oxidized Cr occurs mainly as Cr^{3+}. CIS-spectra of higher gap state show metallic behavior with both Cr- and Ti-like character. CIS-spectra of lower gap-state confirm the existence of Cr^{3+}.

Reference: Christian Winde, Herstellung und Charakterisierung von Cr Schichten auf TiO_2 (110)Oberflächen, PhD Thesis, University of Stuttgart, 2002

O 34: Methods: Atomic and Electronic Structure I

Time: Tuesday 15:45–17:45 Location: H42

O 34.1 Tue 15:45 H42

Calculations for isolated slabs: MgO/Ag(001), Callen effective charge of O in MgO layers, Ag(001) in external electric field — •Ferenc Tasnadi — IFW, Dresden, Germany

The main purpose of the talk is to prove the applicability of our newly developed local scheme for isolated slabs. In this model one can treat systems, like asymmetrically terminated slabs when the two surfaces have different work functions or slabs with polarization along the normal direction, without any additional artificial field and image interaction. The first application gives the complete electronic and geometric analysis of the MgO/Ag(001) insulator metal interface. In the second example the dynamical Callen effective charge of oxygen is calculated for several MgO layers by the finite-difference method. In the third application homogeneous external electric field is applied to calculate the location of the electrostatic mirror plane of several Ag(001) slabs. The results show that our local scheme together with the newly derived two dimensional Ewald method provide an effective method for isolated slabs.

O 34.2 Tue 16:00 H42

The Evaluation of I(V) Curves in Scanning Tunnelling Spectroscopy of Organic Nanolayers Revisited — •Christian Wagner, Robert Franke, and Torsten Fritz — Institut für Angewandte Photophysik; TU- Dresden George-Bähr-Straße 1; 01069 Dresden

In our contribution we want to verify whether the use of *scanning tunneling spectroscopy* (STS) evaluation methods developed for inorganic samples can be justified also for the case of organic nanolayers, or whether modifications are necessary. Here one have to keep in mind that the traditional approaches are derived for the case of bulk samples and low voltages. Since an organic adsorbate on a substrate presents a sample with a more complex structure and is further characterized by a large gap in the eV range, the answer to this question is not *a priori* clear. After discussing relevant quantities, i.e., the sample *density of states* (DOS) and *local density of states* (LDOS), we demonstrate the use of the simple and well known model of a 1D tunnel junction in WKB approximation in order to calculate the sample DOS for several STS results from literature dealing with ultra thin organic layers. In a subsequent discussion we conclude that the model is applicable to the orbital mediated tunneling process 'through' organic molecules and that it can be used to evaluate such STS measurements. By several examples we illustrate a weakness of the normalized differential conductivity as a method of STS I(V) curve evaluation and propose a new normalization algorithm as a solution to the problem.

O 34.3 Tue 16:15 H42

Scanning Tunneling Spectrocsopy of image potential states on NaCl/Ag(100) — •Hans-Christoph Ploigt, François Patthey, and Wolf-Dieter Schneider — Ecole Polytechnique Fédérale de Lausanne, Institut de physique des nanostructures, CH-1015 Lausanne, Switzerland

Image potential states are important two-dimensional electronic states at surfaces the binding energy of which reflects the nature of the substrate, especially the presence of adsorbates. These states are probed by Scanning Tunneling Spectroscopy. We prepared Ag(100) samples which are partially covered by NaCl islands of different thickness and measured dI/dV spectra with closed feedback loop at 50 K and 5 K with different tips (W, PtIr, Ni). The spectra on clean Ag(100) are reproduced with a simple one-dimensional model which includes the electric field of the tunnel junction. In this way, the work function and the radius of curvature of the tip have been determined and introduced as fixed parameters in a 1D model which includes a dielectric layer to calculate the spectra on NaCl/Ag(100). The resulting good agreement between simulation and experiment allows us to extract from the shift of the image potential/field emission states between clean Ag(100) and NaCl covered Ag(100) the work function change of the sample.

O 34.4 Tue 16:30 H42

Enhanced Rashba spin-orbit splitting in Bi/Ag(111) and Pb/Ag(111) surface alloys — •Gustav Bihlmayer[1], Stefan Blügel[1], and Eugene Chulkov[2] — [1]Institut für Festkörperforschung, Forschungszentrum Jülich, D–52425 Jülich, Germany — [2]Donostia International Physics Center, 20018 San Sebastian/Donostia, Basque Country, Spain

We present first-principles calculations of a $(\sqrt{3}\times\sqrt{3})R30^\circ$ Bi/Ag(111) surface alloy. This alloy has recently been investigated experimentally using angle-resolved photoemission spectroscopy [1]. We find that the surface state in the L projected bulk-bandgap shows a Rashba-type spin-orbit splitting which 3 times larger than what has been observed on a clean Bi(111) surface. We explain this large enhancement, which was also found in experiments, by the strong distortion of the surface state wavefunction which is caused by the substantial outward relaxation of the Bi atom. For comparison we report on a similar surface alloy, Pb/Ag(111), where the strong Rashba-type splitting is found in the calculations. Experimentally, the situation seems to be a bit more complicated due to a second, close-by surface state which was also observed. We discuss the dependence of the two-dimensional bandstructure on the surface corrugation and compare to the experimental findings [2].

[1] C. R. Ast et al. arXiv:cond-mat/0509509 (2005)
[2] D. Pacilé et al. Phys. Rev. B **73**, 245429 (2006)

O 34.5 Tue 16:45 H42

Giant spin-orbit splitting in the surface alloy Bi/Ag(111): A theoretical explanation — •Jürgen Henk, Arthur Ernst, and Patrick Bruno — Max-Planck-Institut für Mikrostrukturphysik, Halle (Saale)

The Rashba-Bychkov effect at (111) surfaces of noble metals, in particular Au, results in a spin-orbit splitting of the L-gap surface states, in analogy to a two-dimensional electron gas. Recent photoemission experiments for the surface alloy Bi/Ag(111) also found a spin-orbit splitting but the size of the splitting is unexpectedly large (Chr. Ast *et al*, cond-mat/0509509). Usual explanations of the effect by the atomic contribution to the spin-orbit coupling and by the gradient of the surface-barrier potential fail.

Relativistic first-principles calculations give strong support for a new mechanism. The interplay of the conventional Rashba-Bychkov contribution to the spin-orbit interaction and the in-plane gradient of the surface potential leads to the giant splitting of the Bi-derived surface states. In addition, the spin polarization of these states is considerably rotated out of the surface plane. The latter prediction suggests investigations by means of spin-resolved photoemission.

O 34.6 Tue 17:00 H42

Spin-orbit coupling in the band structures of the layered charge-density-wave compunds 1T-TaS$_2$ and 2H-TaSe$_2$ — •Kai Rossnagel[1] and Neville Smith[2] — [1]Institut für Experimentelle und Angewandte Physik, Universität Kiel, D-24098 Kiel, Germany — [2]Advanced Light Source, Lawrence Berkeley National Laboratory, Berkeley, California 94720, USA

Empirical tight-binding calculations on the layered charge-density-wave materials 1T-TaS$_2$ and 2H-TaSe$_2$ have been performed and are found to replicate the basic phenomenology of the electronic structure near the Fermi level as revealed by angle-resolved photoelectron spectroscopy (ARPES). In the case of 1T-TaS$_2$, the combination of spin-orbit coupling and the $\sqrt{13}\times\sqrt{13}$ reconstruction generates a distinct and very narrow band at the Fermi level [1]. For 2H-TaSe$_2$, the large spin-orbit splitting of the Ta 5d levels causes a significant change of Fermi surface topology and the combination of spin-orbit coupling and the 3×3 reconstruction gives rise to Fermi surface sheet-dependent energy gapping [2]. Our results highlight the importance of spin-orbit interaction in any understanding of the correlation effects and charge-density-wave transitions in these two materials.

[1] K. Rossnagel and Neville V. Smith, Phys. Rev. B **73**, 073106 (2006).
[2] K. Rossnagel and Neville V. Smith, to be published.

O 34.7 Tue 17:15 H42

$1T-TiSe_2$: Semimetal or Semiconductor? — •Julia Rasch, Torsten Stemmler, and Recardo Manzke — Institut für Physik, Humboldt-Universität zu Berlin, Newtonstraße 15, 12489 Berlin

Even though the semimetallic behavior of $1T-TiSe_2$ seemed to be well established by band structure calculations and previous photoemission results (see e.g. [1]), this conclusion has been challenged recently. Two high-resolution photoemission investigations deduced semiconducting behavior, however with a very small band gap [2,3]. But such a conclusion is afflicted, on principle, by the problem of measuring an unoccupied conduction band by photoemission.

In the present contribution this problem is solved by the idea of H_2O adsorption onto the van der Waals-like surface, causing a distinct bending of the bands and resulting in an completely filled lowest conduction band. The detailed analysis yields undoubtedly semiconducting behavior for $1T-TiSe_2$ and interesting new properties of semiconductors with extremely small band gaps.

[1] O. Anderson, R. Manzke, M. Skibowski, Phys. Rev. Letters 55, 2188 (1985) [2] K. Rossnagel, L. Kipp, M. Skibowski, Phys. Rev. B 65, 235101 (2002) [3] T.E. Kidd, T. Miller, M.Y. Chou, T.-C. Yang, Phys. Rev. Letters 88, 226401 (2002)

O 34.8 Tue 17:30 H42

The origin of the Te 4d core level splitting in transition metal dichalcogenides with distorted CdI_2-structure — •Thorsten Zandt, Robert Heimburger, Christoph Janowitz, and Recardo Manzke — Institut für Physik, Humboldt-Universität zu Berlin, Newtonstraße 15, 12489 Berlin

Typically quasi-two-dimensional transition metal dichalcogenides exhibit the charge density wave phenomena. These show up e.g. as a superstructure in electron diffraction (e.g. LEED) or Fermi surface nesting in angular resolved photoemission. In addition, an observed attending splitting of certain core levels has also been interpreted to be caused by the charge density wave.

In this contribution we present a detailed temperature dependent soft x-ray photoemission study of Te 4d core levels of transition metal ditellurides. In some materials with distorted CdI_2-structure we found a splitting of the Te 4d core levels, *but no* superstructure in LEED. It will be argued the core level splitting, at least in the distorted ditellurides, is more likely due to the geometric zig-zag chains of the transition metals than a charge density wave effect.

O 35: Plenary Talk Imamoglu

Time: Wednesday 8:30–9:15 Location: H1

Quantum Dot Spin Manipulation

O 36: Plenary Talk Zabel

Time: Wednesday 9:15–10:00 Location: H1

Magnetic Nanostructures in the Lateral and Perpendicular Direction

O 37: Prize Talk Dadgar (Gaede Prize)

Time: Wednesday 14:00–14:45 Location: H36

Prize Talk O 37.1 Wed 14:00 H36

Gallium-Nitride-on-Silicon: Mission possible! — •Armin Dadgar — Institut für Experimentelle Physik, Fakultät für Naturwissenschaften, Otto-von-Guericke-Universität Magdeburg and AZZURRO Semiconductors AG, Universitätsplatz 2, 39106 Magdeburg

In comparably short time, Gallium-Nitride has developed from an unrulable material in the mid eighties to one of the most important compound semiconductors, starting with first commercial blue LEDs in 1992 to lasers for HD-DVD and Blue-Ray DVD. Main disadvantage is the lack of suited high-quality substrates. Nowadays, only expensive pseudo-substrates are available used mainly for the growth of laser structures. Therefore, LEDs as well as high-performance electronics are grown on sapphire or SiC. Attempts to grow GaN on cheap Si substrates by metalorganic vapor phase epitaxy failed due to the unfavorable thermal expansion, which leads to cracking even for thin layers. At this time, many experts assumed that it is in principle impossible to solve this problem. This viewpoint had to be revised when we showed in 2000 that the thermal incompatibility strain is well controllable and several micron thick, crack-free GaN layers can be grown on silicon. We will present sources of strain in heteroepitaxy and how, by using strain-engineering methods, flat large diameter GaN-on-Si wafers for device applications can be obtained. Additionally, we show examples of application fields where the material combination as well as the lower cost are advantageous for GaN-on-Si.

O 38: Invited Talk Williams

Time: Wednesday 14:45–15:30 Location: H36

Invited Talk O 38.1 Wed 14:45 H36

Fluctuations of nanoscale structures — •Ellen Williams[1], Chenggang Tao[1], William Cullen[1], Timothy Stasevich[1], Theodore Einstein[1], Alexander Bondarchuk[1], Timothy Bole[2], and Philip Rous[2] — [1]MRSEC, U. of Maryland, College Park, MD 20742, USA — [2]Dept. of Physics, UMBC, Baltimore, MD 21250 USA

Thermal fluctuations at electrical contacts in nano- electronic devices will couple to the electrical signal via changes in the local resistivy and electron transmission probabilities. A physical model for such fluctuations is presented by single-layer height steps on surfaces. Temporal variations in step position and and shape have been directly measured on Ag(111) thin films, using STM, as a function of temperature, adhesion of C60 and application of electrical current stress. The time constants and length-scales of the fluctuations, determined from the temporal correlations functions, yield the surprising result that C60 chain-formation along the step edge causes no measurable change in the motion of the Ag atoms along the underlying step. In addition, the signatures of the C60 chain and the Ag step fluctuations are qualitatively different, and occur at different frequencies, in the range of 0.5 to 80 Hz and 0.005 to 0.05 Hz respectively. The coupling of the structural fluctuations to direct current through the sample changes the shape of the correlation function. The results indicate that charge carriers exert average force per diffusing step-edge atom at least an order of magnitude larger than the expected force on freely diffusing surface adatoms. The correlated changes in the surface resisitivity should carry frequency signatures similar to those of the structural fluctuations.

O 39: Nanostructures at Surfaces IV (Dots, Particles, Clusters, Arrays)

Time: Wednesday 15:45–17:45 Location: H36

O 39.1 Wed 15:45 H36

Investigation of the scattering form factor and surface plasmon resonances of metallic nanoparticles by Bragg diffraction — •Manuel Gonçalves, André Siegel, Ralf Ameling, and Othmar Marti — University of Ulm, Inst. Experimental Physics, Albert-Einstein-Allee 11, D-89069 Ulm, Germany

Plasmon resonances in particles of triangular shape on surfaces were investigated by experimental far-field methods and by numerical simulations. The spectral location of these resonances and the associated near-field enhancements are of high relevance for applications like surface enhanced Raman scattering (SERS) and other nonlinear effects. However, these resonances depend on many parameters, like size and shape of the particles, material and illumination conditions. On the other hand, the surface plasmon resonances influence directly the scattering of light, which can be measured in far-field.

The light scattering form factor of particles of different shapes was investigated by measuring the Bragg diffraction patterns of arrays of identical nanoparticles. The relative intensity of the Bragg diffraction orders is very sensitive to the shape and material of the particles. Thus, theoretical models of the scattering form factors of the particles can be checked by simulation of the Bragg patterns and comparison with the experimental data. This method relies on the averaged form factor of the particles and is not sensitive to particular features of single particles.

O 39.2 Wed 16:00 H36

Collective optical properties of silver nanocrystal arrays — •Herbert Wormeester[1], Stefan Kooij[1], Anne-Isabelle Henry[2], Marie-Paule Pileni[2], and Bene Poelsema[1] — [1]Solid State Physics, MESA+ Institute for Nanotechnology, University of Twente, Netherlands — [2]LM2N, Université Pierre et Marie Curie, Paris, France

Silver nanocrystal arrays of 5 nm diameter Ag nanoparticles surrounded by a shell of dodecanethiol are formed by drop-casting. This gives an ordered system of close-packed spherical nanocrystals that enables a thorough analysis of the electromagnetic inter-particle interactions. The position of the two plasmon resonances observed in these nanocrystals is the result of their collective interaction. This collective interaction leads to a low and a high energy plasmon resonance, excited by the electric field components parallel and perpendicular to the interface, respectively. The magnitude of the plasmon resonance splitting previously observed using a variety of different techniques is also found in ellipsometry spectra. We analyzed that the peak separation in the silver nanocrystal arrays is comparable to the optical response of isolated, non-interacting oblate nanocrystals. The optical deformation of the spherical particles as a result of the interaction can be compared with oblate particles that have a depolarization factor of 0.25 parallel to the interface. The ellipsometry measurement shows a better resemblance between calculation and measurement as compared to polarized reflection measurements. Most likely, this is due to the sensitivity for diffuse scattering of the latter technique.

O 39.3 Wed 16:15 H36

Shaping of Triangular Gold Nanoparticles in Periodic Arrays by Nanosecond Laser Pulses — •Rodica Morarescu, Frank Hubenthal, and Frank Träger — Institut für Physik and Center for Interdisciplinary Nanostructure Science and Technology - CINSaT, Universität Kassel, Heinrich-Plett-Sraße 40, D-34132, Germany

In this contribution we present recent results on selective and precise tailoring of triangular gold nanoparticles using ns-pulsed laser light. The reshaping has been investigated as a function of laser fluence and wavelength. In brief, monolayers of triangular gold nanoparticles in a periodic array were prepared by nanosphere lithography. For this purpose, gold atoms were deposited through the nanosphere mask. Subsequently, the mask was removed by sonicating the sample in a solvent, leaving behind periodic arrays of triangular gold nanoparticles.The particles have been reshaped using ns-pulsed laser light with different fluences and wavelengths. The morphological and the accompanying optical changes were investigated by scanning force microscopy and extinction spectroscopy. We demonstrate that laser irradiation is an ideal tool to precisely control the shape of the metal nanoparticles and thus, their optical properties. For example, the position of the surface plasmon resonance of the particles as prepared can be tuned from 732 nm to 532 nm,depending on the applied fluence. The main advantage of laser irradiation in comparisons to, e.g., thermal annealing is that nanoparticles in a well-defined area of the sample can be addressed. Possible applications of such laser tailored nanoparticles, e.g. as anchor points for functional molecular wires, will be discussed.

O 39.4 Wed 16:30 H36

Optical transmission through hexagonal sub-wavelength hole arrays in thin metal films — •Georgios Ctistis, Piotr Patoka, and Michael Giersig — Center of Advanced European Studies and Research (caesar), Ludwig-Erhard-Allee 2, 53175 Bonn, Germany

Nanostructured surfaces exhibit extraordinary optical properties as plasmon assisted transmission through sub-wavelength hole arrays. In this study we present near-field optical results of the light transmission through a nano-hole array in a metal film (gold and aluminium) produced by means of nanosphere lithography. The film thickness varied between 20 and 120 nm while the hole diameter and the inter-hole distance were kept constant at approx. 270 and 500 nm, respectively. Dependent on the thickness, a change in the transmission mechanism could be observed.

O 39.5 Wed 16:45 H36

Ar ion sputtering induced nanostructure on the Ag(110) — •Günther Weidlinger, Lidong Sun, José Manuel Flores-Camacho, Michael Hohage, and Peter Zeppenfeld — Institut für Experimentalphysik, Johannes Kepler Universität Linz, Linz, Austria

The Ag(110) surface was exposed to Ar ion bombardment and its effects on the surface morphology and optical anisotropic response were monitored by means of Atomic Force Microscopy (AFM) and Reflectance Difference Spectroscopy (RDS), respectively. The AFM studies show the formation of well ordered ripple structures. Depending on the sputtering condition either 1D or 2D ripple structures could be created. Especially the 2D ripple structure is quite stable both in Ultra High Vacuum (UHV) and in air at room temperature. The corresponding RD spectra exhibit single (double) pronounced peak for the 1D (2D) ripple structures, which is associated to the coupling of photons with surface plasmon mediated by the diffraction of the ripple structures. The direction and period of the ripple structure determined by the sign and the peak positions of RD spectrum agrees well with what is found from AFM demonstrating that RDS is a powerful tool for the characterization of nanostructured surfaces.

O 39.6 Wed 17:00 H36

An Addressable Supramolecular Rotary Switch Featuring Distinguishable Positions Embedded In A Two-Dimensional Porphyrin-Based Porous Network — •Nikolai Wintjes[1], Hannes Spillmann[1], Andreas Kiebele[1], Meike Stöhr[1], Thomas Jung[2], Davide Bonifazi[3], Fuyong Cheng[3], and François Diederich[3] — [1]Department of Physics, University of Basel, CH-4056 Basel — [2]Paul Scherrer Institute, CH-5232 Villigen PSI — [3]Laboratory for Organic Chemistry, ETH-Zürich, CH-8093 Zürich

In recent years, the attempts to build artificial functional devices from single molecules by the "bottom-up" approach were strongly in the focus of surface nanoscience. First experiments with molecules manually arranged by the STM tip gave first hints on the powerful possibilities of such a device. Nevertheless, a simple way to produce supramolecular devices parallel in vast amounts has never been shown before.

Herein we report on a highly complex supramolecular device that reminds of a mechanical rotary switch fabricated on a Cu(111) surface following the "bottom-up" approach. Self-assembly of a specially designed porphyrin molecule leads to the formation of porous networks featuring chiral cavities which serve as molecular stators for multistate molecular rotors. These can rotate between six stable positions of which three are distinguishable using Scanning Tunneling Microscopy (STM) (see figure 1). The rotation can be induced either thermally or by the STM tip. The energy barrier for rotation was estimated to be 0.28 eV.

O 39.7 Wed 17:15 H36

Creation of open networks from perylene derivatives — •Serpil Boz[1], Manfred Matena[1], Markus Wahl[1], Thomas A.

Jung[2], Lutz H. Gade[3], and Meike Stöhr[1] — [1]Institute of Physics, University of Basel, Switzerland — [2]Paul-Scherrer-Institute, Switzerland — [3]Institute of Inorganic Chemistry, University of Heidelberg, Germany

Self-assembly of molecules on surfaces directed by supramolecular interactions has been widely explored. The perylene derivative (DPDI) we analyzed [1] is modified on the surface in order to achieve self-assemblies. This modification is temperature-induced, thus providing an additional feature to the control of self-assemblies in contrast to usual approaches that make use of molecular properties already inherent to the molecules. Thin films of DPDI were prepared on Cu(111) and investigated with STM. Depending on the coverage before annealing, three different H-bond assemblies are generated, since in a thermally induced reaction the end groups of the molecule are modified and it can then act as both a H-bond donor and acceptor. For a similar perylene derivative (TAPP), an open quadratic assembly is found on Cu(111), which is not based on temperature-induced modification. If both molecules are present on the surface and the sample is annealed, a separation into two porous networks is observed.

[1] M. Stöhr et al., Angew. Chem. Int. Ed., 2005, 44, 7394

O 39.8 Wed 17:30 H36

Self-Assembly of Metal-Organic Coordination Networks at Surfaces with Scalable Nanocavity Size and Aspect Ratio — ●Alexander Langner[1], Steven L. Tait[1], Chandrasekar Rajadurai[2], Nian Lin[1], Mario Ruben[2], and Klaus Kern[1] — [1]Max-Planck-Institut für Festkörperforschung, Stuttgart — [2]Institut für Nanotechnologie, Forschungszentrum Karlsruhe

We report on the rational use of two-dimensional supramolecular self-assembly as efficient bottom-up method for nanoscale patterning of metal surfaces. The controlled self-organization of multi-ligand systems by metal-organic coordination is investigated on Cu(100) under ultra high vacuum (UHV) conditions with scanning tunneling microscopy (STM). Mixtures of dicarboxyl and bipyridyl molecules with vapor deposited iron atoms assemble into arrays of coordination nodes, each consisting of 2 molecules of each functional group termination, coordinated in a cross geometry to a di-iron center. This directional and selective coordination produces ordered rectangular networks in which the size and the aspect ratio of the cavities can be scaled by varying the backbone length of the different linker molecules independently. Investigation of these model systems also gives insight into fundamental properties of self-assembly such as self-recognition or error correction.

O 40: Particles and Clusters I

Time: Wednesday 15:45–17:15 Location: H38

O 40.1 Wed 15:45 H38

Surface strain of Au clusters analysed by transmission electron holography — ●Radian Popescu[1], Erich Müller[1], Dagmar Gerthsen[1], Matthias Wanner[1,2], Marco Schowalter[3], Andreas Rosenauer[3], Arthur Böttcher[4], and Manfred Kappes[4] — [1]Laboratorium für Elektronenmikroskopie and Center for Functional Nanostructures,Universität Karlsruhe, D-76128 Karlsruhe, Germany — [2]Forschungsinstitut für Pigmente und Lacke e.V., D-70569 Stuttgart, Germany — [3]Institut für Festkörperphysik, Universität Bremen, D-28359 Bremen, Germany — [4]Institut für Physikalische Chemie, Universität Karlsruhe, D-76128 Karlsruhe, Germany

We have carried out an accurate quantitative analysis of the dependence of the mean inner Coulomb potential (MIP) on the particles thickness for Au nano-clusters deposited on amorphous carbon (a-C) substrate taking into account the strain relaxation of the cluster surface atoms. It was shown that the high experimental cluster MIP values of about 80 V measured for the 0.5 nm Au clusters radii can be accounted for only by the strain of the surface atoms. The MIP value of Au volume atoms (atoms which have the Au-bulk coordination number) of V=32.1+-3.6 V we have derived, is in good agreement with previous theoretical estimations of the Au bulk MIP values. The theoretical method developed here to calculate the MIP is not only applicable to the special case of Au clusters, but can be extended to any type of metallic materials.

O 40.2 Wed 16:00 H38

Nanosecond and femtosecond laser photodesorption of NO from silver nanoparticles on a thin alumina film — ●Ki Hyun Kim[1], Daniel Mulugeta[1], Kazuo Watanabe[1], Dietrich Menzel[1,2], and Hans-Joachim Freund[1] — [1]Fritz-Haber-Institut der Max-Planck-Gesellschaft, Faradayweg 4-6, 14195 Berlin, Germany — [2]Technische Universität München, 85747 Garching, Germany

Nanosecond (ns) and femtosecond (fs) laser 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. NO was adsorbed on 0.5-nm deposited Ag nanoparticles (∼8 nm particle diameter) at 75 K, resulting in the formation of NO dimers. PD cross sections were calculated from the irradiance dependence of the total PD yield of NO fitted to a single exponential. With ns pulses (∼5 ns) at $h\nu$=3.5 eV in p-polarization, a PD cross section of $5.6.\times10^{-17}$ cm^2, which is about 30 times larger than that on Ag(111), was obtained. Also, the NO mean translational energy (670 K) is larger than in that case. The enhancement is explained by resonant excitation of the Mie plasmon of the Ag nanoparticles at 3.6 eV.

With fs pulses (∼100 fs) at $h\nu$=3.1 eV in p-polarization, off-resonant from the Mie plasmon, a PD cross section of $2.3.\times10^{-16}$ cm^2 was obtained. The mean translational energy of NO was 540 K. The PD yield was proportional to the ∼1.7th power of the laser fluence. A two-photon excitation process or a DIMET (desorption induced by multiple electronic transitions) may be involved in the PD with fs pulses.

O 40.3 Wed 16:15 H38

In Situ Surface Enhanced Infrared Absorption Spectroscopy for the Analysis of the Adsorption and Desorption Process of Au Nanoparticles on the SiO2/Si Surface — ●Dominik Enders[1,2], Tadaaki Nagao[1,2], and Tomonobu Nakayama[1,2] — [1]National Institute for Materials Science (NIMS), 1-1 Namiki, Tsukuba 305-0044, Japan — [2]Nanoscale Quantum Conductor Array Project, ICORP, JST, 4-1-8 Honcho, Kawaguchi, Saitama 332-0012, Japan

The adsorption and desorption of Au nanoparticles (AuNP) in colloidal D2O suspension on the SiO2/Si surface was investigated by in situ ATR-IR spectroscopy. With increasing surface density of AuNP the absorption of the vibrational modes of D2O and of the citrate molecules covering the AuNP increases due to surface enhanced infrared absorption (SEIRA). We show that the adsorption kinetics can be investigated by monitoring the molecular vibrational modes of D2O and the citrate molecules, and furthermore we clarify that the adsorption process can be described very well by a Langmuir-kinetics model. When exposing a saturated AuNP submonolayer to 2-aminoethanethiol/D2O solution, the AuNP are removed from the surface and the IR absorption of the D2O vibrational modes become weaker again. Taking into account the time dependencies of the CH and the OD peaks, we propose a microscopic model explaining the mechanism of the desorption process.

O 40.4 Wed 16:30 H38

Dealloying effects in rotating CuAu nanoclusters - A molecular dynamics study — ●H. Neubauer and S.G. Mayr — I. Physikalisches Institut, Georg-August-Universität Göttingen, Friedrich-Hund-Platz 1, 37077 Göttingen

Dealloying effects in rotating liquid CuAu clusters are investigated with the help of classical molecular dynamics simulations using embeded atom method (EAM) potentials. We employ the model system, CuAu, to investigate the phenomenon as a function of cluster size and composition, i.e. for CuAu, Cu_3Au and $CuAu_3$. In addition to well–established surface energy related effects, we find an enrichment of Au on the surface due to centrifugal forces. An ellipsoid deformation of the cluster occurs, while Au forms a bulge around the rotating cluster. Disturbances occuring during rotational movement, such as thermal fluctuations or oscillations, are found to counteract the dealloying process by mixing the constituents; for long enough times a stationary state is reached. We acknowledge the SFB 602 - TP B3 for financial support.

O 40.5 Wed 16:45 H38

The local tunnelling conductance on cobalt clusters at semiconductor surfaces — •Kristian Sell, Armin Kleibert, Viola von Oeynhausen, and Karl-Heinz Meiwes-Broer — Institut für Physik, Universität Rostock, Universitätsplatz 3, 18051 Rostock

We present scanning tunnelling spectroscopy (STS) and microscopy (STM) measurements on isolated cobalt nanoparticles with diameters ranging from 2 to 12 nm after *in-situ* deposition on Ge(001). The mass-filtered clusters have been deposited under soft-landing conditions (E_{kin}/atom < 0.5eV) using an arc cluster ion source (ACIS).

In the present range of particle sizes the tip folding plays a great role. With the help of a "blind reconstruction method"it is possible to approximate the shape of the tip [1]. After a respective deconvolution of the STM images facetted particles become visible. According to their equilibrium shape - being a truncated octahedron in the case of fcc cobalt - hexagonal and quadrangular facets appear in the images [2]. STS is sensitive to occupied and unoccupied states near the Fermi level and reveals the existence of distinct states in the tunnelling conductivity of the substrate as well as on the clusters. Thus, the richly structured density of states of the germanium surface serves as STM/STS condition test [3]. The tunnelling conductivity measured on the cobalt nanoparticles Ge(001) will be discussed in detail.

[1] J.S. Villarrubia, J. Vac. Sci. Technol. B 14, 1518 (1996), [2] M. Jamet, Phys. Rev. Lett. 86, 4676 (2001), [3] K.-L. Jonas, Appl. Phys. A 82, 131-137 (2006)

O 40.6 Wed 17:00 H38

Resonant Raman Scattering on Functionalized Carbon Nanotubes — •Matthias Müller[1], Janina Maultzsch[1], Christian Thomsen[1], David Wunderlich[2], and Andreas Hirsch[3] — [1]Inst. für Festkörperphysik, TU Berlin — [2]Zentralinst. für Neue Materialien und Prozesstechnik, Univ. Erlangen- Nürnberg, Fürth — [3]Inst. für Organ. Chemie, Univ. Erlangen-Nürnberg, Erlangen

We report Raman measurements on carbon nanotubes functionalized with diverse alkenes and various degrees of functionalisation. Selective reactions of the different tube species (metallic or semiconducting) due to the availability of electrons near the Fermi level were first reported by Strano et al.[1]. Our work focuses on resonant Raman scattering of the radial breathing mode (RBM) concerning the preferred addition of the nuclephile to metallic tubes as suggested by Graupner et al.[2].

Assigning the chiral indices of the tubes by means of the so-called Kataura plot[3] we can study the influence of functionalisation on the transition energies of either metallic and semiconducting tubes in detail. Data of the high energy (HEM)- and defect-mode (D-mode) will also be discussed.

[1] M. Strano et al., Science 301, 1519 (2003) [2] R. Graupner et al., J. Am. Chem. Soc. 128, 6683 (2006) [3] J. Maultzsch et al., Phys Rev B 72, 205438 (2005)

O 41: Metal Substrates: Adsorption II

Time: Wednesday 15:45–17:30 Location: H39

O 41.1 Wed 15:45 H39

Controllable molecular registration state in self-assembly of 3(5)-(9-anthryl) pyrazole molecule on Ag(111) — •Ruifen Dou[1], Arno Tilkorn[1], Dingyong Zhong[1], Wenchong Wang[1], Yue Wang[2], Lifeng Chi[1], and Harald Fuchs[1] — [1]Physikalisches Institut, Universitaet Muenster, 48149 Muenster, Germany — [2]Key Laboratory for Supramolecular Structure and Materials of Ministry of Education, Jilin University, Changchun 130012, China

The highly-ordered molecular structures of 3(5)-(9-anthryl) pyrazole (ANP) have been investigated on Ag(111) by low-energy electron diffraction (LEED) and scanning tunneling microscopy (STM). Through tailoring film preparation, two different superstructures, α and β, corresponding to two different molecular registration states have been obtained on Ag(111). At the low substrate temperature (229 K), the structure α can be prepared, in which the ANP molecule is adsorbed the surface with the anthryl-group plane tilting in respect to the substrate surface. After annealing the sample to room temperature, it is found that the structure α gradually evolves into the structure β with four molecules bound together through the hydrogen bonds among them and the anthryl-group plane parallel to the substrate surface to compromise to forming hydrogen bonds. Our analysis reveals a fact that the adsorbate-substrate interaction dominated in the structure α can change into the hydrogen-bonds prevailed over the structure β as mediating the growth temperature, which is responsible for the variation in the molecular registration states from the anthryl-group plane tilting with the substrate surface to parallel to surface.

O 41.2 Wed 16:00 H39

Different assemblies of a phthalocyanine derivative on metal surfaces — •Tomas Samuely[1], Meike Stöhr[1], Thomas Jung[2], Marco Haas[3], Shi-Xia Liu[3], and Silvio Decurtins[3] — [1]Institut für Physik,Universität Basel, Schweiz — [2]Paul Scherrer Institut, Villigen, Schweiz — [3]Departement für Chemie und Biochemie, Universität Bern, Schweiz

Phthalocyanines have been the subject of intense studies due to their wide range of optical, structural and electronic properties arising from their large π-conjugated system and their assembling into co facially-stacked arrays. We studied a phthalocyanine derivative which features eight ditertiarybutylphenyl substituents attached over an oxygen atom to the peripheral phenyl rings. Ordered assemblies of the derivative were prepared by thermal evaporation, whereas Ag(111) and Au(111) were used as substrates, respectively. The investigations were carried out by means of STM at various temperatures. For coverage less than one monolayer, two different assemblies were observed. At room temperature, a mobile phase was detected next to the ordered islands. Increasing the coverage results in only one ordered phase, while the second layer begins to form before a full monolayer is completed. Applying different bias voltages had a vast effect on the appearance of the imaged molecules. The assembled domains of the derivative could be suitable for subsequent deposition of various molecules: complexes with interesting magnetic, electronic, redox or photo-active properties could be formed.

O 41.3 Wed 16:15 H39

LEED investigations on SAM of biphenylthiols on Au (111) surfaces — •Michel Kazempoor and Gerhard Pirug — Institut für Bio- und Nanosysteme (IBN3) and Center of Nanoelectronic Systems for Informationtechnology (CNI), Forschungszentrum Jülich GmbH, D-52425 Jülich

Organic molecules of 4'-methyl-1,1'-biphenyl-4-alkanethiols (BPn, n = number of alkane spacer) are known to form well ordered so called self assembled monolayer (SAM) structures on metal surfaces. Characterizing the ordering and packing behaviour of BPn is essential for the understanding of the electronic and optical properties. BPn structures are predominantly characterized by STM measurements. In addition a $(2\sqrt{3}$ x $\sqrt{3})$ structure has been proposed for BP3, based on a diffuse LEED pattern (Azzam et. al., Langmuir 19 (2003) 8262). However, there is still an ongoing discussion about different unit cells of BPn molecules on Au (111). In principal, LEED should allow a reliable identification of the unit cell and the determination of its lattice vectors. Therefore we studied the adsorption of BP3 and BP4 on Au(111) surfaces using a micro channel plate (MCP) LEED system, which allows a more gentle examination with reduced electron beam current in the pA regime. The samples were exposed at room temperature to BPn molecules by gas phase deposition. After subsequent annealing up to 423 K we observed unit cells corresponding to a c(16 x $2\sqrt{3}$) and ($5\sqrt{3}$ x $\sqrt{3}$) structure for BP3 and BP4, respectively. Structure models will be discussed under consideration of recent STM findings.

O 41.4 Wed 16:30 H39

Temperature programmed desorption of oligopyridine molecules on HOPG — •Michael Roos, Harry E. Hoster, and R. Jürgen Behm — Institut für Oberflächenchemie und Katalyse, Universität Ulm, 89069 Ulm

As shown in previous STM studies, bis(terpyridine)derivatives (BTP) form highly ordered hydrogen bonded networks on HOPG at the solid/liquid and the solid/gas interface. A reliable method to attain these monolayer networks in UHV is vapor deposition, followed by the desorption of excess material. In this study, we systematically investigate the thermal desorption behavior for varying initial BTP coverage. For a comprehensive understanding, the experimental spectra are compared with spectra attained by simulations based on different models, and are in addition linked to STM images of BTP layers on HOPG with different coverage.

O 41.5 Wed 16:45 H39

Formation of tetrachloroplatinate complexes on Pt(110). — Enrico Donà[1], •Michael Cordin[1], Cesare Franchini[2], Josef Redinger[2], and Erminald Bertel[1] — [1]Institute for Physical Chemistry, University of Innsbruck, Innrain 52a, A-6020 Innsbruck, Austria — [2]Center for Computational Material Science, Gumpendorferstraße 1A, A-1060 Vienna, Austria

The chemisorption of Cl and Br on Pt(110) has been studied as a function of coverage by variable-temperature scanning tunneling microscopy (VT-STM) and low-energy electron diffraction (LEED). For a coverage (Θ) of 0.5 monolayers (ML) Cl and Br form a $p(2 \times 1)$ and a $c(2 \times 2)$ structure, respectively, occupying each second short-bridge (SB) site on the close-packed Pt-rows of the (1×1)-Pt(110) surface. Increasing the coverage leads to the formation of a (3×1) and a (4×1) phase for $\Theta = 0.66$ ML and $\Theta = 0.75$ ML respectively, where both SB and long-bridge (LB) sites are occupied. While these two structures are stable for Br, they are only metastable in the case of Cl. Upon soft annealing (300K < T < 670 K) a transition into a phase with (4×2) periodicity is observed. This phase is characterized by cross-shaped structures, imaged as "clusters"with five bright protrusions by STM. An interpretation of these protrusions entirely in terms of Cl atoms can be excluded by coverage considerations. On the basis of both, experimental arguments and theoretical results the clusters can be identified as tetrachloroplatinate complexes, with the central Pt atom occupying a four-fold hollow site. This implies the onset of Cl induced corrosion on the Pt(110) surface.

O 41.6 Wed 17:00 H39

Racemic mixing in 2D molecular self-assembly — •Thorsten Kampen[1], Rocio Cortes[2], Philipp Martin Schmidt[1], Hugo Dil[1], Arantzazu Mascaraque[2], and Karsten Horn[1] — [1]Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, Germany — [2]Depto. Física de Materiales, Universidad Complutense de Madrid, Madrid, Spain

Inherently achiral molecules may become chiral when adsorbed on surfaces, through the loss of symmetry elements in a 2D structure. Here we show how this effect leads to chiral supramolecular assemblies in 4,4'-stilbene dicarboxylic acid (DCSB) on Cu(110) using scanning tunnelling microscopy. DCSB molecules are found to adsorb on Cu(110) surface via bonding of all four oxygen atoms of the deprotonated carboxylic end-groups to next- neighbour Cu atoms. In the 2D environment of a surface the molecule assumes to enantiomorphous orientation, that is, the molecules become chiral. Due to the chiral character of the adsorbed molecule and intermolecular interactions two chiral adsorption phases are found, namely a cubic and a herringbone phase. While in the metastable "rectangular" phase consists only of right- or left-handed molecules, i.e each domain is enantiomorphously pure, the "herringbone" phase is a "racemic mixture" built up of left- and right-handed molecules. The formation of the herringbone phase is thermodynamically preferred since it decreases the free enthalpy of the self-assembled DCSB islands.

O 41.7 Wed 17:15 H39

On the accuracy of first-principles lateral interactions: Oxygen at Pd(100) — •Yongsheng Zhang, Volker Blum, and Karsten Reuter — Fritz-Haber-Institut, Faradayweg 4-6, D-14195 Berlin, Germany

We employ a first-principles lattice-gas Hamiltonian (LGH) approach to determine the lateral interactions between O atoms adsorbed on the Pd(100) surface. With these interactions we obtain an ordering behavior at low coverages that is in quantitative agreement with experimental data. Uncertainties in our approach arise from the finite LGH expansion and from the approximate exchange-correlation (xc) functional underlying the employed density-functional theory energetics. We carefully scrutinize these uncertainties and conclude that they primarily affect the on-site energy, which rationalizes the agreement with the experimental data. We also investigate the validity of the frequently applied assumption that the ordering energies can be represented by a sum of pair terms. Restricting our LGH expansion to just pairwise lateral interactions, we find that this results in effective interactions which contain spurious contributions that are notably larger than any of the uncertainties e.g. due to the approximate xc functional.

O 42: Methods: Scanning Probe Techniques III

Time: Wednesday 15:45–16:30 Location: H41

O 42.1 Wed 15:45 H41

Infrared Nanofocus Maps Sub-10 nm Particles — •Antonija Cvitkovic[1], Nenad Ocelic[1], Javier Aizpurua[2], Reinhard Guckenberger[1], and Rainer Hillenbrand[1] — [1]Max Planck Institute of Biochemistry, Am Klopferspitz 18, D-82152 Martinsried, Germany — [2]Donostia International Physics Center, Paseo Manuel Lardizabal 4, 20018 Donostia San Sebastian, Spain

Infrared spectroscopy is a powerful tool for material identification based on molecular vibrational fingerprints. However, due to extremely weak scattering cross sections at infrared wavelengths, far-field analysis of individual nanoparticles has not been possible so far.

We demonstrate nanoscale resolved infrared imaging of sub-10 nm gold particles by scattering-type scanning near-field microscopy (s-SNOM). Our s-SNOM is basically an AFM, with the metallized probing tip additionally illuminated by IR light (λ=10 μm). Due to an optical antenna-effect, light is concentrated at the apex of the tip forming a wavelength-independent nanoscale focus. In order to make a detection of sub-10 nm particles possible, we use highly reflecting or polariton resonant materials as sample carriers. That way a strong tip-substrate near-field interaction intensifies the nanofocus illuminating the particles, resulting in the enhanced optical contrasts [1].

Our results already promise a wide application potential in high resolution imaging of nanoscale objects (e.g. gold biolabeling). Combined with spectroscopic mapping, our method opens the door to label-free chemical identification of individual nanocrystals or biomolecules.

[1] A. Cvitkovic et al, Phys. Rev. Lett. 97, 060801 (2006)

O 42.2 Wed 16:00 H41

Plasmons in metallic bilayer wave guides — •Andreas Englisch, Stefan Griesing, and Uwe Hartmann — Institute of Experimental Physics, Saarland University, P.O. Box 15 11 50, D-66041 Saarbruecken

Plasmons constitute a strongly confined electromagnetic field. Plasmon-guiding metal stripes in a planar geometry exhibit a spatial extent of the electromagnetic field of the order of the decay lenght in the dielectric environment (several hundreds of nanometers) perpendicular to the metal surfaces. Cross coupling of different plasmon paths can thus not be avoided for smaller distances. A new geometry is introduced, which consists of two metal films separated by a dielectric layer. The theoretically predicted confinement is now limited by the decay length given for the metal films (50-100 nm). It is possible to construct junctions of arbitrary angles between the plasmon paths. The results of calculations of the field distribution and the power flow are presented as well as those of measurements by Scanning Near-Field Optical Microscopy. The potential of the given geometry to affect the propagation properties of the guided plasmons by a small change of the boundary conditions will be discussed.

O 42.3 Wed 16:15 H41

Elektrische Charakterisierung von Halbleiterstrukturen mittels Electrostatic Force Microscopy — •Markus Ratzke[1], Mario Birkholz[2], Joachim Bauer[2], Detlef Bolze[2] und Jürgen Reif[1] — [1]LS Experimentalphysik II, BTU Cottbus, IHP/BTU JointLab, Konrad-Wachsmann-Allee 1, D-03046 Cottbus — [2]IHP (Institut für innovative Mikroelektronik), lm Technologiepark 25, D-15236 Frankfurt (Oder)

Eine Möglichkeit, elektrische Parameter von Halbleiteroberflächen zu bestimmen, ist die Messung der elektrostatische Kraft zwischen dem leitfähig beschichteten Cantilevers eines Atomkraftmikroskops und der Probe. Verfahren wie Scanning Kelvin Probe Microscopy (SKM) und Scanning Capacitance Microscopy (SCM) erlauben dabei eine Abbildung von Potential- und Ladungsträgerverteilung mit Auflösung im Nanometerbereich.

Wir berichten über die Ergebnisse an n+p-Dotiergittern, die mittels CMOS-Technologie in die Oberfläche von Silizium-Wafern eingeschrieben wurden. Die erreichten Strukturbreiten lagen im Bereich zwischen 100 und 200 nm. Es wurden Potentialdifferenzen zwischen den unterschiedlichen Dotierbereichen von 100 mV ermittelt, was ca. der Hälfte des berechneten Wertes entspricht. Mittels numerischer Lösung der Drift-Diffusions-Gleichungen konnte gezeigt werden, dass der fehlende Potentialbetrag mit der Beleuchtung der Probe während der Messung zu erklären ist. Es ist festzustellen, dass die die genutzten Methoden trotzdem sehr gut geeignet sind, nanoskalige Halbleiterstrukturen in zukünftigen Technologieknoten zu charakterisieren.

O 43: Oxides and Insulators: Adsorption II

Time: Wednesday 15:45–16:45 Location: H42

O 43.1 Wed 15:45 H42

Coadsorption of CO and CO_2 on zinc oxide: from single crystal to powder particles — •Henshan Qiu[1], Yuemin Wang[1,2], Xinyu Xia[2], Martin Muhler[2], and Christof Wöll[1] — [1]Lehrstuhl für Physikalische Chemie I, Ruhr-Universität Bochum, D-44780 Bochum — [2]Lehrstuhl für Technische Chemie, Ruhr-Universität Bochum, D-44780 Bochum

The interaction of CO and CO_2 with ZnO surfaces was studied using high resolution electron energy loss spectroscopy (HREELS), thermal desorption spectroscopy (TDS) and microcalorimetry. Exposing the non-polar ZnO(10-10) surface to CO_2 results in the formation of an unusual tridentate carbonate species with the two carbon dioxide O-atoms being almost equivalently bound to two different Zn surface atoms. Two stable carbonate phases are found: a full (1x1) monolayer with a binding energy of 52 kJ/mol and a half monolayer with (2x1) structure and binding energy of 86 kJ/mol. With regard to CO adsorption on ZnO(10-10), the precoverage of CO_2 leads to an increase of CO binding energy from 30 to 55 kJ/mol and a slight blue-shift of the ν(C-O) peak by 1 meV. The amount of adsorbed CO increases first due to the existence of surfaces carbonates and then decreases because of site blocking effect. The co-adsorbed CO_2 leads also to stronger adsorption of CO on ZnO powder particles, giving rise to an adsorption energy distribution between 45-65 kJ/mol. The increase of interaction strength is attributed to the formation of tridentate carbonates on the most exposed ZnO(10-10) surfaces, which increases the Lewis acidity of the surface.

O 43.2 Wed 16:00 H42

Influence of Electronic Correlations on the Ground-State Properties of Cerium Dioxide Bulk and Surfaces — •Elena Voloshina[1], Carsten Mueller[2], Beate Paulus[1], and Kersti Hermansson[2] — [1]MPI fuer Physik komplexer Systeme, Noethnitzer Str. 38, 01187 Dresden, Germany — [2]Department of Materials Chemistry, The Angstroem Laboratory, University of Uppsala, Box 538, Laegerhyddsvaegen 1, 75121 Uppsala, Schweden

Ceria plays an important role as a component in the active noble metal support in automotive three-way catalytic converters, where NOx, CO, and hydrocarbons are simultaneously removed [1]. The electron-correlation effects on the ground-state properties of bulk CeO2 are studied by ab initio quantum-chemical methods. For this purpose the method of increments is applied. It combines Hartree-Fock calculations for periodic systems with correlation calculations requiring only information of the corresponding finite-cluster calculations. After inclusion of correlations obtained at the CCSD(T) level the calculated values are in good agreement with experiment [2]. With this detailed description of the electronic correlations in bulk CeO2, it is now possible to extend the work to CeO2 surfaces and adsorbed molecules on them. Here we present absorbtion energies of CO and N2O. Especially for these weakly bound molecules an explicitely correlated method is necessary to describe accurately the van der Waals interaction.

[1] J. Kaspar, P. Fornasiero, and M. Graziani, Catal. Today 50, 285 (1999).

[2] E. Voloshina and B. Paulus, J. Chem. Phys. 124, 234711 (2006).

O 43.3 Wed 16:15 H42

Zero-bias conductance anomaly in single Au-CO complexes on a FeO thin film on Pt(111) — •Niklas Nilius, Emile Rienks, Hans-Peter Rust, and Hans-Joachim Freund — Fritz-Haber-Institut der MPG, Berlin

A thin film of FeO grown on Pt(111) forms a hexagonal Moiré pattern due to the 11% lattice mismatch with the metal support that is characterized by a modulated stacking sequence of the Fe ions with respect to the Pt(111) lattice. The spatial inhomogeneity of electronic and chemical properties within the Moire unit cell stimulates a self-organization of Au adatoms into a hexagonal adatom network. Conductance spectra of the adatoms reveal an unoccupied resonance at +0.5 eV, but no features around the Fermi level, as measured by low-temperature STS. After CO adsorption onto the Au monomers, a pronounced zero-bias anomaly appears in the differential conductance of the species. The phenomenon is discussed in terms of the Kondo effect that might be induced by a change of the spin/charge distribution of the Au-CO complex after CO adsorption.

O 43.4 Wed 16:30 H42

Water on ZnO(11$\bar{2}$0): An UPS Study — •Joachim Wider and Christian Pettenkofer — Hahn-Meitner-Institut, Glienicker Strasse 100, 14109 Berlin

In order to understand the growth process of epitaxically grown MOMBE ZnO films on Al_2O_3, we have studied the adsorption of H_2O on a ZnO(11$\bar{2}$0) single crystal. Furthermore it is controversially discussed, whether water adsorbs molecularly or dissociatively on oxide surfaces [1, 2]. Our UV photoemission experiments show that at 95 K water adsorbs both, molecularly and dissociatively on ZnO(11$\bar{2}$0). At increasing exposures, the fraction of dissociatively adsorbed water remains constant, whereas the molecularly adsorbed water forms a ice multilayer. In a second experiment, we annealed the water exposed surface. Between 160 and 180 K, the ice multilayer desorbs, and a layer consisting of H_2O and OH remains on the surface. At 395 K, all adsorbats are desorbed. The adsorption of 20 L H_2O results in a band bending of 0.9 eV. Subsequent annealing decreases band bending. Upon adsorption, the workfunction is constant within 0.1 eV. Annealing the sample yields a sudden incease of the work function at 100 K of 0.2 eV, followed by decrease at 160, and a slow increase between 180 and 340 K of 0.3 eV. At 395 K, the work function has the same value as the clean cooled sample.

[1] G. Zwicker, K. Jacobi, Surf. Sci. 131 (1983) 179.

[2] B. Meyer, D. Marx, O. Dolub, U. Diebold, M. Kunat, D. Langenberg, C.Wöll, Angew. Chem. Int. Ed. 43 (2004) 6642.

O 44: Poster Session II (Semiconductors; Oxides and Insulators: Adsorption, Clean Surfaces, Epitaxy and Growth; Surface Chemical Reactions and Heterogeneous Catalysis; Surface or Interface Magnetism; Solid-Liquid Interfaces; Organic, Polymeric, Biomolecular Films; Particles and Clusters; Methods: Atomic and Electronic Structure; Time-resolved Spectroscopies)

Time: Wednesday 17:00–19:30 Location: Poster C

O 44.1 Wed 17:00 Poster C

A Novel Approach to Measure the Step Line Tension and the Step Dipole Moment on Vicinal Au(001) Electrodes — •Guillermo Beltramo, Harald Ibach, and Margret Giesen — Forschungszentrum Jülich, Institut für Bio- und Nanosysteme IBN 4, D 52425 Jülich, Germany

The step line tension plays a crucial role in the electrochemical deposition and dissolution of metals, and in particular, in the creation of nanostructures and their dynamical properties. In the present work, we introduce a new method to measure the step line tension on metal electrodes, using a theoretical model proposed by Ibach and Schmickler [1]. Vicinal Au(11n) and Au(001) electrodes were investigated by impedance spectroscopy in weakly adsorbing electrolytes. Within the limits of error the shift in the potential of zero charge is proportional to the step density of the electrode surfaces and we determine a dipole moment per step atom of about 6.10^{-3} eÅ for all electrolytes. The line tension of the steps is then calculated from the difference between the surface tension of the stepped and the step free surfaces. In accordance with [1], the step line tension decreases (roughly linear) with the electrode potential in absence of specifically adsorbed ions. Furthermore we are able to give an estimation of the step capacity. The results will be discussed with respect to a recent theoretical model [2].

[1] H. Ibach and W. Schmickler, Physical Rev. Lett. 91 (2003) 016106.
[2] H. Ibach et al., J. Electroanal. Chem. 544 (2003) 13.

O 44.2 Wed 17:00 Poster C

Electron Induced Desorption of Water on Ruthenium(0001) — •Franziska Traeger, Deler Langenberg, YouKun Gao, and Christof Wöll — Physikalische Chemie 1, Ruhr-Universität Bochum, Universitätsstr. 150, 44801 Bochum

When electrons impinge on adsorbed water molecules, desorption, dissociation or structural phase transitions may occur. The system water/Ru has been found to be particularly sensitive, as structures with varying coverage and similar energies have been observed, some of them stabilized by dissociation products (OH and H). In this work the influence of electrons on the adsorbate D_2O/Ru has been investigated by the diffraction of a neutral He atom beam. Without electron impact a high order commensurate structure with 27.3 Å periodicity is found, in contrast to LEED experiments. These results can be explained in terms of a bilayer with slightly larger lattice constant than the bulk ice and which is rotated by 4.7° with respect to the substrate [1]. In further experiments electrons were accelerated with 1000-1200 V onto the surface. The observed changes in the specular He signal and in the He diffraction pattern strongly indicate, that at larger coverages desorption is the dominant mechanism. A quantitative analysis of the He intensity gives a desorption probability of about 0.7 % per electron. Several models for the analysis and their errors are presented. Finally, the results are discussed in comparison with electron induced desorption from the multilayer D_2O/Ru and from ice surfaces.

[1] F. Traeger, D. Langenberg, Y.K. Gao and Ch. Wöll, submitted to Phys. Rev. Lett.

O 44.3 Wed 17:00 Poster C

Controlled immobilization of "device" molecules: self-assembled monolayers of ferrocene-substituted biphenyl ethynyl thiols — Andrey Shaporenko[1], Katrin Rössler[2], Heinrich Lang[2], and •Michael Zharnikov[1] — [1]Angewandte Physikalische Chemie, Universität Heidelberg, 69120 Heidelberg, Germany — [2]Lehrstuhl für Anorganische Chemie, Technische Universität Chemnitz, 09111 Chemnitz, Germany

Homogeneous and mixed (with biphenylthiol: BPT) self-assembled monolayers (SAMs) of ferrocene-substituted biphenyl ethynyl thiols (Fc) were prepared on Au(111) substrates and characterized by several complementary spectroscopic techniques. The mixed films were fabricated either by subsequent immersion of the substrates into the BPT and Fc solutions or by immersion of the substrate into a mixed solution of BPT and Fc. The first procedure resulted in the preparation of high-quality mixed SAMs, in which the Fc molecules were stochastically distributed in the BPT matrix and well separated from each other. The portion of these molecules in such films could be precisely varied from ca. 7 to 42% by selection of the immersion time in the BPT solution. The films prepared from the mixed solution exhibited a phase separation between the Fc and BPT constituents. These films contained mostly the Fc molecules, showing, thus, a significant deviation from the relative content of the target molecules in the primary solution. This means that the Fc molecules, when competing with BPT, preferably adsorb onto Au(111) substrate, suggesting a significant impact of the ferrocene groups onto the structure-building interactions.

O 44.4 Wed 17:00 Poster C

Surface kinetics and structure of thin polymer films — •Christian Vree and S. G. Mayr — I. Physikalisches Institut, Georg-August-Universität Göttingen, Friedrich-Hund-Platz 1, D-37077 Göttingen

Structure formation at surfaces during thin film deposition is of great scientific interest due to the demand for smooth or regularly structured surfaces and interfaces for miniaturized functional films in science and technology. The deposition processes which govern morphology evolution during vapour deposition of polymer films are still poorly understood and need closer investigation.

In the present work this is achieved by a combined experimental - simulational study:

While the kinetics of single chains on polymer surfaces was investigated with MD simulations, experimentally Poly (Bisphenol A carbonate) (BPAPC) thin films were evaporated in a vacuum chamber. Surface morphologies were investigated using scanning force (SFM) and scanning electron microscopy (SEM). Fourier transform infrared spectroscopy (FTIR) and size exclusion chromatography (SEC) were performed for a detailed chemical characterization. It is found, that the rms roughness decreases rapidly, once closed surfaces are obtained at thicknesses as high as 30 nm.

This work was supported by the DFG SFB 602 (TP B3), as well as the GIF No. 1428-303.1/2004.

O 44.5 Wed 17:00 Poster C

In-situ synthesis and reactivity of adsorbed iron(II) and cobalt(II) tetraphenylporphyrins — •Yun Bai, Sven Schöffel, Ken Flechtner, Liam Bradshaw, Hans-Peter Steinrück, and J. Michael Gottfried — Universität Erlangen-Nürnberg, Lehrstuhl für Physikalische Chemie II, Egerlandstr. 3, 91058 Erlangen, Germany

In biological systems, Fe and Co porphyrins play an important role as the active centers of enzymes. Our approach to studying their reactivity is based on well ordered monolayers of these planar metal complexes at a Ag(111) surface. Their reactions with biologically relevant molecules such as O_2 and NO were studied under ultrahigh vacuum conditions with photoelectron spectroscopy and related techniques. Experimental difficulties arise from the extreme oxidation sensitivity of the Fe(II)-porphyrins. Therefore, the commonly employed ex-situ synthesis of the metalloporphyrin and subsequent vacuum deposition was ruled out as a way to prepare Fe(II)-porphyrin monolayers. Instead, we used an approach recently developed for the in-situ synthesis of adsorbed Co(II)-tetraphenylporphyrin [1] and succeeded to metalate monolayers of tetraphenylporphyrin with stoichiometric amounts of vapor-deposited Fe atoms. Supported by the Deutsche Forschungsgemeinschaft through SFB 583.

[1] Gottfried et al., J. Am. Chem. Soc. 2006, 128, 5644.

O 44.6 Wed 17:00 Poster C

STM Investigations on the ordered layers of a Tricarbonyl-(triphenylene)chromium-complex on Ag(111) and Ag(100) — •Christoph Schmitz[1], Iordan Kossev[1], Carola Rang[2], Karl Heinz Dötz[2], and Moritz Sokolowski[1] — [1]Institut für Physikalische und Theoretische Chemie, Universität Bonn, Wegelerstr. 12, 53115 Bonn, Germany — [2]Kekulé-Institut für Organische Chemie und Biochemie, Universität Bonn, Gerhard-Domagk-Strasse 1, 53121 Bonn, Germany

Metal-organic complexes of chromium are interesting as catalysts and also in the role of molecular switches [1]. The switching, i.e., the reversible haptotropic migration of the chromium, has been extensively studied in solution [2]. However, possible technical applications require that the switching process occurs, when the substance is bonded on a surface or in the solid state. Here we show first STM investigations of a monolayer of such metal-organic complex on the Ag(111) and Ag(100) surfaces in ultra-high vacuum. The deposition of the substance was done by sublimation from a home build Knudsen cell. STM measurements at room temperature and low temperatures (80-100 K) reveal long-range ordered structures. Based on the unit cell geometry, the tunneling contrast, and DFT calculations we draw conclusions about the ordering of the molecules in the unit cell. The DFT calculations were kindly provided by Y. Su and F. Neese. This work is supported by DFG, SFB 624. [1] B. L. Feringa, (Ed.), Molecular Switches, Wiley-VCH, Weinheim (2001). [2] H. C. Jahr, M. Nieger and K. H. Dötz, Chemical Communications (2003) 2866.

O 44.7 Wed 17:00 Poster C

SPA-LEED and NIXSW investigations of PTCDA on Ag(100) — •Julian Ikonomov[1], Oliver Bauer[1], Serguei Soubatch[2], Adam Lassise[2], Stefan Tautz[2], and Moritz Sokolowski[1] — [1]Institut für Physikalische und Theoretische Chemie der Universität Bonn, Wegelerstr. 12, 53115 Bonn, Germany — [2]International University Bremen, School of Engineering and Science, P.O. Box 750 561, 28725 Bremen, Germany

We report studies of vacuum deposited PTCDA films on Ag(100). The SPA-LEED (Spot Profile Analysis Low Energy Electron Diffraction) measurements show two ordered structures on Ag(100). Up to one monolayer coverage, PTCDA forms a commensurate c(4×4) structure with two molecules, perpendicularly oriented to each other in the unit cell. The ordered structure is stable up to a sample temperature of 690 K, at which a phase transition to a disordered phase occurs. Cooling the sample back to room temperature recovers the ordered structure. At a coverage above one monolayer the second layer orders in a different structure on top of the c(4×4)-ordered first layer. Herein the molecules are arranged in a herring-bone pattern, and the unit cell is very similar to that of the (102) plane of the PTCDA bulk crystal. NIXSW (Normal Incidence X-Ray Standing Wave) experiments were performed on the monolayer in order to determine the vertical adsorption height and to compare it with values determined earlier for PTCDA on Ag(111) [1]. Supported by SFB 624.

[1] A. Hauschild et al., Physical Review Letters 94 (2005) 036106.

O 44.8 Wed 17:00 Poster C

Looking for optimal Parameters for the self-assembly of linear organic Thiophenes — •Frank Sperka[1], Othmar Marti[1], and Elena Mena-Osteritz[2] — [1]Ulm University, Institute of Experimental Physics — [2]Ulm University, Institute of Organic Cemistry II

Macrocyclic Thiophenes are interesting substances to produce organic semiconductors. The self-assembly-behaviour of various types of macrocycles Cycloterthiophene-diine was studied in the last few years by means of STM. In order to gain a deeper inside into these mechanisms on also has to investigate how the assembly of linear Thiophene-Molecules on a substrate works. In order to do this, we investigated the R,R- and S,S-type of linear molecule Dihexyl-EDOT (EDOT=EthylenDioyThiophene) on mica and grahpite with an AFM in tapping mode. At the beginning it was found that our measurements were inconsistent. In this poster we will describe the influences of several environmental parameters like temperature, humidity and time on the quality of the films. Additionally it was found that the films degrade quite rapidly after formation.

O 44.9 Wed 17:00 Poster C

Interaction of Acetic Acid with Solid Water: A Study with IR Reflection-Absorption Spectroscopy (RAIRS) and Electron Spectroscopies (MIES; UPS) — •Stephan Bahr and Volker Kempter — Institut für Physik und Physikalische Technologien, Technische Universität Clausthal, 38678 Clausthal-Zellerfeld, Germany

The interaction of cyclic dimers of acetic acid, CH_3COOH, with solid water (D_2O) at 120K on polycrystalline Ag was investigated. Metastable Impact Electron Spectroscopy (MIES) and Ultraviolet Photoelectron Spectroscopy UPS(HeII) were utilized to obtain information on the electronic structure of the outermost surface. Infrared Reflection–Absorption spectroscopy (RAIRS) allowed for the identification of the AA species, and provides information on their hydration and the water–induced fragmentation.

The AA species quickly saturate the water OD dangling bonds at the ice surface, even before the first AA layer becomes saturated. For less than 0.3ML coverage the cyclic dimers break up into monomers and linear dimers under the influence of their interaction with the D_2O molecules. For coverages >0.3ML strong lateral interaction between AA monomers increases the linear dimer fraction. The second and following adlayers formed at 120K consist of cyclic dimers, mainly. The results will be compared to theoretical predictions [1,2].

[1] Picaud, S.; Hoang, P.; Peybernès, N.; Le Calvé, S.; Mirabel, P. *J. Chem. Phys.* **2005**, *122*, 194707. [2] Allouche, A.; Bahr, S. *J. Phys. Chem. B* **2006**, *110*, 8640.

O 44.10 Wed 17:00 Poster C

Coverage and temperature dependence of ordered thin pentacene films on Ag(111) investigated with SPA-LEED — •Annegret Hauschild and Moritz Sokolowski — Universität Bonn, Institut für Physikalische und Theoretische Chemie, Wegeler Str. 12, 53115 Bonn

Ultra thin films (1-15 monolayers) of the organic molecule pentacene (C22H14) were deposited with organic molecular beam epitaxy (OMBE) on the Ag(111) surface. Depending on coverage and deposition temperature, different highly ordered structures were found by spot profile low energy electron diffraction (SPA-LEED). For the sub-monolayer, no long range order has been observed. At low temperatures (LT), different to the well known room temperature (RT) phase [1], two further highly ordered structures could be observed in the monolayer. However, by growing multilayers at low temperatures, no change in the LEED patterns was recorded. The LEED spots become only more diffus, this indicates a cluster growth in the Stranski-Krastanov mode. These LT phases are meta stable. By warming up the sample to room temperature, a phase transition to the RT phase occurs.

[1] M. Eremtchenko et al., Phys. Rev. B 72, 1 (2005)

O 44.11 Wed 17:00 Poster C

Charge transfer dynamics in self-assembled monolayers — •Stefan Neppl[1], Ulrich Bauer[1], Peter Feulner[1], Andrey Shaporenko[2], Michael Zharnikov[2], and Dave Allara[3] — [1]Physikdepartment E20, TU-München, Germany — [2]Angewandte Physikalische Chemie, Universität Heidelberg, Germany — [3]Chemistry and Materials Science, Pennsylvania State University, USA

Charge transfer dynamics is a key quantity for the use of self-assembled monolayer as functional interfaces. Utilizing the core hole clock method, we study the endgroup to substrate electron transfer dynamics for cyanide terminated aliphatic thiolates on Au substrates. For aliphatic backbones consisting of 16 methylene groups, we observe pure autoionization spectra for pi-resonant N1s and C1s excitation of the CN endgroup. For resonant CN excitation of short chains of only 2 methylene groups, a mixture of resonant and non-resonant decay indicates endgroup to substrate charge transfer during the lifetime of the core holes. Quantitative results are obtained from the ratios of these contributions. Supported by the DFG (Fe 346/1-3) and the BMBF (05 KS4VHA/4 and 05 ES3XBA/5).

O 44.12 Wed 17:00 Poster C

BINAP's on Au(111) - Electronic interface properties — •Bengt Jaeckel and Bruce Parkinson — Colorado State University; Department of Chemistry; 200 West Lake Street; Fort Collins, CO-80523/USA

Substituted binapthyl-ligands (BINAPs) are important ligands for chiral selective homogeneous catalysis. We are attempting to prepare chiral selective surface by using organic MBE to prepare thin films of various racemic mixtures and enantiomerically pure BINAPs on freshly prepared Au(111)-surfaces. The interface properties were studied by X-Ray- and ultraviolet- photoelectron spectroscopy. Binapthol, the simplest and lightest molecule only forms a sub-monolayer coverage on Au(111) at room temperature. Substituted BINAPs (e. g. with two additional Br-atoms or two substitutional $PC_{12}H_{10}$-groups) show a higher sticking probability and provide interesting insight into the important parameters responsible for the interface formation. By varying the substitution of the basis molecule one can investigate the influence on the physical and chemical interactions with the substrate. Scanning tunneling microscopy studies will be carried out to determine the chiral properties of the molecules on the Au(111)-surface and if it possible to prepare enantiomeric pure surface which can be used for catalysis or sensing applications.

O 44.13 Wed 17:00 Poster C

Subphase dependent (2D) ordering in monolayers of amphiphile molecules — •Saskia Schmacke[1], Bernd Struth[2], Lutz Wiegart[3], Henri Gleyzolle[3], and Metin Tolan[1] — [1]Experimentelle Physik E1a, Universität Dortmund, Otto-Hahn-Str. 4, D-44221 Dortmund — [2]Deutsches Elektronen-Synchrotron DESY, Notkestr. 85, D-22607 Hamburg — [3]ESRF, 6 rue Jules Horowitz, BP 220, F-38043 Grenoble Cedex

Layers of amphiphile molecules on liquid subphases show a different phase behaviour depending on enviromental parameters like temperature, surface pressure and subphase. Gaseous, liquid and solid phases are observable. In this work the influence of different subphases on the crystal structure of the Phospholipid monolayers DPPA (dipalmitoylphosphatidic acid) and DPPC (dipalmitoyl-glycerophosphocholine) was investigated. The crystal structure was determined by using Gracing Incidence X-Ray Diffraction technique (GID) at the beamline ID10b, ESRF. The obtained diffraction patterns are analysed in two steps: First the information about the 2D unit cell of the crystalline phase, e.g. lattice spacings, lattice type (2D Bravais lattice) and the deformation of the lattice was determined. Secondly the intensity dependence on wave vector transfers perpendicular to the surface was analysed leading to information about the scatterer itself, like chain length, diameter, tilt angle and orientation within the lattice of the molecules forming the monolayer. The calculation of the differential cross section using a cylinder model for the lipid molecules shows very good agreement with the experiment for all subphases.

O 44.14 Wed 17:00 Poster C

Complex Structures in Multilayer Polymer-Blends on Glass Substrates — •Hubertus Marbach, Florian Maier, and Hans-Peter Steinrück — Universität Erlangen-Nürnberg, Lehrstuhl für Physikalische Chemie II, Egerlandstraße 3, D-91058 Erlangen, Germany

Recently, multicomponent polymer systems have attracted attention due to their capability to form a wealth of structures in thin films on various substrates. The three-dimensional morphology of these structures depends on the phase separation processes of the polymers involved, and on the corresponding experimental parameters and procedures, such as the polymer mixture, the spin coating parameters, thermal treatments, etc.. In the present paper we focus on layer systems of a mixture of polymethylmethacrylate and polysterene (PMMA/PS) on glass slides. The polymer-blend fims were prepared by a spin-coating technique and interjacent thermal treatments. The resulting rich variety of complex structures was characterized by means of atomic force microscopy under ambient conditions. In addition, the exposure of the PMMA/PS films to cyclohexane leads to the selective dissolution of PS. This enables the identification of the features attributed to PS (or PMMA) and serves as the starting point for the generation of even more complex structures. The main findings of systematic measurements will be presented and the underlying mechanisms will be dicussed.

O 44.15 Wed 17:00 Poster C

Site selective growth of organic molecules — Wenchong wang[1], dingyong zhong[1], jia zhu[1], felix Kalischewski[2], •chuan du[1], andreas heuer[2], harald fuchs[1], and lifeng chi[1] — [1]Physikalisches Institut and Center for Nanotechnology (CeNTech), Universität Münster, 48149 Münster, Germany — [2]Institut für Physikalische Chemie, Universität Münster, 48149 Münster, Germany

Devices with active organic layers are of great interest recently due to their less energy consumable process and potential low cost. However, the future success of these interesting materials in applications will strongly depend on fabrication processes that include patterning. We present a general method to pattern organic molecules by template-directed nucleation control using organic molecular beam deposition. Fully sites selective growth of organic molecules can be controlled at optimized conditions. We use simple Lennard-Jones (LJ) pair potentials to mimic the molecular interactions. The simulation results have good agreements with experimental data. This technique can be applied to fabricate large area uniform organic devices.

O 44.16 Wed 17:00 Poster C

Molecules can climb : Islands formation during organic molecular beam epitaxy — Dingyong Zhong[1,2], •Ruifen Dou[2], Wenchong Wang[2], Harald Fuchs[1,2], and Lifeng Chi[2] — [1]Institut für Nanotechnologie, Forschungszentrum Karlsruhe, 76021 Karlsruhe, Germany — [2]Physikalisches Institut and Center for Nanotechnology, Universität Münster, Wilhelm-Klemm-str. 10, 48149 Münster, Germany

The epitaxial growth of organic thin film has been studied. Islands with sharp edge, flat top and nearly uniform height are formed on metal crystalline substrate at certain range of growth temperatures. To understand the mechanism of the islands formation, a model is proposed in which the binding energy of molecules at the step edge is various at different terraces due to the lattice mismatching of the first monolayer and the three-dimensional island beyond the first monolayer. Both the ascending and descending interlayer transport processes are considered. The numerical simulations of the rate equations based on this model are consistent well with the experimental results.

O 44.17 Wed 17:00 Poster C

Molecular flexibility as a factor affecting the surface ordering of organic adsorbates on metal substrates — •S. Soubatch, R. Temirov, and F. S. Tautz — International University Bremen (Jacobs University Bremen as of spring 2007), Bremen, Germany

The effect of molecular flexibility on the surface ordering of complex organic adsorbates is explored by mean of LEED and STM, using DH4T and mixed DH4T-tetracene phases on Ag(111) as model systems. Above 273 K, DH4T forms a nematic liquid crystalline phase. At 273 K, a reversible phase transition to a long-range ordered, point-on-line coincident phase is observed. However, this ordered state is still affected substantially by the flexible nature of DH4T, which materializes in a large number of local structural defects. If traces of DH4T are co-evaporated with tetracene, inclusions of a 1:1 stoichiometric DH4T-tetracene phase are found in a tetracene/Ag(111) matrix. In this mixed phase, tetracene and the two surface enantiomers of DH4T arrange in a complex stripe structure. The mixed phase shows a higher degree of order than present at the pure DH4T/Ag(111) interface, which also lacks chiral organization. The addition of tetracene molecules as structural templates stabilizes certain conformations of DH4T and thus, by balancing its structural flexibility, allows the surface-induced chirality of DH4T to become a decisive factor in determining the structure of the mixed phase.

O 44.18 Wed 17:00 Poster C

STM Observation of Molecular Chains consisting of Mn_6Cr Single Molecule Magnets on Highly Ordered Pyrolytic Graphite (HOPG) — •Aaron Gryzia[1], Armin Brechling[1], Wiebke Hachmann[1], Marc David Sacher[1], Ulrich Heinzmann[1], Maik Heidemeier[2], and Thorsten Glaser[2] — [1]Faculty of Physics — [2]Faculty of Chemistry, University of Bielefeld, D-33615 Bielefeld

We report on the preparation and characterization of Mn_6Cr-Single Molecule Magnets[1] on a HOPG(0001) surface.

The Mn_6Cr-molecules showed 1D molecular arrangements with many interesting features, such as the occurrence of discrete kink angles in the molecular chains of 30°, only two different molecular orientations, the orientation of the chains along the main crystal axis of HOPG and a much larger molecule-molecule distance than expected from the van der Waals radii of the molecules. The orientation of single Mn_6Cr-molecules in the chain and the orientation of the chain, in respect to the main crystal axis of the HOPG substrate, shows a clear dependence. Segments of the chain with the same orientation of the Mn_6Cr-molecules are parallel to the main crystal axis and parts with an alternating molecular orientation are tilted by 30° in respect to this axis, which is a clear evidence for molecular-substrate interactions.

The observed structures appear to be a very promising model system to study the competition between molecule-molecule interactions and substrate-molecule interactions.

[1] T. Glaser et al., Angew. Chem., **118**, 6179-6183 (2006).

O 44.19 Wed 17:00 Poster C

Valence electronic structure of the PTCDA/Au(111) interface — •Johannes Ziroff, Simon Hame, Frank Forster, Azzedine Bendounan, and Friedrich Reinert — University of Würzburg, Experimental Physics II, Am Hubland, 97074 Würzburg, Germany

We present angular and energy resolved UPS spectra of PTCDA (3,4,9,10-perylene-tetracarboxylic-dianhydride) on the Au (111) surface from the sub-monolayer range to thick films. Using the Shockley state as a probe, one can investigate the substrate-adsorbate interaction of the first monolayer. We will show and discuss changes of binding energy and Rashba term upon adsorption. The valence features of the adsorbed PTCDA molecule, as well as their coverage dependent changes in intensity and binding energy will be addressed. Examples for the use of the surface state as an indicator for the type of thin film growth will also be presented.

O 44.20 Wed 17:00 Poster C

Inelastic electron tunnelling spectroscopy of the ordered PTCDA/Ag(111) interface — •R. Temirov and F.S. Tautz — International University Bremen, Bremen, Germany (Jacobs University Bremen as of spring 2007)

Understanding complex adsorption phenomena is an issue of rising importance. Recently it has been shown that the STM-based Inelastic Electron Tunnelling Spectroscopy (IETS) is a powerful technique for the analysis of adsorption on a single molecular level. Nevertheless the interpretation of the IETS data was shown in general to be far from straightforward. In this contribution we use the well studied case of PTCDA/Ag(111) adsorption as a model system to which the IETS is applied. The results of IETS are compared with HREELS data and theoretically calculated spectra of a free molecule. On the basis of a simple symmetry analysis two vibrational modes are identified. Remarkably, slight variations of the adsorption conditions are found to enhance IETS signal by an order of magnitude. The origin of this enhancement is discussed.

O 44.21 Wed 17:00 Poster C

High-Resolution Photoemission Spectra of Cytosine, Thymine and Uracil — •Andrea Haug, Maria-Benedetta Casu, Heiko Peisert, and Thomas Chassé — Institut für Physikalische und Theoretische Chemie, Auf der Morgenstelle 8, D-72076 Tübingen

In the last decade, significant progress has been made in the use of DNA bases as molecules for electronic applications such as bioorganic field effect transistors and molecular nanowires. Questions arise to which extent they could improve the present status of molecular electronics. These questions can be answered by the investigation of their electronic structure, of their interfaces with metals, and of their growth modes as thin films. In this work we present our investigations on the electronic and molecular structure of the DNA and RNA bases cytosine, thymine and uracil by X-ray photoemission spectroscopy (XPS) and ultraviolet photoemission spectroscopy (UPS). The films were grown by organic molecular beam deposition on polycrystalline gold with different film thickness (between 0.2 and 10 nm and above 20 nm). After each step the sample surface was characterized in situ by monochromatized XPS (Al-Kalpha 1486.6 eV) and UPS (He I, 22.2 eV) under UHV conditions. We have investigated the stability of the bases upon evaporation, the growth mode, and the interface properties.

O 44.22 Wed 17:00 Poster C

Electron spectroscopy on functionalized lignin-like materials — •Lothar Klarhöfer[1], Burkhard Roos[1], Wolfgang Maus-Friedrichs[1], Volker Kempter[1], and Wolfgang Viöl[2] — [1]Institut für Physik und Physikalische Technologien, Leibnizstraße 4, D-38678 Clausthal-Zellerfeld, Germany — [2]Hochschule für angewandte Wissenschaft und Kunst, Fakultät Naturwissenschaften und Technik, Von-Ossietzky-Str. 99, D-37085 Göttingen, Germany

XPS is a common technique for characterizing lignin-like materials, such as pulp and paper or wood surfaces. We combine valence band XPS with MIES (Metastable Impact Electron Spectroscopy) UPS (HeI) (Ultraviolet Photoelectron Spectroscopy) in order to identify functionalities which are difficult to detect with core level XPS due to the small chemical shift. With MIES / UPS it is possible to identify different functional groups of the surfaces, allowing to control surface - modification techniques applied to lignin - like materials, such as the optimization of the plasma treatment of wooden surfaces. Lignin surfaces were characterized by XPS, MIES and UPS. In order to understand the results, additional fingerprint spectra were recorded using the lignin precursors (coniferyl alcohol and sinapyl alcohol), cinnamon alcohol, phenol and benzene. The comparison with the MIES and UPS spectra of these molecules allows the identification of the contributions of the hydroxyl, methoxy and phenol groups the the lignin spectra.

O 44.23 Wed 17:00 Poster C

Characterisation of multi-wall carbon nanotubes functionalised with carboxyl groups — •Marcel Himmerlich, Uwe Ritter, Henry Romanus, Juergen A. Schaefer, Peter Scharff, and Stefan Krischok — Institut für Physik und Institut für Mikro- und Nanotechnologien, TU Ilmenau, P.O. Box 100565, 98684 Ilmenau, Germany

The impact of nitric acid (HNO_3) treatment on the structure, surface composition and surface electronic structure of multi-wall carbon nanotubes (MWCNTs) is investigated employing scanning electron microscopy (SEM) and transmission electron microscopy (TEM) as well as X-ray and ultraviolet photoelectron spectroscopy (XPS, UPS) together with electron energy loss spectroscopy (EELS). The investigated MWCNTs have been synthesised at 900°C by spray pyrolysis using benzene and 1% ferrocene in an Argon flow. After subsequent purification the samples were functionalised by a treatment with nitric acid at 100°C for 2 h. The valence band structures of functionalised and unfunctionalised samples are compared to reference measurements on formic acid (HCOOH) and polyacrylic acid. The analysis of the C1s and O1s core levels together with the observed differences in the valence band structure reveals the formation of carboxyl (-COOH) groups on the nanotubes. TEM measurements indicate that the main reaction takes place at the end of the nanotubes resulting in a cracking of the MWCNT end caps.

O 44.24 Wed 17:00 Poster C

X-ray absorption of spin crossover complexes — •Matthias Bernien[1], Marten Piantek[1], Jorge Miguel[1], Radu Abrudan[1], Heiko Wende[1,2], Wolfgang Kuch[1], Marco Haryono[3], Holger Kämpf[3], and Andreas Grohmann[3] — [1]Freie Universität Berlin, Fachbereich Physik, Arnimalle 14, D-14195 Berlin, Germany — [2]Universität Duisburg-Essen, Fachbereich Physik, Lotharstr. 1, D-47048 Duisburg, Germany — [3]Technische Universität Berlin, Institut für Chemie, Straße des 17. Juni 135, D-10623 Berlin, Germany

Spin crossover (SCO) molecular complexes consist of a central metal ion surrounded by organic ligands. Depending on temperature, pressure, or optical excitation, these complexes can switch between two magnetic states, for which the electrons of the d-orbitals align such that their spins add up (high spin) or compensate partly (low spin) [1].

We report on X-ray absorption (XAS) measurements of thin layers of Fe(II) bispyrazolylpyridine SCO complexes deposited from solution on gold metal surfaces. By means of angle-dependent XAS at the C- and N-K edges we determine the alignment of the molecules on the surface, whereas their spin state is determined by comparing the Fe-L3,2 spectra to measurements on bulk samples. We find that the interaction with the surface plays an important role on the switching phenomenon.

[1] O. Kahn and C.J. Martinez, Science 279, 44 (1998)

O 44.25 Wed 17:00 Poster C

Geometric and electronic structure of azobenze - alkanethiols on gold — •Daniel Brete[1,2], Roland Schmidt[1,2], Sanja Korika[1], Cornelius Gahl[1], and Martin Weinelt[1,2] — [1]Max-Born-Institut, Max-Born-Str. 2A, 12489 Berlin — [2]Freie Universität Berlin, Fachbereich Physik, Arnimallee 14, 14195 Berlin

Azobenzene is a conformational photo-switch. Upon optical excitation at 350 nm and 430 nm geometric changes of the chromophore occur on a sub-picosecond to picosecond timescale. This ultrafast dynamics suggests that switching may even occur when azobenzene is bound to a surface, where charge transfer into the substrate efficiently quenches electronic excitations. Associated with the geometric change of the azobenzene molecule from trans to cis conformation is a shift of the optical π to π^* transition.

We have investigated self-assembled monolayer of azobenzene - alkanethiols adsorbed on gold and their potential as a molecular switch by X-ray absorption as well as by X-ray and VUV photoemission spectroscopy. The molecules are well oriented at 100 K and the azobenzene entity is sufficiently decoupled from the substrate by the alkane chain. The occupied frontier orbitals of non-bonding n and of π character are identified by angle-resolved photoemission and autoionization spectroscopy at the N1s and C1s absorption edges. Their energetics and oscillator strengths are substantially modified by substituants attached to the azobenzene entity. Resultant implications for the switching efficiency will be discussed.

O 44.26 Wed 17:00 Poster C

Molecular distortion upon adsorption: The case of NTCDA/Ag(111) — •Christian Kumpf, Christoph Stadler, Ingo Kröger, Michael Scheuermann, and Eberhard Umbach — Univ. Würzburg, Experimentelle Physik II, Am Hubland, 97074 Würzburg

The properties of many functional materials and electronic devices based on (multi-)layer systems and thin films are dominantly defined by their surfaces and interfaces. This is particularly true for organic thin films and adsorbate systems, the properties of which largely depend on their interaction with the underlying substrate. Therefore a detailed investigation of this interaction is extremely important in order to obtain a comprehensive understanding of these materials.

I this contribution recent results for one of the most important model systems for molecular adsorption on surfaces is presented: 1,4,5,8-naphthalene-tetracarboxylicacid-dianhydride (NTCDA) on Ag(111). Using the techniques x-ray standing waves (XSW) and quantitative low energy electron diffraction (LEED-IV) a significant bending of the molecules was found upon adsorption. The results demonstrate the chemisorptive character of the adsorption.

Furthermore, a novel method for the interpretation of PES- and Auger-based XSW data is presented. The correction of non-dipolar effects in photoemission as well as electron-induced effects in Auger-electron emission was lively discussed within the last years. Using the example NTCDA/Ag(111) we demonstrate how the results from these different detection channels can be reconciled in a self-consistent iterative correction-method.

O 44.27 Wed 17:00 Poster C

Laser-tailoring of the size and shape of gold nanoparticles in solution — •Florian Vogel, Frank Hubenthal, and Frank Träger — Institut für Physik and Center for Interdisciplinary Nanostructure Science and Technology – CINSaT, Universität Kassel, Heinrich-Plett-Strasse 40, 34132 Kassel, Germany

Tailoring of metal nanoparticles with laser light has been a well known technique since several years. Although selective tailoring of certain shapes or sizes of supported metal nanoparticles has been demonstrated with ns-pulsed laser light, tailoring of nanoparticles in solution has remained a challenge.

In this contribution, we present recent studies on tailoring colloidal gold particles prepared by wet chemical reduction of $HAuCl_4$ with trisodium citrate. In general, this method produces elongated particles with relatively broad shape and size distributions. Post-synthesis irradiation with ns-pulsed laser light with photon energies of 1.9 eV and a laser fluence of (52 ± 4) mJ/cm^2 permits reshaping to spherical particles. This is accompanied by a clear reduction of the half width of the plasmon resonance, while the size of the particles remains nearly constant at approximately $R = 25$ nm. In contrast, if a photon energy of 1.4 eV and a comparable fluence is used, particles with axial ratios of about 0.3 are selectively heated and form colloids with radii up to 70 nm by coagulation.

O 44.28 Wed 17:00 Poster C

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 Si_4 this was confirmed in earlier calculations [1]. This leads to the question if these clusters are suited as building blocks for new cluster materials.

These investigations were extended to Si_7. Potential energy curves of two approaching Si_7 clusters were calculated for different reaction channels using Density Functional Theory implemented in the CPMD code available at [2]. It could be shown that the cluster-cluster interaction is either repulsive or there are fusion barriers higher than room temperature.

Since the influence of the surface is important, the next step was to include the graphite surface in the simulations. Also the influence of defects was to be studied.

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

[2] www.cpmd.org

O 44.29 Wed 17:00 Poster C

Kinetics of Ir-cluster lattice formation on a moiré of graphene with Ir(111) — •Tim Plasa[1], Alpha T. NDiaye[1], Josef Mysliveček[2], and Thomas Michely[3] — [1]I.Physikalisches Institut, RWTH Aachen — [2]Institut für Bio- und Nanosysteme IBN-3, Forschungszentrum Jülich — [3]II. Physikalisches Institut, Universität Köln

Highly ordered arrays of Ir clusters can be obtained by depositing Ir on Ir(111) surface covered with a graphene monolayer. The periodicity of these arrays is determined by the moire pattern of graphene on Ir(111) [N'Diaye et al., Phys. Rev. Lett. 97, 215501, 2006]. In order to uncover the mechanisms of Ir-cluster lattice formation on a moiré of graphene with Ir(111) we investigated the average cluster size and the occupation probability of moiré cells as a function of coverage, temperature and annealing time. We used a simple kinetic Monte Carlo simulation to derive atomistic parameters of adatom and cluster motion during the lattice formation. Assuming monomer and dimer mobility only, the data for temperatures up to 400 K may be reproduced fairly well, while at higher temperatures or longer annealing time the effect of the mobility of larger clusters become noticable.

O 44.30 Wed 17:00 Poster C

W_nS_m: Possible material for new fullerene structures — •Wilko Westhäuser[1], Tim Fischer[1], Tobias Mangler[1], Sibylle Gemming[2], Gotthard Seifert[2], and Gerd Ganteför[1] — [1]AG Ganteför, FB Physik, Universitiy of Konstanz, Germany — [2]Institut für Physikalische Chemie und Elektrochemie, University of Dresden, Germany

As the layered semiconductor material WS_2 in bulk is similar to graphite, it is of interest to find out whether this material might form small stable cage-like fullerene structures. In combination with density functional theory calculation and gas phase mass and photoelectron spectroscopy [1,2], certain magic clusters were deposited in soft-landing mode on Ag- and Si-substrates. In gas phase theoretically predicted 2-dimensional triangular shaped platelets of W_nS_m-clusters with n > 5 were detected and similar structures of Mo_nS_m were studied [3]. For first measurements deposited W_1S_3-, W_2S_6- and W_5S_6-clusters known as particularly stable in gas phase experiments were investigated via HREELS and XPS. These data were compared to WS_2 bulk material, additionally.

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

[2] S. Gemming, J. Tamuliene, G. Seifert, N. Bertram, Y.D. Kim and G. Ganteför, Appl. Phys. 82 (2006), 162

[3] B. Bertram, J. Cordes, Y.D. Kim, G. Ganteför, S. Gemming and G. Seifert, Chem. Phys. Lett. 418 (2006), 36

O 44.31 Wed 17:00 Poster C

Ag cluster growth on biaxially oriented PET — •Günther Weidlinger, Lidong Sun, José Manuel Flores-Camacho, Michael Hohage, and Peter Zeppenfeld — Institut für Experimentalphysik, Johannes Kepler Universität Linz, Linz, Austria

Metallic clusters show new and interesting properties different from bulk material, e.g. catalytic effects as well as optical effects. We report our in-situ optical characterization of metal clusters during growth with Reflectance Difference Spectroscopy (RDS). Ag was deposited on biaxially oriented Polyethylene terephthalate (PET) at a constant rate of about 0.1nm/min in Ultra High Vacuum (UHV). Since Ag does not wet the PET surface, the Ag atoms form clusters on the surface and in the surface-near region. Cluster layers with a nominal thickness from 0.1nm to 5nm were investigated. A strong anisotropy of the particle plasmon induced by the biaxially oriented substrate has been observed. Furthermore, this anisotropy shows a strong dependence on the nominal thickness of the silver layer. The relation between the observed optical properties and the size as well as the spacial distribution of the clusters will be discussed.

O 44.32 Wed 17:00 Poster C

CO oxidation and partial oxidation of light alkanes over TiO_2 supported gold catalysts in microreactors — •Guido Walther[1], Sebastian Horch[1], Ulrich Quaade[2], Ib Chorkendorff[2], Søren Jensen[3], and Ole Hansen[3] — [1]CAMD, Department of Physics, DTU, DK-2800 Kgs. Lyngby, Denmark — [2]CINF, Department of Physics, DTU, DK-2800 Kgs Lyngby, Denmark — [3]MIC, Department of Micro and Nanotechnology, DTU, DK-2800 Kgs Lyngby, Denmark

In a new setup, based on microfabricated silicon reactors, oxidation reaction over TiO_2 supported gold catalysts have been studied. In a first experiment size selected gold nanoclusters have been deposited into the microreactor using a cluster source. Here single charge gold clusters were mass selected by a QMS. The cluster beam was focused on the reactor bed using an einzel lens. Hence CO and oxygen were applied at a total flow rate of 0.1 ml min^{-1}, the amount of produced CO_2 was still below the detection limit of the used gas chromatograph. An increased amount of catalyst has been realized in a second experiment. Here a powder catalyst, based on TiO_2 supported 3.5 nm Au particles, was used. Appropriate measurements to CO oxidation gave rise to study partial oxidation of light alkanes over those catalysts. To investigate the reaction products the microreactor was interfaced to a gas chromatograph and a mass spectrometer, as well. Since methane reacts with oxygen in a stoichiometric ratio 1:2, water will be detected associated with CO_2. A significant increase in hydrogen signal marks the onset of the partial oxidation of methane.

O 44.33 Wed 17:00 Poster C

Dynamics of Metal Nanodroplets — Anja Habenicht[1], Paul Leiderer[1], Johannes Boneberg[1], •Moritz Trautvetter[2], Daniel Told[2], Christian Pfahler[2], Alfred Plettl[2], Paul Ziemann[2], Michael Kinyanjui[3], and Ute Kaiser[3] — [1]Universität Konstanz, Fachbereich Physik, 78457 Konstanz — [2]Universität Ulm, Institut für Festkörperphysik, 89069 Ulm — [3]Universität Ulm, Zentrale Einrichtung Elektronenmikroskopie, 89069 Ulm

Liquid metal nanodroplets are generated by a dewetting-induced detachment process: flat metal nanostructures evaporated onto a substrate through colloidal masks or structured by e-beam lithography are illuminated with an intensive ns laser pulse. If heated above the melting point, the liquid structures reduce their surface energy by reforming to spheres. For the small aspect ratios used here this involves a vertical movement of the center of mass and due to inertia the droplets leave the surface. The velocities of the detached nanodroplets are measured with a light barrier technique and compared with the velocity deduced from simple estimations for the dewetting process. Results are shown for different materials, intermediate layers and multilayers. Further we present first results of impact experiments, where the droplets are landed on another substrate. The particles cool down during the flight due to thermal radiation and solidify on the substrate. By catching at different distances, the landing temperature can be varied. Snapshots of different stages of droplet impact are shown. For the latter case, the focused ion beam technique was applied to cut directly through differently formed droplets.

O 44.34 Wed 17:00 Poster C

Electronic structure of iron oxide nanoparticles — •Aladin Ullrich, Daniel Gyasi-Antwi, Marcus Preisinger, Michael Krispin, and Siegfried Horn — Lehrstuhl für Experimentalphysik II, Universität Augsburg, D-86135 Augsburg

We have investigated the electronic structure of nanosized iron oxide and its precursor material apo-ferritin by scanning tunnelling mircroscopy (STM) and spectroscopy (STS) as well as conductive atomic force microscopy (CAFM). The remineralization of apo-ferritin molecules resulted in core sizes varying from 3 – 7 nm depending on the filling quantity of iron. Iron oxide nanoparticles were produced by thermal treatment of remineralized apo-ferritin molecules in air. Depending on the thermal treatment we were able to prepare different phases of nanosized iron oxide resembling α-Fe_2O_3, γ-Fe_2O_3 and mixtures thereof. The electronic structure of remineralized apo-ferritin and iron oxide nanoparticles has been investigated under ambient conditions and will be compared with previous measurements performed in UHV. We show that the band gap can differ from bulk material and is dominated by surface effects.

O 44.35 Wed 17:00 Poster C

Fabrication and Characterization of Gold Nanocrystals on NaCl(001)-Surfaces — •Andreas Winter, Jawad Slieh, Armin Brechling, Wiebke Hachmann, Ulf Kleineberg, and Ulrich Heinzmann — University of Bielefeld, Faculty of Physics, D-33615 Bielefeld

We report on 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(001) surface. The substrate temperature, the averaged thickness and the potential of the sample were studied systematically. After preparation, the gold nanocrystals have been characterized by means of different techniques such as Atomic Force Microscopy (AFM), Transmissions Electron Microscopy (TEM), X-Ray Diffraction (XRD) and Laue Diffraction. Depending on the preparation parameters, the gold grows in clusters with lateral and vertical sizes between 10 nm and 25 nm. XRD-measurements revealed a crystal growth with a preferred orientation of the Au(001)-axis parallel to the NaCl(001)-axis. A second Au(111) orientation, parallel to the NaCl surface normal was observed at a substrate potential between 200 V and 400 V and a substrate temperature of ca. 300°C, only. Estimations of the cluster size, measured by AFM, and the crystal size, measured by XRD exhibit comparable results, which indicate a high amount of single gold crystals. TEM-images, made after dissolving the gold-crystals in an aqueous CHAPS-solution support these results.

O 44.36 Wed 17:00 Poster C

Herstellung und Vermessung von Kobalt-Clustern — Matthias Grube, •Matthias Büenfeld, Frank Schmidl und Paul Seidel — Institut für Festkörperphysik, Friedrich-Schiller-Universität Jena, Germany

Kobalt-Cluster sind wichtige Katalysatoren für Kohlenstoff-Nanoröhren, wobei deren Größe mitbestimmend für den Durchmesser der Röhren ist.

Um die Cluster herzustellen, haben wir durch thermisches Verdampfen eine geschlossenen Kobaltschicht erzeugt, die anschließend getempert wurde. Der Temperprozess erfolgte sowohl an Luftatmosphäre als auch unter Vakuum. Es wurden Clustergrößen in Abhängigkeit von der Temperatur und den Dicken der geschlossenen Schichten untersucht. Als Substrat verwendeten wir Silizium mit und ohne einer zusätzlich gesputterten SiO_2-Schicht.

O 44.37 Wed 17:00 Poster C

Ag islands on C_{60} functionalized Au(111) compared to deposited Ag clusters — •Torsten Richter[1], Stefanie Duffe[1], Thomas Irawan[1], Benedikt Sieben[1], Heinz Hövel[1], Chunrong Yin[2], and Bernd von Issendorff[2] — [1]Universität Dortmund, Experimentelle Physik I, 44221 Dortmund, Germany — [2]Universität Freiburg, Fakultät für Physik, 79104 Freiburg, Germany

We are interested in the electronic structure of clusters in contact with a surface. In addition to experiments with mass selected Ag clusters we grew Ag islands by evaporation of Ag atoms on a C_{60} functionalized Au(111) surface at a temperature below 50 K. The investigation of the silver islands with a low temperature scanning tunnelling microscope shows quite broad height distributions. Tempering the cluster/surface system up to different temperatures leads to a higher mobility of the silver islands and more and more coalescence. We observed a strong coalescence at temperatures above 150 K. These experiments can be compared with experiments of mass selected geometrically magic clusters deposited on C_{60}/Au(111) at room temperature. Here we observed very narrow height distributions. We also studied the position of the clusters relative to the C_{60} molecules. We found out that the size selected clusters are on top of a C_{60} molecule and the grown islands at a position between two C_{60} molecules.

O 44.38 Wed 17:00 Poster C

GISAXS studies of micellar supported Au nanoparticles on TiO_2 — •Nicole Jeutter[1], Didier Wermeille[1], Joachim Bansmann[2], Stefan Kielbassa[2], Christine Fix[2], Ulf Wiedwald[3], Hans-Gerd Boyen[3], and Paul Ziemann[3] — [1]E.S.R.F. , 6 Rue Jules Horowitz, 38000 Grenoble, France — [2]Institute for Surface Chemistry and Catalysis, Ulm University, D- 89069 Ulm — [3]Institute of Solid State Physics, Ulm University , D- 89069 Ulm

Metal oxide supported gold catalysts have attracted considerable attention because of their surprising activity in a number of reactions such as low temperature CO oxidation [1]. The activity of catalysts might be closely related to the morphology and shape changes of the catalysts under different gas environments. Grazing Incidence Small Angle Scattering (GISAXS) experiments can monitor the morphology evolution in-situ and provide the possibility to determine the reaction parameter when shape changes occur.

Au nanoparticles of a nominate thickness of 12 nm have been deposited on a fully oxidized TiO_2 (110) substrate by micellar technique. The characterization of the average size and shape of the catalysts in air before and after annealing to 400°C has been carried out with GISAXS.

First results show that, before the annealing treatment, the average particle to particle distance can be clearly seen in GISAXS. After the annealing procedure the correlation maxima in the GISAXS pattern are broader and weaker than before.

[1] M.Haruta et al, J.Cat.144 (1993) 175

O 44.39 Wed 17:00 Poster C

Tunneling through single atoms — •Martyna Polok, Dmitry Fedorov, Michael Czerner, and Ingrid Mertig — Martin Luther University Halle-Wittenberg, Department of Physics, Institute of Theoretical Physics, 06099 Halle (Saale), Germany

Scanning tunneling microscopy (STM) is of great importance nowadays, since it allows for probing electronic and magnetic properties of surfaces.

In this study we concentrate on the theoretical description of a Cu tip interacting with a Co adatom adsorbed on the Cu (100) surface. The ground state electronic structure of the system was determined by means of density functional theory (DFT) combined with the screened Korringa-Kohn-Rostoker (KKR) Green's function method. It was shown that with the varying tip-surface distance d the geometry of the system undergoes complex structural relaxation[1].

We use Kubo linear response theory in Baranger-Stone formulation to find the conductance of the system for different d. The attention is focused on the value of the tunneling current as a function of d. Additionally we want to determined precisely the tip-surface distance d_0 for which the conductance changes from the tunneling to the contact mode. Results pertaining to tunneling regime will be presented.

[1] R. Z. Huang et al., Phys. Rev. **B** 12, 8169 (2006)

O 44.40 Wed 17:00 Poster C

Experimental band structure of V_2O_5 by angle resolved photoelectron spectroscopy — •Torsten Stemmler, Maximilian Kauert, Helmut Dwelk, and Recardo Manzke — Institut für Physik, Humboldt-Universität zu Berlin, Newtonstr. 15, 12489 Berlin

Due to the manifold of catalytic applications, the vanadium oxides, and among them V_2O_5, came into the scientific focus. For a basic understanding a detailed knowledge of the electronic structure is important. In particulare because the experimental data base on the electronic valence band structure on V_2O_5(010) single crystals is very scarce. Here we present high-resolution angle-resolved photoemission experiments carried out with synchrotron radiation and with the light of a HeI resonance lamp. The results will be compared with theoretical calculations,e.g. from J.C.Parker et al.[1] and A.Chakrabarti et al.[2]. Furthermore the problem of degradation of the surface due to the high reactivity will be discussed.

[1] J.C.Parker, D.J.Lam, Y.-N.Xu and W.YChing, Phys. Rev. B42, 5289 (1990)

[2] A.Chakrabarti, K.Hermann, R.Druzinic, M.Witko, M.Petersen and F.Wagner, Phys. Rev. B59, 10583 (1999)

O 44.41 Wed 17:00 Poster C

Fermi surface map of metallic $MoTe_2$ — •Thorsten Zandt, Robert Heimburger, Christoph Janowitz, and Recardo Manzke — Institut für Physik, Humboldt-Universität zu Berlin, Newtonstraße 15, 12489 Berlin

$MoTe_2$ undergoes a phase transition at about 1125 K from a low-temperature semiconducting α-phase (hexagonal, isostructural with MoS_2) to a high-temperature metallic β-phase (monoclinic, distorted CdI_2). Upon further cooling an additional phase transition is observed at 250 K for monoclinic β-$MoTe_2$. This transition is accompanied by a discontinuous structural change, i.e. the monoclinic angle β of $93°55''$ changes to 90° [1] resulting in an orthorhombic Td-$MoTe_2$ structure, which is isostructural with WTe_2.

Angular resolved photoemission was performed on β- and Td-$MoTe_2$ with HeI radiation and in the photon energy range $50eV < hv < 100eV$ at the U125-2 SGM monochromator at BESSY II. Fermi surface images were obtained by scanning the polar emission angle as well as the photon energy while monitoring the photoemission intensity at the Fermi level. The experimental results will be compared with additional tight-binding band structure calculations.

[1] R. Clarke, E. Marseglia and H.P. Hughes, Phil. Mag. **B38** 121 (1978)

O 44.42 Wed 17:00 Poster C

Spin- and momentum-resolved (inverse) photoemission for *in situ* investigation of the electronic structure of magnetic thin films — •Michael Budke, Tobias Allmers, and Markus Donath — Physikalisches Institut, Wilhelm-Klemm-Str. 10, 48149 Münster

We present a combined experimental set-up for spin- and momentum-resolved photoemission (PE) and inverse photoemission (IPE). This unique combination allows the investigation of the electronic structure below and above the Fermi level E_F of magnetic materials in one chamber on the same sample preparation. The system for PE is commercially available and consists of a gas discharge lamp and an electron analyzer equipped with a SPLEED detector for spin-resolved measurements. Our spin-resolved IPE system is home-made and consists of a spin polarized electron gun and a Geiger-Müller tube filled with acetone vapour for photon detection. The main advantage of our IPE system is its superior energy resolution of 165 meV (FWHM). This is a factor of two better than other state-of-the-art set-ups for IPE and enables us to resolve narrow spectral features not seen before, especially close to E_F. First results will be shown, which demonstrate the improved energy resolution in IPE on the Cu(001) image-potential states. The angular resolution is demonstrated on the surface state of Cu(111). In addition, the advantage of the in situ investigation of the electronic structure below and above E_F will be shown on the system Cr(001) which has been discussed intensely due to a peak right at E_F, previously interpreted as an orbital Kondo resonance [1]. [1] Kolesnychenko *et al.*, Nature **415**, 507 (2002)

O 44.43 Wed 17:00 Poster C

Excited states of matter probed with soft X-rays — •Martin Beye[1], Martin Deppe[1], Alexander Föhlisch[1], Franz Hennies[2], Mitsuru Nagasono[1], Edlira Suljoti[1], and Wilfried Wurth[1] — [1]Institut für Experimentalphysik, Universität Hamburg, Luruper Chaussee 149, D-22761 Hamburg, Germany — [2]MAX-lab, Lund University, Ole Römers väg 1, SE-22100 Lund, Sweden

Resonant soft X-ray spectroscopy allows to determine local electronic structure and binding properties of matter in all aggregate states. Here we present an investigation on crystalline silicon between room temperature and the melting point.

We measured the temperature dependence of the onset of absorption at the silicon L_3 edge in fluorescence yield. We find a shift to lower photon energies with increasing temperature that we attribute to electron-phonon interactions, lattice expansion effects and a change in the electronic screening of the final state.

In RIXS (resonant inelastic X-ray scattering) at low temperatures scattering is coherent and crystal-momentum conserving and shows features related to specific points in the bandstructure. Raising the temperature, coherence is disturbed due to electron-phonon scattering. This leads to bandstructure-integrated spectra showing the density of states. Similar effects can be observed by detuning the incident photon energy relative to the resonance which changes the duration of the scattering process. Shorter scattering duration times supress electron-phonon scattering channels, thus restoring the k-conservation rule and enhancing bandmapping features.

O 44.44 Wed 17:00 Poster C

Matrix-Element Effects in Valence-Band Photoemission of Fe_xTiS_2 using Circularly Polarized Light — •Martin Marczynski-Bühlow[1], Sabrina Lang[1], Jens Buck[1], Kai Rossnagel[1], Lutz Kipp[1], Nathaniel Janke-Gilman[2], Andrew Walter[2], and John Riley[2] — [1]Institut für Experimentelle und Angewandte Physik, Universität Kiel, D-24098, Germany — [2]Physics Department, La Trobe University, Melbourne, Australia

The effect of iron intercalation on the structural, magnetic and electronic properties of the layered transition metal dichalcogenide TiS_2 is an interesting and extensively studied question.

We investigated the valence band structure of Fe_xTiS_2 (x = 0; 0.1; 0.33) by angle-resolved photoemission taking advantage of a second generation toroidal electron spectrometer with fast data acquisition. Particularly, we have studied whether and to what extent Fe intercalation leads to modifications of the host valence band structure, such as increased band filling, hybridization between the Fe 3d orbitals and the host Ti 3d and S 3p orbitals, or new Fe 3d-derived electronic states below the Fermi energy.

Our main aim in this work was to reveal possible spin polarization effects at the Fermi energy by using fully circularly polarized light from beamline U56/2-PGM1 (hν = 89 to 1328 eV) at BESSY. Although we were not able to answer the question concerning spin polarization, interesting matrix-element effects were observed for the iron intercalated as well as for the pristine TiS_2 compound.

This work is supported by the DFG Forschergruppe 353.

O 44.45 Wed 17:00 Poster C

Spatially resolved photoemission measurements using reflective photon sieves — •Matthias Kalläne, Tim Riedel, Dirk Rahn, Sönke Harm, Kai Rossnagel, Jens Buck, Martin Marczynski-Bühlow, Claas Thede, and Lutz Kipp — Institut für Experimentelle und Angewandte Physik, Universität Kiel, D-24098, Germany

A new angle and spatially resolved photoemission experiment is being set up, which exploits a SPECS PHOIBOS 150 analyzer with a 2–dimensional CCD detector, and a grazing incidence photon sieve — a new type of diffraction optics for focusing synchrotron radiation with suppressed side lobes and reduced background [1]. In order to test the

setup before its planned use at the VUV–FEL monochromator beamline at HASYLAB, we carried out experiments at beamline BW3 of the storage ring DORIS III at HASYLAB with a photon energy of 100 eV. The photoemission measurements were done on the transition-metal dichalcogenide misfit compound (PbS)$_{1.13}$TaS$_2$ which consists of layers of cubic PbS and hexagonal 2H–TaS$_2$ subsystems. After cleavage in UHV the surface typically shows islands of both subsystems with sizes in the μm regime. The spatially resolved core level measurements are compared to spatially resolved spectra taken at the photoelectron microscope beamline BL31 at MAX–lab in Lund.
This work is supported by Innovationsfond des Landes Schleswig-Holstein.

[1] L. Kipp, M. Skibowski, R.L. Johnson, R. Berndt, R. Adelung, S. Harm and R. Seemann, Nature **414**, 184 (2001).

O 44.46 Wed 17:00 Poster C

Spin-Orbit Induced Valence-Band Splitting in Mg Thin Films Grown on W(110) and Mo(110) — •Alexander Gottberg, Alexander Helmke, Victor Soltwisch, Günter Kaindl, and Eugen Weschke — Institut für Experimentalphysik, Freie Universität Berlin, Arnimallee 14, 14195 Berlin, Germany

Due to the comparably long penetration depth of its wave function into the bulk [1], the Shockley-like Mg(0001) surface state is strongly influenced in thin films by the substrate. The surface-state band is known to interact with an interface resonance formed at the substrate. This interaction gives rise to a parity-induced energy splitting that depends on the Mg film thickness [2].

Using high resolution angle-resolved photoelectron spectroscopy a second, thickness-independent splitting is observed in Mg/W(110) that is absent in case of Mg/Mo(110). This comparison supports the interpretation of this additional splitting in terms of a Rashba-like spin-orbit effect induced by the W substrate. Since spin-orbit effects scale with the atomic number, this splitting is supposed to be weak in case of Mo, which is in agreement with the experiment.

[1] T. K. Kim *et. al.* Phys. Rev. B **72**, 075422 (2005)
[2] F. Schiller *et. al.* Phys. Rev. B **95**, 126402 (2005)

O 44.47 Wed 17:00 Poster C

Dependence of ultrafast charge transfer on orbital overlap — •Martin Deppe[1], Alexander Föhlisch[1], Franz Hennies[2], Mitsuru Nagasono[1], Martin Beye[1], and Wilfried Wurth[1] — [1]Institut für Experimentalphysik, Universität Hamburg, Luruper Chaussee 149, D-22761 Hamburg, Germany — [2]MAX-lab, Lund University, Ole Römers väg 1, SE-22100 Lund, Sweden

We have determined the dependence of the charge transfer time τ_{CT} on orbital overlap for a chemisorbed S monolayer on a Ru(0001) single crystal substrate by core hole clock spectroscopy. By changing the polarization of the synchrotron light relative to the surface plane S 3p orbitals with different spatial orientations can be selected.

We show that the process is much faster for orbitals with their main symmetry axis perpendicular to the substrate surface (out-of-plane) than for those oriented parallel to the surface plane (in-plane). In both cases the transfer occurs on a timescale faster than 1 fs; in out-of-plane geometry we find $\tau_{CT} = 0.18 \pm 0.04$ fs, while the in-plane case yields $\tau_{CT} = 0.84 \pm 0.36$ fs, both for photon energies directly above the autoionization resonance. This is the direct consequence of the fact that charge transfer is governed by the orbital overlap at the different atomic sites. To achieve the necessary temporal resolution, ultrafast Coster-Kronig autoionization decays are used as internal reference clocks.

O 44.48 Wed 17:00 Poster C

Unbuckling dimers at the Silicon(100) surface — •Christian Eickhoff[1,2], Cornelius Gahl[1], Tanja Giessel[1], Jens Kopprasch[1,2], Irina Ostapenko[1], Helena Prima Garcia[1], Roland Schmidt[1,2], and Martin Weinelt[1,2] — [1]Max-Born-Institut, Max-Born-Straße 2A, 12489 Berlin — [2]Freie Universität Berlin, Arnimallee 14, 14195 Berlin

Electronic structure and electron dynamics at the Si(100) surface have been studied by means of time-resolved photoemission spectroscopy. For low IR pump-laser intensity, i.e. in the limit of single-electron dynamics, electrons excited to the D_{down} dangling-bond band decay exponentially with a lifetime of $\simeq$ 200 ps. At larger excitation densities the decay rate scales quadratically with the population which indicates an effective phonon- and/or defect-assisted surface recombination between the occupied and unoccupied D_{up} and D_{down} dangling-bond bands. Having established significant depletion of the D_{up} and corresponding population of the D_{down}-bands, we observe spectroscopic signatures of atomic motion of the buckled dimers at the Si(100) surface. Time-dependent density functional theory predicts this electronically driven motion to occur on a femtosecond time-scale and to effectively lift the ground-state Peierls distortion of the buckled silicon dimers [1].

[1] J. van Heys, M. Lindenblatt, and E. Pehlke, Phase Transitions **78**, Nos. 9-11 (Sept.-Nov. 2005), 773-786

O 44.49 Wed 17:00 Poster C

Pretreatment of Steel Surfaces — •Christian Holzheu, Matthias Laske, and Othmar Marti — Institute of Experimental Physics, University of Ulm, 89069 Ulm, Germany

Steel is used for many purposes in several industrial fields. To improve the material properties several pretreating methods were tested. Especially laser treating was investigated. The characterization of the effected changes was done by performing different surface measurements. XPS (x-ray photoelectron spectroscopy) and Auger method were used to define the chemical structure, XRD (x-ray diffraction) to characterize the crystalline device. The Roughness was investigated by AFM (atomic force microscope).

O 44.50 Wed 17:00 Poster C

Microscopic picture of adsorption and desorption of D2O processed Au nanoparticles onto amino-terminated SiO2 surface studied by in situ ATR-SEIRA spectroscopy — •Tadaaki NAGAO[1,2], Dominik ENDERS[1,2], and Tomonobu NAKAYAMA[1,2] — [1]National Institue for Materials Science (NIMS), Tsukuba — [2]ICORP-JST

By use of ATR-SEIRA spectroscopy, we revealed the microscopic mechanism of the adsorption and the desorption process of Au nanoparticles onto amino-terminated SiO2 surface. In order to avoid overlapping the faint C-H peak with the strong O-H peak, we used Au nanoparticles produced in D2O solution instead of those processed in normal H2O solution. In this way, we could sensitively detect the C-H signal of the ligand citric molecules directly covering the Au nanoparticles as well as the O-D peaks of the D2O near the nanoparticles. By combining the in situ ATR-SEIRA spectroscopy and the ex situ SEM observations, we successfully explain the reason of the observed Langumuir kinetics of the nanoparticle adsorption, and further we correlate the surface number density of the particles and their morphology (uniform distribution vs. aggregates) to the status of the ligand citrate molecules. When the adsorbed nanoparticles are exposed to the solution of aminoethanethiol (AET: small thiol molecule terminated with amino group), the nanoparticles desorb via two-step substitutional adsorption of the molecules, and are removed completely from the SiO2 substrate.

O 44.51 Wed 17:00 Poster C

Atomic Force Microscopy studies on — •Jörn Wochnowski[1], Thimo Göllnitz[2], Germar Hoffmann[2], Jürgen Heck[1], and Roland Wiesendanger[2] — [1]Institute of Inorganic and Applied Chemistry, University of Hamburg — [2]Institute of Applied Physics, University of Hamburg

The coating of temperature-sensitive substrates, e.g. vitreous substrates in the microtechnology with high melting point materials, is challenging. Organometallic chemical vapour deposition of volatile compounds is one solution. We have developed[1] an experimental set-up for the deposition of elements (metals), element oxides and other functional composites in a glass microreactor (diameter: 70 μm or lower) and in mesoporous material. In a preliminary study numerous organometallic compounds as precursors have been tested as catalytic materials. The catalytic system (CrO$_x$/SiO$_2$) was successfully deposited in a glass microreactor by OMCVD of Cr(CO)$_6$ as precursor for the catalyst and tetraethoxysilane as precursor for the SiO$_2$ support. The deposited layers were investigated by REM and EDX. To study the surface morphology on the nanometer scale we employed Atomic Force Microscopy (AFM). Here, we will present our AFM investigations for surfaces prepared by organometallic chemical vapour deposition. We will discuss the preparation and the analysis of the surfaces with the focus to tailor material properties.

[1] J. Heck, S. Kneip, A. Knöchel, M. Haller, F. Moritz, (FZ Karlsruhe GmbH), DE 19852722, EP 1001050 A2 (2000).

O 44.52 Wed 17:00 Poster C

CO oxidation on modified Pt surfaces — •Regine Streber, Barbara Tränkenschuh, Michael Lorenz, Christian Papp, Reinhard Denecke, and Hans-Peter Steinrück — Lehrstuhl für Physikali-sche Chemie II, Universität Erlangen-Nürnberg, Egerlandstr. 3, 91058 Erlangen

In order to get closer to realistic systems, we studied the CO oxidation reaction not only on Pt(111) [1] but also on stepped Pt surfaces. We investigated the reaction between adsorbed atomic oxygen and CO on Pt(355) and Pt(322), which both have (111) oriented terraces with a width of five atomic rows but different step orientations, (111) vs. (100), respectively. Time-dependent in situ XP spectra in the O 1s and C 1s binding energy region showed that the reaction rate is increased on the stepped surfaces and depends on the step orientation. The preadsorbed atomic oxygen occupies different adsorption sites on both surfaces with different saturation coverages, leading to interesting temperature-dependent phenomena. In order to obtain a more detailed insight, we modified the system by deposition of Ag, which grows in rows along the lower step edges [2]. In this way the oxygen distribution can be modified. However, since higher CO coverages move Ag atoms away from the step edges to form islands on the terraces, the influence of Ag rows can only be studied for the initial period of the oxidation reaction.

The work was supported by the DFG (Ste 620/4-3).

[1] Kinne et al., J. Chem. Phys. 120 (2004) 7113.

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

O 44.53 Wed 17:00 Poster C

Photoinduced catalytic reactions on mars analogous surfaces — •Dominik Schwendt, Burkhard Roos, and Wolfgang Maus-Friedrichs — Institut für Physik und Physikalische Technologien, TU Clausthal, 38678 Clausthal-Zellerfeld, Germany

Many environmental facts about mars are known through NASA missions. Recently, traces of methane as well as formaldehyde in the marsian atmosphere have been found.

The purpose of this work was to find non-biological explanations for the presence of these gases on mars. Thus we tried to find ways to produce methane and formaldehyde on mars-like surfaces under marsian atmospheric conditions. We used Quadrupole Mass Spectroscopy to detect the gases and X-ray Photoelectron Spectroscopy to analyze the substrate. Our research has shown that formaldehyde emerges on watery hematite in a 6 mbar carbon dioxide atmosphere at temperatures around 260 K. Methane forms as well, if ultraviolet irradiation on the hematite is added to the named conditions.

Consequently with this work we present another possible source for the methane and formaldehyde traces in the marsian atmosphere.

O 44.54 Wed 17:00 Poster C

The influence of surface oxygen and oxide layers on adsorption systems on Ni(111) — •Michael Peter Andreas Lorenz, Regine Streber, Fabian Bebensee, Reinhard Denecke, and Hans-Peter Steinrück — Lehrstuhl für Physikalische Chemie II, Universität Erlangen-Nürnberg, Egerlandstraße 3, 91058 Erlangen

During many surface reactions, especially under realistic conditions, oxygen layers and even surface oxides form. We have studied the influence of such surface modifications at Ni(111) on the adsorption of small molecules, such as CO_2 and CH_4. Using in-situ x-ray photoelectron spectroscopy at BESSY II we characterized these oxygen layers by means of O 1s and Ni 2p core levels. In order to facilitate dissociative methane adsorption, we provided molecules with a well-defined kinetic energy (up to 0.8 eV) using a supersonic molecular beam. Interestingly, both the saturated oxygen adlayers as well as a surface Nickel oxide completely prevent dissociative methane adsorption for all energies studied. On the other hand, the physisorption regime seems to be shifted to higher temperatures as compared to clean Ni(111). The same seems to be true for CO_2, which also shows enhanced physisorption in the presence of oxygen.

O 44.55 Wed 17:00 Poster C

Multiple charge states of Ag atoms on ultrathin NaCl films — •Jascha Repp[1,2], Gerhard Meyer[1], Fredrik Olsson[3], Sami Paavilainen[4], and Mats Persson[5] — [1]IBM Research, Zurich Research Laboratory, 8803 Rueschlikon, Switzerland — [2]Institute of Experimental and Applied Physics, University Regensburg, 93053 Regensburg, Germany — [3]Department of Applied Physics, Chalmers University of Technology, 41296 Goteborg, Sweden — [4]Institute of Physics, Tampere University of Technology, 33720 Tampere, Finland — [5]Surface Science Research Centre and Department of Chemistry, The University of Liverpool, Liverpool L69 3BX, UK

So far the observation and manipulation by means of scanning tunneling microscopy (STM) of different charge states of adsorbed atoms have been limited to Au atoms on NaCl films supported by a Cu substrate.

On our poster, we show from a combined STM and density functional calculations study that Ag atoms adsorbed on NaCl bilayers on Cu(111) exhibit charge tristability and can be switched reversibly between the neutral adatom state and the negatively or the positively charged adatom state. Thus, the charge multistability of adatoms is not at all unique for Au adatoms and it is even possible to have more than two different charge states of an adatom. Furthermore, based on a simple model, we identify and discuss the key adatom, film and substrate parameters for the stabilization of multiple charge states. This model can be used as a guide to find other systems of interest.

O 44.56 Wed 17:00 Poster C

Controlling molecular adsorption through domain-patterned lithium niobate — •Alexander Haussmann, Marc Tobias Wenzel, Stefan Grafström, Thomas Härtling, Christian Loppacher, and Lukas Eng — Institut für Angewandte Photophysik, Technische Universität Dresden, D-01062 Dresden

Recent progress in engineering ferroelectric domains has led to the possibility of creating domain patterns on the submicron scale. Because the domain arrangement corresponds to a pattern of opposite surface charges, such structured ferroelectric materials promise interesting applications as templates for the structured adsorption of charged molecules on surfaces. Recent work has reported on the adsorption of noble-metal nanoparticles [1] to such surfaces. Here, we report on the adsorption of λ-DNA to $LiNbO_3$ single-crystal surfaces. The DNA molecules of some 10 μm in length were marked with the fluorescent dye yoyo-1 to facilitate optical tracking of the their distribution on the surface. We found that λ-DNA preferentially adsorbs to c^+ domains. The recently discovered reduction of the coercive field of $LiNbO_3$ under UV illumination [2] offers a promising way for writing arbitrary domain patterns on the micrometer scale. Here, we will report first results on the switching and adsorption behavior observed in a setup in which the sample is mounted in a liquid cell and a focused He-Cd laser beam (at $\lambda = 325$ nm) is used for UV patterning.

[1] J. L. Giocondi and G. S. Rohrer, Chem. Mater. **13**, 241 (2001)

[2] M. Müller, E. Soergel, K. Buse, Appl. Phys. Lett. **83**, 1824 (2003)

O 44.57 Wed 17:00 Poster C

Interaction of different $SrTiO_3$ surfaces with reactive gases — •Florian Voigts[1], Dominik Schwendt[1], Martin Frerichs[2], Christos Argirusis[2], Günter Borchardt[2], and Wolfgang Maus-Friedrichs[1] — [1]Institut für Physik und Physikalische Technologien, TU Clausthal, Leibnizstrasse 4, 38678 Clausthal-Zellerfeld, Germany — [2]Institut für Metallurgie, TU Clausthal, Robert-Koch-Strasse 42, 38678 Clausthal-Zellerfeld, Germany

Donor doped $SrTiO_3$ is well known for its capability as resistive high temperature oxygen sensor. An interesting application of this sensor would be the analysis of automobile exhaust, as it would allow the optimisation of fuel injection and of catalytic oxidation of toxic exhaust, thus reducing fuel consumption and pollution of the environment. Before this application can be implemeted, preliminary studies aiming at the interaction of $SrTiO_3$ with reactive gases must demonstrate the stability of the material in this environment. Also, the influence of these gases on the interation with oxygen must be clarified.

We use Metastable Impact Electron Spectroscopy and Ultraviolet Photoelectron Spectroscopy to analyse the valence band structure of $SrTiO_3$ and its adsorbates. X-ray Photoelectron Spectroscopy is used to check the stoichiometry of the samples. Our results for the interaction of $SrTiO_3$ with CO, CO_2, H_2O, CH_4 and other reactive gases being part of automobile exhaust are presented in this poster. We use $SrTiO_3$(100) as model substance und compare our results with experiments on polycristalline $SrTiO_3$ produced via a sol-gel route.

O 44.58 Wed 17:00 Poster C

Surface properties of indium oxide and its interaction with ozone for the use as gas sensor — •Marcel Himmerlich, Chunyu Wang, Volker Cimalla, Juergen A. Schaefer, Oliver Ambacher, and Stefan Krischok — Institut für Mikro- und Nanotechnologien, TU Ilmenau, P.O. Box 100565, 98684 Ilmenau, Germany

Polycrystalline indium oxide thin films have great potential for low cost and low energy consumption environmental sensors, e.g. for the detection of ozone. We have examined the surface properties of indium oxide films prepared by metal organic chemical vapour deposition using X-ray and ultraviolet photoelectron spectroscopy (XPS, UPS). The influence of the growth temperature on stoichiometry as well as the surface electronic structure is presented. Especially for low temperature (200°C) grown samples strong emission from an up to date unidentified state below the valence band maximum is observed. In order to identify the photoreduction and oxidation mechanisms related to the ozone sensor principle, we have investigated the interaction of indium oxide with ozone and UV radiation. For the interaction with ozone, two adsorbate related states at 6.1 eV and 11.3 eV appear in the valence band together with an increase in the work function and a change in the surface band bending. A model will be proposed to explain the interaction of ozone with the indium oxide surface with respect to the observed drastic changes in resistivity of the samples.

O 44.59 Wed 17:00 Poster C

Stability of $Fe_3O_4(001)$ in a humid environment — •Narasimham Mulakaluri[1], Rossitza Pentcheva[1], and Matthias Scheffler[2] — [1]Section Crystallography, Dept. for Earth and Environmental Sciences, University of Munich — [2]Fritz-Haber-Institut der MPG, Berlin

The interaction of water with a mineral surface is a fundamental process both in nature and technology. We study the influence of water adsorption on the energetics and properties of the $Fe_3O_4(001)$ surface using density functional theory (DFT)-calculations with the FP-LAPW method in the WIEN2k implementation. The surface stability of different terminations as a function of the O_2 and H_2O pressure is compared in the framework of ab initio thermodynamics. On the clean surface a bulk termination containing oxygen and octahedral iron is stabilized through a Jahn-Teller distortion [1]. For this so called modified B-layer as well as the half occupied A-layer termination we vary the degree of hydroxilation of the surface. At water rich conditions where the surface is completely covered by hydroxyl groups a B-layer is found to be favored compared to other models. We investigate also the role of water adsorption on surface reconstruction and find a tendency towards outward relaxation of the surface atoms covered by hydroxyl groups. For the hydroxilated surfaces we obtain metallic behavior compared to the half-metallic bulk, however, the surface states in the majority band gap have a different character compared to the clean surface.

[1] R. Pentcheva et al., Phys. Rev. Lett. 94,126101 (2005).

O 44.60 Wed 17:00 Poster C

α-Fe_2O_3 (0001) surface structure analysis by LEED — •Maike Lübbe and Wolfgang Moritz — LMU, Department für Geo- und Umweltwissenschaften, Theresienstr. 41, D-80333 München

Despite the importance of the haematite, α-Fe_2O_3, surface in chemical and technological applications its structure has not been determined unambiguously up to now although being subject to both theoretical [1, 2] and experimental [3, 4] investigations.

We therefore analysed the (1×1) (0001) surface structure of a bulk α-Fe_2O_3 crystal by low energy electron diffraction.

The polished crystal was installed in an UHV chamber with a base pressure of $2 \cdot 10^{-10}$ mbar and annealed at 500°C in an O_2 atmosphere, $p_{O_2} \approx 3 \cdot 10^{-8}$ mbar, for several hours. The diffraction spots were sharp although a somewhat elevated diffuse background was observed. An I-V-curve data set of 10 symmetrically independent diffraction spots was measured at room temperature in the energy range $E \approx 150 \ldots 500\,\mathrm{eV}$. Measurements at lower electron energies were not possible due to charging effects of the insulating crystal.

Our analysis indicates that the α-Fe_2O_3 (0001) surface is terminated by iron partially occupying two bulk sites when prepared at low oxygen pressure. Relaxation effects along c-axis are quite large and involve several iron double layers.

[1] A. Rohrbach *et al.*, Phys. Rev. B **70**, 125426 (2004) [1] W. Bergermayer, H. Schweiger, Phys. Rev. B **69**, 195409 (2004) [3] G. Ketteler *et al.*, Surf. Rev. Lett. **8**, 661 (2001) [4] S. Chambers, S. Yi, Surf. Sci. Lett. **439**, L785 (1999)

O 44.61 Wed 17:00 Poster C

Temperature dependent femtosecond two-photon photoemission from ultrathin MgO films — •Tobias Gleitsmann, Mihai E. Vaida, and Thorsten M. Bernhardt — Institut für Oberflächenchemie und Katalyse, Universität Ulm, 89069 Ulm, Germany

Due to their chemical and electronical properties, ultra-thin Magnesia films represent an ideal substrate system in order to investigate small deposited metal clusters. Especially the band gap of these isolating films in principle enables the observation of the cluster electronic states near the Fermi level independently from the substrate states whereas avoiding charging effects. The electronic structure of these ultra-thin magnesia films supported on a Mo(100) single crystal surface is investigated as a function of the post-deposition annealing temperature via femtosecond two photon photoemission spectroscopy and electron energy loss spectroscopy. Additionally, the film composition and crystal structure is analyzed by temperature programmed desorption mass spectrometry, Auger electron spectroscopy, and low energy electron diffraction, respectively. Strong evidence is found for the formation of an optical resonance at 4.6 eV with increasing annealing temperature accompanied by a change in the surface work function.

O 44.62 Wed 17:00 Poster C

Surface morphology and surface stress of CaF_2 films on Si(111) — •Markus Neubert, Peter Kury, Friedrich Klasing, and Michael Horn von Hoegen — University of Duisburg-Essen, Institut of Experimental Physics

Thin CaF_2 films with low defect density could be grown epitaxially on Si(111) due to the small lattice mismatch between CaF_2 and Si. Due to the large thermal expansion coefficient ($\alpha_{CaF_2} \approx 19 \cdot 10^{-6} K^{-1}$) of CaF_2 the lattice mismatch increases strongly with temperature ($\alpha_{Si} \approx 2.6 \cdot 10^{-6} K^{-1}$). As a consequence the vertical lattice parameter of thin CaF_2 films increases by tetragonal distortion due to the build-up of compressive stress. We have grown CaF_2 films at temperatures between 600K and 1100K by Molecular Beam Epitaxy (MBE). The resulting surface stress was measured in-situ during deposition by Surface Stress Induced Optical Deflection (SSIOD). The film morphology was investigated by ex-situ non-contact AFM. The thickness of the films was independently calibrated by X-Ray Reflection (XRR) measurements.

O 44.63 Wed 17:00 Poster C

Improvement of the thermal stability of the HfO_2/Si(100) system using a diffusion barrier — •D. Weier[1], A. deSievro[2,3], M. Schürmann[1], C. Flüchter[1], M. Carazzolne[3], A. Pancotti[3], R. Landers[2,3], G. Kleiman[3], and C. Westphal[1] — [1]Experimentelle Physik 1 - Universität Dortmund, Otto-Hahn-Str. 4, D 44221 Dortmund, Germany — [2]Laboratório Nacional de Luz Síncrotron, C.P. 6192, 13084-971 Campinas, SP, Brazil — [3]Instituto de Física - Universidade Estadual de Campinas, C.P. 6165, 13083-970 Campinas, SP, Brazil

The ongoing miniaturisation of transistor devices requires a new gate dielectric to replace silicon oxide (SiO_2) that has been used for the last decades. The possible substitutes have to fulfill several requirements like band gap alignment to the silicon, a good interface quality, and a thermal stability. HfO_2 meets most of the requirements, but it is shown in many studies that it's thermal stability is one of the main problems of the system HfO_2/Si(100) due to silicide formation at high temperature annealing. In this work a film of silicon nitride was deposited on the silicon substrate via sputtering and annealing. The silicon nitride (Si_3N_4) is stable when a high temperature annealing up to approximately 1100 °C is applied. Thus, it can be used as a diffusion barrier for the HfO_2 in the high temperature range. We will show several heating cycles for different diffusion barrier thicknesses and we compare them with similar cycles for HfO_2/Si(100) films without a diffusion barrier. It will be shown that it is possible to increase the thermal stability of HfO_2 with a Si_3N_4 layer.

O 44.64 Wed 17:00 Poster C

Cerium oxide films on TiO_x coated Pt(111)-single crystals — •Thorsten Staudt and Klaus Schierbaum — : Institut für Experimentelle Physik der kondensierten Materie, Abteilung für Materialwissenschaft, HHU Düsseldorf, 40225 Düsseldorf

The epitaxial growth of thin and continuous CeO_2(111) films on metal surfaces suffers from the preferential formation of a 3 D-like morphology, even though epitaxial relationships exist with the substrate lattices. This holds for films prepared by reactive evaporation of Ce in O_2 on Pd(111) and Rh(111)[1], or by oxidation of an ordered surface alloy Pt_5Ce/Pt(111)[2]. One may expect a decreased lattice mismatch if metal surfaces are used that are coated with ultra thin and ordered oxide-based buffer layers. As a candidate we have chosen the "wagon wheel" phase of TiO_x grown on a Pt(111) surface which reveal a hexagonal symmetry and an interatomic spacing of 3.26 Å. This value is closed to the lattice constant of 3.86 Å for CeO_2(111).[3] The film is

1.2 ML thick and shows a continuous morphology in STM.

CeO_x films are subsequently grown by thermal evaporation of cerium in O_2 at RT. The films were analysed by LEED and XPS to determine the geometric structure, chemical composition and stoichiometry. First measurements reveal a change in the stoichiometry of the TiO_x film that is discussed in terms of an interface reaction. Additional information on the initial stages of growth is obtained from STM.

[1]: S. Eck et al., Surf. Sc. 520 (2002), 173-185 and reference therein
[2]: U. Berner and K. Schierbaum, Phys. Rev. B 65 (2002), 235404
[3]: F. Sedona et al., J. Phys. Chem. B 109 (2005), 24411-24426

O 44.65 Wed 17:00 Poster C

EELS investigations of surface color centers in BaO, SrO and lattice matched $Ba_{0.7}Sr_{0.3}O$ on Si(001) — •Dirk Müller-Sajak and Herbert Pfnür — Leibniz-Universität Hannover, Institut für Festkörperphysik, Appelstr. 2, 30167 Hannover, Germany

We investigated the generation of color centers in ultrathin films of BaO and SrO on Si(001) by electron bombardment both as a function of electron energy and of exposure. Both materials grow nanocrystalline on this surface. In a second stage, lattice matched and crystalline layers of $Ba_{0.7}Sr_{0.3}O$ on the same surface are investigated. Electron energy loss spectroscopy was used to identify the color centers formed. These color centers will finally be used as nucleation centers for metal wires and dots.

The dependence of cross sections in the energy range 30-100eV for color center generation on electron energy is compatible with a Knotek-Feibelman generation mechanism. Apart from energetic positions, decay processes and rate dependent behavior were investigated. By controlled oxygen exposure and their extinction as a function of exposure, these defects were clearly identified as oxygen vacancies. Two peaks with characteristic losses at 0.75 and 1.39 eV in the EELS spectra of electron bombarded BaO films decay with the same time constant. They were assigned to surface color centers. A third loss peak at 2.15 eV coincides with that bulk color centers. Correlations with structural properties of the films are discussed.

O 44.66 Wed 17:00 Poster C

In situ STM study of the adsorption and oxidation of sulfide on the Au(1 0 0) surface — •Christian Schlaup, Daniel Friebel, Peter Broekmann, and Klaus Wandelt — Institut für Physikalische und Theoretische Chemie, Wegelerstr. 12, D-53115 Bonn

In contrast to the well described adsorption behavior of sulfide on the Au(1 1 1) surface, the adsorption of sulfide on the Au(1 0 0) surface has not yet been part of extensive investigation. In 0.01 M NaOH / 0.5 mM Na_2S electrolyte, the formation of different ordered sulfide adsorbate layers could be detected. Depending on the applied electrochemical potential a simple p(2 × 2) ($\Theta_S = 0.25$ ML), a more complex c(2 × 6) ($\Theta_S = 0.33$ ML) or a c(2 × 2) ($\Theta_S = 0.5$ ML) overlayer is formed. The well-known Au(1 0 0)-(hex) reconstruction, which could be observed at cathodic potentials, is lifted during the initial stages of sulfide adsorption leading to the formation of small, well oriented gold islands. By increasing the S coverage from initially $\Theta_S = 0.25$ ML, the shape of these islands changes significantly to a serrated form. Thereby a complex bi-layer phase, coexisting with the c(2 × 6) S adlayer, is formed. Upon further oxidation, the characteristic ring-like structure appears, which has already been observed on the S-covered Au(1 1 1) surface at high potentials (EC) and high S coverage (UHV), respectively.

O 44.67 Wed 17:00 Poster C

Surface science approach to study surface and interface properties of room temperature ionic liquids — •Oliver Höfft[1], Stephan Bahr[1], Volker Kempter[1], Marcel Himmerlich[2], Stefan Krischok[2], Maxim Eremtchenko[2], Yonghe Liu[2], Rolf Öttking[2], Anita Neumann[2], Jens Uhlig[2], Pierre Lorenz[2], Imad Ahmed[2], and Jürgen Schaefer[2] — [1]Institut für Physik und Physikalische Technologien, TU Clausthal, 38678 Clausthal-Zellerfeld, Germany — [2]Institut für Physik und Institut für Mikro- und Nanotechnologien, TU Ilmenau, 98684 Ilmenau, Germany

Despite the immense importance of the surface and interface properties of ambient temperature ionic liquids for technical applications, only a few surface sensitive investigations have been performed to date. Therefore, we have chosen the latter approach under well defined ultra high vacuum conditions in order to get some first insight into different surface and interface related properties of liquids like [EMIM]Tf2N. We used ultraviolet and X-ray radiation (20 eV up to 1500 eV), metastable helium atoms and primary electrons by applying a number of techniques like UPS, MIES, XPS, HREELS. The emitted photoelectrons and the elastically and/or inelastically scattered electrons give some first detailed information about the elemental composition, the electronic and vibronic structure and about its radiation induced changes. Some of the experimental results are compared with first principle calculations (DFT-LSDA). Our present status of understanding will be discussed in detail at the conference.

O 44.68 Wed 17:00 Poster C

Corrosion Inhibition by Diphenylviologen on Cu(100) — •Knud Gentz, Peter Broekmann, Simone Kossmann, Barbara Kirchner, and Klaus Wandelt — Institut für Physikalische und Theoretische Chemie, Universität Bonn

The effect of preadsorbed Diphenylviologen (DPV) on the corrosion of a bromide-modified Cu(100) surface in 5mM sulfuric acid has been studied by cyclic voltammetry (CV) and in-situ STM measurements, conducted with a home-built electrochemical STM [3]. In the anodic sweep, the oxidative dissolution of Cu(100) under the given conditions is shifted about 100 mV to more positive potentials with respect to the same surface in the absence of the viologen. Certain structural elements of DPV on the surface lead to the proposal of a tentative model of the mechanism of the corrosion inhibition, that has been developed on basis of DFT calculations of the structure of the viologen. The halide-modification generates a high surface mobility of the copper, leading to ordered step-edges aligned with the <010> directions of the halide lattice. These ordered step-edges induce a structure of the viologen near the edge, which is different from the structures on the terrasses. The compact arrangement of this structure effectively blocks the step-edges as reactive sites for the copper corrosion.

[1] Wilms et al., *Rev. Sci. Instr.,* **70** 7 (1999) 473

O 44.69 Wed 17:00 Poster C

STM results on Electrochemical Surface Electron Transfer Reactions — •Duc Thanh Pham, Knud Gentz, Carolin Zörlein, Peter Broekmann, and Klaus Wandelt — Institut für Physikalische und Theoretische Chemie, Universität Bonn

The structural characterization of 1,1'-dibenzyl-4,4' bipyridinium molecules (dibenzyl-viologen, DBV), adsorbed on a chloride modified Cu(100) electrode is studied by means of Cyclic Voltammetry (CV) and in-situ Scanning Tunneling Microscopy (STM), showing the formation of laterally well-ordered 2D-array of different supramolecular ensembles. By reducing the pre-existing di-cationic DBV^{2+} species to the corresponding radical mono-cation DBV^{*+}, a quasi-reversible phase transition is initiated from a cavitand phase to a stripe pattern. These structural motifs are widely independent on the electronic and structural substrate properties. While each cavitand consists of 4 individual DBV^{2+} sub-units arranged in a circular manner making this supramolecular cavitands chiral, the DBV^{*+} in the stripe pattern are adsorbed with their main molecular axis parallel to the surface in a side-on adsorption geometry. However, by exchanging the pure supporting electrolyte for the viologen-containing solution in the potential regime where this phase transition takes place, it reveals two further metastable phases, which can be irreversibly transformed into the stripe pattern or the cavitand phase. In addition, chloride desorption through the viologen film is discussed as reason for an order-disorder transition within the viologen film at even more negative potentials.

O 44.70 Wed 17:00 Poster C

Potential dependent structures of adsorbed viologens on Cu(100) — •Knud Gentz, Peter Broekmann, Simone Kossmann, Barbara Kirchner, and Klaus Wandelt — Institut für Physikalische und Theoretische Chemie, Uni Bonn

The structures of two different viologens (1,1'-disubstituted 4,4'-Bipyridins) adsorbed on a bromide-modified Cu(100) surface in an electrochemical environment have been studied by cyclic voltammetry (CV) and Scanning Tunneling Microscope (STM) studies. Upon adsorption, both viologens arrange in characteristic structures, dependent on the potential of the electrochemical cell. Via potential variation various structures are accessible and have been characterized. The phase transition are completely reversible between the DBV^{2+} dication and the $DBV^{\bullet+}$ radical cation of Dibenzylviologen and the DPV^{2+} and $DPV^{\bullet+}$ of the Diphenylviologen respectively. For the DPV molecule, this phase transisition proceeds in two steps. First, the bulk phase is oxidized through the adsorbed layer of the $DPV^{\bullet+}$ radical cation. Only at a significantly higher potential the adsorbed viologen is oxidized. In the cathodic sweep a corresponding surface reduction peak can be observed in the cv at higher potential than the bulk reduction peak. The reduction to the neutral DBV and DPV molecules occurs only at low potentials beyond the onset of the hydrogen evolution reaction. Based on DFT calculations of the structure of individual and groups of Viologen molecules, models for the observed structures are proposed.

O 44.71 Wed 17:00 Poster C

Electric field effects at the ice/SiO_2 interface — •Heiko Schröder[1], Sebastian Schöder[1,2], Markus Mezger[1], Harald Reichert[2], Veijo Honkimäki[2], Jörg Bilgram[3], and Helmut Dosch[1] — [1]Max-Planck-Institut für Metallforschung, Heisenbergstr. 3, D-70569 Stuttgart, Germany — [2]ESRF, 6 rue Jules Horowitz, F-38000 Grenoble, France — [3]ETH Zürich, Schafmattstr. 16, CH-8093 Zürich, Switzerland

Since the water molecule has a dipole moment, electric fields are expected to have a strong influence on the water/ice phase transition [1]. A deeper knowledge of the underlying mechanisms could improve our understanding of atmospheric cloud chemistry. To achieve this, we investigate electric field effects at the ice/SiO_2 interface by employing high energy x-ray reflectivity. In earlier experiments, we have studied pre-melting phenomena of ice extensively [2], leading to both a fully established sample preparation technique and a robust experimental setup at a 3rd generation synchrotron source (ESRF, ID15A). Our ice samples are sandwiched between smooth Si(100) substrates to guarantee the application of homogeneous electric fields across the two interfaces. The setup allows voltages up to 40 kV with switchable direction. We show polarization dependent electric field effects leading to structural changes at the ice/SiO_2 interface. Furthermore, our data suggests an influence of substrate preparation on the pre-melting behaviour of buried ice interfaces.

[1] Choi *et al*, PRL **95** 085701 (2005)

[2] Engemann *et al*, PRL **92**, 200401 (2004)

O 44.72 Wed 17:00 Poster C

A x-ray reflectivity study of the structural arrangement of ionic liquids at solid interfaces — •Markus Mezger[1], Harald Reichert[1], Moshe Deutsch[2], Benjamin Ocko[3], Heiko Schröder[1], John Okasinski[1], Sebastian Schöder[1,4], Lilach Tamam[2], Helmut Dosch[1], and Veijo Honkimäki[4] — [1]Max-Planck-Institut für Metallforschung, Heisenbergstr. 3, D-70569 Stuttgart — [2]Bar-Ilan University, Dept. of Physics, Ramat-Gan 52900, Israel — [3]Brookhaven National Laboratory, Upton, NY 11973, USA — [4]European Synchrotron Radiation Facility, F-38043 Grenoble, France

Room temperature ionic liquids (IL) are promising candidates for a variety of new technological processes, ranging from applications as special solvents in green chemistry to catalytic reactions in biotechnology. Although crucial for the understanding of solvent properties, only little is known about the structural rearrangement of anions and cations at solid interfaces. To get access to these deeply buried interfaces, high energy x-ray reflectivity ($\sim$ 70 keV) is an ideal tool. In our systematic study, we observed differently ordered structures, caused by changes in composition, water content, and temperature. By choosing different combinations of anion and cation, we can tune the ion-ion and ion-substrate interaction. Trace amounts of water dissolved in the ILs can interact with the solid surface or the ions, and therefore alter the interfacial properties significantly. By varying the temperature, we can change the ratio between entropy, and interfacial energy, favoring a disordered liquid, or interfacial layering respectively.

O 44.73 Wed 17:00 Poster C

High-resolution in-situ x-ray study of the hydrophobic gap at the water-OTS interface — •Markus Mezger, Harald Reichert, Heiko Schröder, John Okasinski, Sebastian Schöder, and Helmut Dosch — Max-Planck-Institut für Metallforschung, Heisenbergstr. 3, D-70569 Stuttgart

The detailed knowledge of the microscopic structure of water at hydrophobic interfaces is essential for the understanding of key interfacial phenomena in biology, drug design and technology. In order to access such hydrophobic interfaces and extract the microscopic details of the local interfacial structure of water with highest resolution we have applied x-ray reflectivity using high energy x-ray microbeams. The experiments have been carried out with the new HEMD (High Energy Micro Diffraction) setup, which has recently been installed at beamline ID15A (ESRF, Grenoble). We have studied in great detail atomically smooth silicon substrates covered by a native oxide layer which have been functionalized by a densely packed self-assembled monolayer of Octadecy-Trichloro-Silane (OTS). We have obtained high quality scattering data up to $q_z = 0.8$ Å^{-1} from which structural information on a sub-nanometer length scale can be extracted. The experimental data provide clear evidence for the existence of a hydrophobic gap on the molecular scale with an integrated density deficit $\rho d = 1.1$ Å g cm^{-3} at the solid-water interface. In addition, measurements on the influence of gases (Ar, Xe, Kr, N_2, O_2, CO, CO_2), dissolved in the water, have been performed. No effect on the hydrophobic water gap was found. [1] M. Mezger *et al.*, PNAS **103**, 18401-18404 (2006).

O 44.74 Wed 17:00 Poster C

Adsorption of Au on Rutile TiO_2(011)-(2x1) and (110) films grown on Rhenium Host Surfaces — •Susanne Roth, Wilhelmine Kudernatsch, Dirk Rosenthal, and Klaus Christmann — Institut für Chemie und Biochemie, FU-Berlin, Germany

In order to bridge the materials gap in heterogeneous catalysis and to mimic catalyst supports with increasing complexity, we have studied the epitaxy and chemical properties of titanium dioxide films grown with different surface termination on Re($10\bar{1}0$) and Re(0001) host surfaces, respectively. Titania films with a defined stoichiometry and long-range order were prepared by co-deposition of Ti vapor in an O_2 atmosphere at elevated temperatures (T $\geq$ 830 K). Thus, a unique pg(2x2) LEED phase with a characteristic glide mirror plane is formed on Re($10\bar{1}0$), with intermediate faceting. XRD and LEED reveal that the films consist of rutile terminated by a (2x1)-reconstructed (011) phase. On Re(0001), deposition of TiO_2 leads to hexagonal LEED patterns indicating the growth of three domains of rutile(110) rotated by 120° against each other. In a finite coverage range, faceting is observed (as with the Re($10\bar{1}0$) surface) pointing to a Stranski-Krastanov type of growth for both Re surfaces. Model catalyst systems were then prepared by vapor deposition of Au onto the rutile films. Results on the growth and properties of the Au crystallites on TiO_2(110)/Re(0001) using LEIS, XPS and TPD will be presented. Furthermore, we will compare the adsorption of CO, CO_2 and H_2O on the Au-titania surfaces with the respective adsorption on the bare TiO_2(011)-(2x1) films.

O 44.75 Wed 17:00 Poster C

Experimental identification of the "active site" on a nano catalyst: — Thomas Jaramillo[1], Kristina Jørgensen[1], Jacob Bonde[1], Jane Nielsen[1], •Sebastian Horch[2], and Ib Chorkendorff[1] — [1]Center for Individual Nanoparticle Functionality (CINF), NanoDTU, Department of Physics, Technical University of Denmark, DK-2800 Lyngby, Denmark — [2]Center for Atomic-scale Materials Design (CAMD), NanoDTU, Department of Physics, Technical University of Denmark, DK-2800 Lyngby, Denmark

One of the most important problems in heterogeneous catalysis is the identification of the "active site". Only when this site and its relative abundance are known, it is possible to determine turnover-rates per active site (cf. our contribution on CO dissociation on Ni(111)).

We have determined the active site of a well-known model system: single-layered MoS_2 nanoparticles as catalyst for hydrogen evolution. MoS_2 nanoparticles were grown on Au(111) under UHV. Particle sizes were tuned by controlled sintering. Morphological details of the model systems were revealed with STM under UHV. The same samples were subsequently characterized in an electrochemical cell under ambient conditions, where it was found that the electrocatalytic hydrogen evolution scales linearly with the number of *edge sites* of the nanoparticles — and not the *area* of the exposed basal plane — regardless of particle size. These findings are in excellent agreement with theoretical predictions for hydrogen evolution catalysts.

O 44.76 Wed 17:00 Poster C

Thermal and Redox Stability of PdZn Catalysts in Vacuum and During Methanol Adsorption Studied by In-Situ XPS — •Karifala Dumbuya, Reinhard Denecke, and Hans-Peter Steinrück — Lehrstuhl für Physikalische Chemie II, Universität Erlangen-Nürnberg, Egerlandstr. 3, 91058 Erlangen

We have investigated the thermal and redox behaviour of the technically important methanol steam reforming PdZn catalysts between 300-700 K in UHV and during MeOH dosage at 300 K for pressures up to 0.1 mbar. We compare samples from a washcoating process[1] before and after the reduction to PdZn. In both cases, we observed significant structural changes upon heating in the Zn 2p, Pd 3d and O 1s regions, respectively, in agreement with studies on Pd(111)[2]. However, annealing both samples to 700 K led to a significant drop in intensity of the Zn 2p signals, indicating alloy destruction in UHV, accompanied by the emergence of large Mg peaks, which are further enhanced by H_2

exposure of the surfaces at this temperature.

The resulting surface was exposed to MeOH background pressures (1.2*10^{-6}-0.1 mbar) at 300 K and C 1s, O 1s, Pd 3d and Zn 2p spectra were collected. A comparison with similar results on fully intact catalysts[3] show slightly different adsorption behaviour of MeOH. This is relevant, because Mg is known to affect the oxidative methanol steam reforming on Pd/ZnO catalysts.

[1] Pfeifer et al., Appl. Cat. A: 270 (2004) 165. [2] Bayer et al., Surf. Sci. 600 (2006) 78. [3] Pantförder, PhD thesis, Universität Erlangen-Nürnberg, 2004.

O 44.77 Wed 17:00 Poster C

CO oxidation measurements on Au/TiO_2 model catalysts — •Stefan Kielbassa, Joachim Bansmann, and Jürgen Behm — Institute of Surface Chemistry and Catalysis, Ulm University

Au nanoparticles on metal oxide supports exhibit a high catalytic activity for numerous reactions, e.g., the low temperature CO oxidation. It was found, that the activity is not only very sensitive to the size and the shape of the Au particles, but also to the chemical composition of the support. Especially reducible metal oxides, like TiO_2, are known to increase the catalytic activity and thus, they are not only passive spectators.

Planar model catalysts are ideally suited to investigate the influence of structural properties on the catalytic activity by varying the numbers of defects, steps and kinks on the substrate surface. Therefore, different types of planar titania surfaces, from well-ordered single crystal via epitaxially ordered to polycrystalline films, have been prepared and their influence on the CO oxidation activity of Au/TiO_2 model catalysts was studied using a micro-flow reactor attached to the UHV preparation chamber. We found, that significant differences in the catalytic activity can be observed with respect to the surface structure of the support. The results will be discussed with respect to activity data on model catalysts presented previously.

O 44.78 Wed 17:00 Poster C

Enhanced sensitivity and long-term stability for surface stress measurements — •Friedrich Klasing, Peter Kury, and Michael Horn-von Hoegen — University of Duisburg-Essen, Institute for Experimental Physics

Surface stress is one of the most important physical quantities determining the surface structure and morphology due to its large contribution to the total energy. Unfortunately, a direct measurement of surface stress is not possible, but it can be determined via the elastic response of a thin substrate as utilized in bending sample techniques like surface stress induced optical deflection (SSIOD) [1]. A sensitivity of the order of 0.5 Nm^{-1} can easily be achieved, to some extend even with commercially available tools [2].

A strongly enhanced sensitivity down to 0.005 Nm^{-1} (corresponding to stress effects induced by less than a percent of an adsorbate monolayer) together with a long-term stability on a time scale of one hour is only possible with extensive modifications. Still, long-term measurements over several hours suffer under drift effects caused by laser instabilities, ambient air motion and even minor detector nonlinearities. The influence of these effects on the surface stress signal drift is discussed and modifications are presented to reduce the typical drift to below 0.1 $Nm^{-1}hour^{-1}$.

[1]: A. Schell-Sorokin et al., Phys. Rev. Lett. 64(9), 1039 (1990)
[2]: http://www.k-space.com/HTML/Products/mos/
[3]: P. Kury et al., Rev. Sci. Instrum., 76(2), 023903 (2005)

O 44.79 Wed 17:00 Poster C

Depth profiling of thin film solar cell components by synchrotron excited Soft X-Ray Emission Spectroscopy (SXES) — •Harry Mönig[1], Markus Bär[3], Christian Camus[2], Ahmed Ennaoui[2], Alexander Grimm[1], Christian Jung[4], Christian Kaufmann[2], Paul Körber[2], Timo Kropp[2], Iver Lauermann[2], Sebastian Lehmann[2], Martha Lux-Steiner[1,2], Tim Münchenberg[2], Paul Pistor[2], Stefan Puttnins[2], Rodrigo Saez-Araoz[1], Hans-Werner Schock[2], Stefan Sokoll[2], and Christian-Herbert Fischer[1,2] — [1]Freie Universität Berlin — [2]Hahn-Meitner-Institut Berlin — [3]University of Las Vegas — [4]BESSY GmbH Berlin

Depending on the elemental composition of a material, SXES provides an information depth of 50-1000 nm. For studies of thin multilayer structures tuning of this parameter is highly desirable. One possibility is the variation of the excitation energy, which is accompanied by variation of photoionisation cross sections. Alternatively, we performed angle resolved SXES on the solar cell absorber material Cu(In,Ga)Se_2 covered by CdS or Zn(S,O) buffer layers (10-50 nm). Due to our setup geometry, the emission spectra clearly display increased surface sensitivity at small (grazing exit) and large (grazing incidence) exit angles. A model based on Beer-Lamberts law and setup geometry is in reasonable agreement with our experimental data.The presented results show that angle resolved SXES measurements yield depth-dependent information on multilayer structures. The increased surface sensitivity at grazing exit and grazing incidence angles allows the detection of extremely thin cover layers at reasonable recording times.

O 44.80 Wed 17:00 Poster C

Using a scanning tunnelling microscope for pressure measurement — •Thomas Madena and Achim Kittel — Energy and Semiconductor Research Laboratory, Institute of Physics, University of Oldenburg

Changes in mechanical stress distorts the scanning tunnelling microscope (STM) operation during the scanning of the hight information. This effect is the starting point of the idea to use the STM-principle for pressure measurements. A simple tunnelling microscope without xy-scanning stage measures the bending of a membrane due to an applied pressure. The voltage applied to the hight control is now the dependent quantity of the pressure on the rear side of the membrane. The high resolution of the STM makes it possible to see displacement on the nanometer scale. The thickness and the choice of material of the membrane are free parameter to alter the steepness of the pressure sensor. Results of the measurements of the different sensor features are discussed, like the linearity of the characteristics and sensitivity of the sensor. A possible procedure to calibrate the sensor is proposed. Furthermore, the unwanted influence of different interfering quantities was investigated and solutions to reduce their influence are given. For example the influence of a temperature drift can be reduced by the right choice of the used materials.

O 44.81 Wed 17:00 Poster C

PGM-Beamline at the Undulator U55 at DELTA — •Ulf Berges[1,2], Sven Döring[1,2], and Carsten Westphal[1,2] — [1]DELTA, University of Dortmund, Maria-Goeppert-Mayer Str. 2, 44221 Dortmund, Germany — [2]Fachbereich Physik, University of Dortmund, Otto-Hahn-Str. 4, 44221 Dortmund, Germany

A VUV-beamline for linearly polarized synchrotron radiation from a permanent magnet undulator is operated at DELTA, a synchrotron radiation facility at the university of Dortmund, Germany.

The energy range of this PGM-type beamline is 55 to 1500 eV, the calculated focus spot size 70 mum (h) x 30 mum (v). The measured photon flux is about 10ˆ12 photons/s/100 mA at 400 eV and 200 mum exit slit size and cff-value of 2. The beamline can also be operated in a high resolution mode with an expected energy resolution up to 30000. Various measurements concerning energy resolution, flux and beam stability leading towards a characterization of this beamline will be presented. The instrumentation of the beamline will be discussed, too.

O 45: Evening Talk Arzt

Time: Wednesday 20:00–21:00 Location: H1

Adhesion to Micro and Nano Structures: On Geckos, Minimushrooms and Smart Surfaces

O 46: Prize Talk Finley (Walter Schottky Prize)

Time: Thursday 8:30–9:15 Location: H1

Optically Probing Charge and Spin Interactions in Semiconductor Quantum Dots and Molecules

O 47: Invited Talk von Bergmann

Time: Thursday 9:30–10:15 Location: H36

Invited Talk O 47.1 Thu 9:30 H36

Complex magnetic structures on the atomic scale revealed by spin-polarized STM — •Kirsten von Bergmann — Institut für Angewandte Physik, Universität Hamburg, Jungiusstr. 11, 20355 Hamburg

Magnetism in low-dimensions is a fascinating topic: Even in apparently simple systems –such as homoatomic monolayers– the nearest neighbor distance, the symmetry and the hybridization with the substrate can play a crucial role for the magnetic properties. This may lead to a variety of magnetic structures, from the ferromagnetic and antiferromagnetic state to much more complex spin structures.

Spin-polarized scanning tunneling microscopy (SP-STM) combines magnetic sensitivity with high lateral resolution and therefore grants access to such complex magnetic order with unit cells on the nanometer scale. Different previously inconceivable magnetic structures are observed in pseudomorphic homoatomic *3d* monolayers on late *5d* transition metal substrates. For example a hexagonal Fe monolayer on Ir is found to exhibit a novel magnetic unit cell which is nearly square and consists of 15 atoms [1]. Furthermore such monolayers may form spin spirals, where the spin rotates from one atom to the next resulting again in a nanometer sized magnetic period. While in uniaxial systems only one propagation direction is found, in biaxial systems rotational domains of spin spirals are present.

[1] K. von Bergmann *et al.*, Phys. Rev. Lett. **96**, 167203 (2006).

O 48: Invited Talk Schmidt

Time: Thursday 10:15–11:00 Location: H36

Invited Talk O 48.1 Thu 10:15 H36

Semiconductor nanostructures: From self-assembly to self-ordering — •Thomas Schmidt — Institute of Solid State Physics, University of Bremen, Otto-Hahn-Allee 1, 28359 Bremen, Germany

The growth of well ordered, nanoscaled semicondutor structures is of high importance for many fields of application, e.g. for highly efficient light emitting devices. Different mechanisms can lead to spatial ordering of such nanostructures. In order to control their physical properties, an understanding of the ordering mechanisms is essential, which can be obtained by a detailed structural characteriziation. This is illustrated for CdSe/ZnSSe quantum dot stacks [1] and Ge/Si nanostructures [2] which have been investigated by grazing incidence x-ray diffraction and small angle scattering, as well as different electron diffraction and microscopy techniques.

[1] T. Passow *et al.*, Phys. Rev. B **64** (2001) 193311; Th. Schmidt *et al.*, Appl. Phys. Lett. **84** (2004) 4367; Th. Schmidt *et al.*, Phys. Rev. B **72** (2005) 195334.

[2] Th. Schmidt *et al.*, Appl. Phys. Lett. **86** (2005) 111910; Th. Schmidt *et al.*, Phys. Rev. Lett. **96** (2006) 066101.

O 49: Nanostructures at Surfaces V (Self Organization of Molecules)

Time: Thursday 11:15–12:00 Location: H36

O 49.1 Thu 11:15 H36

Insertion of Cu into ordered oligopyridine networks — •Achim Breitruck[1], Christoph Meier[2], Harry E. Hoster[1], Ulrich Ziener[2], and Rolf J. Behm[1] — [1]Institut für Oberflächenchemie und Katalyse, Universität Ulm, 89069 Ulm — [2]Institut für Organische Chemie III, Universität Ulm, 89069 Ulm

The effect of Cu deposition on pre-deposited ordered quasiquadratic networks (QQN) on HOPG was investigated by scanning tunneling microscopy (STM) under ultrahigh vacuum (UHV) conditions. Deposition of small amounts of Cu and subsequent annealing results in the formation of a new hexagonal metal organic network (HMON), coexisting with the ordered oligopyridine precursor layer. The formation of the HMON phase is accompanied by a loss in hydrogen bonds, prevailing in the QQN phase. This loss is overcompensated by the formation of strong Cu-pyridine interactions - the structure determining interactions in the HMON. Hence, the structural transition, from QQN phase to the hexagonal metal organic network is induced by a Cu mediated gain in intermolecular interaction energy.

O 49.2 Thu 11:30 H36

Relaxation of surface stress induced by an organic adsorbate: PTCDA on vicinal Ag(111) — •Florian Pollinger[1], Pavo Vrdoljak[1], Zhen Tian[2], Dirk Sander[2], Dominik Fertig[1], Stefan Schmitt[1], Christian Kumpf[1], Achim Schöll[1], Jürgen Kirschner[2], and Eberhard Umbach[1] — [1]Universität Würzburg, Experimentelle Physik II, Am Hubland, 97074 Würzburg — [2]Max-Planck-Institut für Mikrostrukturphysik, Weinberg 2, 06120 Halle

Self-organization of metallic surfaces on large scales can be induced by the adsorption of organic molecules and has been observed in several experiments [1]. One example is the growth of 3,4,9,10-perylene-tetracarboxylic-acid dianhydride (PTCDA) on stepped (8.5°-vicinal) Ag(111) surfaces. At elevated temperatures, the adsorbate molecules lead to a bunching of substrate steps, which agglomerate to facets of critical sizes. The facets arrange in a coverage-dependent grating-like pattern on a mesoscopic length scale. The resulting order requires a long-range interaction which is mediated by the substrate [2]. It can be explained by a change of surface stress induced by the adsorbate layer. Experimentally, such a change is directly accessible by an optical cantilever bending technique. We monitored the bending of a faceting thin Ag(10 8 7) crystal with this method in order to quantifiy the occurring relaxation of surface stress. [1] J. I. Pascual et al. J. Chem Phys. 120, 11367 (2004) [2] Q. Chen et al., Prog. Surf. Sci. 73, 59 (2003)

O 49.3 Thu 11:45 H36

Chemical nanopatterning of aromatic self-assembled monolayers — •Mark Schnietz[1], Andrey Turchanin[1], Mohamed El-Desawy[1], Harun Solak[2], and Armin Gölzhäuser[1] — [1]Physics of Supramolecular Systems, Department of Physics, University of Bielefeld, D-33615 Bielefeld — [2]Laboratory for Micro and Nanotechnology, Paul Scherrer Institute, 5132 Villigen PSI, Switzerland

Well-defined immobilization of single molecules, molecular arrays and biological objects on solid substrates is of great importance for many areas of fundamental and applied research. Chemically-patterned self-assembled monolayers (SAMs) may play a key role in reaching this goal. We applied extreme UV-interference lithography (EUV-IL) for generation of chemical nanopatterns in 4*-nitro-1,1*-biphenyl-4-thiol (NBPT) SAMs on Au-coated substrates. X-ray photoelectron spectroscopy and atomic force microscopy were employed for characterization. We show that EUV-irradiation converts terminal nitro groups of a NBPT into amino groups while the underlying aromatic groups are dehydrogenated and cross-linked. Large area nitro/amino line/space patterns (1*0.5 mm2) with a line width of about 50 nm were obtained with this approach. We used the resulting chemical nanopatterns for the preparation of biologically relevant interfaces in exchange and grafting type experiments.

O 50: Particles and Clusters II

Time: Thursday 11:15–12:45 Location: H38

O 50.1 Thu 11:15 H38

In-plane optical anisotropy of metal clusters studied by reflectance-difference spectroscopy

— •José Manuel Flores-Camacho, Li Dong Sun, Nadia Saucedo-Zeni, Günther Weidlinger, Michael Hohage, and Peter Zeppenfeld — Institut für Experimentalphysik, Johannes Kepler Universität Linz, A-4040, Linz, Austria

Reflectance-difference spectra of Ag clusters supported on an insulating, uniaxial substrate for Ag coverages in the 0.1 – 4.0 nm nominal thickness range are presented. The observed in-plane optical anisotropy is explained in terms of the splitting of the degeneracy of in-plane polarizations due to the presence of the non-equivalent dipole images in the substrate in quasi-electrostatic approximation. Geometrical sources of anisotropy might be excluded in a first approach since scanning electron and atomic force microscopy images reveal randomly arranged oblate spheroidal particles with in-plane rotational symmetry.

Although the presence of at least one source of in-plane anisotropy is necessary, be it cluster or substrate related, we show that reflectance-difference spectroscopy (RDS/RAS) is very sensitive to a number of particle-plasmon resonance related phenomena such as the cluster geometry, the randomness of the system, shape/size distributions, higher-than-dipole interactions between particles, percolation threshold, and the presence of a dielectric shell. From this we propose RDS/RAS as a reliable tool for the monitoring of cluster growth.

O 50.2 Thu 11:30 H38

Properties of mass selected Ag clusters in comparison to Ag island growth studied by low-temperature STM and STS

— •Stefanie Duffe[1], Thomas Irawan[1], Markus Bieletzki[1], Torsten Richter[1], Benedikt Sieben[1], Heinz Hövel[1], Chunrong Yin[2], and Bernd von Issendorff[2] — [1]Universität Dortmund, Experimentelle Physik I, 44221 Dortmund, Germany — [2]Universität Freiburg, Fakultät für Physik, 79104 Freiburg, Germany

We deposit mass selected Ag clusters on a C_{60} functionalized Au(111) surface at room temperature with a cluster machine consisting of a magnetron sputter gas aggregation source, a differential pumping stage with a cryo pump and a high transmission infinite range mass selector. We especially focus on clusters with closed geometric shells. At room temperature the C_{60} molecules rotate on the surface [1], which may explain the observed mobility of the deposited clusters on the C_{60} surface. For the deposition of Ag clusters with 55, 147 and 309 atoms at room temperature we observed extremely narrow height distributions with a cluster height of 1.7 nm and similar STS spectra for each cluster size. For Ag clusters with 561 and 923 atoms also larger heights were observed. To study the temperature dependent mobility we grew Ag islands on C_{60}/Au(111) by the deposition af Ag atoms at low temperatures.

[1] E.I. Altman, R.J. Colton, Surf. Sci. 295, 13 (1993)

O 50.3 Thu 11:45 H38

Arbitrary-order sum frequency generation scattering from spherical particles

— •Sylvie Roke — Max-Planck-Institut für Metallforschung, Heisenbergstrasse 3, 70569 Stuttgart

Nonlinear optical processes have been widely applied to study materials. The most commonly used techniques rely on second-order processes, such as second harmonic (SHG) and sum frequency generation (SFG). Consequently, SHG, SFG and some higher order techniques (like THG and CARS) have been developed into well-established spectroscopic and microscopic techniques that probe the optical interface- and bulk properties of materials. SHG, SFG and THG have recently been performed in a scattering geometry, in which the interfaces (and bulk) of (nano) particles in solution or embedded in composites can be probed in-situ. This enables one to combine the fields of soft matter and surface science.

To better understand these new developments, we have calculated the expressions for arbitrary-order sum frequency scattering from small particles. We calculate the full 3-dimensional scattering pattern for the case of second-order scattering and specify the selection rules and relations that relate the molecular structure to the scattering process. From these expressions, we can derive useful insights into how molecular order, orientation, and chirality appear in the scattering pattern.

O 50.4 Thu 12:00 H38

Oxidation / reduction cycles of metal nanoparticles

— •A. Stierle, N. Kasper, P. Nolte, N. Y. Jin-Phillipp, and H. Dosch — Max Planck Institut für Metallforschung, Heisenbergstr. 3, D-70569 Stuttgart, Germany

During catalytic reactions, oxide supported transition metal nanoparticles undergo continuously oxidation / reduction cycles. We have performed in-situ x-ray diffraction studies at the MPI-MF beamline at the Ångström Quelle Karsruhe (ANKA) and at beamline BM32 at the European Synchrotron Radiation Facility (ESRF) during the oxidation and reduction of different epitaxial nanoparticle / oxide support systems (Rh, Pd/MgO(100), Rh,Pd/Al_2O_3(0001), Pd/ZnO(0001), particle size 5-10 nm), thereby closing the pressure gap from near-UHV to atmospheric pressures. The oxidation properties of nanoparticles is expected to depend on the support, their orientation and their size and shape. We observe that the particles undergo at 500 K reversible shape changes when changing from reducing to oxidizing conditions and back. Under oxidizing conditions the formation of new facets is observed and in the case of Rh/MgO(100) the evolution of a surface reconstruction. The shape of the nanoparticles is additionally characterized by ex-situ high resolution transmission electron microscopy.

Financial support is acknowledged from the European Union under contract no. NMP3-CT-2003-505670 ($NANO_2$).

O 50.5 Thu 12:15 H38

Photochromic silver nanoparticles embedded in transition-metal oxides

— •Alexander Sprafke, Florian Hallermann, Christoph Straka, Christian Dahmen, Matthias Wuttig, and Gero von Plessen — I. Insitute of Physics (IA), RWTH Aachen University, 52056 Aachen, Germany

Photochromic materials change their color when irradiated with light. We have recently reported on the photochromic transformation of silver nanoparticles embedded in titania. This transformation shows itself in a bleaching of the nanocomposite films at the wavelength of irradiation, and is probably caused by a plasmon-assisted photoemission of electrons from the resonantly excited Ag particles. In the present work, we investigate whether a photochromic effect can also be found in Ag nanoparticles embedded in other transition-metal oxides, such as ZrO_2 and HfO_2. We examine the changes of the optical spectra of the films during laser irradiation, and compare them to the findings of our previous studies on the Ag/TiO_2 system. We discuss to what extent our model of the photochromic transformation can be applied to the Ag/ZrO_2 and Ag/HfO_2 films.

O 50.6 Thu 12:30 H38

Cluster surface interaction probed by resonance photoemission

— Markus Hessler and •Kai Fauth — MPI für Metallforschung, Heisenbergstr. 3, 70569 Stuttgart, Germany

Clusters of the late transmission metals may experience strong modifications of their magnetic moments when exposed to the interaction with surfaces. In particular, the interaction with graphite nearly suppresses the intrinsic magnetism of small Fe, Co and Ni clusters. The present contribution discusses the use of resonance photoemission at the Ni 2p and 3p edges to elucidate details of the cluster substrate interaction. It is found that a gapless electronic structure with low density of states at the Fermi level forms at the cluster substrate interface by hybridization. Loss of magnetization can then be understood as a consequence of the Stoner criterion not being fulfilled. Ni 2p and 3p resonance photoeletron data yield complementary information about cluster surface interaction.

O 51: Metal Substrates: Adsorption III

Time: Thursday 11:15–12:45 Location: H39

O 51.1 Thu 11:15 H39

Sub-surface oxygen in Pd(100): Density-functional theory calculations — •Jörg Meyer and Karsten Reuter — Fritz-Haber-Institut, Faradayweg 4-6, D-14195 Berlin, Germany

We use density-functional theory to investigate a possible incorporation of oxygen into the Pd(100) surface at low coverages. As a first step, we compare the stability of oxygen atoms in high-symmetry sites between the first and second substrate layer with that of oxygen adsorbed on the surface. In agreement with similar results for other (100) and (111) late transition metal surfaces, sub-surface oxygen is found to be significantly less favorable. Calculated barriers show furthermore, that even if populated, sub-surface oxygen will rapidly pop up to the surface at room temperature. We discuss a possible stabilization in the sub-surface sites through nearby on-surface O atoms, and perform molecular dynamics simulations to study the accessibility of sub-surface sites in molecular beam experiments.

O 51.2 Thu 11:30 H39

The Pd(110)-(3x2)-O surface phase investigated by STM and DFT — •Marko Kralj[1,3], Tobias Pertram[1], Nicola Seriani[2], Aleksander Krupski[1], Conrad Becker[1], Georg Kresse[2], and Klaus Wandelt[1] — [1]Institute of Physical Chemistry, University of Bonn — [2]Institute for Material Physics, University of Vienna — [3]Institute of Physics, Zagreb

The catalytic activity of palladium has intrigued researchers to study the interaction of gases with its surfaces for many decades. The complexity of the O-Pd(110) interaction manifests itself in a number of observed surface phases, which depend on oxygen exposures and various surface temperatures. According to LEED measurements six different structures have been reported and surface oxide formation is accompanied by a missing-row restructuring. This type of reconstruction is generally observed with bare and adsorbate covered (110) surfaces of similar metals and is believed to be the most stable reconstruction because it is accompanied by the formation of (111) micro-facets.

Most data about the system have been published in relation to the c(2x4) phase which is easy to prepare and it seems to dominate the phase diagram. Consequently, not much is known about other oxygen overlayer structures. In this study we have used STM in combination with DFT in order to further explore the O/Pd(110) phase diagram. In particular, we have concentrated on the Pd(110)-(3x2)-O surface oxide which corresponds to a low oxygen coverage. Measured and calculated data are in very good agreement and indicate that oxygen atoms are adsorbed in three-fold hollows of the reconstructed surface.

O 51.3 Thu 11:45 H39

In-situ x-ray investigation on the oxidation of platinum (111) surfaces — •Claus Ellinger, Nikolai Kasper, Andreas Stierle, and Helmut Dosch — Max-Planck-Institut für Metallforschung,

We determined the oxide structure on the Pt(111) surface using surface x-ray diffraction. Platinum is one of the most important catalysts for the oxidation of carbonmonooxide and hydrocarbons and is also used as protecting coating material in highly reactive environments. For the understanding of these technological processes a detailed knowledge of Pt oxidation is essential. A important role in the high reactivity of Pt surfaces is attributed to existence of oxide structure phases. At 250 °C and an O_2 pressure of 500 mbar we observe the formation of an oxide similar to α-PtO_2. The determined structure is described by a thin bulk oxide like film consisting of two layers of oxidized platinum. We find that the hexagonal unit cell of the oxide and the Pt(111) are aligned parallel which is in contrast to recent DFT calculations [1]. In addition, specular in-situ reflectivity measurements were carried out during the oxidation of a 100 Å thin Pt(111) film on a sapphire substrate. We demonstrate that an oxide is formed on the platinum film at 300 °C and oxygen pressures from 100 mbar to 500 mbar. Furthermore a material loss during the reaction with oxygen was observed as macroscopic holes appeared locally in the Pt film at an O_2 pressure of 150 mbar and a temperature of 450 °C.

[1] W.X. Li and B. Hammer, Chem Phys Lett **409**, 1-7 (2005).

O 51.4 Thu 12:00 H39

Subsurface oxygen in Ni on ($\sqrt{2}\times 2\sqrt{2}$) R45° O/Cu(001) — •Holger Meyerheim[1], Dirk Sander[1], Radian Popescu[1], Wei Pan[1], Iona Popa[2], Phil Woodruff[3], and Jürgen Kirschner[1] — [1]Max-Planck-Institut f. Mikrostrukturphysik, Weinberg 2, 06120 Halle — [2]ESRF, BP 220, F-38043 Grenoble, France — [3]Univ. of Warwick, Coventry CV4 7AL, UK

Growth, morphology and magnetic properties of Ni deposited on Cu(001) are distictly influenced by preadsorption of oxygen. The pre-oxidized Cu(001) surface exhibits a ($\sqrt{2}\times 2\sqrt{2}$) R45° reconstruction characterized by a "missing row"geometry. Subsequent Ni-adsorption changes the reconstruction to c(2×2) and previous studies indicated that oxygen acts as a surfactant always floating on the surface. The spin re-orientation transition (SRT) from in-plane to out of plane is shifted from ten monolayers (ML) in the case of the non-oxidized Cu substrate to five ML (1 ML= 1.53×10^{15} atoms/cm^2). We present an in-depth surface x-ray diffraction analysis of the interface structure of Ni grown on the reconstructed ($\sqrt{2}\times 2\sqrt{2}$) R45° O/Cu(001) surface in the coverage range between 1.25 and 5.00 monolayers (ML). In contrast to common belief that oxygen atoms always float on the surface, we find an significant fraction (up to ≈0.17 ML) of oxygen located in octahedral interstitial sites below the surface. Surface stress measurements in combination with density functional calculations support this finding. The implications for the understanding of the oxygen induced SRT in the Ni/O/Cu(001) system are discussed.

O 51.5 Thu 12:15 H39

Hindered Spin-Transitions in the Dissociative Adsorption of O_2 on Al(111) — •Christian Carbogno[1], Jörg Behler[2], Axel Gross[1], and Karsten Reuter[3] — [1]Inst. of Theoretical Chemistry, University of Ulm, Germany — [2]Dept. of Chemistry and Applied Biosciences, ETH Zürich, Switzerland — [3]Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, Germany

The low sticking probability for thermal O_2 molecules at Al(111) has recently been related to spin selection rules, which hinder a spin transition from the initial O_2 gas-phase triplet state to the singlet state of the adsorbed O atoms [1]. A constrained density-functional theory (DFT) approach was employed to compute the potential energy surfaces (PESs) of O_2 in different spin-configurations, and the lowered sticking probability was calculated when restricting the O_2 molecule to motion on the spin-triplet PES only. Here, we extend these studies by considering the dissociation dynamics on multiple spin PESs, allowing transitions between them within the quantum-classical fewest-switch algorithm as recently implemented [2], and calculating the non-adiabatic coupling between the PESs with various quantum chemical methods. The established framework enables us to study the adsorption process in detail, both as a function of the incident kinetic energy and incidence angle. Obtaining good agreement with experiment, we critically discuss the effects of the approximate non-adiabatic couplings and the uncertainties underlying the DFT PESs.

[1] J. Behler *et al.*, Phys. Rev. Lett. **94**, 036104 (2005).

[2] C. Bach *et al.*, Israel J. Chem. **45**, 46 (2005).

O 51.6 Thu 12:30 H39

The influence of surface oxides on the hydrogen absorption behaviour of metal hydride alloys — •Mark Schülke[1], Hubert Paulus[2], Martin Lammers[2], Gabor Kiss[3], and Karl-Heinz Müller[1,2] — [1]University of Applied Sciences of South Westphalia, Luebecker Ring 2, 59494 Soest, Germany — [2]Institute for Technology and Knowledge Transfer (TWS), Luebecker Ring 2, 59494 Soest, Germany — [3]Technical University of Budapest, Institute of physics, Chair of atom physics, H-1111 Budapest, Budafoki ut 8, Hungary

Metal hydride alloys are one promising alternative for hydrogen storage. However the influence of their surface on the hydrogen absorption process is not yet understood in detail. Oxygen adsorption from the gas phase as well as oxygen segregation and the segregation of alloy components play an important role in the hydrogen absorption process. The presented investigations are part of a series of experiments dealing with these subjects.

The presented experiments deal with the influence of adsorbed oxygen on the surface composition and the absorption behaviour of a AB_2 Laves phase alloy, namely $Ti_{0.95}Zr_{0.05}Mn_{1.53}V_{0.47}Fe_{0.08}Al_{0.02}$. In order to examine this, the samples were exposed to different doses of oxygen (e.g. 100 L, 1000 L) and analyzed by XPS and SNMS. It is shown that all main alloy components (Ti, Mn, V) are oxidized to certain oxidation states. Also a Mn enrichment at the surface can be observed (oxygen-induced segregation). The influence of these effects on the hydrogen absorption behaviour (capacity, dynamics) is discussed, too.

O 52: Methods: Atomic and Electronic Structure II

Time: Thursday 11:15–12:45 Location: H42

O 52.1 Thu 11:15 H42

Electronic excitations and excited-state forces of the H:Si(001)-(2x1) monohydride surface — Neng-Ping Wang[1], •Michael Rohlfing[2], Peter Krüger[3], and Johannes Pollmann[3] — [1]Institut für Angewandte Physik und Zentrum für Mikrostrukturforschung, Universität Hamburg — [2]Fachbereich Physik, Universität Osnabrück — [3]Institut für Festkörpertheorie, Universität Münster

We investigate electronic excitations of the H:Si(001)-(2×1) monohydride surface using first principles approaches. Density-functional theory is used to calculate the ground state geometry of the system. The quasiparticle band structure is calculated within the *GW* approximation. Taking the electron-hole interaction into account, electron-hole pair states and optical excitations are obtained from the solution of the Bethe-Salpeter equation for the electron-hole two particle Green function. In this work we focus, in particular, on localized excitations of the silicon-hydrogen bonds at the surface layer. These excitations give rise to an outward-directed force on the hydrogen atoms, which may well explain their optically induced desorption from the surface as observed inrecent experiments. The localization of the excitation is described by an artificial confinement potential in addition to standard many-body perturbation theory.

[1] N.-P. Wang, M. Rohlfing, P. Krüger, and J. Pollmann, Phys. Rev. B 74, 155405 (2006).

O 52.2 Thu 11:30 H42

Towards excitation spectra for molecules on surfaces: quasiparticle energy calculations — •Xinguo Ren, Patrick Rinke, Volker Blum, and Matthias Scheffler — Fritz-Haber-Institut der MPG, D-14195, Berlin

To study adsorption-related changes in the electronic structure of molecules from first principles, it is highly desirable to have a computational scheme that can treat both confined (molecules) and extended systems (surfaces) efficiently on equal footing. For present-day excited-state formalisms, achieving this "equal footing"is a challenge. Based on a new highly efficient local-orbital DFT code [1], we have developed a local-orbital based formalism of the *GW* approximation for the many-body self-energy, allowing us to calculate the quasiparticle excitation energies of confined systems efficiently. Focussing on the description of isolated molecules we show for the example of benzene how different local exchange-correlation functionals (LDA, PBE) and non-local (hybrid) schemes (HF, PBE0) affect the atomic and electronic structures of the ground state. In a second step we demonstrate the influence of the ground state functional on the *GW* excitation spectrum and compare this to previous calculations [2].

[1] V. Blum, R. Gehrke, P. Havu, V. Havu, X. Ren, and M. Scheffler, *The FHI Ab Initio Molecular Simulations (AIMS) project*, Fritz-Haber-Institut, Berlin (2006).

[2] M.L Tiago and J.R. Chelikowsky, Solid State Commun. **136**, 333 (2005).

O 52.3 Thu 11:45 H42

Control of dissipative quantum systems — •Erik Asplund and Thorsten Klüner — Institute of Pure and Applied Chemistry, Carl v. Ozzietsky University Oldenburg, Germany

Light interacting with atoms and molecules is not only a source of information about the atoms and molecules studied, it can also initiate charge and energy transfer processes, i.e. chemical reactions. The ability to control quantum systems interacting with their environment and light is investigated. A quantum system interacting with the environment can be separated into a primary system and a bath. This can be done within the framework of the Surrogate Hamiltonian approach [1]. Optimal control theory (OCT) provides a tool to active control of quantum dynamical systems [2]. To gain control of a dissipative system, OCT is combined with the Surrogate Hamiltonian method. It is shown that an effective control of a dissipative system is possible. Theoretical quantum calculations on the benchmark system NO/NiO(100) are provided to illustrate this combined approach and the results are compared with previous studies [3,4].

[1] Roi Baer, and Ronnie Kosloff, J. Chem. Phys. 106, 8862 (1997). [2] Wusheng Zhu, Jair Botina, and Herschel Rabitz, J. Chem. Phys. 108, 1953 (1997). [3] Christiane P. Koch, Thorsten Klüner, Hans-Joachim Freund, and Ronnie Kosloff, J. Chem. Phys. 119,1750 (2003). [4] Sören Dittrich, Hans-Joachim Freund, Christiane P. Koch, Ronnie Kosloff, and Thorsten Klüner, J. Chem. Phys. 124, 024702 (2006).

O 52.4 Thu 12:00 H42

Electron coincidence spectroscopy from surfaces: insulator vs. metal — •Frank Oliver Schumann, Carsten Winkler, and Jürgen Kirschner — Max-Planck-Institut für Mikrostrukturphysik

The effect of electron correlation manifests itself in the creation of the exchange-correlation (xc) hole. This theoretical concept is an important part of modern solid state theory. We have shown previously that the xc-hole is experimentally accessible via electron pair emission from surfaces. In order to assure that the xc-hole can be fully mapped we devised a new time-of-flight set-up with large angular acceptance. This is achieved by means of three channelplate detectors with delay lines anodes. We demonstrate that the xc-hole can now be fully mapped and a material dependent study becomes feasible. This is of general interest for a deeper understanding of the electron-electron interaction. We report on the first experiment aiming to unravel the material dependence of the xc-hole. We compare a Cu(100) surface with an insulator like LiF(100) and find distinctive differences in the electron-electron interaction. The spatial extension of the xc-hole shows a larger size for Cu compared to LiF. We further find that the angular extension of the xc-hole is indepedent of the kinetic energy in both cases. For certain energies of the electrons the xc-hole vanishes. The origin of this behavior is connected to the 2D-energy distributions.

O 52.5 Thu 12:15 H42

Spectro-Microscopy with very high resolution demonstrated at selected surface systems — •Florian Maier[1], Helder Marchetto[2], Ulrich Groh[1], Pierre Levesque[2], Tomas Skala[2], Thomas Schmidt[1], Rainer Fink[3], Hans-Joachim Freund[2], Eberhard Umbach[1], and the SMART-Collaboration[1,2,3,4] — [1]Universität Würzburg, Experimentelle Physik II, 97074 Würzburg — [2]Fritz-Haber-Institut der Max-Planck-Gesellschaft, 14159 Berlin — [3]Univ. Erlangen-Nürnberg, Phys. Chemie II, 91058 Germany — [4]TU Clausthal, TU Darmstadt, ZEISS Oberkochen, BESSY Berlin

The aberration corrected spectro-microscope SMART has been developed for all kinds of photo emission (PEEM) and low energy electron microscopy (LEEM) with outstanding lateral and energy resolution. The recent performance of the well operating instrument is shown, and the capabilities of spectroscopic imaging will be demonstrated for selected sample systems. We will especially concentrate on the adsorption behaviour of the organic molecule PTCDA(3,4,9,10-perylene-tetracarboxylic-acid dianhydride) on Ag(111) and Au(111) surfaces. For example, local work function, spectroscopic information, and even structural differences can be used for image contrast formation. This also allows correlating the substrate morphology with, e.g., the interaction with the organic molecules and even, by taking advantage of the high instrumental transmission, to observe directly, i.e. in real time and in situ, the growth of interface systems. (Funded by BMBF, contract 05KS4WWB/4)

O 52.6 Thu 12:30 H42

Verification of Phase Retrieval Parameters by coherent Measurement itself — •T. Panzner[1], T. Sant[1], G. Gleber[1], I. Vartanyants[2], and U. Pietsch[1] — [1]Festkörperphysik, Institut für Physik, Universität Siegen, Germany — [2]Hasylab-DESY , Hamburg

Monochromatic scattering experiments using a coherent x-ray beam have shown the great potential to get access to atomic resolved results without special preparation of the sample. The big disadvantage of all scattering experiments is the loss of phase information of the scattered signal. Therefore, so called "phase retrieval" procedures are needed to restore the wanted information from the measured intensities. The quality of these procedures strongly depends on additional information about the illuminated area. This information can be given by the size of the illuminated area ("over sampling" [1]) or the illumination function itself (i.e. approximation by Fermi-integrals [2]). In our case (energy-dispersive set-up) we have shown, that the illumination function is well determined by the aperture (pinhole) being equipped in front of the sample. A simple FFT of a measured intensity map is sufficient to reproduce the calculated intensity distribution. The deviation of the reconstructed illumination function from the calculated one, represents the influence of the specimen to the scattering intensity. In case of a reflectivity experiment this information concerns the roughness of surface. Our future work is concentrated on these variations to improve the quality of the phase retrial procedure. [1] J. Miao et al, Phys. Rev. B 67, 174104 [2] I.A. Vartanyants et al, Phys. Rev. B 55, 13193

O 53: Prize Talk Grünberg (Stern Gerlach Medal)

Time: Thursday 13:00–13:45 Location: H1

Spin Transfer Phenomena in Layered Magnetic Structures

O 54: Invited Talk Menzel

Time: Thursday 14:00–14:45 Location: H36

Invited Talk O 54.1 Thu 14:00 H36
Interplay between dimensionality and "exotic" properties: Model systems on surfaces — •Alexander Menzel, Enrico Dona, Mariana Minca, and Erminald Bertel — Institute for Physical Chemistry, University of Innsbruck, Austria

Due to the enhanced many-body interactions in low-dimensional metals, a small change of external parameters may introduce very interesting transitions between various metallic, isolating, magnetic and superconducting phases. Despite intense investigations of various (mostly bulk) model systems, a complete understanding of these phase transitions is still lacking.

The realisation of low-dimensional model systems on a surface rather than in a bulk material has the advantage that the highly advanced surface science tools allow to prepare and change the model system in situ. Additionally, both, electronic structure and geometry can be investigated on a global (ARUPS, LEED) and on a local (STM) level.

While most efforts concentrate on low-dimensional metal structures supported by semiconductor or insulator substrates, it is possible to create low dimensional electronic states also on metal surfaces. Utilizing Pt(110) as a template, it is shown here that strongly anisotropic transition metal surfaces may have peculiar band topologies which support quasi-1 dimensional electronic states with high DOS at the Fermi energy. The surface shows experimental fingerprints typical for low-dimensional metals and other correlated materials and thus indicates a promising new class of model systems.

O 55: Invited Talk Schmidt

Time: Thursday 14:45–15:30 Location: H36

Invited Talk O 55.1 Thu 14:45 H36
Real-time observation of organic layer growth: a spectro-microscopic study — •Thomas Schmidt[1], Helder Marchetto[2], Ullrich Groh[1], Florian Maier[1], Pierre Lévesque[2], Rainer Fink[3], Hans-Joachim Freund[2], and Eberhard Umbach[1] — [1]University of Würzburg, Experimental Physics II, 97074 Würzburg — [2]Fritz-Haber-Institute, Max-Planck-Society, 14195 Berlin — [3]University of Erlangen, Physical Chemistry, 91058 Erlangen

Organic thin films have an increasing importance for electronic devices like organic light emitting diodes, solar cells, field-effect transistors, etc. For the optimization of their functionality and efficiency a deep understanding of the properties of the organic components is required since these properties very much depend on the film growth and interface formation. Compared to the quite well understood atomic growth the growth of organic films tends to be much more complex due to a different bonding behaviour, existence of functional groups, anisotropic molecular structure, larger size, variable molecular orientation, etc. An ideal instrument to study these properties and the influence of the substrate is the spectro-microscope SMART, which combines a photoemission (PEEM, XPEEM) with a low energy (LEEM) electron microscope comprising an imaging energy analyzer and a unique aberration correction system for high spectroscopic and spatial resolution. With this instrument in situ and real-time experiments were performed to investigate, e.g., the temperature dependence of the growth mode, the influence of substrate morphology, the internal structure of crystallites, etc. (Funded by BMBF, contract 05KS4WWB/4)

O 56: Symposium: The Solid-Liquid Interface: A Challenge for Theoreticians I

Time: Thursday 15:45–19:00 Location: H36

Invited Talk O 56.1 Thu 15:45 H36
Computer Simulation of Electrochemical Reactions at the Water / Metal Interface — •Eckhard Spohr — IWV-3, Forschungszentrum Jülich, D-52425 Jülich

The interface between an (aqueous) electrolyte solution and a (noble) metal is the microscopic structural and dynamical heart of many electrochemical phenomena and has over the last 20 years attracted significant efforts in pure theory, electronic structure calculations and atomistic computer simulations. Recently, significant progress has been reached by merging concepts of electronic structure theory with dynamical simulations. At the same time, force field-based simulations will continue to be important, in view of the many-body nature of the interface.

Two topics from recent work in our group will be discussed. (i) A density functional theory / molecular dynamics study of methanol oxidation at the water / platinum interface unambiguously showed that interfacial water on a platinum surface is not only a spectator but actively participates in the oxidation process [1]. (ii) The chemical reaction dynamics was studied during the primary steps of the hydrogen evolution reaction in aqueous environment. The objective, to gain insight into the potential and metal dependence of this reaction, mandated the use of an empirical valence bond force field [2].

[1] C. Hartnig, J. Grimminger and E. Spohr, Electrochim. Acta 52, in press.

[2] F. Wilhelm, W. Schmickler, R. Nazmutdinov and E. Spohr, in preparation.

Invited Talk O 56.2 Thu 16:15 H36

Electric field effects at metal surfaces — •Ali Alavi[1] and Alexander Lozovoi[2] — [1]Department of Chemistry, Cambridge CB2 1EW — [2]School of Mathematics and Physics, Queen's University, Belfast Bt7 1NN

We review our recent work on electric field effects at metal surfaces, concentrating on (a) the relation between first-principles theory and the thermodynamics of charged surfaces [1] (held either at constant charge or constant potential), (b) a practical implementation of suitable for periodic slabs, and (c) new results on the stark effect for CO on Pt(111)[2]. Regarding (a), by generalising Koopman's theorem, we derive expressions for the surface (excess) free energy as a function of charge (or potential) in terms of the neutral surface energy, the workfunction and the position of the image plane. This is used to investigate potential-induced surface reconstructions. We show that a remarkable type of phase-coexistence in which charge-separation occurs. If time permits, we will show results on field effects on surface-relaxation, and adatom diffusion.

[1] A.Y. Lozovoi and A. Alavi, Phys. Rev. B 68 , 245416, (2003).

[2] A.Y. Lozovoi and A. Alavi, J. Electroanalytical. Chem., to appear.

O 56.3 Thu 16:45 H36

Sum-Frequency Vibrational Spectroscopy of Al$_2$O$_3$(0001)/ Water Interfaces — •Björn Braunschweig, Stephan Eissner, and Winfried Daum — Institut für Physik und Physikalische Technologien, TU Clausthal, Leibnizstrasse 4, D-38678 Clausthal-Zellerfeld

Sum-frequency generation (SFG) has been applied to study O-H stretching vibrations of water molecules and hydroxyl groups at Al$_2$O$_3$(0001)/water interfaces. The vibrational spectra of these interfaces strongly depend on the roughness of the Al$_2$O$_3$ surface which was characterized by AFM. O-H stretching bands at 3140 cm^{-1} and 3450 cm^{-1} are assigned to hydrogen-bonded water molecules at the interface with tetrahedral and non-tetrahedral coordination, respectively. A strong pH dependence observed for the intensity of the 3140 cm^{-1} band can be attributed to the interfacial electric field caused by protonation or deprotonation of surface hydroxyl groups. A marked minimum in the pH dependence of this band is related to the isoelectric point of the Al$_2$O$_3$(0001) surface. On rough Al$_2$O$_3$(0001) surfaces we observe an additional narrow band at 3700 cm^{-1} originating from O-H stretching vibrations of free surface hydroxyl groups (aluminol, AlOH). This band is completely absent on smooth Al$_2$O$_3$(0001) surfaces which have been prepared by annealing at 1100 °C and which exhibit atomically flat terraces. The 3700 cm^{-1} band is assigned to hydroxyl groups, presumably adsorbed at defect or step sites, that do not couple to the hydrogen-bonded network of the interfacial water molecules.

30 min. Break

Invited Talk O 56.4 Thu 17:30 H36

Computer simulation of solution/electrode interfaces — •Fernando Fernandes — Department of Chemistry and Biochemistry, Faculty of Sciences, University of Lisboa, Campo Grande, Bloco C8, 1749-016 Lisboa Portugal

In the last few years we have carried out some work on the adsorption and self-assembly of organic molecules (e.g. phenol and alkylthiols solvated by water and ethanol, respectively) on gold electrodes, in collaboration with two experimental groups of interfacial electrochemistry.

Our contributions have been focused towards the atomistic description of structures and processes at the solid-liquid interface. To this end, DFT force fields for the interactions water-Au and ethanol-Au have been proposed and applied to simulations by Monte Carlo techniques. Additionally, we have done preliminary ab initio calculations for the prediction of reactive sites and mechanisms concerned with electropolymerisation processes.

In this talk, we shall review some recent results obtained in our laboratory, from the standpoint of fundamental issues, challenges and possible future developments.

Invited Talk O 56.5 Thu 18:00 H36

Proton Conductors for Fuel Cells: The Role of Interfacial Structure and Dynamics — •Michael Eikerling, Ata Roudgar, and Sudha Narasimachary — Department of Chemistry, Simon Fraser University, Burnaby, BC, Canada

Polymer electrolyte membranes (PEM) are the key components in polymer electrolyte fuel cells. Our work focuses on mechanisms of proton transport in the interfacial region between polymer fibrils and aqueous pathways in PEM. Understanding structure and dynamics at these ion-lined interfaces is of fundamental interest and it could facilitate the rational design of advanced PEM. As a basic model for performing ab-initio quantum mechanical calculations we consider a dense 2D array of ionized surface groups under conditions of minimal hydration. In optimization studies we found a critical separation 7Å of surface groups for the transition between highly ordered and clustered interfacial conformations. The transition from weak to strong binding of additional water molecules occurs also at 7Å. We systematically explore effects of density and chemical architecture of surface groups on conformations, strength of water binding, and interfacial dynamics. Our calculations have identified tilting of surface groups, rotation of acid head groups, and lateral shift of hydronium ions as relevant collective coordinates that control proton motion at the hydrated interface. Currently, we utilize ab-initio molecular dynamics and transition path sampling methods to systematically study free energy profiles along reaction paths and determine relevant transition rates.

O 56.6 Thu 18:30 H36

New aspects of the sulfur electrooxidation on Au(1 1 1) - An in situ STM study — •Christian Schlaup, Daniel Friebel, Peter Broekmann, and Klaus Wandelt — Institut für Physikalische und Theoretische Chemie, Wegelerstr. 12, D-53115 Bonn

We have reinvestigated the nature of the ring-like structure of the S-covered Au(1 1 1) surface, which appears both under electrochemical conditions as well as in UHV, respectively. In contrast to previous electrochemical studies, the HS$^-$ containing alkaline electrolyte was exchanged, after deposition of 0.33 ML sulfur, for a blank 0.01 M NaOH solution, in order to prevent the formation of amorphous bulk overlayers at higher potentials. Subsequently, the structural and morphological changes of the $(\sqrt{3} \times \sqrt{3})R30°$ S layer upon potential increase were studied in situ with STM. Significant Au mass transport perpendicular to the surface with the formation of vacancies and new islands could be observed. The new islands have an ordered rhombic lattice which consists of the known ring-like units. This observation strongly suggests the formation of an Au$_x$S compound in contrast to the traditional view of the formation of S$_8$ species. During the growth of Au$_x$S islands, S atoms are consumed from the $(\sqrt{3}\times\sqrt{3})R30°$ structure. Due to the high electrode potential, S atoms are rather immobile, in particular at upper step edges, which enabled us for the first time to image S-covered $(\sqrt{3} \times \sqrt{3})R30°$ islands along with uncovered (1×1) regions simultaneously.

O 56.7 Thu 18:45 H36

Step Bunching Instability on Stepped Au(1 1 17) Electrodes in Sulfuric Acid Solution — •Margret Giesen, Ernesto Pichardo Pedrero, and Guillermo Beltramo — Institute for Bio- and Nanosystems, IBN 4, Research Centre Juelich, D 52425 Juelich, Germany

We present scanning tunneling microscopy data on the stability of stepped Au(1 1 17) electrodes (vicinal to the Au(001) surface) in sulfuric acid solution. We have analyzed the step-step distance probability distribution as a function of the electrode potential. The width of the probability distribution increases with the (absolute) difference between the electrode potential and the potential of zero charge. Our findings are in agreement with a recent theoretical model [1] showing that all electrode surfaces in contact with an electrolyte are instable against step bunching in a certain potential regime with respect to the potential of zero charge. This is the first quantitative experimental confirmation of the step bunching instability model for metal electrodes. Furthermore, we can deduce an estimate for the step-step interaction constant of 120+/-25 meVÅ. This value is more than an order of magnitude larger than typical values for metal surfaces in vacuum. The reason may lie in the specific adsorption of sulfate ions at the step edges. [1] Surf. Sci. 573 (2004) 24

O 57: Surface Chemical Reactions and Heterogeneous Catalysis II

Time: Thursday 15:45–18:30 Location: H38

O 57.1 Thu 15:45 H38

Determination of the CO adsorption energy on Au/TiO_2 model catalysts at elevated pressures — •Thomas Diemant, Joachim Bansmann, and Rolf Jürgen Behm — Institute of Surface Chemistry and Catalysis, Ulm University, D-89069 Ulm

The adsorption of CO on Au/TiO_2/Ru(0001) model catalysts has been studied by in-situ IR measurements at elevated pressures up to 50 mbar. From a quantitative analysis of the integrated IR intensities it is possible to calculate the CO adsorption energy on the Au particles of the model catalyst surface. We have determined the CO adsorption energy with this method for pure CO and for CO/O_2 mixtures using model catalysts with different Au coverages. Comparing the results for both gas compositions, we can quantify the influence of (co-adsorbed) oxygen on the CO adsorption. From the results for different Au coverages, the influence of the Au particle size on the CO binding strength is derived. The results of this study will be compared to results of UHV studies on the CO adsorption of Au model catalysts using either TPD measurements or a similar analysis of IR results.

O 57.2 Thu 16:00 H38

CO adsorption on a surface oxide: A combined DFT and XPS study — •Jutta Rogal[1], Edvin Lundgren[2], Jesper Andersen[2], and Karsten Reuter[1] — [1]Fritz-Haber-Institut, Faradayweg 4-6, D-14195 Berlin, Germany — [2]Department of Synchrotron Radiation Research, Institute of Physics, Lund University, Box 118, S-221 00 Lund, Sweden

CO adsorption at some transition metal and bulk oxide surfaces is a well-known showcase for the deficiencies of present-day exchange and correlation (xc) functionals in density-functional theory (DFT). Here we investigate whether similar problems in the determination of the proper adsorption site exist for CO adsorption on a so-called surface oxide, i.e. a nanometer thin oxide film. For this we focus on the $(\sqrt{5}\times\sqrt{5})R27^\circ$ surface oxide at Pd(100) and combine DFT with high-resolution x-ray photoemission experiments. Comparing the calculated Pd $3d_{5/2}$ and C $1s$ surface core-level shifts with the experimental data allows to unambiguously identify the bridge site as the adsorption site populated in the experiment. While this is also the most stable adsorption site when using the local-density and several gradient-corrected xc functionals in the DFT calculations, the absolute values of the binding energy at this bridge site is found to vary significantly for the different xc functionals. Suitably combining the computed binding energies and diffusion barriers in kinetic Monte Carlo simulations provides finally first insight into kinetic limitations to the ordering behavior of the CO adsorbates under the low-temperature conditions of the experiment.

O 57.3 Thu 16:15 H38

CO oxidation on RuO_2(110): Temperature programmed reaction spectra from first-principles kMC simulations — •Michael Rieger, Jutta Rogal, and Karsten Reuter — Fritz-Haber-Institut, Faradayweg 4-6, D-14195 Berlin, Germany

The catalytic oxidation of CO over the RuO_2(110) surface has become a frequently studied model system, for which detailed data from steady-state activity measurements and *ex-situ* experiments is available. The steady-state activity of this surface was recently investigated by first-principles kinetic Monte Carlo (kMC) simulations [1], yielding very good agreement with experimental results. Using the same setup, and in particular, the same *ab initio* microscopic parameters, i.e. elementary processes (including desorption, diffusion and reaction events) and process rates based on density-functional theory (DFT) energetics, we now also reproduce detailed temperature programmed desorption (TPD) and reaction (TPR) data for this system [2]. We focus in particular on the experimentally found dependence of the CO_2 yield on the surface coverage, which could not be explained within a simple mean-field picture. Analyzing our simulation results, we can rationalize the observed non-intuitive dependence as the result of a coverage dependent interplay of different possible reaction processes taking place at the surface.

[1] K. Reuter, D. Frenkel, and M. Scheffler, Phys. Rev. Lett. **93**, 116105 (2004); K. Reuter and M. Scheffler, Phys. Rev. B **73**, 045433 (2006).

[2] S. Wendt, M. Knapp, and H. Over, J. Am. Chem. Soc. **126**, 1537 (2004).

O 57.4 Thu 16:30 H38

Is there a "rate determining step" in the catalytic oxidation of CO over RuO_2(110)? — •Hakim Meskine, Karsten Reuter, and Matthias Scheffler — Fritz-Haber-Institut, Faradayweg 4-6, D-14195 Berlin

Out of the several elementary processes in the catalytic cycle, one step is frequently believed to be particularly important, and limiting the overall product formation. We check on this assumption of a rate determining step, using the CO oxidation at RuO_2(110) as a model case. The chemical kinetics is determined with kinetic Monte Carlo simulations, based on rate constants determined by density-functional theory and transition-state theory. The composition and structure of the catalyst surface are computed in reactive environments ranging from ultra-high vacuum (UHV) to technologically relevant conditions (pressures of several atmospheres and elevated temperatures). We employ several forms of sensitivity analyses to identify the rate determining steps under the different environmental conditions. Under UHV conditions we find the catalytic activity indeed predominantly dependent on only one process step, namely the reactant adsorption. However, under catalytically really relevant gas phase conditions, it is not one, but a larger number of elementary processes that contributes equally to the total rate of product formation. The bearings of these findings for the frequently employed approach to extract apparent activation barriers from Arrhenius-type activity plots is critically discussed.

O 57.5 Thu 16:45 H38

Comparison of phenomenological kinetics and kMC modelling of CO oxidation at RuO_2(110) — •Sebastian Matera[1], Hakim Meskine[1], Karsten Reuter[1], Matthias Scheffler[1,2], and Horia Metiu[2] — [1]Fritz-Haber-Institut, Faradayweg 4-6, D-14195 Berlin — [2]University of California at Santa Barbara, Santa Barbara CA 93106

Neglecting the explicit spatial distribution of the chemicals at the catalyst surface is a frequently employed concept in phenomenological kinetics (PK). We scrutinize this concept by comparing with results from kinetic Monte Carlo (kMC) simulations, which do not need to rely on this mean-field approximation. For the model system CO oxidation at RuO_2(110) we compute the surface composition and activity of the catalyst surface in reactive environments ranging from ultra-high vacuum to technologically relevant conditions (pressures of several atmospheres and elevated temperatures). Using the same first-principles rate constants in both approaches, we find the PK modeling to be in serious error, and even failing to identify the correct dominant reaction mechanism. Approaches to improve on this situation, by explicitly including diffusion events and site correlations in the PK modeling, will be discussed.

O 57.6 Thu 17:00 H38

Ultrafast reaction dynamics of the associative desorption of C+O from Ru(001) — •Christian Frischkorn, Steffen Wagner, Henrik Öström, and Martin Wolf — Freie Universität Berlin, Fachbereich Physik, Arnimallee 14, 14195 Berlin

Femtosecond laser excitation of Ru(001) covered with atomic carbon and oxygen results in the recombinative desorption of CO molecules from the surface. A nonlinear fluence dependence of the reaction yield is found for excitation wavelengths of 400 and 800 nm. The higher reaction yield obtained for the 400-nm as compared to the 800-nm excitation can be attributed to the different optical penetration depths in Ru(001). As a consequence, higher surface temperatures rather than significant contributions of non-thermalized hot electrons cause the stronger laser-induced desorption with 400-nm pulses. Furthermore, the reaction mechanism of the CO recombination is investigated with two-pulse correlation measurements which exhibit a FWHM of ≈ 20 ps. However, despite this relatively wide two-pulse correlation (which usually is taken as an indication for a purely phonon-mediated energy flow), all experimental data are only consistently reproduced in the framework of frictional coupling between the substrate and the adsorbate, if both phonon *and* electronic contributions are included.

O 57.7 Thu 17:15 H38

Site specific analysis of CO dissociation on Ni(111) with

STM — •Sebastian Horch, Martin Andersson, Frank Abild-Pedersen, and Jens Nørskov — Center for Atomic-scale Materials Design (CAMD), NanoDTU, Department of Physics, Technical University of Denmark, DK-2800 Lyngby, Denmark

One of the most important problems in heterogeneous catalysis is the analysis of the “active site” (cf. our contribution on the experimental identification of the active site on MoS_2). Only when this site and its relative abundance are known, it is –at least in principal– possible to determine e.g. turnover-rates per active site.

There are not many methods that can perform such site-specific measurements. While STM is the method of choice for atomic-scale visualization of the active site, it is much too slow for a real-time investigation of catalytic reactions at this site. If, however, the reaction leaves a clear footprint at the active site, one might use this to learn more about the reaction itself.

We have used this approach to investigate the dissociation of CO on Ni(111) using STM. The footprint is here the formation of carbide islands at the upper step edges. The steps provide the active site in this process, as can be shown e.g. by step blocking. By measuring the carbon uptake *per step length* for different temperatures and CO pressures, we can learn more about the processes involved and shed some more light onto the long-term debate about the barrier for CO dissociation on Ni surfaces.

O 57.8 Thu 17:30 H38

Dehydrogenation kinetics of methyl on various Pt surfaces as studied by temperature-programmed XPS. — •Christian Papp, Barbara Tränkenschuh, Regine Streber, Reinhard Denecke, and Hans-Peter Steinrück — Lehrstuhl für Physikalische Chemie II, Universität Erlangen-Nürnberg, Egerlandstr. 3, 91058 Erlangen

We studied the reaction of methyl (CH_3) on different platinum surfaces by temperature-programmed XPS at the synchrotron radiation facility BESSY II in Berlin [1]. The quantitative analysis yielded the transition temperatures for the subsequent dehydrogenation steps from CH_3 to CH to atomic C, which depend on the crystallographic orientation of the substrate. Corresponding experiments with deuterated methyl (CD_3) show the same dehydrogenation sequence; however, the transition temperatures are approx. 20 K higher, due to the kinetic isotope effect. By assuming first order reaction kinetics and by applying a simple Redhead analysis [2] to our data, we were able to estimate the activation energies. The difference in the activation barriers for dehydrogenation of deuterated and non-deuterated methyl to methylidyne agrees well with the difference in zero-point energies of the C-H and C-D vibrations. This result is in agreement with expectations from DFT calculations [3], which show that the rate limiting step in methyl dissociation should be the breaking of the first C-H bond.

[1] Papp et al., J. Phys. Chem. C accepted.
[2] Redhead, Vacuum 62 (1962) 203.
[3] Petersen et al., J. Phys. Chem. B 108 (2004) 5909.

O 57.9 Thu 17:45 H38

H laserdesorption experiments from HOPG with VUV photonenergies at the FLASH facility in Hamburg — •Carsten Thewes, Björn Siemer, Tim Hoger, and Marco Rutkowski — Physikalisches Institut, Westfälische Wilhelms-Universität, 48149 Münster

During the past years, the understanding of the interaction of atomic and molecular hydrogen with carbon surfaces has gained new attention for the fields of hydrogen storage [19 and molecular hydrogen formation in the interstellar medium [2, 3]. Our recent experiments concerning the desorption of H and D atoms adsorbed on highly oriented pyrolytic graphite (HOPG) will be surveyed. The experiments are performed at the Free Electron Laser facility FLASH at DESY using 32.5 nm XUV photons. The recording of arrival time distributions via a delayable laser detection scheme (hydrogen 2s ← 1s excitation REMPI process), information about possible reaction mechanisms is accessible. Based on this background an insight to the so far evaluated data and results will be given. The analysis of the kinetic energy distribution of the desorbing neutral hydrogen atoms reveals different contributions peaking at around 2, 8 and 25 meV. The new experimental data is discussed in the model of Hammer et al. [3]. [1] L. Schlapbach, A. Züttel, Nature 414, 353 (2001) [2] N.Rougeau, D. Teillet-Billy and V. Sidis, Chem. Phys. Let., 431, 135138 (2006) [3] L. Hornekær, E. Rauls, W. Xu, Z. Sljivančanin, R. Otero, I. Stensgaard, E. Lægsgaard, B. Hammer, F. Besenbacher, Phys. Rev. Let. 97 (18), 186102 (2006)

O 57.10 Thu 18:00 H38

Surface studies of simple and complex ionic liquid systems using XPS — •Manuela Killian[1], Christian Potzner[1], Till Cremer[1], Jörg Michael Gottfried[1], Natalie Müller[2], Dirk Gerhard[2], Peter Wasserscheid[2], Florian Maier[1], and Hans-Peter Steinrück[1] — [1]Lehrstuhl für Physikalische Chemie II, Universität Erlangen, Egerlandstr. 3, 91058 Erlangen — [2]Lehrstuhl für Chemische Reaktionstechnik, Universität Erlangen

Ionic liquids (ILs) - organic salts with melting points below 100°C - represent a new class of materials in liquid phase physics and chemistry. In surface science, ILs open up unprecedented possibilities for surface studies of phenomena related to liquids in general because of their negligible vapour pressures even at elevated temperatures. Our studies focus on two ILs consisting of the same cation but different anions, namely 1-ethyl-3-methylimidazolium ethylsulfate (EMIM EtSO4) and 1-ethyl-3-methylimidazolium bis(tri-fluoromethane-sulfon)amide (EMIM BTA). To determine surface composition and molecular orientation, angle dependent XP spectra were recorded for the pure ILs, their mixtures, and solutions comprising a dissolved platinum salt as model catalyst. In the latter case, we demonstrate a selective enrichment of the platinum cation at the surface.[1] The basic understanding of surface/interface enrichment effects is important for all kinds of multiphasic catalysis operations employing ionic liquids. This work was supported by the DFG through SPP1191.

[1] F. Maier et al., Angew. Chem. Int. Ed. 45 (2006) 7778.

O 57.11 Thu 18:15 H38

Plasma modified bimetallic nanocolloid arrays - a model system for structural and order effects in particle catalysis — •Bernhard Gehl[1], Jan Ingo Flege[2], Vesna Aleksandrovic[3], Thomas Schmidt[2], Sigrid Bernstorff[4], Jens Falta[2], Horst Weller[3], and Marcus Bäumer[1] — [1]Institut für Angewandte und Physikalische Chemie, Universität Bremen, Leobener Strasse NW2, 28359 Bremen, Germany — [2]Institut für Festkörperphysik, Universität Bremen, Otto-Hahn-Allee, 28359 Bremen, Germany — [3]Institut für Physikalische Chemie, Universität Hamburg, Grindelallee 117, 20146 Hamburg, Germany — [4]Sincrotrone Trieste, Strada Statale 14, km 163.5, in Area Science Park, 34012 Basovizza / Trieste, Italy

The high surface to volume ratio and special chemical properties of nanoparticles have made them a very common class of materials for catalytic coatings. Well-defined monolayers of nanoparticles were obtained by spin-coating of bimetallic colloidal particles on oxidic substrates. Plasma treatment and thermolysis were applied to strip the particles of the organic ligands serving as stabilizers in the liquid phase and as spacers during deposition. With SEM, GISAXS, and XPS the structural and chemical changes induced by both cleaning methods were examined.

O 58: Metal Substrates: Adsorption IV

Time: Thursday 15:45–18:15 Location: H39

O 58.1 Thu 15:45 H39

On the interaction between etheylene and defect-sites on the Cu(111) surface — Martin Binder, •Olaf Skibbe, and Annemarie Pucci — Kirchhoff-Institut für Physik, Im Neuenheimer Feld 227, D-69120 Heidelberg

It is well-known, that ethylene adsorbed on rough copper surfaces shows a strong chemical enhancement in the surface enhanced Raman scattering (SERS). In former research, these Raman-active vibrational bands also have been detected also with infrared reflection absorption spectroscopy (IRRAS) on cold deposited and hence rough copper films. They were therefore referred to as defect sites (annealable sites). By evaporating small amounts (sub-monolayers) of copper to the cold surface, we could show that the occurence of such Raman-active absorption bands in IRRAS of ethylene on a smooth Cu(111) surface is related to defect sites. Surprisingly, not only the intensity of the Raman-active bands was increasing with the amount of evaporated copper, but an unforeseen strong decrease in intensity of the infrared-active out-of-plane vibration (CH_2 wagging mode) was also detected. In order to understand the morphology of the roughened surface and the nature of the interaction between the copper adatoms and the ethylene molecules, we used high-resolution electron energy loss spectroscopy (HREELS) to examine the vibrational modes of the copper adatoms on the surface and those of the adsorbed ethylene. By doing so, we found that the CH_2 wagging mode of ethylene is still present on the roughened surface. The loss in dipole-activity of this vibration is an unexpected result. We try to give an explanation.

O 58.2 Thu 16:00 H39

Tuning the interaction of fullerenes with metal surfaces by molecular self-assembly — •Katharina Jennifer Franke[1], Gunnar Schulze[1], Isabel Fernández-Torrente[1], Nils Henningsen[1], Sebastian Zarwell[2], Karola Rück-Braun[2], Nicolás Lorente[3], and José Ignacio Pascual[1] — [1]Freie Universität Berlin, Fachbereich Physik, Germany — [2]Technische Universität Berlin, Institut für Chemie, Germany — [3]Université Paul Sabatier, Toulouse, France

Frequently, thin insulating layers are used to electronically decouple molecules from metallic substrates. In an alternative approach we show here, that intermolecular interactions can be employed to create supramolecular structures, which decrease the electronic coupling of fullerenes to a metallic substrate. By low-temperature scanning tunnelling microscopy (STM) we find that the co-adsorption of molecular tripods (1,3,5,7-tetraphenyladamantane) and fullerenes on Au(111) leads to the formation of two basic self-assembled building blocks, which hierarchically arrange in larger structures. One of them is a triangular shaped tetramer consisting of three tripods with a C_{60} in their centre. The second one results in rows of alternating adamantane and fullerenes. In both cases scanning tunnelling spectroscopy shows that the presence of the tripod linkers modify the electronic configuration of the fullerene cage. In particular, the tunnelling spectra show a negative differential resistance characteristic for a weaker electronic coupling to the Au(111). DFT calculations indicate that the tripods lift the C_{60} from the surface, thus allowing the tunability of the fullerene-metal interaction.

O 58.3 Thu 16:15 H39

Controlled Contact to a C60 Molecule — •Neel Nicolas, Kröger Jörg, Limot Laurent, and Berndt Richard — Institut für Experimentelle und Angewandte Physik CAU Kiel

The tip of a low-temperature scanning tunneling microscope is approached towards a C60 molecule adsorbed on Cu(100) to form a tip-molecule contact. Beyond the tunnelling regime the conductance rapidly increases in a transition region to contact regime. At contact formation, a conductance well below a quantum of conductance is observed. The conductance increases slowly upon further approach of the tip until a jump to one quantum of conductance occurs. The contact properties depend on the adsorption geometry of the molecule on the surface. Ab-initio calculations within density functional theory and non-equilibrium Green's function techniques explain the experimental data in terms of the conductance of an essentially undeformed C60. The conductance at the transition from tunneling to contact is strongly affected by structural fluctuations which modulate the tip-molecule distance.

O 58.4 Thu 16:30 H39

Substrate dependent bonding distances of PTCDA - A comparative X-ray standing-wave study on Cu(111) and Ag(111) — •Alexander Gerlach[1], Stefan Sellner[1], Frank Schreiber[1], Norbert Koch[2], and Jörg Zegenhagen[3] — [1]Institut für Angewandte Physik, Universität Tübingen, Auf der Morgenstelle 10, 72076 Tübingen, Germany — [2]Institut für Physik, Humboldt-Universität zu Berlin, Newtonstr. 15, 12489 Berlin, Germany — [3]European Synchrotron Radiation Facility, 6 Rue Jules Horowitz, BP 220, 38043 Grenoble Cedex 9, France

We study the adsorption geometry of 3,4,9,10-perylene-tetracarboxylic-dianhydride (PTCDA) on Ag(111) and Cu(111) crystals using X-ray standing waves. The element-specific analysis shows that the carbon core of the molecule adsorbs in a planar configuration, whereas the oxygen atoms experience a non-trivial and substrate dependent distortion. On copper (silver) the carbon rings resides 2.66 Å (2.86 Å) above the substrate. In contrast to the conformation on Ag(111), where the carboxylic oxygen atoms are bent towards the surface, we find that on Cu(111) all oxygen atoms are above the carbon plane at 2.73 Å and 2.89 Å, respectively.

O 58.5 Thu 16:45 H39

Interface characterization of TTF-TCNQ on metal surfaces — •Isabel Fernandez-Torrente[1], Sergio Monturet[2], Katharina Jennifer Franke[1], Nils Henningsen[1], Nicolás Lorente[2], Jordi Fraxedas[3], and José Pascual[1] — [1]Institut für Experimentalphysik, Freie Universität Berlin, Germany — [2]Université Paul Sabatier, Toulouse, France — [3]ICMAB, Campus UAB, Bellatera, Spain

Molecular charge transfer (CT) complexes are defined as the association of donor and acceptor molecules. The self-assembling properties of molecules open the possibility of building different donor-acceptor stacking structures which rule the electronic funcionality of the compound. Tetrathiafulvalene 7,7,8,8-tetracyanoquinodimethane (TTF-TCNQ) is an example of a CT complex which shows a metal conducting behaviour. The stacking of TTF and TCNQ forms in bulk one-dimensional partially occupied energy bands that gives rise to the metalicity. By means of Low Temperature Scanning Tunneling Microscopy/Spectroscopy we have characterised for the first time the mixed growth of TTF and TCNQ on a metallic surface in submonolayer and monolayer regimes. The self-assembled growth is governed by donor-acceptor recognition. In particular a one dimensional phase with alternating lines of TTF and TCNQ is formed and can be considered as the precursor stage for the bulk structure. By Scanning Tunneling Spectroscopy we associate electronic resonances with the Highest Occupied Molecular Orbital (HOMO) and the Lowest Unoccupied Molecular Orbital (LUMO) of TTF and TCNQ and the self-assembled TTF-TCNQ.

O 58.6 Thu 17:00 H39

Copper-Phthalocyanine on Ag(111) - A SPA-LEED study — •Ingo Kröger, Christoph Stadler, Christian Kumpf, and Eberhard Umbach — Universität Würzburg, Experimentelle Physik II, Am Hubland, 97074 Würzburg

The adsorption of Copper-Phthalocyanine (CuPc) on Ag(111) has been studied by Spot Profile Analysis Low Energy Electron Diffraction (SPA-LEED). Three different phases were found in the submonolayer regime, differing in coverage and temperature.

At coverages below 0.8 layers and at room temperature no long-range order was observed. However, from diffuse rings in LEED we could still determine an average distance between the molecules which decreases *continuously* with increasing coverage.

Between 0.8 and 1.0 layers CuPc forms incommensurate superstructures. The unit cell size shrinks *continuously* from $216\mathring{A}^2$ (0.8 ML) to $196\mathring{A}^2$ (1.0ML). These measurements show that the molecules (at RT) always occupy the maximum surface area, a behaviour which is only compatible with a repulsive intermolecular interaction and a relatively small influence of the substrate.

Furthermore, at coverages between 0.7 -0.8 layers a low temperature phase was found, which is commensurate with the substrate. Very recently the same behaviour was found for SnPc on Ag(111).

O 58.7 Thu 17:15 H39

Self-organization of cobalt-phthalocyanine on a vicinal gold surface revealed by scanning tunnelling microscopy — •J. Kröger, H. Jensen, N. Néel, and R. Berndt — Christian-Albrechts-Universität zu Kiel, D-24098 Kiel, Germany

Adsorption of cobalt-phthalocyanine on Au(788) in the sub-monolayer coverage regime leads to a preferential occupation of step edges with the molecule plane tilted such as to bridge adjacent terraces. Molecules which adsorb on terraces leave the surface reconstruction of Au(788) unchanged and exhibit the propensity to occupy face-centered cubic stacking domains. Tunnelling spectroscopy in the centre of the molecule reveals cobalt d-orbital related features, while spectroscopy on the benzene rings shows the lowest unoccupied molecular orbital.

O 58.8 Thu 17:30 H39

Conformational switching in the self assembling process of azobenzene on Au(111) — •Nils Henningsen[1], Katharina Jennifer Franke[1], Isabel Fernandez-Torrente[1], Gunnar Schulze[1], Beate Priewisch[2], Karola Rück-Braun[2], and José Ignacio Pascual[1] — [1]Institut für Experimentalphysik, Freie Universität Berlin, Germany — [2]Institut für Chemie, Technische Universität Berlin, Germany

Here we present low temperature scanning tunneling microscopy studies of 3,3'-Carboxymethylester-Azobenzene (CMA) adsorbed on a Au(111) surface. Two different adsorption geometries are observed, which differ from each other by the rotation of one phenylene ring. The two CMA isomers selectively assemble in two different structures: highly ordered densely packed islands and chains of interlocked molecules. Both molecular structures are stabilised by hydrogen bonds. The ratio of the two conformers has been studied dependently of coverage and adsorption temperature and shows that the selective assembly is not only influenced by conformational recognition during diffusion processes but furthermore by conformational changes while assembling. This proves that intra-molecular conformational dynamics can govern self assembly processes.

O 58.9 Thu 17:45 H39

Tracking the chiral recognition of adsorbed dipeptides at the single molecule level — •Giovanni Costantini[1], Magalí Lingenfelder[1], Giulia Tomba[2], Lucio Colombi Ciacchi[3], Alessandro De Vita[2], and Klaus Kern[1] — [1]MPI-FKF, Stuttgart, Germany — [2]Physics Department, King's College London, UK — [3]Fraunhofer IWM, Freiburg, Germany

We report on the direct observation of chiral recognition events of diphenylalanine adsorbed on Cu(110) by scanning tunneling microscopy (STM). We monitor the self-organization of co-deposited di-L-phenylalanine (L-Phe-L-Phe) and its stereoisomer D-Phe-D-Phe and rationalise the observed steps of the system's dynamical evolution using first principles and classical molecular dynamics techniques.

We demonstrate that the adsorbed dipeptides must undergo both a conformational change and a chemical rearrangement (into a zwitterionic form) in order to assemble into stable supramolecular structures. The process is successfully completed if the approaching dipeptides have the same chirality, and fails otherwise, so that the final structures are in all cases strictly homochiral.

Our analysis shows that a static three-point-model is in general not sufficient for a complete description of chiral recognition. We prove the importance of mutually induced conformational changes in the chiral recognition process, thereby visualizing at the single molecule level a 50 years old prediction of L. Pauling.

O 58.10 Thu 18:00 H39

Adsorption von Ethen auf Pt(111)- und Pt$_x$Sn- Oberflächenlegierungen. Eine vergleichende HREELS- und DFT-Studie. — •Jan Markus Essen, Jan Haubrich, Conrad Becker und Klaus Wandelt — Institut für Physikalische und Theoretische Chemie, Universität Bonn, Wegelerstr. 12, 53115 Bonn

Durch Zulegieren eines Fremdmetalls können die Eigenschaften von Katalysatoren gezielt beeinflusst werden. Es werden unerwünschte Reaktionswege unterdrückt, das Zielprodukt kann so in höherer Ausbeute und Reinheit erhalten werden. Es wurde das Adsorptionsverhalten von Ethen, als kleinster Repräsentant ungesättigter Kohlenwasserstoffe auf Pt(111) sowie den Oberflächenlegierungen Pt$_3$Sn und Pt$_2$Sn auf Pt(111) mittels thermischer Desorptions-Spektroskopie (TDS) und hochauflösender Elektronen-Energie-Verlustspektroskopie (HREELS) untersucht. Die erhaltenen Adsorptionsenergien und Schwingungsspektren werden mit Ergebnissen von Dichte-Funktional-Theorie (DFT) Rechnungen verglichen und interpretiert.Ethen adsorbiert auf allen drei Oberflächen bevorzugt in einer di-σ -Konformation, zeigt aber ein völlig verschiedenes Desorptionsverhalten. Als Mindermengen-Komponente konnte durch Vergleich mit den Rechnungen, erstmalig auf diesen Oberflächen eine π -gebundene Ethen Spezies nachgewiesen werden.Durch diese vergleichende Betrachtung der experimentellen Messungen mit den theoretischen Rechungen können Reaktionswege, Intermediate und Oberflächenspezies aufgeklärt und der Legierungseinfluss des Zinns bei der unterdrückten Dehydrierung des Ethens auf diesen Oberflächen verstanden werden.

O 59: Oxides and Insulators: Clean Surfaces

Time: Thursday 15:45–18:45 Location: H41

O 59.1 Thu 15:45 H41

Structure of the $(\sqrt{67}\times\sqrt{67})$R12.2° surface oxide on Ni$_3$Al(111) — •Michael Schmid[1], Georg Kresse[2], Evelyn Napetschnig[1], and Peter Varga[1] — [1]Institut für Allgemeine Physik, TU Wien, Österreich — [2]Institut für Materialpyhsik, Universität Wien, Österreich

With a unit cell size of 4.16 nm, the surface oxide on Ni$_3$Al(111) is one of the largest well-defined inorganic surface structures known today [1]. We have studied this oxide by high-resolution scanning tunneling microscopy (STM) and obtained atomic resolution of the topmost oxygen layer. This information, together with the building rules of the surface oxide on NiAl(110) [2] allowed us to build a raw model of the surface oxide, which was refined by density functional theory calculations. Although the structure is oxygen deficient, there are very few sites where the bonding environment of the individual atoms deviates from the rules found on NiAl(110). The most intriguing structural feature is a regular array of "holes" in the oxide, which explains the excellent properties of the structure as a template for growth of ordered arrays of clusters [3].

[1] S. Degen et al., Surf. Sci. 576, L57 (2005).
[2] G. Kresse et al., Science 308, 1440 (2005).
[3] G. Hamm et al., Nanotechnology 17, 1943 (2006).

O 59.2 Thu 16:00 H41

Disorder and Complexity in the Surface Structure of Alumina on Ni3Al(111) — •Sebastian Gritschneder[1], Holger Schnieder[1], Conrad Becker[2], Klaus Wandelt[2], and Michael Reichling[1] — [1]Fachbereich Physik, Universität Osnabrück, Barbarastraße 7, 49069 Osnabrück, Germany — [2]Inst. für Phys. u. Theo. Chemie, Universität Bonn, Wegelerstraße 12, 53115 Bonn, Germany

An alumina surface with several outstanding properties is that of a thin film grown on the (111) surface of a Ni3Al substrate. The dominant phase of this oxide film has early been identified as an excellent template for the controlled growth of nanostructures. Templating on the alumina film is facilitated by a dot and a network super-structure that can readily be prepared but have not been understood at the atomic scale. By dynamic force microscopy, we reveal that this phase is build up from a hexagonal lattice of 0.29 nm periodicity, that is commensurate to the aluminum sub-lattice of the substrate. The complex interaction between oxide film and substrate leads to the formation of the two super-structures. By comparison of highly resolved images of the dominant phase with images of another phase of the oxide film, we reveal that their basic structural elements are identical, and therefore we speculate that different substrate conditions are responsible for the adoption of either of the phases.

O 59.3 Thu 16:15 H41

Self-Assembled Sub-Surface Oxygen Vacancy Arrays on Reduced CeO$_2$(111) — •Stefan Torbrügge[1], Michael Reichling[1], Seizo Morita[2], and Oscar Custance[2] — [1]Fachbereich Physik, Universität Osnabrück, Barbarastr. 7, 49076 Osnabrück, Germany — [2]Graduate School of Engineering, Osaka University, 2-1 Yamadaoka, Suita, Osaka, Japan

In this contribution, we present atomic resolution dynamic scanning force microscopy (SFM) measurements of the reduced CeO$_2$(111) surface performed at 80 K. We have been able to clearly recognize surface and sub-surface oxygen vacancies and to corroborate the topographic heights predicted by previous theoretical calculations [1,2]. A detailed structural analysis of these two types of oxygen vacancies, as well as other surface defects, is presented. We found that some terraces of the prepared CeO$_2$(111) surface are dominated by sub-surface oxygen vacancies. By the combined analysis of two complementary SFM signals, namely topography and dissipation, we are able to clearly locate each sub-surface oxygen vacancy. Our findings suggest that sub-surface oxygen vacancies do not cluster together but tend to self-assemble in ordered arrays leading to a (2x2) locally reconstructed surface. Thus, we present experimental evidences that single sub-surface vacancies, ordered in arrays at high concentration, are energetically more favorable than sub-surface vacancy clusters.

[1] F. Esch et al., Science **309**, 752 (2005)
[2] S. Fabris et al., J. Phys. Chem. B **109**, 22860 (2005)

O 59.4 Thu 16:30 H41

Stability, atomic and electronic structure of reduced Fe_3O_4(111) surfaces — •Markus Paul[1], Michael Sing[1], David Schrupp[2], Ralph Claessen[1], and Victor Brabers[3] — [1]Lehrstuhl für Experimentelle Physik IV, Universität Würzburg, Germany — [2]Lehrstuhl für Experimentalphysik II, Universität Augsburg, Germany — [3]Department of Physics, Eindhoven University of Technology, The Netherlands

Polar faces of ionic materials present a challenge for the determination of the atomic structure. Underlying difficulties are the relative stability and variability of such surfaces which can cause a poor reproducibility in the experiment or the coexistence of different structures on the same surface. In this work Magnetite(111) single crystal surfaces have been studied by STM, LEED and XPS under different *in situ* preparation conditions and stoichiometries, accordingly. The coexistence of several surface structures has been detected confirming only small differences in their relative stabilities . An unusual superstructure has been found for a reduced $Fe_{1-x}O$-like surface layer. It is explained as originating from elastic strain formation due to lateral mismatch between Fe_3O_4 substrate and $Fe_{1-x}O$-like overlayer.

O 59.5 Thu 16:45 H41

Stabilization of thin ZnO films by surface depolarization — •Christian Tusche, Holger L. Meyerheim, and Jürgen Kirschner — MPI für Mikrostrukturphysik Halle, D-06120 Halle, Germany

Heterostructures of the oxide semiconductor ZnO attracted interest for application in ultra violet laser diodes and spintronic devices. Theoretical predictions rely on detailed information on the film and interface structures. Scanning tunneling microscopy (STM) and surface x-ray diffraction (SXRD) was used to study morphology and structure of ultra thin ZnO films on Ag(111).

ZnO films, 0.3 to 5 monolayers (ML) in thickness, were grown by pulsed laser deposition in 10^{-7} mbar O_2 atmosphere on Ag(111) at 300 K, followed by annealing at 680 K. SXRD indicates that the film is (0001) oriented, and the hexagonal lattice vectors are aligned parallel with the Ag(111) surface. While single crystal (0001) or $(000\bar{1})$ surfaces are polar, and extended flat regions (> 10 nm) are not stable, the 2 ML thick ZnO films form a flat double-layer over the whole surface.

Stabilization is achieved by a transition of the Wurtzite- towards a graphite like structure with reduced polarity, i. e., O ions move to the plane of Zn ions: SXRD shows an in-plane expansion of the ZnO lattice by 1.6 % compared to bulk (3.30 Å vs. 3.25 Å), corresponding to a 7/8 coincidence with the Ag substrate (Ag: 2.89 Å). In parallel, Zn-O bonds (bulk: 1.97 Å) within the hexagonal plane shorten to 1.92 Å and intra-plane Zn-O bonds expand to 2.20 Å. The ions change their four-fold coordination (Wurtzite structure) to a three-fold one.

O 59.6 Thu 17:00 H41

Identification of reactive oxygen sites at surfaces of MoO_3 by polarization–resolved NEXAFS spectra: theoretical studies — •Matteo Cavalleri and Klaus Hermann — Fritz-Haber-Institut der MPG, Faradayweg 4-6, 14195 Berlin, Germany

The identification of reactive oxygen sites at metal oxide surfaces and the characterization of their physical properties is of great importance for an understanding of the catalytic activity of such materials and, thus, for a rational design of more efficient and selective catalysts. Here we evaluate Near–Edge X–Ray Absorption Fine Structure (NEXAFS) spectra, based on density functional theory and appropriate surface clusters, to study and discriminate non–equivalent oxygen centers present at surfaces of catalytically relevant molybdenum oxides. For the (010) surface of bulk MoO_3 this technique is able to unambiguously distinguish between singly coordinated molybdenyl oxygen covering the topmost molybdenum layers and other oxygen centers of similar local environment, differing only by their spatial orientation in the crystal. Theoretical predictions are also successfully used to identify and interpret characteristic features in the NEXAFS spectrum that arise from defects and oxygen vacancies[1]. Upon comparison between measured and computed NEXAFS spectra for different photon polarization directions it is also possible to validate proposed structures of thin MoO_3 films at the Au(111) surface.

[1] M. Cavalleri, K. Hermann, S. Guimond, Y. Romanyshyn, H. Kuhlenbeck and H.–J. Freund, submitted to Cat. Today (2006)

O 59.7 Thu 17:15 H41

Lattice Dynamics of RuO_2: Bulk and (110) Surface — •Klaus-Peter Bohnen[1], Rolf Heid[1], and Omar de la Pena Seaman[2] — [1]Forschungszentrum Karlsruhe, Institut für Festkörperphysik — [2]Department of Applied Physics, CINVESTAV-Mérida, Yucatán, Mexico

Although RuO_2 has been studied as a prototype catalyst for CO oxidation no careful study of the lattice dynamics for this material has been presented so far. Using modern ab-initio methods we obtain the phonon dispersion and the generalized density of states (GDOS). Inelastic neutron scattering experiments allow for an experimental determination of the GDOS. In contrast to what is known from structural studies, we find that the local density approximation gives a much better description of the phonon spectrum than the generalized gradient corrected form. This is also consistent with Raman measurements. Besides the bulk we have also studied the lattice dynamics for the (110) surface. Unfortunately, no complete experimental phonon study of this surface has been carried out so far, however, our results are consistent with the available experimental information. These calculations allow for the first time for the determination of the bulk and surface part of the phononic contribution to the free energy, a quantity which is essential for the determination of thermodynamic properties.

O 59.8 Thu 17:30 H41

Tensor LEED study of the dynamics of the NaCl(100) surface — •Jochen Vogt — Chemisches Institut der Otto-von-Guericke-Universität Magdeburg, Universitätsplatz 2, 39106 Magdeburg

A wealth of theoretical studies dealt with the dynamics of the NaCl(100) surface, e.g. in relation to its melting behaviour, friction, or the simulation of image contrast in atomic force microscopy. Accurate experimental information on the temperature dependent vibrational amplitudes of ions in different layers is missing so far, although it could serve as a critical test for the various potential models applied to this prototype material. This contribution reports LEED experiments at various temperatures between 25 K and 300 K, in which beam intensities were recorded as a function of electron energy. The experimental I(E) data were analyzed using the tensor LEED approach. At all investigated temperatures the NaCl(100) surface exhibits the same relaxation, characterized by a static inward shift of the topmost Na^+ ion of 0.09 ± 0.03Å. The dynamics of the topmost layer is significanlty higher than those of the second layer, where the measured amplitudes are close to literature bulk values. Above 100 K, Na^+ and Cl^- ions in the topmost layer have nearly the same amplitudes, while the amplitudes of the cations in the second layer are larger than those of the anions. In this temperature range the mean square amplitudes of the ions at the surface are in good agreement with previously reported lattice dynamics studies.

O 59.9 Thu 17:45 H41

Photon Mapping of MgO thin Films with an STM — •Hadj-Mohamed Benia, Niklas Nilius, and Hans-Joachim Freund — Fritz-Haber-Institut der MPG, Berlin

The light emission from an STM junction consisting of an MgO thin film on Mo(001) and an Au tip is analysed with respect to its spatial distribution for various excitation conditions. The spectral characteristic of the light is compatible with an emission mechanism mediated by tip-induced plasmons that are excited by inelastic tunnel processes involving field emission resonances in the tip-sample gap. For MgO islands of distinct topographic height, the local emission yield can be tuned by changing the sample bias. This interrelation reflects the dependence of field emission resonances on the MgO work function, which in turn is a function of the number of MgO layers covering the Mo support.

O 59.10 Thu 18:00 H41

Structural and electronic properties of bulk earth alkali oxides and their surfaces — •Björn Baumeier, Peter Krüger, and Johannes Pollmann — Institut für Festkörpertheorie, Universität Münster, Wilhelm-Klemm-Str. 10, 48149 Münster

Earth alkali oxides play a vital role in a number of technological applications, most prominently as supports in catalysis.

While structural properties of BeO, MgO, CaO, SrO and BaO are quite well described within the local density approximation of density functional theory, the calculated electronic structure suffers from well-known shortcomings, most noticeably the significant underestimate of the band gap and conduction band energies. We present results of DFT calculations using self-interaction-corrected (SIC) pseudopotentials for the aforementioned earth alkali oxides. Bulk electronic properties are in very good agreement with experimental data and – where available – with results of considerably more elaborate quasiparticle calculations. To investigate the properties of nonpolar low-index surfaces of these oxides we apply the very same SIC pseudopotentials and find that the SIC effect on the surface is comparable to that on the bulk electronic structure. The surface bandstructure of MgO(001) resulting within the SIC approach is practically identical to the one resulting from GWA calculations, while the required computational effort in SIC remains at the LDA level. We infer from this good agreement for MgO(001) that our calculations for the other earth alkali oxide surfaces are of similar quality. These results consitute a solid quantitative basis for further studies, e.g., for investigations of optical spectra or adsorbate systems.

O 59.11 Thu 18:15 H41

Imaging the muscovite mica surface by means of high resolution dynamic scanning force microscopy — •Frank Ostendorf, Carsten Schmitz, Sabine Hirth, and Michael Reichling — Fachbereich Physik, Barbarastrasse 7, 49076 Osnabrück

Muscovite mica is a widespread substrate for many applications, for instance in biology and material science. Mica is famous for its large atomically flat terraces after cleavage and its atomic scale structure has been studied by dynamic force microscopy performed in a liquid environment [1]. We investigated air and UHV cleaved mica surfaces in detail by a dynamic force microscope operated in the non-contact mode under ultra-high vacuum conditions. We adapted several appropriated recipes for air cleaved mica preparation techniques from the literature and varied two major parameters, namely degassing temperature and degassing period. It has been found that none of the recipes leads to a true atomically flat and clean surface, even after degassing the sample for several hours at temperatures above 500 Kelvin. On regularly shaped flat nanostructures found on the surface, two different types of atomic scale patterns were observed.

[1] Fukuma T. et al. Appl. Phys. Lett. 87 (2005) 034101

O 59.12 Thu 18:30 H41

Band mapping the $ZnO(11\bar{2}0)$ surface by angle-resolved photoelectron spectroscopy — •Stefan Andres, Christian Pettenkofer, Wolfgang Bremsteller, and Joachim Wider — Hahn-Meitner-Institut GmbH, Berlin, Deutschland

Zinc oxide (ZnO) is a transparent, piezoelectric semiconductor. Its large band gap of about 3.4eV and high exciton binding energy of about 60meV render ZnO an interesting material for optoelectronic devices in the UV-regime. Furthermore the piezoelectric properties can be utilized in SAW-devices.

Recent studies have shown that the $ZnO(11\bar{2}0)$ surface is a promising candidate for such devices.

We present angle resolved photoemission data from an in-situ cleaved, $(11\bar{2}0)$ oriented ZnO single crystal as well as from epitaxially grown thin $ZnO(11\bar{2}0)$ films. The spectra were recorded at the TGM7 beamline at BESSYII synchrotron light facility in Berlin.

It is shown, that the surface electronic structure of both the epitaxially thin films and the single crystal coincide with each other. The band dispersion along $k_\perp$ and $k_\parallel$ is discussed in accordance with theoretical band structure calculations.

For the $\overline{\Gamma} - \overline{X'}$ direction a new band, centered at $\overline{X'}$ is observed which is tentatively assigned to a surface-Umklapp process.

O 60: Time-Resolved Spectroscopies

Time: Thursday 15:45–18:30 Location: H42

O 60.1 Thu 15:45 H42

2PPE measurements of PTCDA on Ag(111) — •Christian Schwalb[1], Sönke Sachs[2], Achim Schöll[2], Eberhard Umbach[2], and Ulrich Höfer[1] — [1]Fachbereich Physik und Zentrum für Materialwissenschaften, Philipps-Universität Marburg, D-35032 Marburg, Germany — [2]Universität Würzburg, Experimentelle Physik II, D-97074 Würzburg, Germany

Electron transfer at a metal-molecule interface plays an important role in many chemical disciplines, ranging from molecular electronics to surface photochemistry. We present measurements using time-resolved two-photon photoemission (2PPE) to probe the energetics and dynamics of electronically excited states in epitaxial 3,4,9,10-perylenetetracarboxylic acid-dianhydride (PTCDA) thin films on a Ag(111) surface for a thicknessrange from one to ten monolayers. These measurements allow the identification and determination of the energetic positions for the lowest unoccupied molecular orbital (LUMO), and LUMO + 1. Angle-resolved 2PPE-measurements show a weak dispersion for the LUMO of ˜150 meV. Our experiments indicate that the excitation process for the LUMO is mainly done by electrons from the Ag(111) substrate. Time-resolved measurements probing the dynamics of the system show an increasing of lifetime for the LUMO for increasing layer thickness from 40 to 80 fs.

O 60.2 Thu 16:00 H42

Photoemission Electron Microscopy Study of Anthracene Thin Film Growth on Si(111) — •Niemma Buckanie and Frank Meyer zu Heringdorf — Universität Duisburg-Essen, Lotharstraße 1, 47057 Duisburg

The organic molecule anthracene consists of three linearly fused aromatic rings and has been successfully used in Organic Light Emitting Devices (OLED).The efficiency of the OLEDs depends strongly on the crystalline structure of the anthracene films. The frequency (color) of the emitted light is determined by an Exciton in the molecule.

We used linear and non-linear Photoemission Electron Microscopy (PEEM)to study the growth and the electronic properties of anthracene thin films on Si(111). Anthracene forms fractal-shaped islands with standing up molecules on top of a wetting layer that consists of flat-lying molecules. The illumination of the films with fs-laser pulses (E = 3.1 eV) enables us to determine the azimuthal alignment of the molecules in the textured films by using two photon-photoemission (2PPE). In 2PPE, a first photon excites the singlet exciton S1. The absorption of a second photon leads to the photoemission. The S1 state can only be excited with an electric field along the b-axis of the anthracene unit cell.

O 60.3 Thu 16:15 H42

Femtosecond electron dynamics in atomic wires: Si(557)-Au — •Tilman K. Rügheimer[1,2], Franz Himpsel[2], and Thomas Fauster[1] — [1]Lehrstuhl für Festkörperphysik, Universität Erlangen-Nürnberg, Staudtstr. 7, 91058 Erlangen — [2]Department of Physics, University of Wisconsin-Madison, 1150 University Ave, Madison WI 53706, USA

Atomic wires of noble metals such as gold on silicon surfaces serve as a model system for the investigation of one-dimensional electron systems. Recent experiments on Si(557)-Au have proven the existence of a spin-split surface state band below E_F [1] and have provided first information on the unoccupied part of the electronic band structure [2,3]. The dynamics of electrons has not been investigated so far.

We have carried out time-resolved two-photon photoemission experiments using femtosecond laser pulses. The lifetime of the previously reported image-potential resonance [2] is found to be smaller than 10 fs. At energies in the bulk band gap, the $I(\Delta t)$ curves are strongly asymmetric and cannot be explained by a single state and one decay channel. An interpretation using electron scattering between surface states in the gap is used to fit the data and reveals several lifetimes on the femtosecond and the picosecond scale.

[1] I. Barke et al., Phys. Rev. Lett. 97, 226405 (2006)
[2] J. A. Lipton-Duffin et al., Phys. Rev. B 73, 245418 (2006)
[3] T. K. Rügheimer et al., submitted

O 60.4 Thu 16:30 H42

Photoemission at the Si(001)-Ga surface using femtosecond lasers — Daniel Kampa, •Andrea Melzer, Jinxiong Wang, and Thomas Fauster — Lehrstuhl für Festkörperphysik, Universität Erlangen-Nürnberg, Staudtstr. 7, D-91058 Erlangen

The Si(001) (2×2)-Ga surface was used to investigate time-dependent Ga(3d) core-level shifts by pumping electrons from the valence to the conduction band. The pump-probe experiments were done by exciting the carriers with 1.59 eV laser pulses and probing the Ga(3d) core level with higher harmonics. These were generated 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. For the 25th harmonic used, the time resolution of the experiment was ~ 400 fs after the grating monochromator. The band bending of about 110 meV of the p-doped Si(001) (2×2)-Ga surface is completely lifted by illumination of the surface with the 1.59 eV laser pulses. The Ga(3d) core level shows a slow time-dependent shift attributed to the build-up (∼ 1 ns) and decay (∼ 100 ns) of the photovoltage. The Ga(3d) core-level shift in the subpicosecond range is determined to be < 12 meV at the used pump pulse intensity of 10 mJ/cm^2.

O 60.5 Thu 16:45 H42

Ultrafast Vibrational Dynamics of CO/Ir(111) — •Heike Arnolds, Ian Lane, and David King — Department of Chemistry, University of Cambridge, Lensfield Road, Cambridge CB2 1EW, UK

We present a set of experiments that provide a complete mapping of coherent and incoherent vibrational relaxation times for a saturated layer of CO on a metal surface, Ir(111). Using femtosecond infrared pump - sum frequency probe spectroscopy, we measure the vibrational spectrum, the free induction decay and the vibrational lifetime. We also present the first measurement of a mid-infrared photon echo from a metallic surface, some fifteen years after the analogous measurement on a semiconductor surface. We find that the spectral linewidth (∼5 cm^{-1}) in this strongly dipole-coupled system is dominated by lifetime broadening and inhomogeneity, with only a small contribution from pure homogeneous dephasing due to coupling with low frequency modes. In addition, we see a change in echo peak shape with delay time, which shows that the inhomogeneity in this system is not static, instead frequency fluctuations contribute on different time scales.

O 60.6 Thu 17:00 H42

Femtosecond laser induced diffusion of CO on vicinal Pt(111)-surfaces — •Marco Lawrenz, Krisztina Stépán, Jens Güdde, and Ulrich Höfer — Fachbereich Physik und Zentrum für Materialwissenschaften, Philipps-Universität Marburg, D-35032 Marburg, Germany

Femtosecond laser induced surface diffusion of CO from step edges onto terraces of a vicinal Pt(111) surface has been studied at low substrate temperature using optical second harmonic generation (SHG) as a sensitive probe of the step coverage. We have investigated the diffusion rate as a function of laser fluence and delay between two time-delayed excitation pulses in a two-pulse correlation scheme. Compared to our previous studies on the diffusion of atomic oxygen on vicinal Pt(111) [1], we observe a weaker nonlinear dependence of the diffusion rate on laser fluence ($\propto F^6$) in a fluence range of $F = 2$–4 mJ/cm^2. The two-pulse correlation, on the other hand, has a narrower width of only ≈500 fs, which unambiguously show that the excitation mechanism for CO diffusion is also mediated by the substrate electron- rather than the phonon-system. As in the case of oxygen, the narrow two-pulse correlation can be described within the generalized one-dimensional electronic friction model only, if we assume an electron-temperature-dependent friction coefficient.

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

O 60.7 Thu 17:15 H42

Spin-dependent lifetimes of hot electrons in Co/Cu(100) revisited — •Ilja Panzer[1,3], Andreas Goris[1,3], Martin Pickel[2], Anke Schmidt[1,3], Fabian Giesen[1], Markus Donath[2], and Martin Weinelt[1,3] — [1]Max-Born-Institut, Max-Born-Straße 2A, 12489 Berlin — [2]Physikalisches Institut, Universität Münster, Wilhelm-Klemm-Straße 10, 48149 Münster — [3]Freie Universität Berlin, Arnimallee 14, 14195 Berlin

There is an ongoing controversy over hot electron lifetimes in ferromagnetic metals from the experimental as well as the theoretical point of view [1,2]. From the various experimental approaches to measure the lifetimes of excited electrons no consistent picture of the underlying processes has emerged. For ferromagnetic thin films it is widely accepted that the lifetime of excited electrons is spin dependent, but the ratio between majority and minority lifetimes is still not settled.

We have measured the spin-dependent lifetimes of hot electrons between 250 and 750 meV above E_F for 20 ML Co/Cu (100) with time-resolved two-photon photoemission. Hot electrons are created by a 1.5 eV IR pulse of 3 nJ and probed with a significantly weaker UV pulse with the UV photon energy tuned slightly below the work function thus reducing the background of direct photoemission. We find significantly different lifetimes for minority and majority electrons. The implication for ultrashort magnetic switching will be discussed.

[1] Aeschlimann et al., Phys. Rev. Lett. **79**, 5158 (1997)

[2] Zhukov et al., Phys. Rev. Lett. **93**, 096401 (2004)

O 60.8 Thu 17:30 H42

The Laser-Assisted Photoelectric Effect on Surfaces — •Aeschlimann Martin[1], Luis Miaja-Avila[2], Guido Saathoff[2], Margaret M. Murnane[2], and Henry C. Kapteyn[2] — [1]Department of Physics, University of Kaiserslautern, Kaiserslautern, Germany D-67663 — [2]Department of Physics and JILA, University of Colorado, Boulder, CO 80309-0440

While the laser-assisted photoelectric effect (LAPE) in atoms is well established for the characterization of femtosecond EUV pulses, the equivalent process in the original manifestation of the photoelectric effect -photoemission from surfaces- has not therefore been studied.

In the present work, we present the first observation of the LAPE process in two-color surface photoemission [1]. In our experiment, IR pulses of 30 fs duration and 1.5 mJ at 780 nm are produced by a Ti:sapphire laser system and split into probe and pump. The probe beam is upconverted to the EUV using phase-matched high harmonic generation in a hollow fiber. A pair of Si:Mo multilayer mirrors spectrally selects the 27th harmonic (30 nm). The pump beam is directed through an optical delay arm and spatially and temporally overlapped with the EUV beam on a Pt(111) sample. A time-of-flight detector then measures the kinetic energy of the photoemitted electrons. In the presence of the pump pulse, these electrons can either absorb or emit an IR photon leading to sidebands in the EUV photoelectron spectrum. This ‘dressing‘ of the continuum states is visible as steps in the Fermi edge.

[1] L. Miaja-Avila et al, Phys. Rev. Lett. 97, 113604 (2006)

O 60.9 Thu 17:45 H42

Space-,Time- and Energy- resolved PEEM at deposited Clusters — •Martin Rohmer, Carsten Wiemann, Michael Bauer, and Martin Aeschlimann — Department of Physics, University of Kaiserslautern, Kaiserslautern, Germany D-67663

Photoemission electron microscopy (PEEM) is a common technique to map the lateral distribution of the photoemission yield from micro- and nanostructured samples with sub-micron spatial resolution. Energy-resolved PEEM combined with the time-resolved two-photon photoemission technique (TR 2PPE) enables us to probe at the same time the ultrafast dynamics of electron excitations at surfaces (Lifetime mapping).

In this presentation we show that this setup is capable to identify very small differences (1-3 fs) in the excited state lifetime of supported clusters as result of lateral variations in the coupling efficiency to the underlying HOPG substrate. The high sensitivity of time-resolved PEEM to these temporal inhomogenities is related to the parallel acquisition mode of this technique, which significantly reduces the resolution limiting influence of systematic error arising from temporal fluctuations in the experimental parameters.

O 60.10 Thu 18:00 H42

Laser-induced ultrafast modification of electronic structure studied by femtosecond x-ray spectroscopy — •Niko Pontius, Christian Stamm, Torsten Kachel, Marko Wietstruk, Hermann A. Dürr, and Wolfgang Eberhardt — BESSY m.b.H., Albert-Einstein-Str. 15, 12489 Berlin, Germany

Femtosecond laser-induced excitation and relaxation processes of valence electrons in metals have so far been intensely studied by time-resolved techniques exclusively probing the valence electron response. However, including core level electrons in the probing process by using ultrashort x-ray pulses we demonstrate that additional, novel information about the transient modification of the electronic structure can be obtained.

In a laser-pump and x-ray-probe experiment at the BESSY ‘femtosecond slicing’ source we found for Ni that upon optical excitation the L_3 absorption line undergoes a ∼200 meV shift to lower energies. This shift occurs within the experimental temporal resolution of 150±50 fs. Comparing the experimental data with cluster calculations suggests that the observed L_3 absorption line shift is associated with an increase of valence electron localization inducing a shift of the 2p-core level to lower binding energy. This localization effect could be caused by enhanced scattering of itinerant electrons with electron-hole excitations. Such a modification of the electronic structure as a result of the electronic system perturbation has so far been unknown.

O 60.11 Thu 18:15 H42

A soft x-ray energy-dispersive beamline for NEXAFS and other CFS/CIS studies — •D. R. Batchelor[1], Th. Schmidt[1], R. Follath[2], Ch. Jung[2], R. Fink[3], M. Knupfer[4], B. Büchner[4], and E. Umbach[1] — [1]Universität Würzburg, Experimentelle Physik II

— [2]BESSY GmbH, Berlin — [3]Physikalische Chemie II, Universität Erlangen-Nürnberg — [4]IFW Dresden

Energy-dispersive near edge x-ray absorption fine structure (NEXAFS) spectroscopy is a well-known technique in the hard x-ray regime. By combining the photon energy dispersion of a plane-grating XUV monochromator with the imaging properties of a hemispherical electron energy analyzer, soft x-ray energy dispersive electron spectroscopy is possible. This multiplex technique allows not only NEXAFS without time-consuming scanning of the photon energy but also high-resolution CFS/CIS spectroscopic studies such as Auger/autoionization spectroscopy and photoelectron diffraction. We present the design for an upgrade of the BESSY UE52-PGM beamline and the results of a pilot experiment. Data from copper and its oxides together with phthalocyanines will be presented. Besides the common photoemission and Auger lines and the known participator and spectator decay channels the extensive, quasi-3-dimensional data sets clearly show that other excitations, such as “shake-up”, play an important role in both, the normal and resonant Auger processes. The new technique provides data with much more accuracy and detail than hitherto achieved by simply stepping the photon energy.

Financial support is under BMBF 05KS4WWC/2

O 61: General Meeting of the Surface Science Division

Time: Thursday 19:30–20:00 Location: H36

Report of the Chairman of the DPG Surface Science Division; Miscellaneous

O 62: Post Deadline Session

Time: Thursday 20:00–21:00 Location: H36

4 contributed talks to be determined

O 63: Surface Science Symposion

Time: Thursday 21:00–24:00 Location: H36 hallway

Informal get-together

O 64: Plenary Talk Joanny

Time: Friday 8:30–9:15 Location: H1

Active gels: toward a generic approach of cell mechanics

O 65: Plenary Talk Nørskov

Time: Friday 9:15–10:00 Location: H1

Catalysis from First Principles

O 66: Nanostructures at Surfaces VI (Surface Reconstructions)

Time: Friday 10:15–12:00 Location: H36

O 66.1 Fri 10:15 H36

Morphology and growth of hafnium silicide on Si(111) — •Eva Henschel[1], Mark Schürmann[1], Christian Flüchter[1,2], Daniel Weier[1,2], Axel Beimborn[1], and Carsten Westphal[1,2] — [1]Experimentelle Physik 1 - Universität Dortmund, Otto-Hahn-Str.4, D 44221 Dortmund, Germany — [2]DELTA -Universität Dortmund, Maria-Goeppert-Mayer-Str. 2, D 44221 Dortmund, Germany

The structure and growth of hafnium on Si(111) were studied by scanning tunneling microscopy (STM). Hafnium was deposited by electron beam evaporation onto a clean Si(111) surface under UHV-conditions. The sample was heated in several steps to 900°C. A growth of elongated nanosized structures was observed. Since it is known that hafnium on silicon forms silicide compounds [1], the islands are assumed to consist of $HfSi_2$. The islands were found to grow in three main directions, related to the symmetry of the (111) surface.

The morphology of these silicide islands is affected by the annealing temperature. The first structures were observed after annealing at 450°C and the first free standing islands were found at 650°C. The islands grow in all three dimensions simultaneously, although the growth of length, width and height starts at different temperatures.

With increasing island volume the island number decreases. An analysis of the mean coverage was performed which indicated a possible decrease of the hafnium amount on the surface. Furthermore, the influence of step edges on the island distribution was studied.

[1] A. de Siervo et al., Phys. Rev. B **74** (7), (2006) 075319

O 66.2 Fri 10:30 H36

AFM studies of the systems Hf/Si(100) and HfO_2/Si(100) — •Axel Beimborn[1], Mark Schürmann[1], Christian Flüchter[1,2], Daniel Weier[1,2], Eva Henschel[1], and Carsten Westphal[1,2] — [1]Experimentelle Physik 1 - Universität Dortmund, Otto-Hahn-Str.4, D 44221 Dortmund, Germany — [2]DELTA -Universität Dortmund, Maria-Goeppert-Mayer-Str. 2, D 44227 Dortmund, Germany

The ongoing down-scaling of silicon based structures in the semiconductor industry leads to the demand of new gate dielectrics with high-k values in order to replace the currenty used SiO_2. One of the most promising candidates is HfO_2. In this work the thermal stability of thin films of Hf on Si(100) was studied with *in situ* (conductive)-AFM and LEED investigations. At temperatures above 700°C a (2x1) LEED pattern indicates large parts of the uncovered Si substrate surface. Further HfO_2 was evaporated onto Si(100) substrates. The oxide films were stepwise heated from 400°C up to 900°C. After each annealing process the surface morphology and the growth of the $HfSi_2$ islands was investigated by AFM and LEED.

O 66.3 Fri 10:45 H36

Static Speckle Experiments with White Synchrotron Radiation — •Tushar Sant[1], Tobias Panzner[1], Wolfram Leitenberger[2], Gudrun Gleber[1], and Ullrich Pietsch[1] — [1]Solid State Physics, University of Siegen, 57068 Siegen, Germany — [2]Institute of Physics, University of Potsdam, 14415 Potsdam, Germany

Static speckle experiments were performed using white synchrotron radiation at EDR beamline at BESSY-II. It has been shown that for coherent scattering experiments in reflection geometry the knowledge of the illumination function incident on the sample is important[1]. In order to prove the inter play between the illumination function and a real sample the coherent reflectivity has been recorded from the surface of technologically smooth GaAs wafer. Besides periodic oscillations which are caused by the scattering from incident pinhole other features appear which are associated with the sample surface profile. The illumination function calculated by means of Lommel formalism matches well with the measured function and will be used for further surface reconstruction from speckle maps. For further examination speckle map of reflection from a laterally periodic structure like GaAs grating is studied [2]. Under coherent illumination the grating peaks split into speckles which correspond to fluctuations on the sample surface. The surface morphology of the grating is reconstructed from this coherent scattering so as to determine local height fluctuations. 1.Pietsch U, et al. Physica B- Condensed Matter, 357 (2005) 45. 2.Pietsch U, et al. Physica B- Condensed Matter, (2007) in press.

O 66.4 Fri 11:00 H36

A Simplified Model for FIB Structuring I — •Andreas Stadler — Institut für Angewandte Physik und Zentrum für Mikrostrukturforschung, Jungiusstr. 11, 20355 Hamburg

Within the wide field of Nano-Technology, methods - as Focused Ion Beam (FIB) - which allow a well defined structuring of any material, have an outstanding position. Therefore the primary aim must be to minimize the producible structure-diameters. While a lot of effort has been undertaken to focus the ion beam, we have focused on the investigation of the influence of substrate parameters on structure diameters.

A 'non-numerical' model has been developed to comprehensibly interpret the measured structures. So called internal and external re-depositions have been taken into account for dots, lines and two-dimensional structures.

Besides the parameters current and diameter of a Gaussian beam profile the influence of substrate parameters as density, molar mass and aspect ratio (structure depth versus beam diameter) on structure topography are shown. The effect of typical parameters for FIB processes as dose, step width and write cycle repetition on the morphology have been investigated.

O 66.5 Fri 11:15 H36

Nanostructuring of metallic thin films — •Stefan Griesing, Andreas Englisch, Joachim Sukmanowski, and Uwe Hartmann — Institute of Experimental Physics, Saarland University, P.O. Box 15 11 50, D-66041 Saarbruecken

Several methods are established for micro- and nanostructuring of metallic and dielectric films: Focused ion beam milling, ultraviolet and electron beam lithography and nanoimprint techniques. In this context, we introduce a new method of structuring metallic thin films: A focused electron beam is used for directly melting metallic films. Charge carrier densities in the range of 10ˆ6...10ˆ8 muC/cmˆ2 in conjunction with beam currents of 0.1...1.5 nA are applied. The applicability on different substrate-metal systems is demonstrated. Structures of different geometry in the sub-100-nanometer range can be achieved by this method. Scanning electron microscopy and atomic force microscopy were used for topographical characterization. The excitation and propagation of surface plasmons in structures of different sizes and geometries was checked by scanning optical near-field microscopy.

O 66.6 Fri 11:30 H36

Low pressure Hydrogen Loading of Pd nanoparticles and films using a Hydrogen plasma — •Hans-Gerd Boyen[1], Paul Ziemann[1], Anitha Ethirajan[1], Luyang Han[1], Ulf Wiedwald[1], Andriy Romanyuk[2], and Peter Oelhafen[2] — [1]Institut für Festkörperphysik, Universität Ulm, D-89069 Ulm} — [2]Institut für Physik, Universität Basel, CH-4056 Basel

The loading of metals with atomic Hydrogen is usually performed in (molecular) Hydrogen atmospheres at elevated pressures (several bars) in order to overcome the problem of small dissociation rates at the surface of the corresponding metal. Here, we present an experimental study for the in-situ loading with atomic Hydrogen of Pd nanoparticles of different size (10nm,3nm, prepared by a micellar method) as well as of a Pd bulk reference sample using a Hydrogen plasma (0.1mbar). The chemical state of the different samples is studied by means of X-ray photoelectron spectroscopy (XPS) allowing to identify the interdiffusion of Hydrogen atoms into the metal by means of an hydride-induced chemical shift of the Pd-3d core levels. First results for the loading/unloading behaviour of the different samples (bulk, nanoparticles) will be presented.

O 66.7 Fri 11:45 H36

DFT Studies on Ir(210)-Surface Faceting Induced by Oxygen Adsorption — •Payam Kaghazchi, Timo Jacob, and Matthias Scheffler — Fritz-Haber-Institut der MPG, D-14195 Berlin, Germany

Some atomically rough surfaces show facet formation in presence of strongly interacting adsorbates. STM and LEED studies demonstrated that the initially planar Ir(210) surface becomes faceted when exposed to oxygen and annealed to temperatures above 600K. The facets that form have been identified to have a pyramidal shape showing (311) and (110) faces. While the (311) faces are smooth and unreconstructed the (110) faces are rough and consist of both 1×1 terraces and a stepped double-missing-row superstructure [1]. Using density functional theory calculations together with the *ab initio* atomistic thermodynamics we studied the adsorption of oxygen on those surfaces, being involved in the facet-formation. In agreement with the experiment our calculated (p, T)-surface phase diagram shows that while at the experimental oxygen partial pressure and temperatures above ≈900K the planar O/Ir(210) surface is stable, at lower temperatures the facets are thermodynamically more stable. Those combine two O/Ir(311) faces and one face of either O/Ir(110)-regular or O/Ir(110)-superstructure. Due to the relatively small difference in stability our calculations support the picture of a coexistance of the regular and the superstructured Ir(110). We are now in the process of investigating contributions from step-edges, kinks and phonons. [1] I. Ermanoski, C. Kim, S. P. Kelty, T. E. Madey, *Surf. Sci.*, **596**, 89 (2005).

O 67: Symposium: The Solid-Liquid Interface: A Challenge for Theoreticians II

Time: Friday 10:15–13:00 Location: H38

Invited Talk O 67.1 Fri 10:15 H38

Interfacial Properties of Transition Metal Oxides — •Elisabet Ahlberg, Zareen Abbas, and Sture Nordholm — Department of Chemistry, Göteborg University, 412 96 Göteborg, Sweden

Catalytic and electrocatalytic ability of transition metal oxides is commonly related to the nature of the metal cation and its coordination. However, in aqueous solution the pH rather than potential determines their interfacial chemistry and surface complexation models have been successfully used to describe interfacial properties by including specific chemical surface interactions besides electrostatic effects. We have used corrected Debye-Hückel (CDH) analysis to clarify the mechanisms at work in surface complexation. Ion size in the ion-ion interactions is accounted for in the diffuse screening and a layer of condensed counterions are introduced to treat nonlinear electrostatic response close to the surface. In the CDH theory the particle is considered to be a sphere which can have any size.

Recently, the effect of particle size on the surface charge density was investigated. The results show an increase in surface charge density as the size decreases. This sharp rise in the surface charge density may be explained by the increasing curvature of the double layer as the particle size decreases. The screening becomes more efficient as the size of the particles decreases due to accumulation of ions around the small particles.

In my talk surface complexation at oxide surfaces will be treated from both theoretical and experimental point of view. The implication on electrocatalytic properties will also be discussed.

Invited Talk O 67.2 Fri 10:45 H38

Modeling the Electrochemical Potential of the Aqueous-Electrode Interface within Periodic Density Functional Theory — •Sally Wasileski[1], Christopher Taylor[2], Michael Janik[2], and Matthew Neurock[2] — [1]Department of Chemistry, Univer-

sity of North Carolina at Asheville, Asheville, NC 28804 USA — [2]Departments of Chemical Engineering and Chemistry, University of Virginia, Charlottesville, VA 22904 USA

Ab-initio methods such as density functional theory (DFT), used extensively in modeling the structure and reactivity of adsorbates at vacuum interfaces, are now capable of probing energies and pathways for complex metal/solution environments and are proving to be a good complement to experimental efforts. A model has been developed to include the influence of the tunable electrochemical potential at the aqueous-electrode interface within the periodic density functional theory methodology [Taylor, CD, Wasileski, SA, Filhol, J-S, Neurock, M, "First principles reaction modeling of the electrochemical interface: Consideration and calculation of a tunable surface potential from atomic and electronic structure" Phys. Rev. B (2006) 73, 165402/1-165402/16]. Specific aspects of the model will be addressed in detail along with examples of using the methodology to investigate electrocatalytic reactions such as potential-dependent water dissociation at VIII and IB surfaces and potential-dependent methanol dehydrogenation and carbon monoxide oxidation (relevant chemistry to direct methanol fuel cells).

O 67.3 Fri 11:15 H38

Structural stability and OH adsorption properties of Au/Pt(111) surfaces — •Yoshihiro Gohda and Axel Gross — Institute of Theor. Chemistry, Ulm Univ., 89069 Ulm/Germany

Platinum-based bimetallic electrodes are of current interest for electrochemical and electrocatalytic applications to fuel cells for example. The structural stability of such electrodes is one of the most important prerequisites. Furthermore, OH groups adsorbed on the electrode surface are produced in the initial stage of the oxygen reduction at the cathode. The OH adsorption could also be of importance during the consumption of water in the electro-oxidation of methanol at the anode. A fundamental understanding of OH adsorption properties should thus be helpful for a better description of such reactions on the atomic scale.

Here we report first-principles calculations on the structural stability of Au/Pt(111) surfaces and the OH adsorption on them. We have found that 1-monolayer (ML) thick surface alloys on Pt(111) are energetically preferred compared to the decomposition into the clean Pt(111) surface and Au droplets. They are also more stable than 2-ML thick alloys with the same Au concentration, too, because Au atoms that are larger than Pt atoms prefer to be located in the uppermost layer where they reduce the surface stress which is in general tensile. This bimetallic surface system favors separating into two phases at 0 K: the clean Pt(111) surface and the Au/Pt(111) overlayer. In contrast, stable surface alloy formation due to entropy effects is seen for the $Au_{0.5}Pt_{0.5}$ composition at 800 K. Calculations for the OH adsorption will also be reported.

O 67.4 Fri 11:30 H38

d-Band Catalysis in Electrochemistry — •Sonja Bartenschlager[1], Wolfgang Schmickler[1], and Elizabeth Santos[2] — [1]Universität Ulm, Institut für Theoretische Chemie, Albert-Einstein-Allee 11, 89069 Ulm — [2]Zentrum für Sonnenenergie und Wasserstoff-Forschung, Helmholtzstr. 8, 89081 Ulm

Understanding the mechanism of electrocatalysis is of primary importance for the development of efficient fuel cells. We present the first theory for electrochemical electron transfer reaction that can account for specific catalytic effects caused by the interaction of the reactants with the d-band of a metal electrode. It is based on a model Hamiltonian that combines elements of the Anderson-Newns theory with tight binding and with the Marcus theory.

We have applied this model to the breaking of a bond in a diatomic molecule; this is a particularly important case, since generally bond breaking requires a strong catalytic effect of the electrode. Specifically, we have performed calculations based on a simple, semi-elliptic form of the d-band. In this way, we were able to demonstrate and understand a number of qualitative effects: the change in the density of states as the reaction proceeds and the system passes the saddle point; the importance of a high density of d-band states near the Fermi level, which interact with the anti-bonding orbital as it passes the Fermi level; the loss of symmetry between the anodic and cathodic direction; the decrease in the energy of activation with increasing interaction, which in extreme cases can result in dissociative adsorption without barrier.

O 67.5 Fri 11:45 H38

Theoretical study of the dynamics of gold islands on Au(100) — •Kay Pötting[1], Paola Quaino[1], Wolfgang Schmickler[1], and Timo Jacob[2] — [1]Institut für Theoretische Chemie, Universität Ulm, 89069 Ulm, Germany — [2]Fritz-Haber-Institut der Max-Planck-Gesellschaft, 14195 Berlin-Dahlem, Germany

Nanostructures on metal electrodes are presently the subject of intensive investigations because they are expected to play an important role in future nanotechnologies. Their stability and dynamics has been found to depend exponentially on the electrode potential, an effect which we ascribe to the interaction of local dipole moments with the electric field of the double layer. In order to verify the validity of this conjecture, and to clarify the details of the underlying mechanism, we have investigated the dynamics of gold island on Au(100), which has been the subject of intense experimental investigations, by a combination of DFT calculations and kinetic Monte Carlo simulations. For this purpose, we have calculated the diffusion barriers and associated dipole moments for several important elementary processes by DFT. These results were combined with embedded atom potentials in order to generate the rates for all possible steps, which were then used as the basis for kinetic Monte Carlo simulations. In this way we have investigated both the dynamics of single islands and the Ostwald ripening of two islands of different sizes. Preliminary results indicate a strong effect of the field on energetic parameters like the step line tension and the kink energy, and on the rate of particle exchange and Ostwald ripening.

O 67.6 Fri 12:00 H38

DFT-Studies on the Potential-Induced Lifting of the Au(100) Surface Reconstruction — •Sudha Venkatachalam, Timo Jacob, and Matthias Scheffler — Fritz-Haber-Institut der MPG, D-14195 Berlin, Germany

The study of potential-induced changes of single crystal surface morphologies is of great interest because of its diverse application in electrocatalysis and nanostructuring. In case of Au(100), different surface sensitive techniques show the lifting of stable hexagonal-reconstructed Au(100)-hex to the regular Au(100)-(1×1) structure at electrode potentials >0.55V in 0.01M $HClO_4$ and at >0.32V in 0.1M H_2SO_4 [1]. Although various theoretical and experimental investigations have hitherto been carried out, the rationale behind the lifting of reconstruction is still not clear. In order to study this effect, we performed DFT calculations on Au(100)-hex and Au(100)-(1×1), first neglecting the electrolyte and studying the influence of the electrode potential by applying an external electric field. For both electrolytes ($HClO_4$ and H_2SO_4) we were able to reproduce the experimentally measured transition potentials after correlating the applied electric field to the electrode potential using experimental capacity curves. While this already implies a major role of surface charging, we are now in the process of investigating the influence of ion adsorption. [1] D. M. Kolb, *Prog. Surf. Sci.*, **51**, 109 (1996).

O 67.7 Fri 12:15 H38

Theoretical Studies on the Electro-Oxidation of Pt-electrodes — •Timo Jacob and Matthias Scheffler — Fritz-Haber-Institut der MPG, D-14195 Berlin, Germany

Using an extension of the *ab initio* atomistic thermodynamics approach to electrochemical systems the interfacial structure and composition of Pt-electrodes in aqueous electrochemical environments was studied. Focusing on positive electrode potentials, at which first electro-oxidation and then oxide-formation occurs, we evaluated the full (p, T, ϕ)-surface phase diagram. Assuming experimental temperature and pressure conditions, we find that after forming a (2×2) structure at 0.95 V, the bulk-oxide is thermodynamically stable above 1.20 V. Consequently, the assumption of a plain Pt-electrode, often used in the modeling of electrochemistry, is clearly incomplete. Instead, the surface structure and composition is significantly modified. To further investigate the oxide-formation, we focused on bulk-oxide systems and calculated the stability of the low-index surfaces of α-PtO_2, β-PtO_2, and PtO bulk-oxides. On the basis of formation energies we first deduced the stability ranges at which the bulk-oxides are the thermodynamically stable phase. Afterwards for each of the considered bulk-oxides the corresponding (p, T, ϕ)-phase diagram of surface structures was obtained, showing a preference for α-PtO_2(001), β-PtO_2(110), and PtO(100) respectively, which all have PtO_2 bulk-like compositions even on their surfaces. However, in case of thin oxide layers a PtO composition might also be relevant.

O 67.8 Fri 12:30 H38

Surface stress and surface tension at charged solid-liquid interfaces — •Dominik Kramer[1] and Jörg Weissmüller[1,2] — [1]Institut für Nanotechnologie, Forschungszentrum Karlsruhe, Postfach 3640, 76021 Karlsruhe, Germany — [2]Technische Physik, Universität des Saarlandes, 66041 Saarbrücken, Germany

Most experimental and theoretical results of surface stress changes of electrodes support either the view that the variations of surface stress are identical or similar of that of surface tension, i.e. have essentially a quadratic dependence on the potential, or that the basic dependence is a linear function of the charge. By using a simple model of the solid surface and using both the Lippmann equation (which describes the potential dependence of surface tension) and Shuttleworth's equation (which relates stress and tension) we demonstrate that the surface stress can be considered as a sum of two terms. The first one is a linear function of the surface tension; the second one is a linear function of the surface charge density. This comprehensive description allows explaining of the different results and their seeming discrepancies without assuming experimental errors or fundamental thermodynamic problems.

O 67.9 Fri 12:45 H38

Räumlich aufgelöste IR Spektroskopie und elektrochemische Messungen zur nichtlinearen Dynamik der Elektrooxidation von H$_2$,CO Gemischen an Pt-Elektroden — •Philipp Bauer, Nilüfer Baba, Johannes Bolten, Jan Siegmeier und Katharina Krischer — Technische Universität München, Physik-Department E19, James Franck Str.1, 85748 Garching

Bei Niedertemperaturbrennstoffzellen vermindert die herstellungsbedingte Kohlenmonoxidverunreinigung des Wasserstoffgases den Wirkungsgrad erheblich. Wir verfolgen den Ansatz, mit Hilfe von Methoden der nichtlinearen Dynamik diesen negativen Effekt zu minimieren.

Berechnungen mit einem System von gekoppelten Differentialgleichungen [1], das die Oxidation von H$_2$,CO an einer Platinelektrode beschreibt, sagen von monostabilem Verhalten über Oszillationen und Domänenbildung bis hin zu komplexer Dynamik, eine Vielzahl von zeitlichen und räumlichen Mustern voraus. Wir stellen experimentell ermittelte Bifurkationsdiagramme, die aus globalen potentiostatischen Messungen gewonnen wurden vor und zeigen erste Ergebnisse zur räumlichen Musterbildung. Hierfür findet ein Infrarotspektrometer mit Focal-Plane-Array in ATR-Konfiguration (abgeschwächte Totalreflexion) Verwendung, mit dem raumzeitliche Muster in der CO Bedeckung abgebildet werden können.

Wir diskutieren, inwiefern durch Kontrolle der Parameter ausgewählte Muster eingestellt werden können, die auch in Gegenwart von CO eine hohe Effizenz der Wasserstoffoxidation erlauben.

[1] J. Siegmeier, Diplomarbeit, Physik Department, TU-München, München (2005)

O 68: Metal Substrates: Adsorption V

Time: Friday 10:15–11:45 Location: H39

O 68.1 Fri 10:15 H39

Argon adsorbed on Ag(111) — •Thomas König, Markus Heyde, Hans-Peter Rust, and Hans-Joachim Freund — Fritz-Haber-Institute of the Max-Planck-Society, Faradayweg 4-6, D-14195 Berlin, Germany

The adsorption of Xe on Ag(111) has been a an interesting task since many years [1,2]. We found that investigations about Ar on Ag(111) are less spread. Here we present the preparation and scanning tunnelling microscopy (STM) characterization of Ar on Ag(111). Our employed setup is similar to the one developed by P.S. Weiss et al. [3] and used by Rust et al. [4]. Characteristic of this setup is a pendulum. The pendulum is thermally coupled to a liquid helium dewar. The preparation of the Ar on Ag(111) was accomplished in a special manner. An Ag(111) sample at room temperature was transferred in the cold microscope located at the end of the pendulum. The pendulum and microscope was pre-dosed by Ar before. The hot Ag(111) sample warms the sample holder from where Ar desorbs. Ar-islands or an Ar-film that covers the surface fully can be observed depending on the concentration of Ar. The electronic structures are mapped by STM measurements. A statistical analysis of the Ar-islands and their formation will be shown. The closed Ar-film shows symmetry properties that will be discussed.

[1] J. Unguris, L.W. Bruch, E.R. Moog, M.B. Webb, Surf. Sci. 109, 522 (1981). [2] M. Caragiu, G.S. Leatherman, Th. Seyller, R.D. Diehl, Surf. Sci. 475, 89 (2001). [3] P.S. Weiss, D.M. Eigler, NATO ASI Series E, 235, 213 (1993). [4] H.-P. Rust, J. Busisset, E.K. Schweizer, L. Cramer, Rev. Sci. Instrum. 68, 129 (1997).

O 68.2 Fri 10:30 H39

Quasi-periodic arrangement of one-dimensional defects in iodine adlayers on Pt(100) — •Björn Braunschweig, Alexej Mitin, and Winfried Daum — Institut für Physik und Physikalische Technologien, TU Clausthal, Leibnizstrasse 4, D-38678 Clausthal-Zellerfeld

Long one-dimensional defects in iodine adlayers on a Pt(100) surface, prepared by flame annealing and subsequently quenching in iodine vapor, have been studied by scanning tunneling microscopy (STM). On Pt(100) iodine forms $(\sqrt{2} \times 5\sqrt{2})\mathrm{R}45^\circ$ adlayers consisting of closed-packed, defect-free domains and domains with line defects in [010]-direction, parallel to the Pt steps. The density of the line defects depends on the adsorption temperature. Three types of defects have been identified for adsorption temperatures between 870 K and 1300 K. Based on atomically resolved STM images, structural models for the different defect patterns which consist of iodine rows displaced perpendicular to the [010]-direction have been derived. Iodine adsorption at 1100 K leads to the formation of a pattern with a long-range, quasi-periodic arrangement of line defects.

O 68.3 Fri 10:45 H39

Carbon monoxide adsorption sites on roughened Au(111) — •Tobias Nowitzki[1], Wai-Leung Yim[2], Mandus Necke[3], Hanno Schnars[3], Jürgen Biener[4], Monika Biener[4], Volkmar Zielasek[1], Katharina Al-Shamery[3], Thorsten Klüner[2], and Marcus Bäumer[1] — [1]Institut für Angewandte und Physikalische Chemie, Universität Bremen — [2]Institut für Reine und Angewandte Chemie, Theoretische Chemie, Universität Oldenburg — [3]Institut für Reine und Angewandte Chemie, Physikalische Chemie, Universität Oldenburg — [4]Lawrence Livermore National Laboratory

Since Au turned out to be an active catalyst for the oxidation of carbon monoxide, the adsorption properties on various Au surfaces have been studied. Interestingly, a comparable behavior has been revealed for a wide range of surfaces from supported particles to rough single-crystals: two desorption states above 100 K and one infrared signal. The atomistic origins for this behavior have not yet been clarified completely.

To study this effect, we prepared a rough surface by ion-bombarding a Au(111) single-crystal in ultrahigh vacuum and characterized the system by scanning tunneling microscopy, temperature-programmed desorption and infrared spectroscopy. Furthermore, density functional theory calculations were performed for a Au(332) surface exhibiting similar adsorption properties as the roughened Au(111). The results indicate that two distinct kinds of low-coordinated atoms can explain the experimental findings.

O 68.4 Fri 11:00 H39

Adsorption of CO on stepped Rh(553) — •Hans Peter Koch, Priyanka Singnurkar, and Robert Schennach — Graz University of Technology, Institute of Solid State Physics, Graz, Austria

The adsorption of CO on stepped surfaces has so far only been investigated on a limited number of systems. On Pt (112) and (335) for example distinct desorption peaks for CO from the steps and from the terraces were reported [J. Xu, J. Yates Surf. Sci. 327(1995)193]. In this work we show that CO adsorption on the stepped Rh(553) surface behaves surprisingly different. Thermal desorption spectroscopy (TDS) does not show a peak that can be attributed to CO adsorbed on the steps. Angle resolved thermal desorption data show a simple cosine distribution, as would be expected from a (111) surface. Nevertheless, reflection absorption infra red spectroscopy (RAIRS) shows vibrational features that can be attributed to CO molecules adsorbed on the steps. Apparently, the difference in the desorption energy of CO bound on terraces and on steps is not very different according to the TPD results. However, the binding of the CO molecules on the steps and terraces is different enough to show unique vibrational features in RAIRS. The experimental results will be discussed in the light of recent density functional theory calculations.

O 68.5 Fri 11:15 H39

Adsorption of Deuterium and CO on PdRu surface alloys studied by temperature programmed desorption — •Heinrich Hartmann, Thomas Diemant, Joachim Bansmann, and Juergen Behm — Institute of Surface Chemistry and Catalysis, Ulm University, D-89069 Ulm

The adsorption properties of Pd/Ru surface alloys on Ru(0001) were investigated by Temperature Programmed Desorption using D_2 and CO as probe molecules. The surface alloys were created by depositing Pd on a Ru(0001) crystal and subsequent annealing to 1100 K. This results in the replacement of Ru by Pd atoms in the first surface layer. Earlier STM experiments showed a tendency for phase separation between Pd and Ru in the alloy surface. The TPD experiments showed a lower adsorption energy for CO and D_2 on the bimetallic alloy surfaces with respect to Ru(0001) and Pd(111) surfaces, this has been attributed to electronic and ensemble effects on the Pd/Ru surface. Concomitantly the saturation coverage and initial sticking coefficients of D_2 were found to decrease for higher Pd-contents, indicating an activation barrier for D_2 adsorption on the bimetallic surfaces, whereas the saturation coverage and initial sticking coefficients of CO remained unchanged with respect to adsorption on Ru(0001). Concurrently, a shift of the high-temperature end of the spectra to lower temperatures was observed for both adsobates, indicating a destabilization of the remaining Ru adsorption sites or a faster desorption process due to diffusion between adsorption sites of different bonding strength.

O 68.6 Fri 11:30 H39

STM study of the adsorption of Au and Pb on Mo(110) — •Aleksander Krupski[1], Wojciech Linhart[1], Adam Paruszewski[1], Izabela Cebula[1], Zbigniew Jankowski[1], and Tomasz Kobiela[2] — [1]Institute of Experimental Physics, University of Wrocław, Poland — [2]Institute of Physical and Theoretical Chemistry, University of Bonn

Scanning tunneling microscopy (STM) has been used for the first time to investigate the growth of ultrathin Au and Pb films on the Mo(110) surface.

O 69: Metal Substrates: Clean Surfaces

Time: Friday 10:15–11:45 Location: H41

O 69.1 Fri 10:15 H41

First-principles based prediction of composition and substitutional ordering in the $Pt_{25}Rh_{75}$(100) surface — •Philipp Welker, Ole Wieckhorst, and Stefan Müller — Universität Erlangen-Nürnberg, Lehrstuhl für Festkörperphysik, Staudtstr. 7, D-91058 Erlangen, Germany

The clean (100) surface of the disordered $Pt_{25}Rh_{75}$ alloy shows a strong tendency towards Pt segregation. Whereas the segregation profile is well known from both, STM- and LEED-investigations [1,2], only little progress has been made in understanding the energetics that lie behind the observed segregation behaviour. We find almost the same Pt enrichment in the first layer as already predicted for the (111) surface [3]. This result can be explained in terms of the difference in surface energies of the two components, being almost the same for both the (111) and the (100) surface. However, the underlying layers in the (100) surface consist mainly of Rh, in contrast to the (111)-surface that shows an oscillatory depth profile. The difference in the layer dependent Pt concentration can be explained by the segregation energies, i.e. the energy gain for the exchange of a Pt atom from the bulk with a Rh atom from the surface. Moreover, the combination of density functional theory (DFT) and cluster expansions with Monte-Carlo-simulations allows for the prediction of the temperature dependence of the substitutional ordering behaviour in the $Pt_{25}Rh_{75}$(100) surface.
[1] E. Platzgummer et al., Surf. Sci. 419 (1999) 236.
[2] E. L. D. Hebenstreit et al., Surf. Sci. 441 (1999) 441.
[3] S. Müller et al., Appl. Phys. A 82 (2006) 415.

O 69.2 Fri 10:30 H41

Influence of defects in the NiAl(100) surface on structure and energy — •Kerrin Dössel, Daniel Lerch, Stefan Müller, and Klaus Heinz — Festkörperphysik, Universität Erlangen-Nürnberg, Staudtstr.7, D-91058 Erlangen

The ordered B2-phase of NiAl is stable over a wide composition range around the 1:1 stoichiometry. Therefore, atomic defects such as vacancies or antisites must exist, whose concentration - especially at grain boundaries and surfaces - may heavily influence the stability of the alloy with respect to segregation phenomena. We studied the atomic structure and energetics of the NiAl(100) surface in view of the existence of vacancies and antisites by first-principles calculations and quantitative Low-Energy Electron Diffraction (LEED). The influence of defects on the surface formation and structure and their correlation to segregation will be discussed by use of DFT-based results. The enthalpy of surface formation and the surface structure have been calculated using Density Functional Theory for the ideal surface as well as for different defect types and configurations. The results will be compared to the best-fit structure resulting from our LEED structure analysis.

O 69.3 Fri 10:45 H41

Image-potential states examined by a "Display-Type Analyzer" — •Matthias Gubo and Thomas Fauster — Lehrstuhl für Festkörperphysik, Universität Erlangen-Nürnberg, Staudtstr. 7, 91058 Erlangen

The Rydberg-like series of image-potential states is a prototype system for loosely bound electrons at a metal surface. The electronic structure and the femtosecond dynamics of these states are studied by energy- and time-resolved two-photon photoemission.

A two-dimensional, multi-angle energy analyzer is used for electron detection. It consists of an ellipsoidal mirror low pass filter, a retarding field high pass filter, microchannel plates as an area detector and an image processing system for data acquisition [1].

The image-potential states on the clean Cu(001) surface were successfully imaged. The results are in good agreement with previous measurements using hemispherical analyzers. Several methods to analyze the multidimensional data sets are discussed.
[1] D. Rieger, R. D. Schnell, W. Steinmann und V. Saile, Nucl. Instr. Methods 208 (1983) 777

O 69.4 Fri 11:00 H41

Real-space observation of the Kondo-effect on deeply burried Co-Atoms — •Alexander Weismann, Martin Wenderoth, and Rainer Ulbrich — IV. Physikalisches Institut Universität Göttingen; Friedrich Hund Platz 1; 37077 Göttingen

Isolated Co Atoms beneath the Cu(100) surface were prepared by simultaneous deposition of host-metal and impurity-compound under UHV-conditions. Scanning Tunnelling Spectroscopy performed at 6K shows highly anisotropic bulk Friedel-oscillations around the impurities which can be detected even for impurity depths of 15 ML. Due to the real-space properties of the single electron propagator, which depends decisively on details of the host-metals Fermi-surface, the electron density is only influenced in narrowly defined directions from the impurity (electron focusing). A distinct phase-shift of the LDOS-oscillations can be observed around zero bias as a direct consequence of the Kondo resonance of the Co impurity. dI/dU(U) spectra exhibit Fano-lineshapes with a spatially dependent asymmetry. These can be observed only within the regions of high LDOS-modulation while no spectral feature is present directly above a deep Co-Atom.

O 69.5 Fri 11:15 H41

Electron pair emission from surfaces excited with photons and electrons — •Frank Oliver Schumann, Carsten Winkler, and Jürgen Kirschner — Max-Planck-Institut für Mikrostrukturphysik

It has been shown theoretically that the double photoemission (DPE) intensity from an electronic system consisting of independent electrons vanishes. A non-zero DPE intensity requires electron-electron interaction. However, apart from the simultaneous ejection of two electrons upon photon absorption, another pathway of pair emission exists. It is possible that the photon is absorbed by a single electron. This electron eventually scatters from another electron, which can also lead to pair emission. The question arises to what extent the total coincidence intensity comes from a DPE process. We have addressed this issue by studying the pair emission from a Cu(111) surface excited by 50 eV photons as well as primary electron of 45 eV, which means that the maximum sum energy of the emitted pair is in both instances 40 eV. The experiments were performed with a time-of-flight spectrometer using two channelplate detectors with delay line anodes. As pulsed light source we used the BESSY storage ring in the single-bunch mode. For in-house experiments we employed a pulsed electron gun. We find that the 2D-energy distributions for photon excitation are markedly different from those obtained from electron excitation. Qualitatively this can be understood by the selection rule for double photoemission. Hence, the DPE intensity comes from the absorption of a photon followed by the ejection of an electron pair.

O 69.6 Fri 11:30 H41

Die elektronische Struktur der Ni(111) Oberfläche — •Kai-Felix Braun — Freie Universität Berlin, Arnimallee 14, 14195 Berlin

Mit Hilfe von Rastertunnelspektroskopie wurde bei tifen Temperaturen die Ni(111) Oberfläche untersucht. Punkt- und Flächenspektroskopie wurden auf der reinen und mit Einzelatomen bedeckten Oberfläche aufgenommen. Die Auswertung im Fourierraum ergibt eine hohe Auflösung eines Oberflächenzustandes. Feinstruktur und Aufspaltungen werden diskutiert. Lebensdauern der Oberflächenelektronen wurden über das Abklingverhalten der reflektierten Elektronenwellen an einer Stufenkante bestimmt. Die vergleichbar kleinen Werte sind nicht symmetrisch zur Fermienergie.Eine Oberflächenresonanz unterhalb des Oberflächenzustandes konnte nur an der Stufenkante beobachtet werden.

O 70: Methods: Atomic and Electronic Structure III

Time: Friday 10:15–12:00 Location: H42

O 70.1 Fri 10:15 H42

Positron annihilation induced Auger electron spectroscopy (PAES) of thin metal layers on Cu and Si — •Jakob Mayer[1], Christoph Hugenschmidt[1,2], Philip Pikart[1], and Klaus Schreckenbach[1,2] — [1]Technische Universität München, Physikdepartment E21, James-Franck-Str., 85748 Garching — [2]Technische Universität München, ZWE FRM-II, Lichtenbergstr. 1, 85748 Garching

The high intense positron source NEPOMUC at the FRM-II in Munich provides an intensity of $\geq 10^7$ moderated (15 eV) positrons/s. This facility enables measurement times for positron annihilation induced Auger electron spectroscopy (PAES) of a few hours/spectrum. In contrast to the usual ^{22}Na based lab beams with a measurement time of several days, at NEPOMUC a spectrum can be obtained after only three hours. Compared with conventional EAES, PAES has a much higher surface sensitivity and due to the low positron energy even weakly bound atoms/molecules at the surfaces are not destroyed by the incident positron beam. Another advantage of PAES is the low background in the energy region of the Auger peaks.

The primarily high electron background due to surrounding experiments in the experimental hall of the FRM-II has been eliminated and hence background free experiments have become possible. Measurements of single crystalline silicon, polycrystalline copper and Cu coated Si are presented and compared with EAES respectively. The results reveal the advantages and the surface sensitivity of PAES.

O 70.2 Fri 10:30 H42

Electronic band structure of the layered dichalcogenide β-MoTe$_2$ — •Robert Heimburger, Thorsten Zandt, Christoph Janowitz, and Recardo Manzke — Humboldt-Universität zu Berlin, Institut für Physik, Newtonstraße 21, 12489 Berlin

The transition metal dichalcogenide β-MoTe$_2$ grown by chemical vapour transport (CVT) at temperatures above 1175 K and cooled to room temperature shows a layered structure that can be described as stacked sandwiches of the tree layers Te-Mo-Te. One molybdenium atom is surrounded by six tellurium atoms forming an octahedron which is slightly distorted because of the molybdenium atom beeing displaced from the centre. Therefore strong metal-metal bonds are found which form zigzag chains along the crystallographic b-direction. Upon cooling below 250 K the material undergoes a structural phase transition where the β phase (monoclinic) changes to an orthorhombic Td-structure.

In this contribution we present a detailed temperature dependent study of electronic band structure and Fermi-surface of β-MoTe$_2$ performed by angle-resolved photoemission spectroscopy (ARPES). The measurements were carried out at BESSY II. It results that the dispersion of the valence bands along the different high-symmetric directions of the Brillouin zone are extremely weak. These bands reveal close insight into the low temperature and phase transition behaviour of quasi-two dimensional materials like β-MoTe$_2$. Fermi level crossings are studied by Fermi-surface maps. The experimental findings will be compared with tight-binding band structure calculations.

O 70.3 Fri 10:45 H42

Exploiting "local" in local orbital based all-electron electronic structure theory: How near can we get? — •Paula Havu, Ville Havu, Patrick Rinke, Volker Blum, and Matthias Scheffler — Fritz-Haber-Institut, Faradayweg 4-6, D-14195 Berlin, Germany

Numeric atom-centered local orbitals (NAO) are efficient basis sets for all-electron electronic structure theory. A strict localization of NAOs can be exploited to render (in principle) all operations of the self-consistency cycle $O(N)$. This is straightforward for 3D integrals using domain decomposition into spatially close subsets ("domains") of integration points, enabling critical computational savings that are effective from ∼tens of atoms (no significant overhead for smaller systems) and make large systems (hundreds of atoms and beyond) computationally feasible. Using a new all-electron NAO-based code,[1] we investigate the quantitative impact of basis orbital localization on three distinct physical classes of systems: Extended light-element biomolecules, compact transition metal clusters, and periodic bulk/surface systems. Strictly confined NAOs are achieved by imposing a cutoff potential with an onset radius r_c, and exploited by appropriately shaped integration domains. Conventional tight $r_c \leq 3$Å have no measurable accuracy impact in Alanine-based polypeptides, but introduce inaccuracies of 20-30 meV/atom in Cu$_n$ clusters. We show how a rigorous exploitation of NAO localization is critical in dense periodic systems.

[1] V. Blum, R. Gehrke, P. Havu, V. Havu, X. Ren, M. Scheffler, *The FHI Ab Initio Molecular Simulations (aims) Project*, Fritz-Haber-Institut, Berlin (2006).

O 70.4 Fri 11:00 H42

Sampling of stable and metastable cluster structures by a first-principles Monte Carlo approach — •Ralf Gehrke, Volker Blum, Karsten Reuter, and Matthias Scheffler — Fritz-Haber-Institut, Faradayweg 4-6, D-14195 Berlin

Size-selected nano-scale atomic clusters are now systematically becoming accessible in experiment, but characterizing their ground-state and metastable isomer ensemble averages from first principles requires a global and local exploration of vast configuration spaces. We here explore a first-principles Monte Carlo scheme to efficiently sample the minima of the corresponding total energy landscapes. The energetics is obtained at the density-functional theory level, using an all-electron local orbital based first principles code,[1] which allows to switch seamlessly from minimal size effective tight-binding like to meV-level chemically accurate basis sets within a single fundamental framework. The sampling strategies rely on basin hopping, using single and multiple atomic moves to create new trial structures. We demonstrate the reliability and performance of the approach for Cu and Si clusters, discussing in particular the suitability of minimal basis set runs for a coarse screening of the total energy landscapes.

[1] V. Blum, R. Gehrke, P. Havu, V. Havu, M. Scheffler, *The FHI Ab Initio Molecular Simulations (aims) Project*, Fritz-Haber-Institut, Berlin (2006).

O 70.5 Fri 11:15 H42

Efficient treatment of segregation phenomena at alloy surfaces: The UNCLE code — •Ole Wieckhorst and Stefan Müller — Universität Erlangen-Nürnberg, Lehrstuhl für Festkörperphysik, Staudtstr. 7, D-91058 Erlangen

The success of the Cluster Expansion (CE) method in alloy surface problems depends heavily on the number of Density Functional calculations (DFT) necessary to stabilize the CE Hamiltonian. That is, a "good choice" of input structures, as well as pair- and multibody figures, plays a crucial role for the efficiency of the method. In strongly ordering and symmetry-lowering systems, (surfaces, e.g.), it may even happen that other modern CE's fail to predict the system's properties. We show that our new UNCLE code efficiently selects and reduces the number of relevant layer-dependent pair and multibody interactions. Consequently, the necessary number of DFT calculations is greatly decreased. This is accomplished by use of a mixed-space representation for the bulk and a separate treatment of relaxation energies in the CE Hamiltonian. We will demonstrate that, even with these smaller input sets, the code quantitatively predicts segregation phenomena at alloy surfaces.

O 70.6 Fri 11:30 H42

Band structure mapping and calculations of $CuInS_2(001)$ — •Carsten Lehmann[1], Christian Pettenkofer[1], and Volker Eyert[2] — [1]Hahn-Meitner-Institut, SE6, Glienicker Strasse 100, 14109 Berlin, Germany — [2]Universität Augsburg, Inst. f. Physik, Universitätsstrasse 1, 86135 Augsburg, Germany

The ternary compound semiconductor $CuInS_2$ is used as an absorber material for thin film solar cells. A better understanding of the detailed electronic structure might lead to an improvement of the junction properties with respect to the still limited photo voltage of the present devices. We report on band structure mapping via ARUPS on thin epitaxial layers of $CuInS_2(001)$ 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. Samples were prepared and precharacterized in a dedicated UHV deposition and analysis system. ARUPS measurements were conducted at the beamline TGM7 at BESSY II. We will discuss the experimentally determined band structure in comparison to recent augmented spherical wave (ASW) calculations as based on density functional theory and the local density approximation (LDA). Beside earlier calculations presented by Zunger for some high symmetry directions along $k_{perpendicular}$ our calculations include for $k_{parallel}$ the experimental parameters of an ARUPS experiment thus allowing a direct comparison with our experimentally derived data rather than an idealistic run on the boundary of the brillouin-zone. Additionally we derive the effective mass from the valence band curvature.

O 70.7 Fri 11:45 H42

Geometric Analysis of Etch Pits for Intrinsic Defect Studies in Optical Crystals — •Christian Motzer and Michael Reichling — Fachbereich Physik, Universität Osnabrück, Barbarastr. 7, 49076 Osnabrück

Calcium fluoride is the material of choice in optical devices applying deep ultraviolet light. Intrinsic crystal defects, e.g. dislocations, may cause birefringence and reduce the laser damage threshold. Such defects, therefore, impose major limitations on optical lithography in the semiconductor industry. By etching the crystal surface such defects exhibit an enhanced reactivity and a characteristic etching figure remains that allows a characterisation of defects in the crystal. We have investigated the dimensions and geometry of etch pits created with hydrochloric and phosphoric acid on (111) CaF_2 cleavage plates by means of contact mode scanning force microscopy (SFM). By comparing geometric data, we can differentiate between two basic types. One etch pit type is related to dislocation defects terminating on the surface. Our measurements showed that the depth of those etch pits relates to the angle between the surface and the direction of dislocations. The other etch pit type is related to nm-sized local defects and has a typical geometric characteristic which differs from that of dislocation etch pits. High resolution SFM images reveal that there is a distinct transition when the core of these defects is dissolved. By comparing geometric data, we can differentiate between combinations of dislocations and these local defects.