OBERFLÄCHENPHYSIK (O)

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ÜBERSICHT DER HAUPTVORTRÄGE UND FACHSITZUNGEN

(Hörsäle TU EB107, TU EB202, TU EB301, TU EB407, TU EB420, TU H3005, TU A151)

Hauptvorträge

O 1.1	Fr	09:45	(TU EB301)	**Ultrafast dynamics of coherent lattice and spin excitations at the Gd(0001) surface**, Uwe Bovensiepen
O 8.1	Fr	14:00	(TU EB301)	**Dimensionality-dependent magnetic properties: from single atoms at surfaces to 1D and 2D structures**, Pietro Gambardella
O 9.1	Fr	14:45	(TU EB301)	**Structure and stability of binary alloy surfaces: Segregation, relaxation, and ordering from first-principles calculations**, Stefan Müller
O 16.1	Sa	09:00	(TU EB301)	**Low-dimensional electrons at silicon surfaces**, Franz J. Himpsel
O 17.1	Sa	09:45	(TU EB301)	**Order-disorder Surface Phase Transitions from First-principles**, Catherine Stampfl, M. Borg, A. Mikkelsen, J. Gustafson, E. Lundgren, M. Scheffler, J.N. Andersen
O 23.1	Sa	14:00	(TU EB301)	**Electron dynamics at surfaces**, Pedro M. Echenique
O 29.1	Mo	09:45	(TU EB301)	**Femtosecond dynamics of adsorbate-surface interactions studied by means of time-resolved photoelectron spectroscopy**, Michael Bauer
O 35.1	Mo	14:00	(TU EB301)	**Die Bayes'sche Variante**, Volker Dose
O 37.1	Di	09:45	(TU EB301)	**Silicon Carbide Surfaces: Metallization versus Passivation**, Patrick Soukiassian
O 43.1	Di	14:00	(TU EB301)	**Structure and growth of thin films of aromatic molecules on solid surfaces**, Gregor Witte
O 44.1	Di	14:45	(TU EB301)	**Diamond surfaces: familiar and amazing**, Jürgen Ristein
O 51.1	Mi	09:45	(TU EB301)	**Electronic structure of organic interfaces**, Thorsten Ulrich Kampen

Fachsitzungen

O 1	**Hauptvortrag Bovensiepen**	Fr 09:45–10:30	TU EB301	O 1.1–1.1
O 2	**Organische Dünnschichten I**	Fr 10:45–13:00	TU EB301	O 2.1–2.9
O 3	**Oberflächenreaktionen I**	Fr 10:45–13:00	TU EB420	O 3.1–3.9
O 4	**Epitaxie und Wachstum I**	Fr 10:45–13:00	TU EB202	O 4.1–4.9
O 5	**Zeitaufgelöste Spektroskopie I**	Fr 10:45–13:00	TU EB107	O 5.1–5.9
O 6	**Grenzfläche fest-flüssig**	Fr 10:45–13:00	TU EB407	O 6.1–6.9
O 7	**Symposium Recent Progress in Scanning Probe Methods**	Fr 11:00–13:00	TU H3005	O 7.1–7.4
O 8	**Hauptvortrag Gambardella**	Fr 14:00–14:45	TU EB301	O 8.1–8.1
O 9	**Hauptvortrag Müller**	Fr 14:45–15:30	TU EB301	O 9.1–9.1
O 10	**Adsorption an Oberflächen I**	Fr 15:45–17:00	TU EB301	O 10.1–10.5
O 11	**Elektronische Struktur I**	Fr 15:45–17:00	TU EB420	O 11.1–11.5
O 12	**Nanostrukturen I**	Fr 15:45–17:00	TU EB202	O 12.1–12.5

O 13	**Magnetismus**	Fr	15:45–17:00	TU EB107	O 13.1–13.5
O 14	**Struktur und Dynamik reiner Oberflächen**	Fr	15:45–16:45	TU EB407	O 14.1–14.4
O 15	**Postersitzung (Adsorption an Oberflächen, Epitaxie und Wachstum, Organische Dünnschichten, Oxide und Isolatoren, Rastersondentechniken, Zeitaufgelöste Spektroskopie, Methoden)**	Fr	17:00–20:00	Poster TU D	O 15.1–15.84
O 16	**Hauptvortrag Himpsel**	Sa	09:00–09:45	TU EB301	O 16.1–16.1
O 17	**Hauptvortrag Stampfl**	Sa	09:45–10:30	TU EB301	O 17.1–17.1
O 18	**Adsorption an Oberflächen II**	Sa	10:45–13:00	TU EB301	O 18.1–18.9
O 19	**Nanostrukturen II**	Sa	10:45–13:00	TU EB420	O 19.1–19.9
O 20	**Organische Dünnschichten II**	Sa	10:45–13:00	TU EB202	O 20.1–20.9
O 21	**Elektronische Struktur II**	Sa	10:45–13:00	TU EB107	O 21.1–21.9
O 22	**Rastersondentechniken I**	Sa	10:45–13:00	TU EB407	O 22.1–22.9
O 23	**Hauptvortrag Echenique**	Sa	14:00–14:45	TU EB301	O 23.1–23.1
O 24	**Teilchen und Cluster I**	Sa	15:00–17:00	TU EB301	O 24.1–24.8
O 25	**Zeitaufgelöste Spektroskopie II**	Sa	15:00–17:00	TU EB420	O 25.1–25.8
O 26	**Oxide und Isolatoren I**	Sa	15:00–17:00	TU EB202	O 26.1–26.8
O 27	**Phasenübergänge**	Sa	15:00–16:45	TU EB107	O 27.1–27.7
O 28	**Methodisches (Exp. und Theorie)**	Sa	15:00–17:00	TU EB407	O 28.1–28.8
O 29	**Hauptvortrag Bauer (Gaede-Preis)**	Mo	09:45–10:30	TU EB301	O 29.1–29.1
O 30	**Adsorption an Oberflächen III**	Mo	10:45–13:00	TU EB301	O 30.1–30.9
O 31	**Organische Dünnschichten III**	Mo	10:45–13:00	TU EB420	O 31.1–31.9
O 32	**Nanostrukturen III**	Mo	10:45–13:00	TU EB202	O 32.1–32.9
O 33	**Teilchen und Cluster II**	Mo	10:45–13:00	TU EB107	O 33.1–33.9
O 34	**Rastersondentechniken II**	Mo	10:45–13:00	TU EB407	O 34.1–34.9
O 35	**Hauptvortrag Dose (R.W. Pohl-Preis)**	Mo	14:00–14:45	TU EB301	O 35.1–35.1
O 36	**Postersitzung (Elektronische Struktur, Grenzfläche fest-flüssig, Halbleiteroberflächen und -grenzflächen, Nanostrukturen, Oberflächenreaktionen, Teilchen und Cluster, Struktur und Dynamik reiner Oberflächen)**	Mo	15:00–18:00	Poster TU F	O 36.1–36.79
O 37	**Hauptvortrag Soukiassian**	Di	09:45–10:30	TU EB301	O 37.1–37.1
O 38	**Halbleiteroberflächen und -grenzflächen**	Di	10:45–13:00	TU EB301	O 38.1–38.9
O 39	**Nanostrukturen IV**	Di	10:45–13:00	TU EB420	O 39.1–39.9
O 40	**Adsorption an Oberflächen IV**	Di	10:45–13:00	TU EB202	O 40.1–40.9
O 41	**Elektronische Struktur III**	Di	10:45–13:00	TU EB107	O 41.1–41.9
O 42	**Oberflächenreaktionen II**	Di	10:45–13:00	TU EB407	O 42.1–42.9
O 43	**Hauptvortrag Witte**	Di	14:00–14:45	TU EB301	O 43.1–43.1
O 44	**Hauptvortrag Ristein**	Di	14:45–15:30	TU EB301	O 44.1–44.1
O 45	**Organische Dünnschichten IV**	Di	15:45–18:30	TU EB301	O 45.1–45.11
O 46	**Adsorption an Oberflächen V**	Di	15:45–18:30	TU EB420	O 46.1–46.11
O 47	**Rastersondentechniken III**	Di	15:45–18:30	TU EB202	O 47.1–47.11
O 48	**Oxide und Isolatoren II**	Di	15:45–18:30	TU EB107	O 48.1–48.11
O 49	**Epitaxie und Wachstum II**	Di	15:45–18:30	TU EB407	O 49.1–49.11
O 50	**Postdeadline-Session**	Di	20:00–21:00	TU A151	O 50.1–50.4
O 51	**Hauptvortrag Kampen**	Mi	09:45–10:30	TU EB301	O 51.1–51.1
O 52	**Elektronische Struktur IV**	Mi	10:45–13:00	TU EB301	O 52.1–52.9
O 53	**Organische Dünnschichten V**	Mi	10:45–13:00	TU EB420	O 53.1–53.9
O 54	**Adsorption an Oberflächen VI**	Mi	10:45–13:00	TU EB202	O 54.1–54.9
O 55	**Epitaxie und Oberflächenreaktionen**	Mi	10:45–13:00	TU EB107	O 55.1–55.9

Mitgliederversammlung des Fachverbands Oberflächenphysik

Di 19:30–20:00 A151 (Architekturgebäude)

Vorläufige Tagesordnung:

- Bericht des Fachverbandsvorsitzenden
- Verschiedenes

HINWEISE:

Postersitzung O7 am Freitag (17:00-20:00) im Bereich TU D (HG 3. OG)
Die Poster können ab Freitagmorgen aufgehängt werden und sollen nach der Postersitzung entfernt werden.
Der Abend wird unterstützt von **Omicron Vakuumphysik GmbH**.

Postersitzung O36 am Montag (15:00-18:00) im Bereich TU F (PN unten)
Die Poster können ab Montag 8:00 Uhr aufgehängt werden und sollten nach der Postersitzung entfernt werden.

Postdeadlinesitzung O50 am Dienstag von 20:00-21:00 Uhr im Hörsaal TU A151 (Architekturgebäude), von 21:00-23:30 Uhr im Foyer des Architekturgebäudes
Deadline für die Einladung ist der 15. Februar 2004.
Die Sitzung wird unterstützt von **SPECS GmbH** zusammen mit **BESTEC GmbH**, **VTS CREATEC GmbH** und **Oxford Scientific Ltd**.

GEMEINSAME VERANSTALTUNGEN UND SYMPOSIEN MIT ANDEREN FACHVERBÄNDEN:

O7 Symposium Recent Progress in Scanning Probe Methods
Freitag, 04.03.2005, 10:15-13:00 Uhr, Hörsaal TU HE101 (1. Vortrag Rugar, gemeinsam mit SYQL)
Fortsetzung 11:00 Uhr, Hörsaal TU H3005

DS21 Symposium Optical Spectroscopy of Thin Films and Interfaces
Dienstag, 08.03.2005, 09:45-13:30 und 14:30-16:45 Uhr, Hörsaal TU H110

SYSR Symposium Highlights in Synchrotron Radiation Research
Samstag, 05.03.2005, 08:30-13:00 Uhr, Hörsaal TU HE101

SYOO Symposium Optoelectronics and Photonics
Montag, 07.03.2005, 14:00 Uhr, Hörsaal TU HE101

Fachsitzungen

– Haupt-, Fach-, Kurzvorträge und Posterbeiträge –

O 1 Hauptvortrag Bovensiepen

Zeit: Freitag 09:45–10:30 Raum: TU EB301

Hauptvortrag

O 1.1 Fr 09:45 TU EB301

Ultrafast dynamics of coherent lattice and spin excitations at the Gd(0001) surface — •Uwe Bovensiepen — Freie Universität Berlin, Fachbereich Physik, Arnimallee 14, 14195 Berlin

The dynamics of collective excitations of electrons, spins and phonons are of fundamental interest to develop a microscopic understanding of elementary interactions and relaxation mechanisms of these quasiparticles. Based on magnetoelasticity, magnon-phonon interaction is usually attributed to spin-orbit coupling which transfers a displacement of ion cores in the lattice to the spin system and vice versa. However, a microscopic picture is generally not available. Here, ferromagnetic Gd(0001) characterized by a very weak spin-orbit coupling and its exchange-split d_{z^2}-surface state serves as a model system for such coupled phonon-magnon modes, which can be excited coherently by femtosecond laser pulses. Gd(0001) is investigated by complimentary pump-probe-experiments of non-linear optical second harmonic generation (SHG) and time-resolved photoemission (TRPE). SHG separates electron/lattice and spin dynamics by their symmetry with respect to magnetization reversal. A coherent phonon-magnon mode at 2.9 THz is observed in the transient SHG response, which is driven by electronic excitation of surface and bulk states and is damped by scattering with electrons as well as thermalized phonons and spin waves. TRPE adds information on the interaction mechanism. We find that the binding energy of the surface state oscillates at 3 THz as well, which suggests a parametric phonon-magnon-coupling by modulation of the exchange splitting, contrary to the conventional type mediated by spin-orbit-interaction.

O 2 Organische Dünnschichten I

Zeit: Freitag 10:45–13:00 Raum: TU EB301

O 2.1 Fr 10:45 TU EB301

Investigating the stability of the tetracene/Al_2O_3-interface with high-resolution electron energy loss spectroscopy and LEED — •R. Temirov[1], A. Langner[2], M. Sokolowski[2], and F.S. Tautz[1] — [1]International University Bremen, School of Engineering and Science, PO Box 750761, D-28725 Bremen — [2]Institut für Physikalische und Theoretische Chemie, Universität Bonn, Wegelerstr. 12, D-53115 Bonn

Surprisingly, fluorescence of tetracene molecules in contact with a sapphire substrate is quenched, in spite of the fact that the high band gap of Al_2O_3 should provide an effective barrier to charge delocalisation [1]. The reappearance of luminescence after annealing thin tetracene layers to 240 K can be explained by a reduction of the tetracene/substrate interaction, either by molecular reorientation or dewetting of the interface. Here we report an HREELS investigation of the interface between thin epitaxial Al_2O_3-layers on $Ni_3Al(111)$ and tetracene. Our experiments show that under the current deposition conditions (thermal evaporation onto a sample at T=80K) at least some tetracene molecules are oriented with their molecular plane parallel to the substrate. The maximized contact area between molecule and substrate may be an important factor in understanding the observed luminescence quenching. Our data also suggest that after annealing, contact area is minimized by the formation of three-dimensional tetracene islands. [1] M. Schneider, E. Umbach, A. Langner, M. Sokolowski, Journal of Luminescence 110, 275-283 (2004).

O 2.2 Fr 11:00 TU EB301

Tripod Liganden für starre und geordnete selbstorganisierte Monolagen auf Gold — •T. Weidner[1,2], A. Krämer[3,2], U. Siemeling[3,2] und F. Träger[1,2] — [1]Institut für Physik, Universität Kassel, Heinrich-Plett-Str. 40, 34132 Kassel — [2]Center for Interdisciplinary Nanostructure Science and Technology - CINSaT, Universität Kassel, Heinrich-Plett-Str. 40, 34132 Kassel — [3]Institut für Chemie, Universität Kassel, Heinrich-Plett-Str. 40, 34132 Kassel

Selbstorganisation maßgescheiderter Moleküle auf Oberflächen ist ein verbreitetes und vielversprechendes Konzept, hoch geordnete funktionelle monomolekulare Schichten auf Edelmetalloberflächen zu präparieren. Entscheidend für Anwendungen in Katalyse, Sensorik und Datenspeicherung ist es, eine definierte und stabile Anordnung der funktionellen Einheiten zu gewährleisten.

Um dieses Ziel zu erreichen, haben wir äußerst starre, tripodale Tris[(methylthio)-methyl]silyl Ankergruppen synthetisiert. Untersuchungen der Phenyl- und Biphenylderivate dieser "dreibeinig" aufgebauten Ankergruppe auf Goldsubstraten mit Infrarotspektroskopie und Rastertunnelmikroskopie, sowie der Adsorptions- und Ordnungskinetik mit optischer Frequenzverdopplung und Ellipsometrie zeigen deutlich, dass beide Verbindungen auf Gold adsorbieren. Darüber hinaus konnte die Entstehung sehr stabiler und geordneter Phenyl- und Biphenyl-Monolagen in situ verfolgt werden.

O 2.3 Fr 11:15 TU EB301

Molekulare Magnete auf Oberflächen — •Miriam Klusmann, Andrea Kahlen und Marika Schleberger — Universität Duisburg-Essen, Fachbereich Physik, 45117 Essen

Durch geeignete Präparationstechniken wurden die magnetischen Moleküle Ti4 und Mo72Fe30 auf die Schichtsubstrate Glimmer und HOPG aufgebracht. Untersuchungen mit den Rastersondenmethoden AFM (*Atomic Force Microscopy*, Rasterkraftmikroskopie) und STM (*Scanning Tunneling Microscopy*, Rastertunnelmikroskopie) zeigen eine Ausbildung von Ti4-Inseln auf Glimmer sowie die Selbstorganisation von Mo72Fe30 auf HOPG. Da das Lösungsmittel Dichlormethan, welches zur Deponierung von Ti4 auf Glimmer verwendet wird, einen ungünstigen Einfluss auf das Substrat nimmt, ist eine qualitative Auswertung der aus AFM-Messungen gewonnenen Topographie-Daten nur unter Berücksichtigung der simultan aufgezeichneten Signale der Frequenzverschiebung und der Dämpfung der Cantilever-Oszillation möglich. Die Adsorption von Mo72Fe30 ist abhängig von der Konzentration der Moleküle in Lösung, so dass sich verschiedene Strukturen auf dem HOPG-Substrat ausbilden - von Ringen über Ketten bis hin zu Einfach- oder Mehrfachlagen.

O 2.4 Fr 11:30 TU EB301

Aliphatic selenolates on gold and silver substrates — •Andrey Shaporenko[1], Avi Ulman[2], Andreas Terfort[3] und Michael Zharnikov[1] — [1]Angewandte Physikalische Chemie, Universität Heidelberg, Im Neuenheimer Feld 253, 69120 Heidelberg, Germany — [2]Department of Chemical Engineering, Polytechnic University, Brooklyn 11201, New York, USA — [3]Anorganische und Angewandte Chemie, Universität Hamburg, 20146 Hamburg, Germany

We studied self-assembled monolayers (SAMs) formed from didodecyl diselenide (C12SeSeC12) and didodecyl selenide (C12SeC12) on (111) Au and Ag substrates. C12SeSeC12 was found to form contamination-free, densely-packed, and well-ordered C12Se SAMs on both substrates, whereas the adsorption of C12SeC12 occurred only on Au and resulted in the formation of a SAM-like C12SeC12 film with a low packing density and a conformational disorder. The properties of the C12Se SAMs were compared with those of dodecanethiolate (C12S) SAMs. The packing density, orientational order, and molecular inclination in C12Se/Au and C12S/Au were found to be very similar. In contrast, C12Se/Ag exhibited significantly lower packing density, a lower degree of the conformational and orientational order, and a larger molecular inclination than C12S/Ag. The results suggest a sp^3 bonding configuration for the selenium atom on Au and Ag and indicate a larger corrugation of the headgroup-substrate binding energy surface in C12Se/Ag than in C12S/Ag.

O 2.5 Fr 11:45 TU EB301

Periodical density functional theory study of the bonding of aromatic organic molecules containing carboxylate group on metal surfaces — •Nicolae Atodiresei, Azadeh Farahzadi, Kurt Schroeder, and Stefan Blügel — Institut für Festkörperforschung, Forschungszentrum Jülich, D-52425 Jülich, Germany

The family of five-membered heterocycles and its derivates is of basic importance in chemistry and physics. Much work is now undertaken in molecular self-assembly experiments which lead to oriented growth of organic films. We study the structure of adsorbed carboxylic acids containing furan, thiophene, selenophene and tellurophene aromatic rings in a (2x1) cell on Cu(110) surface by ab initio calculations. In the stable configuration the molecules sit perpendicular in bridge position above the first Cu-surface layer with the carboxylate group oriented along to the $[1\bar{1}0]$ direction. In the gas phase the single molecule has a planar geometry with an extended π-system over the five-membered ring and carboxylate group. The adsorption of the molecules breaks this planarity. Due to the strong lateral interactions between the hydrogen atoms of neighboring adsorbed molecules the rings are rotated by $\sim 24°$ relative to the carboxylate group.

O 2.6 Fr 12:00 TU EB301

Growth of thin para-sexiphenyl films on Cu(110) and Cu(110)-(2x1)O — •K. Maschek, Y. Hu, L.D. Sun, M. Hohage, and P. Zeppenfeld — Institut für Experimentalphysik, Johannes-Kepler-Universität Linz, Austria

Para-sexiphenyl (P6P) has attracted considerable interest as a promising candidate for future organic opto-electronic applications. Its molecular structure consists of a linear chain of six linked benzene rings showing strong π bond delocalization in the direction of the chains. Previous research shows that the optical absorption of P6P films depends strongly on the molecular orientation. On the other hand, Reflectance Difference Spectroscopy (RDS) has been demonstrated to be a powerful tool to measure the optical anisotropy at normal incidence. Here, we present a RDS investigation of para-sexiphenyl thin film growth on Cu(110) and Cu(110)-(2x1)O. The RDS spectra show a pronounced anisotropy of the P6P films formed on both substrates at room temperature, indicating preferential orientation of P6P molecules on these two atomically well defined substrates: On Cu(110), the P6P molecular chains align in the $[1\bar{1}0]$ direction, i.e., along the Cu atomic rows, while on the Cu(110)-(2x1)O surface, the molecules align in the orthogonal [001] direction, i.e., along the Cu-O rows formed on Cu(110). Additionally, the evolution of the RDS signal at different photon energies during growth provides detailed information about the growth mode of P6P on both substrates.

O 2.7 Fr 12:15 TU EB301

Ab-initio investigation of organic molecules on metal surfaces:3-nitrothiophen/selenophen/tellurophen on Cu(110) — •Azadeh Farahzadi[1,2], Nicolae Atodiresei[1], Stefan Blügel[1], and Kurt Schroeder[1] — [1]Institut für Festkörperforschung, Forschungszentrum Jülich, 52425 Jülich — [2]I.Physikalisches Institut, RWTH-Aachen Sommerfeldstraße 14, 52074

The future of nanoelectronics may consist in hybrid structures build of organic molecules and inorganic materials. The interesting family of five-member heterocycles which includes thiophen/selenophen/tellurophen rings, plays an important role in constructing the charge carrier polymers. Based on the density functional theory (DFT) in the generalized gradient approximation (GGA), we have optimized the geometric structure of the single molecules, 3-nitrothiophen/selenophene/tellurophen and the dense-packed structure ((2×1) unit cell) of these molecules on the Cu(110) surface. In the stable configuration the molecules sit perpendicular to the surface with the nitro group ($-NO_2$) along the [110] direction. In the gas phase the single molecules have a planar geometry but the adsorption of the molecules breaks this planarity. We discuss the electronic structure and the binding energy of the molecule at the surface. The calculations have been carried out using the PAW-method EStCoMPP.

O 2.8 Fr 12:30 TU EB301

Transfer and amplification of chirality in hydrocarbon monolayers — •Karl-Heinz Ernst, Manfred Parschau, Roman Fasel, and Sara Romer — Empa-Materials Science and Technology, 8600 Duebendorf, Schweiz

We present a new form of chirality transfer and amplification observed in two-dimensional monolayers. In the first case, a special surface enantiomorphism is observed via STM after adsorption of the enantiomers of a helical aromatic hydrocarbon on Cu(111) at 50 K. Instead of crystallization into homochiral domains on the surface, racemic mirror domains are observed, i.e., they possess an equimolar content of left- and right-handed molecules. In this situation, a small excess of one chiral species is sufficient to create domains of a single handedness throughout the whole surface layer. In the second case, homochirality was induced in monolayers of achiral molecules after chiral doping. Achiral molecules can become chiral when adsorbed at surfaces because of the reduced symmetry in the molecule or the adsorbate lattice. Adsorbed on Cu(110), succinic acid forms equal numbers of left- and right-handed domains and the surface is globally achiral. Doping with small amounts of left- or right-handed tartaric acid, however, creates homochirality and the opposite mirror domains are not observed anymore in the LEED pattern. Our findings are explained by cooperative interactions and will be discussed in the frame of a one-dimensional random-field Ising model.

O 2.9 Fr 12:45 TU EB301

STM investigations of ordered monolayers of tetralactam macrocycles on Au(111) — •Iordan Kossev and Moritz Sokolowski — Institut für Physikalische und Theoretische Chemie, Universität Bonn, Wegelerstr. 12, 53115 Bonn, Germany

Rotaxanes and catenanes are of interest for the investigation on mechanically interlocked molecules [1]. A large tetralactam - macrocycle (905.05 amu), very often used as a building block for catenanes, was deposited onto the Au(111) surface in UHV from a thermal evaporation cell. STM images were taken for different coverages at room temperature. At a coverage around one monolayer, different long range ordered monolayer structures were observed with submolecular resolution on the terraces. After annealing to 400 K, in addition to the two dimensional structures, chains of well ordered molecules adsorbed at step edges were observed. We explain these STM images by structure models based on a weak interaction of the molecules to the Au(111) surface and a considerable intermolecular interaction due to hydrogen bonds. The macrocycles were kindly supplied by C. Schalley and F. Vögtle. This work was supported by the DFG (SFB 624).

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

O 3 Oberflächenreaktionen I

Zeit: Freitag 10:45–13:00 Raum: TU EB420

O 3.1 Fr 10:45 TU EB420

Investigation of Au/TiO_2 model catalysts prepared from micellar stabilized gold particles — •S. Kielbassa[1], F. Weigl[2], A. Ethirajan[2], H.G. Boyen[2], P. Ziemann[2] und R.J. Behm[1] — [1]Abt. Oberflächenchemie und Katalyse, Universität Ulm, 89069 Ulm — [2]Abt. Festkörperphysik, Universität Ulm, 89069 Ulm

Metal oxide supported Au catalysts have attracted considerable interest over the last years because of their high activity for low-temperature oxidation and hydrogenation reactions. For studying particle size and transport effects, we prepared model systems with a narrow distribution for particle sizes and particle separations by depositing Au loaded diblock copolymer micelles onto atomically smooth TiO_2 (110) rutile substrates. Removing of the polymer shells in an oxygen plasma leads to a hexagonal arrangement of Au particles. The stability of these model systems in typical activation and reaction atmospheres/temperatures as well as their activity for CO oxidation under high pressure conditions was investigated for different particle sizes and seperations. Consequences on the reaction mechanism are discussed.

O 3.2 Fr 11:00 TU EB420

Catalytic properties of UHV-prepared Au/TiO_2-model systems at elevated pressures up to 100 mbar — •Thomas Diemant, Zhong Zhao, Hubert Rauscher, and R. J. Behm — Abt. Oberfächenchemie und Katalyse, Universität Ulm, 89069 Ulm

Oxide supported Au catalysts have found increasing interest because of their high activity for various oxidation and reduction reactions. For model studies under realistic reaction conditions we performed in-situ IR spectrocopy (PEM-IRAS) and rate measurements for CO oxidation on structurally (STM) [1] and chemically (XPS, CO-TPD) well-defined model catalysts, prepared by Au deposition on thin TiO_2 films at pressures up to 100 mbar. Results for various Au particle sizes, temperatures, and partial pressures are presented and discussed in comparison with data obtained on real catalysts. Consequences for the reaction mechanism are derived.

[1] Zhong Zhao et al., DPG-Frühjahrstagung AKF Oberflächenphysik, Berlin (2005)

O 3.3 Fr 11:15 TU EB420

Reduction of the Surface Oxide Layer on Rh(111) by CO and H_2 — •Jan Klikovits[1], Michael Schmid[1], Edvin Lundgren[2], Jasper N. Andersen[2], Lukas Köhler[3], Georg Kresse[3], and Peter Varga[1] — [1]Institut für Allgemeine Physik, TU Wien, A-1040 Wien, Austria — [2]Department of Synchrotron Radiation Research, Lund University, Box 118, S-221 00, Sweden — [3]Inst. f. Materialphysik, Universität Wien, A-1090 Wien, Austria

We have studied the surface oxide on Rh(111) and its reduction by CO and H_2. The structure of the surface oxide has already been solved [1]. Reducing the oxide by CO requires temperatures of about 100 °C. Essentially all CO adsorbs at reduced areas, thus the reduction rate increases while the amount of oxide decreases at the surface. STM images show that the reduction starts at step edges and islands. A (2 x 2) superstructure is observed in the reduced areas. We argue that the CO molecules are immobilized by a oxygen superstructure which is in thermodynamic equilibrium with the oxide. The reduction of the surface oxide by H_2 was observed in-situ by STM. It starts already at room temperature, almost exclusively in stepped areas. We can also initiate the reduction process by deliberately creating defects with the STM tip allowing us to examine the reduction kinetics in detail. At low H_2 pressures or small reduced areas the reduction rate is limited by the hydrogen adsorption on the reduced area. For large reduced areas the reduction rate is limited by the processes at the border of the reduced area.

[1]: J. Gustafson et al., Phys. Rev. Lett 92, 126102, (2004).

O 3.4 Fr 11:30 TU EB420

Hydrogen Transfer Reaction on the Surface of an Oxide catalyst — •Daniela Crihan, Marcus Knapp, and Herbert Over — Phys.Chem.Institut, Justus Liebig Univ. Giessen, D-35392 Giessen

RuO_2(110) exposes two kinds of active surface species (acidic and basic centers) which govern the interaction of the gas phase in contact with the catalysts surface. Here we will elucidate the cooperative interplay of these two active surface sites for a simple model reaction, namely the water formation over RuO_2(110) catalysts when supplying hydrogen and oxygen from the gas phase. The bridging O atoms harvest the hydrogen from the gas phase, while the on-top O atoms picks up those adsorbed hydrogen atoms from the bridging O atoms to form water. This mechanism of hydrogen transfer is mediated by a strong hydrogen bond. Hydrogen transfer is expected to play a vital role for the whole class of catalyzed hydrogenation and dehydrogenation reactions of hydrocarbons over RuO_2(110).

O 3.5 Fr 11:45 TU EB420

Interaction of Hydrogen with RuO_2(110) Surfaces — •Yuemin Wang[1,2], Jinhai Wang[2], Chaoyang Fan[2], Karl Jacobi[2], and Gerhard Ertl[2] — [1]Lehrstuhl für Physikalische Chemie I, Ruhr-Universität Bochum — [2]Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin

The adsorption and reaction of hydrogen on the stoichiometric and oxygen-rich RuO_2(110) surfaces - the latter exposing a weakly bound atomic oxygen species (O-cus) on-top of the unsaturated Ru atom (Ru-cus) - was studied using high-resolution electron energy-loss spectroscopy (HREELS) and thermal desorption spectroscopy (TDS). On the stoichiometric RuO_2(110) surface two hydrogen adsorption states are identified at 85 K [1]: Molecular hydrogen at Ru-cus and dissociated hydrogen forming a dihydride with O-bridge, the other unsaturated surface oxygen besides O-cus. The dihydride is transformed into monohydride by release of hydrogen at 350 K. On oxygen-rich RuO_2(110) surfaces hydrogen reacts with O-cus forming H_2O-cus. This species undergoes desorption instead of dissociation with heating to higher temperatures. The reaction mechanisms of hydrogen with O-bridge and O-cus are derived.

[1] Wang, J.; Fan, C. Y.; Sun, Q.; Reuter, K.; Jacobi, K.; Scheffler, M.; Ertl, G. Angew. Chem. Internat. Edition 2003, 42, 2151.

O 3.6 Fr 12:00 TU EB420

Interaction of supported Pd nanoparticles with H, O and C — •Günther Rupprechter, Matthias Morkel, Marta Borasio, and Hans-Joachim Freund — Fritz-Haber-Institut, Faradayweg 4-6, 14195 Berlin

Vibrational sum frequency generation (SFG) spectroscopy, thermal desorption spectroscopy (TDS) and photoelectron spectroscopy (XPS) were utilized to examine the interaction of Al_2O_3 supported Pd nanoparticles with hydrogen, oxygen and methanol. Experiments were performed both under ultrahigh vacuum (UHV) as well as mbar pressure. The Pd nanoparticles had a mean size of 5 nm and exhibited mostly (111) facets.

Pd-hydride formation was observed to proceed predominantly via minority sites on Pd nanoparticles, i.e. defects and (100) faces. Explosive hydrogen desorption through a CO overlayer originates from the confinement of dissolved hydrogen within the limited nanoparticle volume. The oxidation of Pd nanoparticles under UHV and mbar pressure also seems to be strongly influenced by defects. Carbonaceous deposits that appear during methanol decomposition and oxidation are located both in surface and subsurface positions. A possible involvement of CH_x species in the oxidation reaction is discussed.

O 3.7 Fr 12:15 TU EB420

Surface Diffusion and Fluctuations on Catalyst Nanoparticles — •Mathias Laurin[1], Viktor Johánek[1], Ann W. Grant[2], Bengt Kasemo[2], Jörg Libuda[1], and Hans-Joachim Freund[1] — [1]Fritz-Haber-Institut der Max-Planck-Gesellschaft, Faradayweg 4–6, 14195 Berlin, Germany — [2]Department of Applied Physics, Chalmers University of Technology, 41296, Göteborg, Sweden

The CO oxidation and oxygen diffusion kinetics are investigated using molecular beam methods under ultrahigh vacuum (UHV). We employ oxide supported Pd nanoparticles prepared by physical vapor deposition (PVD) and electron beam lithography (EBL) covering a large range of particle sizes (1–500 nm).

The angular resolved distribution of CO_2 depends on the reaction conditions and particle size. In combination with the experiments, microkinetic simulations give information on the mobility of the adsorbed species under reaction conditions and on the local reaction rates on the particle surface.

A macroscopic bistability of the reaction is observed at low temperatures on the big particles. It is however quenched on small nanoparticles. This is attributed to fluctuation induced transitions, accelerated in the presence of defect sites.

O 3.8 Fr 12:30 TU EB420

In-situ high resolution XPS study of the CO oxidation on Pt(355) — •Barbara Tränkenschuh, Thomas Fuhrmann, Christian Papp, Daniel Kiessling, Reinhard Denecke, and Hans-Peter Steinrück — Lehrstuhl für Physikalische Chemie II, Universität Erlangen-Nürnberg, Egerlandstr. 3, 91058 Erlangen

The oxidation of CO on the stepped Pt(355)=[5(111)x(111)] surface was studied by in-situ high resolution XPS experiments at BESSY II. The different species and adsorption sites (O, CO on-top/bridge) on steps and terraces are clearly distinguishable in O 1s or C 1s spectra. In the experiments first an oxygen layer was prepared using a procedure, which leads to a p(2x2)-O-LEED pattern on Pt(111). On Pt(355), however, no ordered adsorbate structure was observed. Therefore, the coverages of the reactants (O, CO) were estimated by comparing the XPS intensities with those observed on Pt(111) [1]. CO was dosed by a supersonic molecular beam, which allows to vary the CO pressure on the sample. The oxidation was studied as a function of reaction temperature and CO pressure on the sample by recording time-dependent O 1s and C 1s intensities. Measurable reaction rates on Pt(355) are observed at much lower temperatures than on Pt(111) (200 vs. 270 K, respectively) [1]. The reaction product CO_2 was additionally detected by mass spectrometry. Supported by the DFG (STE 620/4-2).

[1] M. Kinne et al., J.Chem. Phys. 120 (2004) 7113.

O 3.9 Fr 12:45 TU EB420

Messungen an einer YSZ/Pt-Gasreferenzzelle zur elektrochemischen Promotion katalytischer Reaktionen — •Tobias Neubrand[1], Sebastian Günther[2] und Ronald Imbihl[1] — [1]Institut für Physikalische Chemie und Elektrochemie, Universität Hannover, Callinstraße 3-3a, 30167 Hannover — [2]LMU München, Department Chemie, Butenandstr.11 E, 81377 München

Während elektrochemischen Pumpens ändert sich bei Festelektrolyt/Metall-Systemen die Austrittsarbeit des Metalls. Es wurde eine 1:1 Beziehung zwischen Austrittsarbeitsänderung und eingestellter Spannung postuliert, die aber nur teilweise durch Messergebnisse bestätigt werden konnte. Zur Klärung dieser Frage wurde eine gasdichte elektrochemische Zelle für den Einsatz im UHV aufgebaut, bei der auf einem YSZ-Festkörperelektrolyten die Elektroden durch Aufsintern einer Pt-Paste aufgebracht wurden. Ein fester Sauerstoff-Referenzdruck verhindert das Verschieben des Referenzpotentials durch Anreduktion von YSZ. An dieser Zelle konnten Ratenmessungen der katalytischen CO-Oxidation an Pt mit Messungen der Austrittsarbeit korreliert werden, die integral über eine Kelvin-Sonde und lokal über Photoelektronenemissionsmikroskopie (PEEM) bestimmt wurden. Die verschiedenen Beiträge zu Kelvinsondenmessungen der Austrittsarbeit konnten damit identifiziert werden: Ein elektrostatischer durch Aufladung der Elektroden und ein ëchter", der durch SSpillover"von O-Ionen von YSZ zur Pt-Oberfläche zustande kommt.

O 4 Epitaxie und Wachstum I

Zeit: Freitag 10:45–13:00 Raum: TU EB202

O 4.1 Fr 10:45 TU EB202

Unidirectional patterning of transition-metal films on Ir(100) — •Chiara Giovanardi, Andreas Klein, Andreas Schmidt, Lutz Hammer, and Klaus Heinz — Lehrstuhl für Festkörperphysik, Universität Erlangen Nürnberg, Staudtstr. 7, D-91058 Erlangen

We report and compare the unidirectional patterning of Fe, Ni and Co ultrathin films deposited on the hydrogen-stabilized substrate Ir(100)-(5×1)-H. This template develops by exposure of the Ir(100)-(5×1)-hex phase to hydrogen and consists of long, regularly spaced and defect-free Ir monoatomic wires residing on the (1×1) structured Ir substrate. The space between the wires can be filled by deposition of the transition metals (TM) Fe, Co and Ni. We show by STM that this filling process is rather different for the three metals but eventually results, at 0.8 ML coverage, in lateral superlattices {TM_4Ir}. The crystallographic structure of the three compounds was determined by quantitative LEED, which also reveals that there is no intermixing of TM atoms with the Ir wires. By further TM deposition, the superlattice is covered by pure TM in a layer-by-layer growth mode. In the second and third layer, atoms deviate from the ideal quadratic arrangement as induced by the 1-dim. corrugated structure of the {TM_4Ir} interface. The vertical buckling of the interface is imprinted in the TM film, with a maximum amplitude of e.g. 0.11 Å in the third Ni layer. Laterally, the atomic rows above the Ir chains of the interface have a larger separation and, under special conditions, can be decorated by further TM adatoms leading to well separated chain structures on top of the film.

O 4.2 Fr 11:00 TU EB202

Strain relaxation in ultrathin Ni films grown on Ir(100)-(1x1) and Ir(100)-(5x1)-H — •Andreas Klein, Bernd Gumler, Lutz Hammer, and Klaus Heinz — Lehrstuhl für Festkörperphysik , Universität Erlangen-Nürnberg, Staudtstr. 7, D-91058 Erlangen

We report on the growth of Ni films both on the metastable (1x1) phase and on the hydrogen-induced (5x1)-H phase of the Ir(100) surface in the coverage regime 4-10 monolayers (ML) applying STM and LEED. Whilst the (1x1) phase corresponds to the bulk-like truncated crystal, the (5x1)-H phase consists of long Ir wires of single atomic width which reside on this (1x1) phase in (on average) 5-fold lateral periodicity. On both templates an almost perfect layer-by-layer growth in the low coverage regime is followed by strain-relief controlled growth above 4 ML coverage. In this regime islands of 5 atoms width grow only one-dimensionally and eventually form irregular grids on the surface. Only with the completion of a layer the spaces within the grids are filled so that flat and homogeneous, but strained layers are formed. With film thicknesses in the range 6-8 ML the layerwise growth becomes less perfect and, at about 10 ML, dislocations are formed. For the (1x1) substrate the structures mentioned extend in both the [011] and [01-1] directions, whereas on the (5x1)-H phase the Ir wires at the film-substrate interface impose their unidirectionality on the higher coverage films. Only above a coverage of about 10 ML this differences between the two phases disappear and the nickel films exhibit similar patterns of strain relief.

O 4.3 Fr 11:15 TU EB202

Morphology and structure of pseudomorphic Ni-films grown on the Ir(100)-(1x1) surface — •Bernd Gumler, Andreas Schmidt, Andreas Klein, Lutz Hammer und Klaus Heinz — Lehrstuhl für Festkörperphysik, Universität Erlangen - Nürnberg, Staudtstr. 7, D-91058 Erlangen

Recent investigations of the epitaxial growth of Ni on the hexagonally reconstructed (100) surface of iridium, Ir(100)-(5x1)-hex, have shown that the reconstruction is lifted at very low Ni coverage leading to strong intermixing at the interface resulting in a rather limited order of the film. Therefore we used the surface's 1x1-structure, which can be prepared as metastable phase, as a template instead of the reconstructed phase. Scanning tunnelling microscopy (STM) and (quantitative) low-energy electron diffraction (LEED) were applied in the investigation. The Ni-Ir epitaxial misfit is as large as 8.2% so that layer-by-layer growth should not be expected. Indeed, we did not succeed to prepare a perfectly flat and closed 2 monolayers film. Surprisingly, yet, deposition of a third Ni layer yielded an almost ideal 3 layers film, i.e. the system seems to return to layer-by-layer growth. In fact, also the 4th layer grows accordingly. The films structures were determined and verified by excellent LEED theory-experiment fits. Structures were found to be tetragonally distorted with layer spacings of about 1.55 Å which are very close to the prediction of elastic theory. The structural influence of hydrogen adsorption on the films was investigated, too.

O 4.4 Fr 11:30 TU EB202

Nucleation in the presence of adatom insertion: Co / Pt(111) — •Philipp Buluschek, Stefano Rusponi, Mehdi El Ouali, Emmanuel Vargoz, Klaus Kern, and Harald Brune — Institute of the Physics of Nanostructures, Ecole Polytechnique Fédérale de Lausanne, CH-1015 Lausanne, Switzerland

We used variable temperature STM to study submonolayer nucleation of Co / Pt(111). Our experiments show that insertion of Co adatoms into the topmost layer of the Pt surface sets in at temperatures as low as 180 K. By relieving the tensile stress of the Pt surface, insertion leads to the formation of double partial dislocation lines. These take the shape of three branched stars.

With the insertion and the associated reconstruction, the Co / Pt(111) system makes a transition from homogeneous to heterogeneous nucleation. The behavior of the island density as a function of deposition temperature has been modeled in kinetic Monte-Carlo simulations. We show that the partial dislocations act as repulsive line defects with a diffusion energy barrier $E_d > 670\,\mathrm{meV}$. The comparison between simulations and experiment also enables access to the energy barriers for surface diffusion and the density of included adatoms in the surface.

O 4.5 Fr 11:45 TU EB202

Growth of Copper on Nickel (111) - a Scanning Tunneling Microscopy Study — •Florian Maier, Reinhard Lindner, and Hans-Peter Steinrück — Lehrstuhl Physikalische Chemie II, Universität Erlangen-Nürnberg, Egerlandstr. 3, D-91058 Erlangen

Controlled growth of bimetallic structures on a nanometer scale is of crucial interest in many fields. Therefore, the initial growth stage of copper on Ni(111) (0.05 ML < θ_{Cu} < 1.5 ML) as a model system was studied with scanning tunneling microscopy (STM). Copper was deposited using an electron beam evaporator that produced a flux of neutral atoms accompanied by a small fraction of ions. The latter was controlled by a countervoltage. The island size distribution was investigated as a function of substrate temperature (100 K or room temperature), concomitant copper ions, preadsorbed layers of water, and preadsorbed carbon monoxide.

In summary, room temperature promotes two-dimensional growth (due to kinetic effects), ion assisted deposition yields small islands (due to enhanced nucleation center formation), deposition on preadsorbed water layers results in a morphologie analogous to Stranski-Krastanov growth (due to "soft landing" of preformed copper clusters), and CO coadsorbtion prohibits island fusion (due to reduced diffusion length and/or step stabilisation).

O 4.6 Fr 12:00 TU EB202

Electronic structure of Zn on Pd(111) during growth and alloying — •Andreas Bayer, Ken Flechtner, Dieter Borgmann, Reinhard Denecke, and Hans-Peter Steinrück — Lehrstuhl für Physikalische Chemie II, Universität Erlangen-Nürnberg, Egerlandstr. 3, D-91058 Erlangen

Hydrogen as energy carrier can be produced by steam reforming of methanol over Pd/ZnO catalysts. The high activity and selectivity of the catalysts is attributed to the in-situ formation of Pd-Zn alloys as one of the active components [1]. Therefore, we investigated the growth of thin Zn layers (0-3 ML) on Pd(111) at 105 K and the changes in electronic structure during subsequent annealing to higher temperatures (up to 1000 K) by high-resolution X-ray photoelectron spectroscopy (XPS) with monochromized Al K_α radiation, ultraviolet photoelectron spectroscopy (UPS), and low energy electron diffraction (LEED). The formation of Pd-Zn alloys above 300 K can clearly be seen in XP spectra, as new Zn $2p_{3/2}$ and Pd $3d_{5/2}$ peaks evolve. The temperatures, at which these alloys form, strongly depend on the amount of adsorbed Zn. An ordered alloy was only observed for annealing 1 ML of Zn to 400-600 K. UPS measurements show a reduction in the density of states near the Fermi edge during alloying, explaining the Cu-like catalytic behaviour.

Supported by the DFG (Schwerpunktsprogramm 1091, Ste620/3-3).

[1] N. Iwasa, S. Masuda, N. Ogawa, and N. Takezawa, Appl. Catal. A 125 (1995) 145

O 4.7 Fr 12:15 TU EB202

Temperature dependent evolution of Au/Pd(110) structure — •Marko Kralj[1], Stefan Degen[1], Aleksander Krupski[1], Conrad Becker[1], Klaus Wandelt[1], Aude Bailly[2], Marie-Claire Saint-Lager[2], Pierre Dolle[2], and Robert Baudoing-Savois[2] — [1]Institut für Physikalische Chemie, Bonn, Germany — [2]Laboratoire de Cristallographie, Grenoble, France

Ultra thin gold films on Pd(110) are studied by surface x-ray diffraction (SXRD) and scanning tunneling microscopy (STM). The focus is set to a 2.5 atomic layers thick gold film. The evolution of the room temperature deposited film structure and morphology is investigated as a function of annealing temperature in the range of 300-580 K. With increasing temperature the film order increases and the surface plane exhibits a (1×2) missing row reconstruction. Also, after 500 K, a competitive process of alloying with the palladium substrate takes place. A diffuse component is observed when performing transverse SXRD scans along the (01L) crystal truncation rod. This diffuse intensity is present only in one direction and is thus induced by "defects" of anisotropic form. We propose a consistent model which clearly relates this effect to the STM data.

O 4.8 Fr 12:30 TU EB202

Bcc-like crystal structures in ultrathin "fcc"Fe films on Cu(111) — •Albert Biedermann, Werner Rupp, Michael Schmid, and Peter Varga — Institut für Allgemeine Physik, Vienna University of Technology, 1040 Vienna, Austria

Growing ultrathin Fe films on fcc substrates can stabilize the fcc structure of Fe. More often, however, distorted bcc-like structures are found instead. Fe/Cu(100) films are very flat and show relatively well defined fcc and bcc-like phases, among them a "nanomartensitic"bcc-like phase [1]. In contrast, Fe/Cu(111) films grown by thermal deposition are relatively rough, favoring Cu surface segregation and hampering standard LEED-I/V analyses. We have used atomically resolved STM and STS of clean and H-covered bi- and multi-layer islands together with XPD data by Kief and Egelhoff [2] to show the presence and conditions of stability of strained bcc-like phases in Fe/Cu(111) films. Our results are compared to published magnetic measurements [3] and first principles predictions [4], which favor an ideal fcc phase for very thin films.

[1] A. Biedermann, R. Tscheließnig, M. Schmid, and P. Varga, Appl. Phys. A 78 (2004) 807.

[2] M. T. Kief, W. F. Egelhoff, Jr, Phys. Rev. B 47 (1993) 10785

[3] P. Ohresser, J. Shen, J. Barthel, M. Zheng, C. V. Mohan, M. Klaua, and J. Kirschner, Phys. Rev. B 59, 3696 (1999).

[4] Spišák and J. Hafner, PRB 67 (2003) 134434

O 4.9 Fr 12:45 TU EB202

Growth and electronic structure of ultrathin chromium films on iridium(111) investigated by scanning tunneling microscopy and spectroscopy — •Felix Marczinowski, Kirsten von Bergmann, and Roland Wiesendanger — Institut für Angewandte Physik, Universität Hamburg

Magnetic materials are showing interesting properties when prepared as thin films. Bulk Cr has bcc structure and is antiferromagnetic. Instead, if grown as a hexagonal monolayer film, the antiferromagnetic alignment of neighbouring atomic moments is impossible and a frustrated spin-structure will be formed [D. Wortmann et al., Resolving Complex Atomic-Scale Spin Structures by Spin-Polarized Scanning Tunneling Microscopy, PRL(2001)]. To study this spin-structure on an atomic level, Cr films of various coverages were deposited on an Ir(111) substrate by means of molecular beam epitaxy (MBE). The growth up to three monolayers was studied by scanning tunneling microscopy and spectroscopy. Indeed, the Cr monolayers grow pseudomorphically on the Ir(111) substrate and hence have hexagonal symmetry. Interestingly, we find a coexistence of faulted and unfaulted Cr-monolayer areas with distinct morphology and slightly different electronic properties. For higher coverages, a modified Volmer-Weber growth mode is observed. For coverages above two monolayers the Cr film relaxes towards its bulk structure and shows an epitaxial relationship according to the Kurdjumov-Sachs orientation.

O 5 Zeitaufgelöste Spektroskopie I

Zeit: Freitag 10:45–13:00 Raum: TU EB107

O 5.1 Fr 10:45 TU EB107

Ultrafast adaptive nano-photonics — •Walter Pfeiffer[1], Tobias Brixner[1], Johannes Schneider[1], and F.J. García de Abajo[2] — [1]Physikalisches Institut, Universität Würzburg, Am Hubland, 97074 Würzburg, Germany — [2]Centro Mixto CSIC-UPV/EHU, Apartado 1072, 20080 San Sebastián, Spain

The time-resolved investigation of nanoscale transport phenomena requires localizing pump and probe excitation both for different times and at different locations. This requires a method for controlling independently the electric field evolution at closely neighboring locations. Here we present a rather general scheme that allows us to achieve this control over the spatial and temporal field distribution below the diffraction limit in the optical near field of a metal nanostructure. The scheme is based on interferences of optical near-field modes that are controlled by the excitation with polarization-shaped laser pulses. It is demonstrated that the interaction of optimally polarization-shaped femtosecond laser pulses with metal nanostructures allows controlling the spatial and temporal evolution of the electromagnetic near field. This control with simultaneous but independent nanometer length and femtosecond time resolution opens a new realm for ultrafast spectroscopy on the nanoscale and will allow novel quantum control schemes.

O 5.2 Fr 11:00 TU EB107

Ultrafast Photoemission Microscopy — •Frank-J. Meyer zu Heringdorf, Dagmar Thien, Liviu I. Chelaru, Oliver Heinz, Ping Zhuo, Dietrich von der Linde, and Michael Horn-von Hoegen — Institut für Experimentelle Physik, Universität Duisburg-Essen (Campus Essen), 45117 Essen, Germany

The combination of ultrafast spectroscopy with photoemission microscopy is a rather challenging venture, that has so far only been attempted at few places around the world. Here we describe a novel experimental setup at the University of Duisburg-Essen that combines photoemission electron microscopy (PEEM) with pulsed fs-laser sources to study the energy dissipation of excited electrons in self organized nanostructures. The presentation describes the recent status of the setup and first experimental results of self-organized Ag nanostructures on Si(001).

O 5.3 Fr 11:15 TU EB107

Second-harmonic generation from nanoscopic metal tips: Generalized symmetry selection rules for single nanostructures — •Catalin C. Neacsu[1], Georg A. Reider[2], and Markus B. Raschke[1] — [1]Max-Born-Insitut für Nichtlineare Optik und Kurzzeitspektroskopie, D-12489 Berlin — [2]Institut für Photonik, Technische Universität Wien, A-1040 Wien

Second-harmonic generation from individual nanoscopic metal tips has been investigated. As a partially asymmetric (∞mm) nanostructure with the mirror symmetry broken in the axial direction the tip geometry allows for the first time to directly distinguish otherwise inseparable local surface and nonlocal bulk second-harmonic polarizations. Distinct second-harmonic-emission directions and polarization selection rules are observed that are different compared not only to linear light scattering but also compared to SHG from both, planar interfaces as well as spherical or ellipsoidal nanoparticles. In addition, the local field enhancement at the tip apex has been quantified ranging from 8 to 25 for Au tips with radii of 50 nm down to 10 nm and drops significantly for W or PtIr as tip material. The large sensitivity of SHG with respect to this local field enhancement together with the new selection rules being generally applicable to partially asymmetric nanoscopic systems provide new degrees of freedom for surface-specific second-harmonic investigations of nanostructures and the optical coupling in scattering-type near-field microscopy.

O 5.4 Fr 11:30 TU EB107

Photoemission from surface states using higher harmonic radiation — •Andrea Melzer[1], Jinxiong Wang[1], Alvaro Wulff[1], Martin Weinelt[2], and Thomas Fauster[1] — [1]Lehrstuhl für Festkörperphysik, Universität Erlangen-Nürnberg, Staudtstr. 7, D-91058 Erlangen — [2]Max-Born-Institut, Max-Born-Str. 2A, D-12489 Berlin

Photon energies up to 45 eV are generated by focussing pulses from a multipass amplifier into argon. The laser provides pulses with 1.4 mJ energy at 770 nm wavelength at a repetition rate of 1 kHz. The pulse length is 30 fs leading to an intensity of $\sim 5\times10^{14}$ W/cm^2 at the focus. A grating monochromator with two interchangable toroidal gratings (250 and 950 lines/mm) is used to select the individual harmonics. Photoelectron spectra from surface states on fcc(111) surfaces are measured to characterize the photon energy, linewidth, polarization, intensity, and pulse length of the higher harmonic photon source. One-photon photoemission spectra can be recorded at gas pressures below 10 mbar with no detectable pressure increase in the ultrahigh vacuum chamber of the electron spectrometer.

O 5.5 Fr 11:45 TU EB107

Two-Photon Photoemission Spectroscopy of Thiophenol Self-Assembled Monolayers on Gold(111) — •S. Dantscher, T. Schutzmeier, C. Kennerknecht, and W. Pfeiffer — Physikalisches Institut, Universität Würzburg, Am Hubland, 97074 Würzburg

The aromatic molecule thiophenol forms ordered self assembled monolayers (SAM) on gold surfaces. Using two-photon photoemission spectroscopy we investigate the influence of this surface modification on the occupied and unoccupied electronic structure of both the substrate and the adsorbate.

The samples consist of 600Åthick gold(111) films on mica that have been evaporated in UHV. The preparation of the SAMs from an ethanolic solution takes place in an inert nitrogen atmosphere. Femtosecond laser pulses with wavelengths of 400nm and 266nm are used for the photoemission measurements.

The adsorption of thiophenol results in a decrease of the work function of the sample from 4.8eV to 3.7eV. The photoemission spectra exhibit peaks related to the SAM formation that shift with applied laser intensity. These peaks are attributed to electronic states in a physisorbed molecular overlayer on the chemisorbed monolayer. This overlayer can easily be charged by injection of excited electrons.

Accompanying these experiments, density functional theory calculations of free and adsorbed thiophenol molecules were performed. The calculated static dipole moment of thiophenol on a small gold cluster is in agreement with the observed work function change.

O 5.6 Fr 12:00 TU EB107

Ultrafast electron dynamics in C_6F_6/Cu(111) analyzed with time-reslved photoelectron and resonant Auger-Raman spectroscopy — •P. Kirchmann[1], P. Loukakos[1], U. Bovensiepen[1], M. Wolf[1], V. Sethuraman[2], A. Pietsch[2], F. Hennies[2], M. Nagasono[2], A. Föhlisch[2] und W. Wurth[2] — [1]Freie Universität Berlin, Fachbereich Physik, Arnimallee 14, 14195 Berlin — [2]Universität Hamburg, Institut für Experimentalphysik, Luruper Chaussee 149, 22761 Hamburg

Ultrafast charge transfer processes in molecules adsorbed on a metal surface can be investigated by resonant Auger-Raman spectroscopy [1] and femtosecond time-resolved two-photon-photoemission (2PPE) [2]. To systematically compare both techniques we investigated the system C_6F_6/Cu(111). This study reveals a qualitatively different coverage dependence of the decay rate of the lowest unoccupied molecular resonance. In addition the decay rate for monolayer coverages measured by the two methods is different by a factor of five. This is attributed to the fact that Auger-Raman spectroscopy detects intra-molecular charge delocalization as well as the delocalization between the molecule and its environment. In contrast, 2PPE probes the intraband scattering within delocalized states of the molecular adlayer as well as the population decay by interband scattering to the substrate. Thus different relaxation channels are measured with the two approaches. The project was funded by the DFG through SPP 1093.

[1] W.Wurth and D.Menzel, Chem. Phys. 251, 141 (2000)

[2] C.Gahl, K. Ishioka, Q. Zhong, A. Hotzel and M. Wolf, Faraday. Discuss. 117, 191 (2000)

O 5.7 Fr 12:15 TU EB107

Vibrational dynamics of the C-O stretching mode of CO:Si(100) — •Kristian Lass, Xu Han, and Eckart Hasselbrink — Fachbereich Chemie, Physikalische Chemie, Universität Duisburg-Essen, Standort Essen, Universitätsstr. 5, D-45141 Essen

Surface infrared-visible sum frequency generation (SFG) spectroscopy (using ps laser pulses) has been utilised to study the vibrational dynamics of the internal stretching mode of CO molecularly adsorbed on a Si(100) surface. The structure of the CO-adsorbed Si(100) surface is not known in detail; however, two slightly different adsorbed species have been suggested in the past. With our IR laser linewidth of 9 cm^{-1}, only one resonance was distinguishable, whose linewidth was significantly lower than our laser linewidth. Using a IR-pump-SFG-probe setup, the vibrational lifetime of the system could be determined to be about 2 ns. This value is unexpectedly short, in view of the fact that the vibrational excitation cannot couple to electron-hole pairs because of the large bandgap in Si. The lifetime appears to be independent of the carrier density of the Si crystal (within the accuracy of our experiment), as judged from the vibrational lifetime measured on crystals with different dopant densities.

O 5.8 Fr 12:30 TU EB107

Mechanism of femtosecond laser induced diffusion of oxygen on vicinal Pt(111) — •K. Stépán, J. Güdde, and U. Höfer — Fachbereich Physik und Zentrum für Materialwissenschaften, Philipps Universität Marburg, D-35032 Marburg

Laser-induced diffusion of atomic oxygen from step edges onto terraces of a vicinal Pt(111) surface has been studied by exploiting the sensitivity of optical second-harmonic generation (SHG) on surface symmetry. The excitation mechanism of the diffusion process has been investigated by measuring the diffusion rate as a function of fluence and delay between two femtosecond pump pulses. The strong nonlinear fluence dependence ($\propto F^{15}$) and a width of 1.5 ps in the two-pulse-correlation measurements show that the diffusion process can be understood within the same framework as the well studied phenomena of desorption induced by multiple electronic transitions (DIMET). For a quantitative modeling of the data we approximate the detailed coupling of adsorbate modes and excited substrate electrons with an electronic friction coefficient [1]. In contrast to the situation in most laser-induced desorption experiments, a friction coefficient that depends on the excitation density is required in to describe the whole data set. We interpret this dependence in terms of an indirect electronic excitation mechanism of the frustrated translation leading to diffusion. We suggest that the electronic excitation of the substrate couples primarily to the O-Pt stretch vibrations which then excite frustrated translations via an anharmonic coupling of modes.

[1] M. Brandbyge *et al.* Phys. Rev. B. **52**, 6042 (1995)

O 5.9 Fr 12:45 TU EB107

Dynamics of Electron Transfer, Trapping, and Solvation in D_2O/Ru(001) — •Julia Stähler, Uwe Bovensiepen, Cornelius Gahl, and Martin Wolf — Fachbereich Physik, Freie Universität Berlin, Arnimallee 14, 14195 Berlin, Germany

The dynamics of excess electrons photo-injected into ultrathin ice layers on Ru(001) has been studied by femtosecond time-resolved two photon photoelectron (2PPE) spectroscopy. The electrons' residence time in the adlayer is limited due to the transfer matrix element between substrate and adsorbate. In amorphous ice layers, this leads to subps-lifetimes of the solvated electrons. These are initially injected into the ice conduction band before they start to stabilize 2.9eV above the Fermi level [1]. In contrast, we observe excess electrons within crystalline D_2O/Ru(001) that present lifetimes up to several minutes before they relax back to the metal. Variation of the UV excitation energy shows that these electrons are transferred to the delocalized image potential state within the ice layer before they localize more than 2eV above the Fermi level into preformed traps. During their extremely long lifetime an increase of binding energy is observed, which is attributed to a rearrangement of the polar environment. The notable temperature dependence of binding energy and photoelectron intensity will be discussed.

[1] U. Bovensiepen et al., Isr. J. Chem. 45 (2005), in press

O 6 Grenzfläche fest-flüssig

Zeit: Freitag 10:45–13:00 Raum: TU EB407

O 6.1 Fr 10:45 TU EB407

Surface Stress – Charge Coefficient for Charged Nanoporous Platinum — •Viswanath Raghavan Nadar[1], Dominik Kramer[1], and Jörg Weissmüller[1,2] — [1]Forschungszentrum Karlsruhe, Institut für Nanotechnologie, Karlsruhe — [2]Universität des Saarlandes, Fachrichtung Technische Physik, Saarbrücken

If porous, nanostructured metals immersed in an electrolyte are charged electrically, volumetric expansion and contraction is induced in phase with the applied potential[1,2], with strain amplitudes comparable to those of commercial piezoceramics. Several microscopic interactions contribute to the potential dependence of the surface stress and the corresponding interfacial properties: electrostatic repulsion in the space−charge layers, changes in the bonding between metal atoms, and forces between neighboring adsorbate atoms or between adsorbates and the metal. The relative contributions of these interactions are so far not well understood. The present study is to obtain insight into this issue by studying the electrolyte concentration dependence of the surface stress − charge coefficient ζ for platinum. We compute ζ from the volumetric strain measured from in−situ dilatometer experiments and discuss the influence of specific adsorption. [1] J. Weissmüller et al, Science 300 (2003) 312; [2] D. Kramer, R. N. Viswanath, J. Weissmüller, Nano Letters 4 (2004) 793

O 6.2 Fr 11:00 TU EB407

Kompression der Au(111) Oberflächenschicht während homoepitakitischer elektrochemischer Abscheidung — •Jochim Stettner, Ahmed Ayyad und Olaf Magnussen — Institut für Experimentelle und Angewandte Physik, Christian-Albrechts-Universität Kiel, Leibnizstraße 19, 24098 Kiel

Die strukturelle Untersuchung von Metalloberflächen unter reaktiven Bedingungen ist von hoher Bedeutung für das Verständnis elektrochemischer Prozesse. Wir haben die homoepitaktische elektrochemische Abscheidung von Au(111) in wässrigen Elektrolytlösungen untersucht. Dieses System ist für grundlegende Studien aufgrund der potentialabhängigen $(p \times \sqrt{3})$ Rekonstruktion der Au(111)-Oberfläche besonders interessant. In-situ Oberflächen-Röntengenbeugungsexperimente unter streifendem Einfall zeigen im Vergleich zu entsprechenden Experimenten in Au-freien Elektrolyten oder unter UHV Bedingungen ($p \approx 22$) eine signifikant erhöhte Kompression der obersten Au-Monolage. Die Kompression nimmt zu negativeren Potentialen hin zu und erreicht im gewählten Potentialbereich ein Maximum von 5.5% ($p \approx 18$). Mit Hilfe eines thermodynamischen Modells kann der Kompressionseffekt semiquantitativ durch den Abbau potential-induzierter mechanischer Spannungen in der Au-Oberfläche erklärt werden.

O 6.3 Fr 11:15 TU EB407

Quantitative in-situ Video-STM study of the lateral displacements of isolated reconstruction strings on Au(100) electrodes — •Miguel Labayen, Christian Haak, and Olaf Magnussen — Institut fur Experimentelle und Angewandte Physik, Leibnizstrasse 19, Universitaet Kiel, Kiel 24098, Deutschland

The dynamic behavior of the reconstructed Au(100) surface has been studied in Cl- containing solution via in-situ electrochemical high-speed scanning tunneling microscopy (Video-STM), at image acquisition rates of 15 - 20 frames per second. The Au(100)(1x1) surface structure undergoes reconstruction of the top-most layer to a hexagonal close-packed structure at negative potentials. The elemental units of this reconstructed surface are parallel strings separated 14.5 Å. We have focused our study to the high mobility of isolated strings perpendicular to the main direction[1]. Jump distribution functions for individual strings indicate contributions by at least two different processes (jumps by one and two atomic distances). String jumps can be ascribed to small atomic displacements in the strings induced by propagating kinks. The mechanisms of kink nucleation and propagation and the corresponding energy barriers, obtained from temperature-dependent measurements, are discussed.

[1] M.Labayen, C.Ramirez, W.Schattke, O.M.Magnussen, Nature Materials 2, 783 (2003).

O 6.4 Fr 11:30 TU EB407

In Situ Observation of Adsorbates Diffusion on Au(111) using Electrochemical Video-STM — •Koji Suto and Olaf Magnussen — Institut für Experimentelle und Angewandte Physik, Universität Kiel, Kiel, Germany

The diffusion and interaction of molecular adsorbates on solid-liquid interface is an important fundamental subject of surface physics, due to its relevance for numerous surface processes, e.g. catalytic reactions, growth, or the formation of self-assembled adlayers. This time we report investigation of adsorbates motion at metal electrode - liquid electrolyte interfaces by an electrochemical Video-STM, capable of recording up to 30 images per sec and with atomic scale resolution. Full coverage of sulfate adlayers were observed to form well defined structure of $(\sqrt{3} \times \sqrt{7})$ on Au(111)-(1 × 1) surfaces at 0.8 V vs. SCE in sulfuric acid solution as reported before [1], which fluctuated strongly in slightly negative potential region due to pronounced migration of the adsorbates between neighboring domains. 1,4-butanedithiol, a strong chemisorbed organic species, were found to migrate individually on the reconstructed Au(111) surface (at 0.3 V vs. SCE) at low coverage in acidic solution. The diffusion process could not be described by simple hopping migration, but involved rotational motion and translational motion of the adsorbates on the surface.

[1] O. M. Magnussen, J. Hageboeck, J. Hotlos, R. J. Behm, Faraday Discuss., 94 (1992) 329.

O 6.5 Fr 11:45 TU EB407

Elektrochemisch präparierte ultradünne Kupfersulfidfilme auf Au(111)-Oberflächen — •Christian Schlaup, Daniel Friebel, Peter Broekmann und Klaus Wandelt — Institut für Physikalische und Theoretische Chemie, Universität Bonn, Wegelerstr. 12, D-53115 Bonn

In alkalischen Lösungen wurde die Adsorption von Sulfid ($S^{\,2-}$) auf ultradünnen Kupferfilmen durch *in-situ* Rastertunnelmikroskopie in Verbindung mit zyklischer Voltrammetrie untersucht. Hierzu wurde auf einem Au(111)-Einkristall durch Unterpotential-Abscheidung entweder eine $(\sqrt{3} \times \sqrt{3})R30^\circ$ 2/3-Monolage oder eine vollständige (1 × 1) Cu-Monolage erzeugt. Auf den so erzeugten Cu-Filmen wurde anschließend Sulfid aus 0.1 M Natronlauge (pH ≈ 13) adsorbiert. Die dabei gebildeten potentialabhängigen Adsorbatstrukturen unterscheiden sich grundlegend von den bekannten Adsorbatstrukturen von Sulfid auf Au(111) bzw. Cu(111)-Oberflächen und werden im Folgenden vorgestellt und charakterisiert.

O 6.6 Fr 12:00 TU EB407

Potentialabhängige Tracer-Diffusion von Sulfidadsorbaten auf Cu(100)-Elektroden in HCl Lösung — •Tunay Tansel und Olaf Magnussen — Institut für Experimentelle und Angewandte Physik, Christian-Albrechts-Universität Kiel, Leibnizstrasse 19, D-24098 Kiel, Germany

Die Oberflächendiffusion von Adsorbaten an Phasengrenzen zwischen elektrolytischen Flüssigkeiten und Metallelektroden spielt eine wichtige Rolle in vielen Grenzflächenprozessen, wie z.B. (elektro-) katalytischen Reaktionen, galvanischer Abscheidung und der Bildung geordneter Adsorbatschichten. Es ist bekannt, dass Transportprozesse an elektrochemischen Grenzflächen häufig stark vom Elektrodenpotential abhängen. Hier stellen wir erste detaillierte Messungen zum zugrunde liegenden Elementarprozess, der Tracer-Diffusion einzelner Adsorbate, am Beispiel von Sulfidadsorbaten auf der c(2x2)-Cl bedeckten Cu(100) Oberfläche in 0.01M HCl vor. In-situ Untersuchungen auf der atomaren Skala mittels elektrochemischer Hochgeschwindigkeits-Rastertunnelmikroskopie (Video-STM) bei Sad-Bedeckungen 0.01 bis 0.03 ML zeigen eine Hopping-Diffusion zwischen Plätzen des c(2x2)-Cl Koadsorbatgitters. Die über eine Sprungverteilungs-Analyse der Videos ermittelten Sprungraten zeigen eine starke, exponentielle Abhängigkeit vom Potential mit einem Koeffizienten von 19.5 V-1. Dies lässt sich in einem einfachen Modell erklären, in dem der effektive Ladungszustand des Adsorbats vom Adsorptionsplatz abhängt.

O 6.7 Fr 12:15 TU EB407

Catalysis of CO and H_2 electrooxidation on UHV prepared PtAu/Ru(0001) model surfaces — •H.E. Hoster, E. Filonenko, and R.J. Behm — Abteilung Oberflächenchemie und Katalyse, Universität Ulm, 89069 Ulm

Utilizing an electrochemical flow cell setup for single crystals we have evaluated the electrocatalytic activity of a series of PtAu model electrodes for CO oxidation and H_2 oxidation/evolution. The electrodes consist of PtAu monolayers of varying compositions on a Ru(0001) substrate and Au-decorated Pt/Ru(0001) submonolayer structures. The surfaces were prepared under UHV conditions, and their morphology and distribution of surface atoms was quantitatively determined by STM [1]. The variation of the catalytic activity is quantitatively related to the distribution of surface atoms in order to evaluate the activity of atomic ensembles. The influence of Au decoration on the activity of Ru and Pt steps in bimetallic Pt/Ru(0001) surfaces is tested and discussed. [1] E. Filonenko, H.Hoster, H.Rauscher, R.J. Behm, 'Zweidimensionale Legierungsbildung in PtAu Monolagenschichten', pesented at this conference

O 6.8 Fr 12:30 TU EB407

Mikroelektrochemisches Verhalten von Aluminiumlegierungen der Familie AlMgSi — •Fabian Eckermann[1,2], Patrik Schmutz[2], Jörg F. Löffler[1] und Peter J. Uggowitzer[1] — [1]Laboratory of Metal Physics and Technology, ETH Zurich, 8093 Zurich, Switzerland — [2]Laboratory for Corrosion and Materials Integrity, EMPA, 8600 Dubendorf, Switzerland

Aufgrund galvanischer Kopplung und veränderter Oxidschicht beeinflussen Intermetallische Phasen (IMP) in hohem Masse das Korrosionsverhalten technischer Aluminiumlegierungen. Mikroelektrochemische Untersuchungen ermöglichen eine qualitative und quantitative Bewertung. Das elektrochemische Verhalten unterschiedlicher IMP unter Berücksichtigung der umgebenden Matrix wurde mit Stromdichte-Potential Kurven charakterisiert. Die elektrochemische Mikrokapillar-Messzelle bietet hier die Möglichkeit, die elektrochemische Natur der inhomogenen Oberflächenstruktur gezielt zu analysieren. Mit der hohen lateralen Auflösung dieser Technik und Messflächen von wenigen Quadratmikrometern konnte auf einzelnen Bereichen verschiedener Phasenzusammensetzung der Einfluss verschiedener Intermetallischer Phasen auf die elektrochemischen Reaktionen mit einer Auflösung von 10 fA bewertet werden. Die Oberflächenveränderungen aufgrund des Kontaktes mit NaCl-Lösung wurden zudem mit der Auger-Elektron-Spektroskopie und der Mikrosonde untersucht.

O 6.9 Fr 12:45 TU EB407

In Situ STM study of the intercalation of organic molecules in 1-T TaS$_2$ — •Sujit Kumar Dora and Olaf Magnussen — Institut für Experimentelle und Angewandte Physik, Universität Kiel, Kiel, Germany

It has been know for more than 20 years that transition metal dichalcogenides are ideal host materials for the intercalation of large organic molecules, resulting in materials with strongly modified structural and electronic properties. However, little is known on the atomic-scale mechanisms of the intercalation process. In this study, the electrochemical intercalation/ deintercalation of pyridine and octylamine (0.01 M solutions, pH 4) in 1T-TaS$_2$ was investigated by in-situ electrochemical STM and cyclic voltammetry. The STM observations show characteristic structural changes in the surface morphology during these processes, illuminating the important role of surface defects, such as holes and steps. In particular, the growth of holes and the formation of layers with fractional step heights (1/2 of the 1-T TaS$_2$ layer spacing) were observed.

O 7 Symposium Recent Progress in Scanning Probe Methods

Zeit: Freitag 11:00–13:00 Raum: TU H3005

Fachvortrag

O 7.1 Fr 11:00 TU H3005

From Spins to Phonons: Mapping Local Excitations with Atomic Resolution — •Klaus Kern — Max-Planck-Institut für Festkörperforschung, Heisenbergstr. 1, 70569 Stuttgart

Recent experimental advances have provided the unique ability to investigate matter with sub-Ångstrom precision. Scanned probes not only allow us to image and manipulate individual atoms and molecules adsorbed at surfaces with unprecedented resolution but also to probe their electronic and vibrational states by tunneling spectroscopy. In this talk we demonstrate the power of elastic and inealastic tunneling spectroscopy for detecting and mapping local excitations with atomic resolution. As examples we will discuss the phonon spectromicroscopy of single walled carbon nanotubes and the spin detection and manipulation of adatoms and molecules on metallic surfaces.

Fachvortrag

O 7.2 Fr 11:30 TU H3005

Spin Mapping on the Atomic Scale: From 2D Antiferromagnets to Single Impurities — •Roland Wiesendanger — University of Hamburg, Institute of Applied Physics, Jungiusstr. 11, 20355 Hamburg

Spin-polarized Scanning Tunneling Microscopy (SP-STM)[1] and Spectroscopy (SP-STS)[2] have allowed the visualization of atomic-scale spin structures [3,4] and the investigation of the spin-dependent local density of states spatially resolved [5]. In a recent SP-STM experiment we could prove that a single monolayer of Fe on a W(001) substrate exhibits a c(2x2) antiferromagnetic ground state with perpendicular anisotropy in contrast to a single Fe monolayer on W(110) which is ferromagnetic with in-plane anisotropy [6]. Spin-dependent scattering at single oxygen impurities on Fe/W(110) was visualized in real-space reflecting the orbital nature of the electronic states involved as well as their spin character [7]. Finally, applications of SP-STM and SP-STS for studying spin states of single magnetic impurities will be discussed. [1]R. Wiesendanger et al., Phys. Rev. Lett. 65, 247 (1990). [2]M. Bode, M. Getzlaff, R. Wiesendanger, Phys. Rev. Lett. 81, 4256 (1998). [3]R. Wiesendanger et al., Science 255, 583 (1992). [4]S. Heinze et al., Science 288, 1805 (2000). [5]O. Pietzsch et al., Phys. Rev. Lett. 92, 057202 (2004). [6]O. Pietzsch et al., Phys. Rev. Lett. 84, 5212 (2000). [7]K. von Bergmann et al., Phys. Rev. Lett. 92, 046801 (2004).

Fachvortrag

O 7.3 Fr 12:00 TU H3005

Force microscopy experiments of single molecules on insulators — •Ernst Meyer, Laurent Nony, Enrico Gnecco, Anisoara Socoliuc, Lars Zimmerli, Sabine Maier, and Oliver Pfeiffer — Institute of Physics, Klingelbergstr. 82, CH-4056 Basel, Switzerland

So far, most of the high resolution SPM studies of molecules were restricted to metallic substrates. However, insulating surfaces are necessary to avoid coupling between the molecule electrons and the substrate. Apart from the advantage to be independent of the conductance of the substrate, AFM offers the possibility to perform local force vs. distance curves [1]. The application of force microscopy on single molecules of Cu-tetra (3,5 di-t-butylphenyl) porphyrines revealed that different molecular conformations can be detected. In addition, the energetics of these simple molecular switches can be studied in a quantitative manner. Here, we present force microscopy investigations of molecules deposited on insulators. The surface of KBr(001) is structurized by electron beam irradiation. Small pits of some nanometers in diameters are formed. The decoration with perylene and sub-phtalocyanine molecules shows that the pits act as molecular traps [2].

[1]Ch. Loppacher, M. Guggisberg, O. Pfeiffer, E. Meyer, M. Bammerlin, R. Luethi, R. Schlittler, J. K. Gimzewski, H. Tang and C. Joachim, Phys. Rev. Lett. 066107 (2003).

[2] L. Nony et al., to appear in Nanoletters (2004).

Fachvortrag O 7.4 Fr 12:30 TU H3005

Recent Progress in Friction Force Microscopy — •Roland Bennewitz — Physics Department, McGill University, Montreal, Canada

The development of Scanning Force Microscopy has provided us with tools to study friction and wear on the nanometer scale. The atomic granularity of matter shows up in the lateral force which is necessary to slide a small contact over a flat surface. Also, mechanical damage of a sample surface can be monitored with monolayer resolution. I will discuss the laws which determine the dependence of atomic friction on normal load or velocity, and in what respect they differ from the ones we have learned to describe macroscopic friction. For small scales, a regime of ultra-low friction has long been suggested which recently has been experimentally realized.

O 8 Hauptvortrag Gambardella

Zeit: Freitag 14:00–14:45 Raum: TU EB301

Hauptvortrag O 8.1 Fr 14:00 TU EB301

Dimensionality-dependent magnetic properties: from single atoms at surfaces to 1D and 2D structures — •Pietro Gambardella — Institut de Physique des Nanostructures, Ecole Polytechnique Fédérale de Lausanne, CH-1015 Lausanne, Switzerland

The magnetic moment of gas-phase transition-metal atoms deposited on nonmagnetic substrates undergoes significant changes depending on the surface electronic structure, morphology, and coupling to magnetic neighbours [1]. The controlled assembly of metal nanostructures on crystalline surfaces combined with x-ray magnetic circular dichroism experiments in strong magnetic fields is used here to track the evolution of the spin and orbital magnetization from single adatoms to one-dimensional nanowires and two-dimensional clusters on nonmagnetic substrates. Giant magnetic anisotropy energy values are reported for single adatoms, while scaling with the orbital magnetic moment and atomic coordination is observed in finite-sized clusters [2]. Unusual oscillations of the easy axis of magnetization and magnetic anisotropy energy are observed in one-dimensional atomic wires constructed on a Pt vicinal surface as a function of the wire transverse width [3], an effect attributed to the filling of d-orbitals with different symmetry [4]. Finally, we will discuss the conception of novel metal-organic magnetic networks at surfaces in analogy with supramolecular grid structures.

[1] P. Gambardella et al., Phys. Rev. Lett. 88, 047202 (2002). [2] P. Gambardella et al., Science 300, 1130 (2003). [3] P. Gambardella et al., Phys. Rev. Lett 93., 077203 (2004). [4] J. Dorantes-Dávila and G.M. Pastor, Phys. Rev. Lett 81., 208 (1998).

O 9 Hauptvortrag Müller

Zeit: Freitag 14:45–15:30 Raum: TU EB301

Hauptvortrag O 9.1 Fr 14:45 TU EB301

Structure and stability of binary alloy surfaces: Segregation, relaxation, and ordering from first-principles calculations — •Stefan Müller — Universität Erlangen-Nürnberg, Lehrstuhl für Festkörperphysik, Staudtstr. 7, D-91058 Erlangen

Although modern computer codes based on density functional theory (DFT) allow the reliable prediction of many surface properties, they often cannot be applied when the problem of interest demands a consideration of huge configuration spaces or model systems containing many thousand atoms. An important example are binary alloy surfaces where substitutional ordering phenomena on a mesoscopic scale and surface segregation are involved. The latter describes the deviation of the surface region's stoichiometry from that of the bulk. Consequently, a successful theoretical description of this phenomenon demands the consideration of both, bulk and surface properties leading to model slabs consisting of hundreds, if not thousands of atoms. Moreover, in general first-principles methods based on DFT cannot take configurational enthalpies into account and, therefore, are not able to describe the segregation of atoms at all. In this contribution, our recent developments, possibilities and limitations to study surface segregation and ordering phenomena in metal alloys based on first-principles methods will be discussed. It will be demonstrated how the combination of DFT calculations with so-called cluster expansions and Monte-Carlo simulations allows for a quantitative prediction of alloy surface properties from the miscroscopic to the mesoscopic scale without any empirical parameters (supported by DFG).

O 10 Adsorption an Oberflächen I

Zeit: Freitag 15:45–17:00 Raum: TU EB301

O 10.1 Fr 15:45 TU EB301

The Adsorption of Triptycene on Au(111): a bilayer growth stabilised by intermolecular π-π interactions — •I.F. Torrente[1,2], N. Henningsen[1], and J. I. Pascual[1] — [1]Institut für Experimentalphysik, Freie Universität Berlin, Arnimallee 14, D-14195 Berlin, Germany — [2]Institut Català de Nanotecnologia, Campus UAB, Bellaterra, Barcelona, Spain

The adsorption of triptycene molecules (C20H14) on Au(111) is studied by means of Low-Temperature Scanning Tunnelling Microscopy and Spectroscopy. Triptycene is a model system to investigate the balance between the tendency of the aromatic units to bond flat, parallel to a metal surface, and the intermolecular π-π interactions. In planar aromatic molecules, the interaction of π states with the metal electronic states usually dominates. The structure of triptycene frustrates partially such planar configuration. As a result, triptycene interaction with the Au(111) metal surface is described by a weak physisorption. As soon as the substrate temperature is above a few tenths of K, Triptycene ensemble in self-assembled molecular islands with a characteristic bilayer structure. The interpretation of such growth mechanism is done on the basis of the dominant role of stronger intermolecular interactions respect to physisorption energies.

O 10.2 Fr 16:00 TU EB301

Manipulation und Adsorptionsplatzbestimmung von einzelnen Pentazen-Molekülen auf Cu(111) — •Stefan Fölsch[1], Kiyoshi Kanisawa[2] und Jérôme Lagoute[1] — [1]Paul-Drude-Institut für Festkörperelektronik, Hausvogteiplatz 5-7, D-10117 Berlin — [2]NTT Basic Research Laboratories, NTT Corporation, Atsugi-shi, Kanagawa 243-0198, Japan

Atomare und molekulare Manipulation mittels Tieftemperatur-Rastertunnelmikroskopie läßt sich als analytisches Werkzeug für die Oberflächenphysik einsetzen. Wir demonstrieren dies anhand der Adsorptionsplatzbestimmung einzelner Pentazen-Moleküle auf Cu(111) bei 7 K. Pentazen (C22H14) ist ein aromatischer Kohlenwasserstoff bestehend aus fünf linear angeordneten Benzolringen. Das Einzelmolekül adsorbiert in planarer Geometrie, wobei die lange Molekülachse stets parallel zu den dichtgepackten Cu-Reihen in der Oberflächenebene ausgerichtet ist. Attraktive Wechselwirkungen zwischen Molekül und STM-Spitze können dazu ausgenutzt werden, um kontrollierte laterale Translationen des Moleküls entlang verschiedener hochsymmetrischer Richtungen auszuführen. Durch kombinierte Manipulation sowohl des Moleküls als auch einzelner Cu-Adatome finden wir, daß die Benzoleinheiten des adsorbierten Moleküls stets über hexagonal-dichtgepackten (HCP-) Plätzen der Cu(111)-Oberfläche zentriert sind.

O 10.3 Fr 16:15 TU EB301

Coulombic amino-group–metal bonding: Adsorption of adenine on Cu(110) — •Martin Preuss, Wolf Gero Schmidt, and Friedhelm Bechstedt — Institut für Festkörpertheorie und -optik, Max-Wien-Platz 1, 07743 Jena

The knowledge of the interaction between biologically active molecules such as proteins or nucleic acid and solid surfaces is relevant to the preparation of biocompatible materials and biosensors. The adsorption of small organic molecules, in particular amino acids or nucleic acid bases, on metal surfaces thereby serves as a model case for the understanding of more complex systems as well as reactions between organic molecules. The bonding of molecular amino groups to metal surfaces is of particular interest and has given rise to a number of interpretations. Here we analyze the adsorption of adenine on Cu(110) using *first principles* calculations. A directional bonding between the amino-group nitrogens and copper surface atoms is found to emerge that cannot simply be explained by covalent or ionic contributions. Instead we propose the established bond to be a result of mutual polarization of the amino-group N lone pair of electrons and the metal substrate. To rationalize this notion we decompose the Coulombic interaction energy due to the charge transfer into monopole and dipole terms.

O 10.4 Fr 16:30 TU EB301

Electronic interaction between a single molecular wire and a metallic nanostructure — •Leonhard Grill[1], Francesca Moresco[1], Ping Jiang[2], Sladjana Stojkovic[2], Christian Joachim[2], Andre Gourdon[2], and Karl-Heinz Rieder[1] — [1]Institut für Experimentalphysik, Freie Universität Berlin, Arnimallee 14, 14195 Berlin — [2]Nanoscience Group, CEMES-CNRS, 29 rue J.Marvig, 31055 Toulouse, France

We have studied organic so-called Lander molecules with low temperature STM. On Cu(110) these molecules act as templates for the formation of characteristic copper nanostructures, two atoms wide and seven atoms long. By manipulation with the STM tip the molecules can be shifted laterally along these nanostructures where they adapt to various stable conformations. The characterization and control of the electronic contact between a molecule and an electrode is of fundamental importance for future molecular electronics. In the present work an electronic contact, i.e. additional contribution to the tunneling current, between the molecular board and the metal atoms is observed, in particular if the Lander is brought to the end of the copper nanostructure by STM manipulation. We have studied the dependence of this electronic interaction on the molecular position and conformation, the height of the molecular wire and the chemical properties of its end group. Experimentally determined results are compared with calculations.

O 10.5 Fr 16:45 TU EB301

Mediated Co-Adsorption of Hydrogen-Bound Molecular Monolayers — •Lorenz Kampschulte, Markus Lackinger, Stefan Griessl, and Wolfgang M. Heckl — Department for Earth- and Environmental Sciences, Ludwig-Maximilians-University Munich, Theresienstr. 41, D-80333 Munich, www.nano-science.de

Self-assembled monolayers (SAMs) are an important grounding for future applications of long range ordered molecular structures in nanotechnology. Hence it is of general interest to understand the parameters determining the growth and stability of these systems.

By means of Scanning Tunneling Microscopy (STM) based experiments we try to learn more about driving forces for molecular self-assembly and the influence of external parameters. Stable adsorption of TPT (1,3,5-tris(4-pyridyl)-2,4,6-triazin) molecules at the liquid-solid interface (which normally do not adsorb in an equilibrium situation) was observed by STM. Adsorption of TPT was made possible with the aid of H-bonding "glue-molecules" like TMA (1,3,5-benzene-tricarboxylic acid - trimesic acid) or TPA (1,4-benzene-dicarboxylic acid -terephthalic acid). With this method it was possible to prepare SAMs of TPT co-adsorbed with either TMA or TPA which were stable during the observation time of approximately 30 min. For continuative investigations the same molecular systems were prepared under Ultra-High-Vacuum (UHV) conditions.

O 11 Elektronische Struktur I

Zeit: Freitag 15:45–17:00 Raum: TU EB420

O 11.1 Fr 15:45 TU EB420

Oxygen 1s NEXAFS spectra of differently terminated $V_2O_3(0001)$ surfaces: ab initio DFT cluster studies for the $V'OV$ and $O_tV'O$ terminations — •Christine Kolczewski and Klaus Hermann — Fritz-Haber Institut der Max-Planck Gesellschaft, Faradayweg 4-6, 14195 Berlin, Germany

In the present work we use model clusters and ab initio density functional theory (DFT) together with gradient corrected functionals to obtain theoretical 1s core excitation spectra of differently coordinated oxygen appearing near the $V_2O_3(0001)$ surface. Here we consider both the intrinsic half metal layer, $V'OV$, and the vanadyl termination, $O_tV'O$. Comparison of the theoretical spectra with those from recent NEXAFS experiments [1] spectra yields overall good agreement. This allows us to assign spectral details in the experiment to specific O 1s core excitations where final state orbitals are determined by the local binding of the differently coordinated oxygen centers. The strong dependence of peak positions and relative intensities on the photon polarization direction found in experiment is also described well by the present theoretical spectra. As a result, a combination of the present theoretical spectra with experimental NEXAFS data enables an identification of differently coordinated surface oxygen species at the $V_2O_3(0001)$ surface.

[1] A.-C. Dupuis, M. Abu Haija, B. Richter, H. Kuhlenbeck, and H.-J. Freund, Surface Science, 2003, vol. 539(1-3), 99-112

O 11.2 Fr 16:00 TU EB420

Electronic structure of alkaliated transition metal oxides used as battery cathodes — •Andreas Thissen[1], Francisco Javier Fernandez Madrigal[1], Qi-Hui Wu[2], Stefan Laubach[3], Peter C. Schmidt[3], and Wolfram Jaegermann[1] — [1]FB Material- und Geowissenschaften, FG Oberflächenforschung, TU Darmstadt, Petersenstr. 23, D-64287 Darmstadt — [2]Lehrstuhl für Physikalische Chemie I, Ruhr-Universität Bochum, Universitätsstr. 150, D-44780 Bochum — [3]FB Physikalische Chemie, FG Festkörpertheorie, TU Darmstadt, Petersenstr. 20, D-64287 Darmstadt

Electronic structure of (Li, Na)xV2O5 and (Li, Na)xCu2.33V4O11 has been studied by XPS, UPS, ResPES and XAS. V2O5 thin films have been prepared by PVD and RF magnetron sputtering. From ResPES partial valence band density of states has been derived, giving a V3d-admixture to the valence band of 12 percent, comparing well to recent DFT calculations. From that value real oxidation numbers are calculated to V+2.5 and O-1. Adsorption of lithium and sodium at room temperature leads to spontaneous intercalation until alkali saturation concentrations of Li2.4V2O5 and Na2V2O5 are reached. O.32 electrons per lithium and 0.42 electrons per sodium atom are transferred to V3d states, reducing the formal oxidation state of the V-ion from 5+ to 4+. The Fermi-level is shifted upwards due to the charge transfer and the V3d states are stabilized by localization indicating the breakdown of the rigid band model. A model is shown, to correlate the electronic structure to battery voltages against Li/Li+ from electrochemical measurements. This work is funded by DFG(SFB595), EU(INTERCALNET) and BMBF.

O 11.3 Fr 16:15 TU EB420

Electronic structure of Li-inserted V_6O_{13} battery cathodes: rigid band behaviour and effects of hybridization — •V. Eyert[1], U. Schwingenschlögl[1], T. Schmitt[2], and L.-C. Duda[2] — [1]Institut für Physik, Universität Augsburg — [2]Department of Physics, Uppsala University

The electronic properties of $Li_xV_6O_{13}$ battery cathodes are studied by means of resonant soft x-ray emission spectroscopy and *ab initio* calculations as based on density functional theory using the augmented spherical wave (ASW) method. For $x = 0, \ldots, 6$ we observe both experimentally and theoretically a rather rigid shift of the V $3d$ bands centered about the Fermi energy. However, lithiation leads to an overall weakening of the V $3d$-O $2p$ hybridization. These findings conform with the observed high crystal structure stability upon insertion of Li, which is essential for the desired use as a battery cathode material.

O 11.4 Fr 16:30 TU EB420

Analysis of the SrTiO$_3$ Valence Band Structure by X-ray Standing Wave Measurements and Ab-Initio Calculations — •Sebastian Thiess[1], Tien-Lin Lee[1], François Bottin[2], Bruce C.C. Cowie[1], and Jörg Zegenhagen[1] — [1]ESRF, Grenoble, France — [2]CEA, Bruyères-le-Châtel, France

We have determined the Sr, Ti and O components of the SrTiO$_3$ valence band (VB) by site-specific X-ray photoelectron spectroscopy employing the X-ray Standing Wave (XSW) method. Decomposition into angular-momentum resolved density of states for each element was achieved by comparision with *ab initio* calculations based on norm-conserving pseudopotentials within the local density approximation.

Lattice site-specific electronic information - which is not available from standard XPS - is obtained by utilising the spatial intensity modulation of an XSW interference field, generated by the coherent superposition of an incident and a Bragg-reflected x-ray beam. By proper positioning the antinodes of the XSW within the STO unit cell, photoemission from specific lattice sites can be preferentially excited and their valence electronic contribution identified.

XSW fields were generated by the STO(111) and STO(112) reflections at photon energies of 2.75 and 3.89 keV. XSW modulated, high-resolution core and valence-electron emission spectra were recorded from an in-situ UHV annealed STO single crystal at beamline ID32 at the ESRF.

O 11.5 Fr 16:45 TU EB420

Electronic Structure of decagonal Al-Cu-Co quasicrystals — •Jan Hugo Dil[1], JeongWon Kim[1], Eli Rotenberg[2], Karsten Horn[1], and Wolfgang Theis[3] — [1]Fritz-Haber-Institut der MPG, Berlin — [2]Advanced Light Source, Lawrence Berkeley Lab — [3]Fachbereich Physik der FU Berlin

An analysis of the electronic structure of quasicrystals is important for an explanation of the unusual structural and physical properties of these materials. Progress has been made in understanding the band structure in the lower s-p region of the valence levels in decagonal quasicrystalline alloys. However, an identification of the dispersion relation of bands near the Fermi level in these solids, which lack translational symmetry, is still missing. Here we characterize the electronic levels in decagonal Al-Cu-Co through photoemission data from the tenfold and twofold symmetric surfaces. Al-Cu-Co is a useful material from the point of view of photoemission experiments since the Cu and Co d bands are well separated, and the influence of either d metal can thus be identified. We compare strongly dispersing features in the region near E_F with LEED data to identify those reciprocal lattice vectors which give rise to dominant features in the photoemission intensity maps, and compare our data with results from Al-Ni-Co where the Ni and Co bands overlap.

O 12 Nanostrukturen I

Zeit: Freitag 15:45–17:00 Raum: TU EB202

O 12.1 Fr 15:45 TU EB202

PEEM as a tool for the investigation of optical near fields — •M. Cinchetti[1], A. Gloskovskii[1], S. Nepijko[1], G. Schönhense[1], M. Kreiter[2], H. Rochholz[2], D. Bayer[3], C. Wiemann[3], M. Bauer[3], and M. Aeschlimann[3] — [1]Institut für Physik, Johannes Gutenberg-Universität Mainz — [2]MPI für Polymerforschung Mainz — [3]Institut für Physik, Universität Kaiserslautern

Photoemission electron microscopy (PEEM) was used to image the electrons photoemitted from specially tailored Ag nanoparticles (crescents, dots, rods) deposited alternatively on a Si substrate with its native oxide (SiO$_x$) or on an ITO substrate. Photoemission was induced by illumination with a Hg UV-lamp (photon energy cutoff $\hbar\omega_{UV} = 5.8\,\mathrm{eV}$, wavelength $\lambda_{UV} \geq 220\,\mathrm{nm}$) and with a Ti:Sa femtosecond laser ($\hbar\omega_l = 3.0\,\mathrm{eV}$, $\lambda_l = 400\,\mathrm{nm}$), respectively. Upon illumination at energies above the Ag plasmon frequency the photoemission from the nanoparticles appears rather homogeneous. In contrast, at lower photon energies a strongly spatially localized photoemission signal is recorded. For 400 nm laser radiation the electron emission results from two-photon photoemission as was previously demonstrated by PEEM spectromicroscopy [1]. The results are interpreted as a signature of the local electrical field thus providing a tool to map the optical near field with the resolution of emission electron microscopy.

[1] M. Cinchetti *et al.* , Appl. Phys. Lett. **83** (2003) 1503 and J. El. Spectr. Rel. Phen. **137-140** (2004) 249.

O 12.2 Fr 16:00 TU EB202

Alloy formation of supported Gold nanoparticles at their transition from clusters to solids: Does size matter? — •H.-G. Boyen[1], A. Ethirajan[1], G. Kästle[1], F. Weigl[1], P. Ziemann[1], G. Schmid[2], M.G. Garnier[3], M. Büttner[3] und P. Oelhafen[3] — [1]Abteilung Festkörperphysik, Universität Ulm, D-89069 Ulm — [2]Institut für Anorganische Chemie, Universität Duisburg-Essen, Universitätsstrasse 5-7, D-45117 Essen — [3]Institut für Physik, Universität Basel, Klingelbergstr. 82, CH-4056 Basel

Gold nanoclusters of a size approaching the molecular limit (<3nm) were prepared on Si substrates in order to study alloy formation on the nanometer scale. For this purpose, Indium atoms are deposited on top of the gold particles at room temperature and the formation of AuIn$_2$ is studied by X-ray Photoelectron Spectroscopy (XPS) in situ. It is observed that the alloy formation takes place independent of whether the particles electronically are in an insulating molecular or in a metallic state. Most important, however, closed packed full-shell clusters containing 55 Au atoms are found to exhibit an outstanding stability against alloying despite a large negative heat of formation of the bulk Au-In system. Thus, Au$_{55}$ clusters may play a significant role for the design of nanoscaled devices where chemical inertness is of crucial importance.

O 12.3 Fr 16:15 TU EB202

Collective Surface Plasmon Modes in Ensembles of Gold Particles — •Phillip Olk[1], Jan Seidel[1], Stefan Grafström[1], Lukas Eng[1], Marcell Ott[2], and Martin Möller[2] — [1]Institut für Angewandte Photophysik, TU Dresden, 01062 Dresden — [2]Dt. Wollforschungsinstitut an der RWTH Aachen, 52062 Aachen

The optical properties of self-arranged spherical gold nanoparticles are studied by means of scanning near-field optical microscopy (SNOM) and white-light spectroscopy. Films were prepared by plasma etching of self-arranged monolayers of inverted micelles which were loaded with gold salt[1]. Continuous decoration of both glass and silicon substrates is possible, resulting in typical inter-particle distances of 120 nm and sphere diameters of 10 nm.

When exciting the cluster array in a Kretschmann-Raether-like total-internal-reflection set-up, we find surface-bound optical modes very similar to surface plasmon polaritons on flat continuous metal films. We detect such modes by scanning a dielectric SNOM tip across the surface and recording the amount of evanescent light above the sample surface.

Although our films are far from being *continuous* metal films, the modes are found to decay in intensity with a decay length measuring $> 20\ \mu\mathrm{m}$, comparable to the decay length of surface plasmon polaritons in dense metal films. Moreover, the decay length is found to depend on wavelength and in-plane **k** component, indicating the existence of a material-dependent optical band structure.

[1] J. P. Spatz et al., *Langmuir* **16**, 407–415 (2000)

O 12.4 Fr 16:30 TU EB202

Long range order of 2D C_{60} islands on Au(788) — •Nicolas Neel, Jörg Kröger, and Richard Berndt — Institut für Experimentelle und Angewandte Physik Universität Kiel

Submonolayer coverages of C_{60} on Au(788) were investigated by low-temperature scanning tunnelling microscopy. At 0.5 ML coverage self-organized two-dimensional C_{60} islands occur and form well ordered rectangular arrays which extend over distances of hundreds of nanometres. Judging by a large number of images recorded througout the crystal surface we estimate that the arrays cover more than 95 percent of the total area. The formation of the periodic array and observed homogeneity of the island shape are discussed within a model which involves initial nucleation of C_{60} at step edges and preferential adsorption on FCC domains of the gold surface. This adsorption system appears to be a useful template for further deposition of functional units.

O 12.5 Fr 16:45 TU EB202

Single-molecule chemical field-effect transistors with nanometer-sized gates: demonstration and tests — •Frank Jäckel[1], Zhaohui Wang[2], Mark D. Watson[2,3], Klaus Müllen[2], and Jürgen P. Rabe[1] — [1]Humboldt-Universität zu Berlin, Institut für Physik, Newtonstr. 15, 12489 Berlin, Germany — [2]Max-Planck-Institut für Polymerforschung, Ackermannweg 10, 55128 Mainz, Germany — [3]University of Kentucky, Department of Chemistry, Lexington KY 40506-0055, USA

We present a prototypical three-terminal single-molecule device in which the current through a hybrid molecular diode, made from a single molecule in the junction of a scanning tunneling microscope, is modified by the presence of oriented organic charge transfer complexes covalently attached to the molecule in the gap. The set-up represents the first single-molecule transistor with nanometer-sized gates [Phys. Rev. Lett. 92 (2004) 188303]. The observed change in the current-voltage characteristics is explained with an interface dipole originating from the charge transfer complexes. We present tests of this model with respect to the orientation of the dipoles.

O 13 Magnetismus

Zeit: Freitag 15:45–17:00 Raum: TU EB107

O 13.1 Fr 15:45 TU EB107

Nanomagnet arrays fabricated on self-organized semiconductor templates — •C. Teichert[1], A.M. Mulders[2], M.A. Niño[3], S. Heun[4], A. Locatelli[4], C. Hofer[1], N. Mikuszeit[3], J. Camarero[3], A. Fraile Rodriguez[2], J.J. de Miguel[3], and R. Miranda[3] — [1]Inst. of Physics, University of Leoben, A-8700 Leoben, Austria — [2]Dept. of Physics, Uppsala University, S-75121 Uppsala Sweden — [3]Dept. of Condensed Matter Physics and Institute of Materials Science N. Cabrera Univ. Autónoma de Madrid, Cantoblanco, 28049-Madrid, Spain — [4]Sincrotrone Trieste, in AREA Science Park, 34012 Basovizza, Trieste, Italy

Self-organized nanofaceted semiconductor surfaces are attractive candidates to be used as large-area templates for the growth of magnetic nanostructures. By shadow deposition onto selected facet types, arrays of isolated nanomagnets can be fabricated. Using this technique we prepared Co nanomagnets on SiGe templates at the Nanospectroscopy Beamline of the synchrotron ELETTRA. X-ray magnetic circular dichroism (XMCD) measurements using a photoemission electron microscope reveal the in plane magnetization of the 7 monolayer thick Co nanomagnets. Their base size of about 200 nm x 25 nm corresponds to the facet size of the templates as determined by atomic-force microscopy. Although the nanomagnets are isolated, XMCD reveals several micrometer large areas within which the nanomagnets have correlated magnetization. The magnetic coupling is preferentially along the easy axis of the nanomagnets in agreement with micromagnetic simulations.

O 13.2 Fr 16:00 TU EB107

Quantum-Well States and Spin Polarization in Ni/Cu Thin-Film Structures — •Volker Renken, Dehong Yu, Georgi Rangelov, and Markus Donath — Physics Institute, University of Münster, Wilhelm-Klemm-Str. 10, 48149 Münster, Germany

Spin- and angle-resolved inverse photoemission was used to study the unoccupied quantum-well states in ultrathin Ni films on Cu(001). Three quantum-well features are clearly resolved that disperse to higher energies with increasing Ni overlayer thickness. The transition from two- to three-dimensional behaviour is followed by observing the bulk sp-band being formed from discrete quantum-well states. The dispersion of the quantum-well states as a function of the wave vector parallel to the surface agrees well with the corresponding sp-band dispersion. Our results are discussed in comparison with results for Co on Cu(001) [1] with respect to energy dependence and magnetic exchange splitting.

[1] Yu et al., Phys. Rev. B 68 (2003) 155415.

O 13.3 Fr 16:15 TU EB107

Spin polarization and electron confinement in nanoscale Co islands on Cu(111) — •Oswald Pietzsch, André Kubetzka, Stefan Heinze, Matthias Bode, and Roland Wiesendanger — Institute of Applied Physics,University of Hamburg,Jungiusstrasse 11, 20355 Hamburg, Germany

Spin-polarized scanning tunneling spectra (SP-STS) of nanoscale ferromagnetic Co islands on Cu(111) show that the spin polarization (SP) is strongly dependent on the energy in the vicinity of the Fermi level [1]. In particular, the sign of SP is reversed several times within the observed energy window. We discuss possible explanations based on first principles spin-resolved band structure calculations.

Similar to the Cu surface, the Co islands exhibit a standing wave pattern in the local density of states (LDOS) which can be observed by STM [2]. A comparison of the Co and Cu patterns as a function of energy reveals the essential difference: while the latter shows two-dimensional (2D) free electron gas behavior, the former is determined by lateral electron confinement. We compare our results with models based on an exact solution of the particle-in-a-triangular-box problem and a multiple scattering approach. signature of the island rim which is yet different from that of both Co and Cu.

[1] O. Pietzsch *et al.*, Phys. Rev. Lett., **92**, 057202 (2004).
[2] L. Diekhöner *et al.*, Phys. Rev. Lett. **90**, 236801 (2003).

O 13.4 Fr 16:30 TU EB107

Complex magnetism of small 3d transition metal clusters on Ni and Cu surfaces — •Phivos Mavropoulos, Samir Lounis, Rudolf Zeller, Stefan Blügel, and Peter H. Dederichs — IFF, Forschungszentrum Jülich, D-52425 Jülich, Germany

We present ab-initio calculations of magnetic clusters on non-magnetic or magnetic substrates. Firstly, we study small clusters (1-9 atoms) of Fe, Cu, and Ni on Ni and Cu surfaces. Emphasis is given on the dependence of the spin moments on cluster shape and size. For Fe we derive a quantitative rule connecting the moment of each Fe atom linearly to its coordination number. Thus the moment of an arbitrary cluster can be readily found if the positions of the atoms are known. For Co clusters the rule holds to a lesser extent, and much less so for Ni clusters.

Secondly, we focus on small magnetic Mn and Cr clusters, where a competition between ferro– and antiferromagnetic interactions can lead to noncollinear spin structures. The size and orientation of the local moments and the stabilization of noncollinear magnetic state are investigated.

Work supported by the DFG Schwerpunktsprogramm “Clusters in contact with Surfaces” (SPP 1153).

O 13.5 Fr 16:45 TU EB107

Evidence for canted spin structures for small mass selected deposited chromium clusters? — •Matthias Reif, Leif Glaser, Michael Martins, and Wilfried Wurth — Institut für Experimentalphysik, Universität Hamburg, Luruper Chaussee 149, 22761 Hamburg

The magnetic properties of small (N=1..13) Cr_N clusters deposited on ultrathin Fe films on a Cu(100) substrate magnetized normal to the surface plane have been investigated. To determine the element specific magnetic spin and orbital moments, we have measured X-ray Magnetic Circular Dichroism (XMCD) spectra at the BESSY II storage ring. Soft landing conditions have been used for cluster deposition.

A strong decrease of the spin magnetic moments with increasing cluster size is observed. The spin moments per d-hole decrease from a value of $0.4\mu_B$ for the monomer down to values of $0.1\mu_B$ for the Cr_{13} clusters. The orbital magnetic moments are close to zero for the various cluster sizes except for the Cr_4 cluster. Here, an orbital moment coupled antiparallel to the spin moment is observed and the spin moment is strongly enhanced compared to Cr_3 or Cr_5.

The strong decrease of the spin magnetic moments with increasing cluster size suggests a non collinear alignment of the individual spin moments of the atoms in the larger clusters.

This work was supported by the German ministry for education and research (BMBF) under grant KS1 GUB/5.

O 14 Struktur und Dynamik reiner Oberflächen

Zeit: Freitag 15:45–16:45 Raum: TU EB407

O 14.1 Fr 15:45 TU EB407

Time-resolved low energy electron diffraction from large molecules on surfaces — •Claudio Cirelli[1,2], Matthias Hengsberger[1], Andrei Dolocan[1], Hansjörg Neff[1], Jürg Osterwalder[1], Herbert Over[2], and Thomas Greber[1] — [1]Physik-Institut, Universität Zürich, CH-8057, Switzerland — [2]Physikalisch-Chemisches Institut, Justus-Liebig-Universität, Heinrich-Buff-Ring 58, D-35392 Gießen, Germany

In order to observe dynamics of molecules adsorbed on solid surfaces in real time, it is necessary to develop a technique which combines both temporal and spacial resolution on the scale of molecular motion. This task is tackled with a pump-probe experiment, where Low Energy Electron Diffraction (LEED) probes the collective response of a surface on a laser pump pulse as a function of time delay between pump and probe. We present an electron gun that produces ultra-short electron pulses by two-photon photoemission process when 400nm laser light pulses are focused onto a gold cathode (20nm thick film deposited on sapphire substrate): the electron yield is about 0.5 electron/pulse with 0.5nJ laser pulses with a measured energy resolution of 0.7eV at 100eV. This results in a nominal time resolution of 3ps. As a molecular system we investigate one monolayer of C_{60} on Ag(111), that forms a $2\sqrt{3}x2\sqrt{3}$ R30° structure. This system has a low Debye temperature of about 50K and is thus, together with the large mass of C_{60}, well suited for our purpose. First results will be presented and compared to results of static LEED experiments.

O 14.2 Fr 16:00 TU EB407

Temporal evolution of surface structures after fs-laserpulse excitation — •B. Krenzer, A. Janzen, and M. Horn-von Hoegen — Fachbereich Physik, Universität Duisburg-Essen, Universitätsstr. 5, 45117 Essen

Studies of surface-dynamics with fs-timeresolution are very well established using optical methods, e.g. SHG, SFG. Structural informations of the investigated systems, however, are only indirectly accessible. Using ultrashort X-ray pulses a direct determination of bulk structures and their dynamics is possible [1]. The highly enhanced surface sensitivity and higher scattering amplitude of electrons made the development of timeresolved electron diffraction for surface studies desirable. Recently, the construction of electron guns providing fs-electron pulses has been achieved. This progress allows studies of structural changes of thin metal films and adsorbate systems on a ps- to sub-ps timescale [2].

We built an electron diffraction system capable to study surface dynamics. Short electronpulses are directed at glancing angle on surfaces excited by a fs-laserpulse. Depending on the delay between pumping laserpulse and probing electronpulse on the surface the temporal evolution of surface structures can be determined on a ps-timescale (ps-RHEED). In this talk we will present first results obtained with the new system. These investigations were conducted on clean and Bi-covered Si(001)-surfaces.

[1] K. Sokolowski-Tinten et. al., Nature **422**, 286 (2003).

[2] B.J. Siwick et. al., Science **302**, 1382 (2003), C.-Y. Ruan et. al., Science **304**, 80 (2004).

O 14.3 Fr 16:15 TU EB407

Atomically resolved imaging of Stoichiometric CeO_2 (111) — •S. Gritschneder[1], Y. Namai[2], A.S. Foster[3], Y. Iwasawa[2], and M. Reichling[1] — [1]Fachbereich Physik, Universität Osnabrück, Barbarastraße 7, 49076 Osnabrück, Germany — [2]Department of Chemistry, The University of Tokyo, 7-3-1 Hongo, Bunkyo-ku, Tokyo 113-0033, Japan — [3]Laboratory of Physics, University of Helsinki, P.O. Box 1100, 02015 HUT, Finland

The (111) surface of CeO_2 in various oxidation states is important for catalytic activity and some of its details relating to surface oxygen atoms have already been studied with dynamic scanning force microscopy. For an in-depth understanding of the surface chemistry of CeO_2(111), it is most interesting to gain insight into the details of surface structural features and to yield an unambiguous interpretation of contrast features observed in dynamic scanning force microscopy results obtained on CeO_2(111). While atomic resolution can routinely be achieved nowadays, interpretation of atomic contrast images is still a non-trivial task. As CeO_2 exhibits the same fluorite structure as the prototype material CaF_2 and contrast formation on CaF_2(111) is quantitatively well understood, we compare atomic contrast formation on both surfaces. On flat terraces, surface ions mostly appear as disk-like features but also other contrast feature like triangular patterns are observed. When scanning at smallest distance, the predominant contrast pattern is a stable honeycomb structure. By theoretical modelling of the imaging process we aim to assign the different contrast patterns to the anionic and the cationic sub-lattices, respectively.

O 14.4 Fr 16:30 TU EB407

Zweidimensionale Legierungsbildung in PtAu Monolagenschichten — •Eleonora Filonenko, Harry Hoster, Hubert Rauscher und R.J. Behm — Abt. Oberflächenchemie und Katalyse, Universität Ulm

Im Rahmen einer Studie zu den (elektro-) katalytischen Eigenschaften wohldefinierter Pt-Au Oberflächen wurde das 2D-Mischungsverhalten der beiden Metalle in Monolagenschichten mittels hochauflösendem STM untersucht. Als Modellsysteme dienten i) Au auf Pt(111) und ii) Pt und Au auf Ru(0001), präpariert durch (sequenzielles) Aufdampfen und nachfolgendes Heizen. Quantitative Analysen atomar aufgelöster STM-Bilder fur verschiedenen Zusammensetzungen zeigen, dass die für das Volumen bekannte schlechte Mischbarkeit von Pt und Au sich in beiden Modellsystemen auch für den zweidimensionalen Fall wiederfindet. Die Resultate werden mit dem Verhalten anderer 2D-Oberflächenlegierungen unterschiedlicher Mischbarkeit verglichen. Thermodynamische und kinetische Aspekte der 2D-Mischbarkeit werden diskutiert.

O 15 Postersitzung (Adsorption an Oberflächen, Epitaxie und Wachstum, Organische Dünnschichten, Oxide und Isolatoren, Rastersondentechniken, Zeitaufgelöste Spektroskopie, Methoden)

Zeit: Freitag 17:00–20:00 Raum: Poster TU D

O 15.1 Fr 17:00 Poster TU D

Compression of submonolayer goldfilms by CO adsorption on a Re($10\bar{1}0$) surface — •C. Pauls and K. Christmann — Inst. f. Chemie, FU Berlin, Takustr. 3, 14195 Berlin

We have studied the adsorption of carbon monoxide on the clean and partially gold-covered Re(10-10) surface by means of LEED, thermal desorption (TPD) and work function change ($\Delta\Phi$) measurements. On the Re(10-10) surface, increasing coverages of Au produce a variety of (1xn) LEED superstructures in the submonolayer regime (n = 3, 4, 5, 6), until a pseudomorphic (1x1) phase is formed at a complete Au monolayer. This phase has been subjected to a quantitative LEED analysis and clearly reveals a continuation of the Re lattice by a double layer of Au atoms in the 'A' termination of the Re(10-10) surface. Still larger Au coverages lead to a (1x8) LEED phase which is surprisingly stable in the multilayer regime. Interesting effects become apparent, if CO is adsorbed into the submonolayer Au phases: Apparently, CO is able to compress the rows of Au atoms in [0001] direction, i.e., perpendicular to the troughs, since the low-coverage (1x3) and (1x4) Au phases undergo transitions to the (1x4) and (1x5) phases, respectively, in the presence of coadsorbing CO. So far, similar effects have only been reported for coadsorption of oxygen and gold on a ruthenium (10-10) surface [1].

[1] S. Poulston, M. Tikhov, and R.M. Lambert, Langmuir 13 (1997) 5356

O 15.2 Fr 17:00 Poster TU D

Density-functional theory study of oxygen adsorption at vicinial Pd surfaces — •Yongsheng Zhang, Jutta Rogal, and Karsten Reuter — Fritz-Haber-Institut, Faradayweg 4-6, D-14195 Berlin

The contact with our O-rich atmosphere can lead to the formation of oxides at transition metal surfaces, and therewith significantly alter the surface properties and functionality. Although atomic steps are generally believed to play a prominent role in this oxide formation process, most of our atomic-scale understanding derives to date from studies concentrating on low-index surfaces. As a first step to explicitly address the effect of atomic steps, we use density-functional theory to investigate the adsorption of oxygen at vicinal Pd(11N) surfaces (N=3,5,7), exhibiting (111) steps and (100) terraces of varying width. Oxygen adsorption close to the steps induces strong changes in the geometric relaxation of the surfaces, that before followed a clear trend with contraction of all surface layers with undercoordinated atoms. Adsorption at the steps is energetically preferred compared to the terrace sites, and we find the geometric, energetic and electronic properties of the center terrace sites at Pd(117) to be already almost indistinguishable from those at a low-index Pd(100) surface.

O 15.3 Fr 17:00 Poster TU D

Interaction of Formic Acid with Surfaces of Solid Water between 80 and 200K — •S. Bahr[1], O. Höfft[1], A. Borodin[1], V. Kempter[1], F. Borget[2], T. Chiavassa[2], and A. Allouche[2] — [1]Institut für Physik und Physikalische Technologien, TU Clausthal, Leibnizstr. 4, D–38678 Clausthal–Zellerfeld — [2]Physique des Interactions Ioniques et Moléculaires, CNRS-UMR6633 Université de Provence, Campus St. Jérôme, Marseille France

The interaction of formic acid (HCOOH) with solid water, deposited on tungsten at 80K, was studied witch metastable impact electron spectroscopy (MIES), UPS(HeI and II), IR-Spectroscopy and TPD. In MIES and UPS the emission from the outermost $1b_1$, $3a_1$, $1b_2$ MOs of water and the weakest–bonded π– and σ–type MOs of formic acid (FA) were monitored. The results are interpreted witch the help of cluster DFT calculations. FA/water interfaces were prepared at 80K, namely FA layers on thin films of solid water and H_2O adlayers on thin FA films; they were annealed between 80 and 200K. It is concluded that an H–bonded FA–network forms on the solid water surface, suggesting that the lateral interaction between FA species is stronger that between FA and water. In the entire studied temperature range the FA species remain in the surface layer although a partial solvation takes place above 120K. After the desorption of water (155K TPD peak maximum), weak features of FA can be seen up to about 170K. Under the studied conditions no de–protonation of FA can be detected. Results for the deposition for H_2O on FA films at 80K will also be presented.

O 15.4 Fr 17:00 Poster TU D

Interaction of Cs Halides with the surface of Solid Water between 80 and 200K. — •O. Höfft, A. Borodin, S. Bahr, and V. Kempter — Institut für Physik und Physikalische Technologien, TU Clausthal, Leibnizstr. 4, D–38678 Clausthal–Zellerfeld

The interaction of the Cs halides (CsX) with X=: F, Cl, and I with solid water was investigated with Metastable Impact Electron Spectroscopy (MIES) and UPS(HeI and II) and TPD between 80 and 200K. In MIES and UPS the emission from the outermost H_2O MOs $1b_1$, $3a_1$, $1b_2$ and from the npX–states of X (n=2,3,5 for F, Cl and I, respect.) was monitored. We have prepared CsX/water interfaces, namely CsX layers on thin films of solid water and H_2O adlayers on thin CsX films; they were annealed between 80 and 200K. At 80K closed CsX layers were obtained on H_2O and vice versa; no interpenetration of the two components H_2O and CsX could be observed. However, ionic dissociation of CsX takes place when H_2O and CsX do interact directly. Above 105K we find that solvation of these ionic species becomes significant. Our results are compatible with a transition of ionic species from a surface site to an energetically favored water–separated site, where the species are solvated. Desorption of the water molecules, not involved in the solvation process, becomes sizeable above 135K. On the other hand, the temperature for desorption of H_2O molecules interacting with salt ions depends strongly on the particular anion X^- (120, 140, and 190K for F, Cl and I, respect.).

O 15.5 Fr 17:00 Poster TU D

Low Temperature STM investigation of pentacene molecule on $Cu_3Au(100)$ — •Micol Alemani, Francesca Moresco, Leo Gross, and Karl-Heinz Rieder — Inst. für Exp.physik, FU Berlin, Arnimallee 14, D-14195

The adsorption geometry of pentacene molecules on $Cu_3Au(100)$ is studied by means of a Low-Temperature Scanning Tunneling Microscope. The $Cu_3Au(100)$ is terminated by the gold-rich plane, as already known and as probed by atomic resolution images. Depending on the substrate geometry the molecules exhibit two different orientations and conformations. Thanks to the stability of the system at low temperature (7 K), it has been possible to perform controlled manipulation of single pentacene molecules. The study of the manipulation of pentacene on $Cu_3Au(100)$ is presented.

O 15.6 Fr 17:00 Poster TU D

Neutron Reflectometry from Thin Liquid Layers (Foam Films) — •R. Krastev[1,2], Th. Gutberlet[3], N. C. Mishra[1], and H. Möhwald[1] — [1]Max-Planck Institute of Colloids and Interfaces, 14424 Potsdam, Germany — [2]Hahn-Meitner Institute, Berlin, Glienicker Str. 100, 14109 Berlin, Germany — [3]Paul Scherrer Institute, 5232 Villigen PSI, Switzerland

The properties of liquids confined in small volumes deviate from that of the bulk material. Foam films have been widely used as model system to study interactions between fluid interfaces but they may be also used as a tool to study the properties of liquids in confined volumes. A foam film is formed by two monolayers of surfactant molecules with the hydrophobic parts facing the air and the hydrophilic head groups in contact with a central aqueous core. Film thickness can be tuned by the physicochemical parameters of the bulk solution from which films are formed while their surfaces always stay parallel each other. This way formation of structures with well defined geometry is assured. We used neutron reflectometry to study the composition of the layers which form a foam film. Films were prepared from solutions of surfactants in D2O. The layers of surfactant and aqueous core were discriminated due to different scattering length densities (SLD). The SLD of the surfactant layers does not depend on the distance between the film surfaces while that of the film central aqueous layer depends on the film thickness. SLD similar to that of D2O was measured in the case of thick films. It decreases when the two surfaces approach each other. The experimental results are shown and future work is discussed.

O 15.7 Fr 17:00 Poster TU D

Study of the effect of electrolyte ions on the forces between hydrophobic polymer surfaces in aqueous solutions — •Astrid Drechsler and Karina Grundke — Leibniz-Institut für Polymerforschung e.V., Hohe Straße 6, 01069 Dresden

Interfacial phenomena are strongly influenced by adsorption processes. In aqueous environments, even simple electrolyte ions modify the interactions of polymer surfaces. In the present study, the forces between a flat polystyrene surface and a colloidal polystyrene sphere have been measured directly in water and solutions of KCl and KOH using a scanning force microscope. At distances > 5...50 nm, all force-distance curves show an electrostatic repulsion caused by an electrical double-layer of electrolyte ions adsorbed to the surface. The surface potential of the polystyrene surface calculated from the force-distance curves coincides with its zeta potential. The decay lenght of the electrostatic repulsion diminishes with increasing electrolyte concentration due to the screening of the surface potential by the mobile ion layer. At distances < 5...20 nm, in most of the solutions an attractive force of variable range and strength dominates, the so-called 'hydrophobic force'. We attribute it to the existence of nanoscopic air bubbles on the hydrophobic polymer surfaces. It is not affected by the KCl concentration. In KOH concentrations <= 10-4 M, this attraction disappears. Instead, a "soft"steric repulsion occurs. The adhesion force decreases steadily with increasing KOH concentration. It is not clear if these phenomena are caused by air nanobubbles or if the nanobubbles are replaced by a strongly adsorbed layer of OH– and counterions.

O 15.8 Fr 17:00 Poster TU D

Particle Size Effects in TPD: Adsorption of CO_2 on Clean and Oxygen-Precovered Au(110)-(1x2) — •J.M. Gottfried[1,2] and K. Christmann[1] — [1]Institut fuer Chemie der Freien Universitaet Berlin, Takustr. 3, D-14195 Berlin — [2]Lehrstuhl fuer Physikalische Chemie II, Universitaet Erlangen-Nuernberg, Egerlandstr. 3, D-91058 Erlangen

Temperature programmed desorption (TPD) spectra of CO_2 on Au(110)-(1x2) exhibit overlapping submonolayer and multilayer peaks, indicating that the intermolecular CO_2-CO_2 attraction is of similar strength as the CO_2-gold interaction. Thus, layer-by-layer growth and three-dimensional growth are equally favoured. Accordingly, the TPD spectra show two anomalies: i) A low-temperature and a high-temperature state grow simultaneously, and ii) the second-layer TPD peak appears at a lower temperature than the multilayer peak. This behavior can be explained by three-dimensional growth of the Stranski-

Krastanov type. For small CO_2 aggregates, the surface energy contribution to the total energy increases the CO_2 vapour pressure and, hence, the desorption rate (Kelvin effect), whereas larger crystallites inhibit the desorption by excluding a certain fraction of the total coverage from desorption. Semi-quantitative simulations of the TPD spectra, supplemented by UPS and work function measurements, support our growth and interaction model of the CO_2 adsorbate on clean and oxidized gold.

O 15.9 Fr 17:00 Poster TU D

Adsorption properties of pyridine molecules on TiO_2 surfaces — •M. Dürr, A. Yasuda und G. Nelles — Materials Science Laboratories, Sony Int. (Europe) GmbH, D - 70327 Stuttgart

Photochemical solar cells based on nano-crystalline TiO_2 which is sensitized by organic dye molecules (dye-sensitized solar cells) have been shown to exhibit a strongly increased open circuit voltage and thus improved power conversion efficiency upon the addition of *tert*-butylpyridine to the electrolyte. This improvement of the cell performance was earlier attributed to a suppression of electron transfer between the TiO_2 conduction band and the redox couple in the electrolyte.

For a better understanding of the underlying mechanisms, the adsorption of pyridine molecules on TiO_2 was investigated by means of quartz crystal microbalance techniques and ultraviolett photoemission spectroscopy (UPS). A clear correlation between pyridine adsorption and the increase of open circuit voltage was observed. Moreover, it could be shown that only a small fraction of the total surface area is covered by the pyridine molecules at saturation coverage. The results are interpreted in terms of adsorption at defect sites and are correlated to adsorption-induced changes in the electronic structure as observed by means of UPS.

O 15.10 Fr 17:00 Poster TU D

Adsorption of Methanol on $Pd_3Sn/Pd(111)$ Surface- Alloy — •Christian Breinlich, Thomas Schmidt, Conrad Becker, and Klaus Wandelt — Institut für Physikalische Chemie, Wegelerstr.12, 53115 Bonn

Over the last decade several experimental UHV- studies have been published, describing the decomposition of methanol, adsorped on Pd(111)-surfaces, into carbon monoxide and hydrogen. We have investigated the adsorption of methanol on a palladium tin surface alloy with a $p(2 \times 2)$ superstructure. The idea behind this is to reduce the reactivity of the palladium surface by alloying it with a less noble metall. We investigated the geometric and electronic properties of the surface by AES, LEED and UPS. TDS showed a desorption of methanol from the multilayer at 140 K. At 160 K the monolayer desorbs intact. Neither CO nor hydrogen were detected in significant amounts, so that in contrast to the bare Pd surface, methanol does not decompose on this alloy. These results were supported by UPS data and work function measurements. There was no evidence, that carbon monoxide or surface carbon were formed. A Redhead analysis of the TDS data resulted in an adsorption energy of the multilayer of about 0.36 eV, which is similar to that on Pd (111). For the monolayer we found an adsorption energy of about 0.41 eV. These data agree with our studies on the corresponding $(\sqrt{3} \times \sqrt{3})R30^\circ\ PdSn_2/Pd(111)$ surface alloy.

O 15.11 Fr 17:00 Poster TU D

Study of conductivity and surface morphology during adsorption of silver atoms on a smooth Ag(111) film — •Giriraj Jnawali, Boris Krenzer, and M. Horn-von Hoegen — Institute for Laser and Plasma Physics, University of Duisburg-Essen, Essen, Germany

The conductivity of ultra-thin metal film has great relevance to technological applications. In contrast to thin metal film, the surface morphology has an enhanced impact on the electronic transport through the film.

In this poster we'll present the results of conductivity measurements along with morphology study of ultra-thin metal films. The conductivity measurements were performed by four-point resistance measurements and the morphology was studied by SPA-LEED.

Ultra-thin Ag(111) films were prepared by depositing silver atoms on Si(100) substrate at 80K and annealed the film carefully until it turned into flat surface. The quality of flatness was checked by SPA-LEED measurements. Subsequently the film was exposed to a low dose silver atoms at different substrate temperatures ranging from 80 to 200K. An increase in resistance due to scattering at adsorbate atoms was observed. The resistance measurements were accompanied by SPA-LEED to determine the surface roughness.

O 15.12 Fr 17:00 Poster TU D

'Pulse injection': A non-destructive way of depositing large organic molecules under ultrahigh vacuum conditions — •Ingeborg Stass, Leonhard Grill, Francesca Moresco, and Karl-Heinz Rieder — Institut für Experimentalphysik, Freie Universität Berlin, Arnimallee 14, 14195 Berlin

A fundamental problem in the deposition of molecules from a Knudsen cell is the heating procedure: When the molecules are getting larger the temperature must be increased which results in the dissociation of molecular bonds. We present a low temperature STM study of porphyrin-based molecules on copper surfaces. In order to deposit intact molecules onto the substrate we have used the so-called pulse injection method. Molecules (in solution) are injected by a valve with very short aperture times (few ms). Residual solvent contamination can be desorbed from the surface by heating of the sample, but the chemical structure of the molecules must be maintained. We used various solvents, which differ in their chemical properties, and obtained information on the adsorption and desorption behaviour of the solvents on the metal substrate. The results are compared and discussed by means of the ideal deposition conditions.

O 15.13 Fr 17:00 Poster TU D

Organische Moleküle auf Oberflächen — •Alexander Barth, Manfred Albrecht, Günter Schatz, and Frank Treubel — Universität Konstanz, Fachbereich Physik, 78457 Konstanz

Zur Nanostrukturierung von van der Waals-Oberflächen wurden organische Moleküle durch Organic-MBE-Technik in einem UHV-System aufgebracht. Diese weisen eine langreichweitige selbstorganisierte Ordnung auf. Als Materialien wurden Moleküle wie TMA, TPA und TDA verwendet, die alle aus einem Grundgerüst aus Benzolringen bestehen, an denen Carboxylgruppen chemisch gebunden sind. Über Wasserstoffbrückenbindungen zwischen den Molekülen bildet sich dann die selbstorganisierte Ordnung aus. Als Substrate dienten HOPG und Schichthalbleiter, wie Wolframdiselenid, aber auch Cu(111)-Keimschichten auf Al_2O_3(0001)-Substraten. Ziel dieser Arbeit ist es geordnete Ensembles von magnetischen Nanostrukturen zu erzeugen, indem die organischen Moleküle als Monolage eine selbstorganisierte Aufdampfmaske zur Nanostrukturierung bilden. Zur strukturellen Untersuchung wurden AFM und STM benutzt. Aber auch die Selbstorganisation dicker Filme wurde mittels RHEED untersucht.

O 15.14 Fr 17:00 Poster TU D

Investigation of thin hexane films using coherent X-rays — •Robert Fendt[1], Simone Streit[1], Michael Sprung[2,1], Christian Gutt[3,1], Anders Madsen[4], and Metin Tolan[1] — [1]Experimentelle Physik 1, Universität Dortmund; Otto-Hahn-Str. 4, 44227 Dortmund, Germany — [2]8ID/IMMY-XOR-CAT, APS/ANL, Argonne, IL, 60439, USA — [3]Department of Physics 0350, University of California, San Diego, 9500 Gilman Drive, La Jolla, CA 92093-0350, USA — [4]ID10A, ESRF, B.P. 220, F-38043 Grenoble, France

Very thin hexane films were prepared on a silicon substrate via condensation from a vapour phase. Using this method, it is possible to produce thin films of different thickness (about 20-200 angstroms) by changing the sample temperature. The films were first investigated by means of X-ray photon correlation spectroscopy to measure the spectrum of the capillary waves which were expected on the liquid surface. However, all XPCS measurements showed no dynamics at all on the investigated length and time scales (i.e., a few μm and 10^{-6} to 1000s). As a consequence, static diffuse scattering scans of the surface were made, revealing pronounced speckle structures. These speckles were proven to be stable at least on time scales of up to 20 minutes. The pattern changes slightly when changing the film thickness slowly, and very drastically after quick thickness changes. We believe that this corresponds to different growth modes of the sample on the substrate.

O 15.15 Fr 17:00 Poster TU D

Coverage dependent details of benzene adsorption on Ni (111) studied by XPS — •Papp C., Fuhrmann T., Tränkenschuh B., Steinrück H.-P., and Denecke R. — Lehrstuhl für Physikalische Chemie II, Universität Erlangen-Nürnberg, Egerlandstr. 3, 91058 Erlangen.

We studied the adsorption of benzene and fully deuterated benzene on Ni(111) by in-situ XPS at the synchrotron radiation facilities BESSY II, Berlin and MAX II, Lund. The spectra show some significant differences occurring during the adsorption process, which are observed for the first time, due to the high energy resolution achieved. To determine the nature of the spectral features giving rise to these differences, we also studied the adsorption of substituted benzenes (e.g. chlorobenzene) and benzene coadsorbed with CO and NO. Based on a quantitative analysis of the spectra and their features, models are proposed, which can explain the observed differences. The aim of these models is to distinguish between conformational and electronic effects. Supported by the DFG (STE 620/4-2) and a European Community ARI program (HPRI-CT-2001-00135).

O 15.16 Fr 17:00 Poster TU D

Engineering the Adsorption of Latex Spheres on Charged Surfaces II: Switching the Surface Charge by Adsorption of Layered Double Hydroxides on Mica — •D. Rapp[1], H. Gliemann[2], P.G. Weidler[1], R. Nüesch[1], Th. Schimmel[2,3], Y. Mei[4], A. Wittemann[4], G. Sharma[4], and M. Ballauff[4] — [1]ITC-WGT, Forschungszentrum Karlsruhe, 76021 Karlsruhe — [2]INT, Forschungszentrum Karlsruhe, 76021 Karlsruhe — [3]Institut für Angewandte Physik, Universität Karlsruhe, 76128 Karlsruhe — [4]Institut für Physikalische Chemie I, Universität Bayreuth, 95447 Bayreuth

Layered Double Hydroxides (LDH) are rare in nature but easy to synthesize in the laboratory. Because of their positive layer charge LDH can be used to modify negatively charged surfaces or to adsorb negatively charged particles (e.g. polymer particles). The applications of polymer nanoparticles (like coatings or paints) are based on the adsorption of the particles on organic or inorganic surfaces. Therefore the investigation of the adsorption behavior of spherical core-shell polymer particles with negatively charged chains (anionic SPB) on different charged inorganic surfaces was aim of this work. As negatively charged substrate we used freshly cleaved mica. AFM investigations of anionic SPB adsorbed on mica showed the formation of a densely packed particle layer with a two-dimensional long-range order. By the adsorption of LDH on mica the surface charge of the substrate was switched from negative to positive. On this modified surface anionic SPB adsorb as single particles.

O 15.17 Fr 17:00 Poster TU D

Adsorption and Surface Mobility of Cinchonidine on Pt(111) studied by STM — •Markus Wahl[1], Matthias von Arx[1,2], Thomas A. Jung[1,3], and Alfons Baiker[2] — [1]Institute of Physics University of Basel, Switzerland — [2]Department of Chemistry and Applied Biosciences, ETH Zürich, Switzerland — [3]Paul-Scherrer Institute, Villigen, Switzerland

The investigation of complex organic molecules on metal surfaces by scanning probe microscopies has become a topic of great interest. Most of this research has been focussed on rather unreactive metal surfaces. Here we report [1] on the adsorption of cinchonidine (CD) on Pt(111) in the presence and absence of hydrogen. This investigation is of particular interest due to its relevance to asymmetric heterogeneous catalysis [2].

The time resolved studies revealed that the CD molecules are immobile at low hydrogen pressure, whereas considerable mobility was observed at higher hydrogen pressure. Based on different adsorption geometries and surface mobility different species could be distinguished.

[1] Matthias von Arx et al., Phys. Chem. Chem. Phys., 2005, 7, Advance Article

[2] A. Baiker, H.-U. Blaser in Handbook of Heterogeneous Catalysis, VCH, Weinheim 1997, Vol. 5, 2422.

O 15.18 Fr 17:00 Poster TU D

Adsorptionsexperimente von Acrylnitril und Allylcyanid auf der Si(001)-2x1 Oberfläche — •Ralf Funke[1], Guido Piaszenski[1], Martin Kneppe[1], Ulrich Köhler[1], Sylvie Rangan[2], Fabrice Bournel[2], Stefan Kubsky[2] und Francois Rochet[2] — [1]Experimentalphysik IV / Oberflächenphysik, Ruhr-Universität Bochum, 44780 Bochum — [2]Laboratoire de Chimie Physique Matiere et Rayonnement, Universite Pierre et Marie Curie, Paris, Frankreich

Das Adsorptionsverhalten zweier organischer Moleküle mit Nitril-Gruppen - Acrylnitril und Allylcyanid - auf der Si(001)-2x1 Oberfläche wurde mit STM, XPS und NEXAFS untersucht. Bei Acrylnitril zeigen für niedrige Bedeckungen ($< 10^{13}$ Moleküle / cm^2) STM-Aufnahmen nur eine Adsorptionsgeometrie: das Molekül überbrückt den Zwischenraum zweier benachbarter Dimerreihen und bindet an zwei *dangling bonds* des Siliziums. Untersuchungen mit XPS und NEXAFS bei Bedeckungen im Bereich von 10^{13} bis 10^{14} Molekülen / cm^2 geben Hinweise auf zwei zusätzliche Adsorptionsgeometrien. Im Fall von Allylcyanid erlauben NEXAFS und XPS Spektren die Identifizierung von ebenfalls drei Adsorptionsgeometrien, auch STM zeigt mehrere Bindungsplätze. In allen Fällen werden hier die Adsorptionsplätze auf zwei benachbarten Dimeren einer Reihe gebildet.

O 15.19 Fr 17:00 Poster TU D

Experimental study of the specific adsorption of DNA on the surface of ferroelectric crystals. — •Marc Tobias Wenzel — Institute of Applied Photophysics (IAPP), Dresden

At present, many research groups study the metallisation of DNA in order to use it as a conducting nanowire. For the integration into electronic systems, the DNA needs to be bound to contacts or surfaces.

Our intention is to clarify the mechanisms of adsorption of DNA at the surface of ferroelectric barium titanate $BaTiO_3$ [100] and to investigate which effects the adsorption has on the properties of the DNA. For this purpose, 16 μm long double-stranded lambda-DNA is deposited on the ferroelectric surface from an aqueous solution. The DNA is labelled by the selective yoyo-1 fluorescence dye for observation. Subsequently, the system is examined by scanning confocal microscopy and scanning force microscopy.

For the investigation of the interaction between the DNA and the charged surface of the ferroelectric, confocal Raman spectroscopy of the DNA is planned in the future.

O 15.20 Fr 17:00 Poster TU D

Structure of a thin oxide film on Rh(100) — •Wilhelm Hofer[1], Christof Klein[1], Michael Schmid[1], Peter Varga[1], Lukas Köhler[2], Georg Kresse[2], Johan Gustafson[3], Anders Mikkelsen[3], Mikael Borg[3], Jesper Andersen[3], and Edvin Lundgren[3] — [1]Allgemeine Physik, TU Wien — [2]Materialphysik, Uni Wien — [3]Synchrotron Radiation Research, Lund (Sweden)

We have studied the surface oxide of Rh(100) with different experimental and theoretical methods: STM (scanning tunneling microscopy), LEED (low energy electron diffraction), HRCLS (high resolution core level spectroscopy) and DFT (density functional theory). The HRCLS measurements indicated a trilayer RhO_2 structure with two oxygen layers and one Rh layer in-between. STM and quantitative LEED revealed a close-to-hexagonal surface with a c(8×2) periodicity. In order to coincide with the square Rh(100) substrate, the hexagonal oxide overlayer is slightly distorted, resulting in a c(8×2) structure. The structural details were obtained by quantitative LEED (Pendry R-factor = 0.16) and DFT calculations. It was found that every seventh of the lower O atoms of the trilayer surface oxide resides in on top positions of the Rh(100) substrate. Ab initio DFT calculations give almost perfect agreement with the LEED results in all atomic coordinates. We therefore regard the trilayer surface oxide model as confirmed and thus the oxygen induced c(8×2) structure as solved. [J. Gustafson et al., submitted to Phys.Rev.B]

O 15.21 Fr 17:00 Poster TU D

Untersuchung atomarer Stapelfolgen und Versetzungen in Co Doppel- und Tripellagen mittels Rastertunnelspektroskopie — •Marco Pratzer und Hans-Joachim Elmers — Institut für Physik, Staudingerweg 7, Universität Mainz, D-55099 Mainz

Die Untersuchung der elektronischen Struktur von ultradünnen ferromagnetischen Filmen, insbesondere der elektronischen Interface-Zustände, ist von entscheidender Bedeutung für zukünftige Spintronik-Anwendungen. Eine wichtige Rolle spielt hierbei die Homogenität der Grenzfläche. Mittels MBE wurde ein System aus Co Doppel- und Tripellageninseln auf einem W(110)-Einkristall präpariert und die elektronische Struktur mittels Rastertunnelspektroskopie (STS) untersucht. Bei einer Präparation bei $T = 420$ K wachsen die Tripellageninseln dicht gepackt entweder mit hcp- oder fcc-Stapelfolge. Diese lassen sich anhand der unterschiedlichen elektronischen Struktur mit Hilfe von STS leicht unterscheiden. Auch bei der Doppellage können zwei verschiedene Stapelfolgen vorliegen (AB oder AC), die, auch wie die Stapelfolgen ABA und ACA in der Tripellage, elektronisch äquivalent sind. Wachsen während der Präparation zwei Doppellageninseln mit unterschiedlicher Stapelfolge zusammen, so bildet sich eine Versetzungslinie, in deren Bereich die elektronische Struktur leicht geändert ist. Im Spektroskopiebild findet man zwei verschiedene Versetzungstypen, die sowohl in der Doppel- als auch in der Tripellage in Abhängigkeit von der Kristallrichtung auftreten und die mit Hilfe eines Hartkugelmodells erklärt werden können. Mit dieser Information ist es nun möglich, die atomaren Stapelfolgen in den Doppel- und Tripellageninseln zu bestimmen.

O 15.22 Fr 17:00 Poster TU D

Self-ordering of hexa-peri-hexabenzocoronene and derivatives on Cu(111) — •Leo Gross[1], Francesca Moresco[1], Pascal Ruffieux[2], André Gourdon[3], Christian Joachim[3], and Karl-Heinz Rieder[1] — [1]Institut für Experimentalphysik, Freie Universität Berlin, Arnimallee 14, D-14195 Berlin, Germany — [2]Swiss Federal Laboratories for Materials Testing and Research, Überlandstrasse 129, 8600 Dübendorf, Switzerland — [3]The Nanoscience Group, CEMES-CNRS, 29 rue J. Marvig, P.O. Box 94347, F-31055 Toulouse Cedex, France

An LT-STM study of the submonolayer growth of hexa-peri-hexabenzocoronene (HBC) and three custom designed derivates on Cu(111) is presented. Thanks to the systematic choice of molecules it was possible to assign properties of adsorbates to specific chemical groups inside the molecule. We find that tert-butyl side groups induce intermolecular attraction, while their influence on the molecule-substrate bonding is negligible. The planar aromatic HBC core is on the other hand strongly bound to the substrate inducing a fixed molecular orientation. Best monolayer ordering has been found for a molecule with tert-butyl side groups and a molecular core that bounds only at the central position, allowing a rotation in the absence of other pinning centres.

O 15.23 Fr 17:00 Poster TU D

New phases of NaCl monolayers on Ag(100) — •Hans-Christoph Ploigt, François Patthey, Marina Pivetta, and Wolf-Dieter Schneider — Institut de Physique des Nanostructures, École Polytechnique Fédérale de Lausanne, CH-1015 Lausanne, Switzerland

We used low-temperature scanning tunneling microscopy and scanning tunneling spectroscopy to characterise the growth mode of ultrathin NaCl layers on cold Ag(100) substrates. NaCl was evaporated from a Knudsen cell at substrate temperatures between 0 °C and -120 °C. As a function of decreasing temperature three different atomic arrangements for a NaCl monolayer were found: (i) the square structure of the NaCl(100) plane, (ii) an oblique lattice and (iii) a hexagonal lattice.

O 15.24 Fr 17:00 Poster TU D

DEPES/DAES investigations of the Pb/Ni(111) adsorption system — •Aleksander Krupski[1,2], Marek Nowicki[1], and Stefan Mróz[1] — [1]Institute of Experimental Physics, University of Wrocław, pl. Maxa Borna 9, PL 50-204 Wrocław, Poland (Permanent address) — [2]Institut für Physikalische und Theoretische Chemie, Uinversität Bonn, Wegelerstr. 12, D-53115 Bonn, Germany

The crystalline structure of ultrathin Pb layers deposited on the Ni(111) surface in ultrahigh vacuum was investigated with the use of directional elastic peak electron spectroscopy (DEPES) and directional Auger electron spectroscopy (DAES). Experimental DEPES data recorded for the primary electron beam energies in the range 1.0-1.9 keV were compared with theoretical profiles obtained with the use of single scattering cluster (SSC) calculations for clean and covered Ni(111). Similar intensity maxima reflecting the crystalline structure of the Ni(111) sample were observed on experimental and theoretical profiles. Results obtained after deposition of 10 ML of Pb on Ni(111) at the substrate temperature T=150 K exhibit intensity maxima corresponding to two mutually rotated Pb(111) domains. The populations of two possible Pb domains were determined by an R-factor analysis. The growth of one domain was found to be preferred, which can be rationalised by the miscut of the Ni(111) sample and the resulting step orientation.

O 15.25 Fr 17:00 Poster TU D

Electrospray ion beam deposition in UHV: experimental development and first results — •Stephan Rauschenbach[1], Frank Stadtler[1], Egenio Lunedei[1], Sergei Koltsov[2], Nicola Malinovski[1], Giovanni Costantini[1] und Klaus Kern[1] — [1]Max-Planck-Institut für Festörperforschung, D-70569 Stuttgart — [2]Institute for Analytical Instrumentation, Russian Academy of Sciences, 19813 Saint Petersburg

To avoid the intrinsic limitations in vapor deposition of organic molecules a novel ion beam source using Electro Spray Ionization (ESI) was constructed. The single molecular particle beam is formed from charged droplets due to iterative Coulomb explosion. High- and low-pressure radio frequency (RF) quadrupoles and electrostatic ion optics guide the ion beam through four differential pumping stages from ambient pressure to 10^{-6} mbar at the substrate position.

The composition of the ion beam can be adjusted using the quadrupole ion guides as mass filters. Beam properties, particularly kinetic energy, mass and spatial distribution were characterized. The incidence energy could be measured between 5eV and 20eV per charge. A time-of-flight mass spectrometer was integrated.

Particle beams produced by the ESI source were used in a preliminary deposition setup in high vacuum. The samples were analyzed with atomic force microscopy (AFM) under ambient conditions. Organic molecules (Rhodamin m=443 amu) and Albumin (BSA, m=66000 amu) as well as Gold colloids (diameter=3.6-6.5 nm) were deposited on highly ordered pyrolytic graphite (HOPG) or Silicon substrates.

O 15.26 Fr 17:00 Poster TU D

X-ray Standing Wave Imaging: the Growth of the First Monolayer $YBa_2Cu_3O_{7-\delta}$ on $SrTiO_3(001)$ — •Sebastian Thiess, Tien-Lin Lee, Bruce C.C. Cowie, and Jörg Zegenhagen — ESRF, Grenoble, France

For structure determination the X-ray Standing Wave (XSW) technique can be used as an element specific Fourier technique, which allows determining amplitude *and phase* of the Fourier coefficients of atomic distribution functions $\rho(\mathrm{r})$. In order to obtain the $(\mathrm{hkl})^{th}$ Fourier coefficient of $\rho(\mathrm{r})$, the photoemission from a sample is recorded while the X-ray photon energy is simultaneously scanned through the energy range of the (hkl) Bragg reflection. A real space image of $\rho(\mathrm{r})$ is rendered by back transforming a sufficient number of Fourier coefficients.

We have studied the nucleation of the first monolayer YBCO on the STO(001) surface. 3D Fourier reconstructed images show the crystallographic distribution of all constituent elements of a 1 ML and a 0.5 ML YBCO film grown in situ by pulsed laser deposition. XSW measurements were carried out in UHV at beamline ID32 at the ESRF for 7 different STO(hkl) reflections at photon energies between 2.7 and 5.5 keV.

O 15.27 Fr 17:00 Poster TU D

STM Untersuchung der Interdiffusion an den Grenzflächen Fe/Nb(110) und Nb/Fe(110) — •Isabelle Rauschenbach, Claudia Wolf und Ulrich Köhler — Experimentalphysik IV / Oberflächenphysik, Ruhr-Universität-Bochum, 44780 Bochum

Rastertunnelmikroskopie bei unterschiedlichen Substrattemperaturen (Raumtemperatur bis 900K) wurde angewendet, um das heteroepitaktische Wachstum von Eisenschichten auf Nb(110) und Niobschichten auf Fe(110) zu untersuchen. Bei Raumtemperatur zeigen beide Systeme keine Anzeichen von Interdiffusion, das Vorhandensein einer Schwoebel-Ehrlich-Barriere verhindert jedoch ein glattes Schichtwachstum. Die Relaxation der unterschiedlichen Gitterkonstanten erfolgt ab der dritten Lage durch Ausbildung eines geordneten Versetzungsnetzwerks. Bei dem Wachstum unter erhöhter Probentemperatur verdrängen aufgebrachte Nb-Atome die Fe-Atome aus der ersten Fe(110)-Lage und führen zur Bildung von Eisen-Adinseln. Die Wechselwirkung der in die Oberfläche eingelagerten Nb-Atome führt zu einer linienförmigen Anordnung. Im Falle der Fe auf Nb(110)-Abscheidung äußert sich eine Interdiffusion durch die Koexistenz zweier unterschiedlicher Inseltypen auf der Oberfläche.

O 15.28 Fr 17:00 Poster TU D

Growth of ultra-thin Fe films on Cu(111) — •Werner Rupp, Albert Biedermann, Michael Schmid, and Peter Varga — Institut für allgemeine Physik, Technische Universität Wien

Using scanning tunneling microscopy (STM), scanning tunnelling spectroscopy (STS) and low-energy electron diffraction (LEED) we have characterized ultra-thin films of Fe on Cu(111). The films were grown by thermal deposition (TD) at room temperature (RT). Whereas bulk Fe is normally bcc (α-Fe) at temperatures below 1186 K, fcc Fe (γ-Fe) can be stabilized in ultra thin films on fcc substrates. Analysing these TD-films, we find a pseudomorphic growth at low coverages [1]. With atomically resolved STM images we show the initial formation of strained bcc domains at low coverages (3ML) on flat Fe islands. This strain decreases with the thickness of the film. The bcc domains have Kurdjumov-Sachs orientation in agreement with LEED [2]. With STS measurements we show that the Cu covers the Fe islands decorating the step edges already during the deposition process. Correlated with this Cu coverage is the formation of 1ML high vacancy islands near the step edges of the substrate [3].

[1] J.Shen et al, Phys. Rev. B 56, 11134 [2] P. Ohresser et al, Phys. Rev. B. 59, 3696 [3] A. Brodde et al, Phys. Rev. B 47, 6609

O 15.29 Fr 17:00 Poster TU D

Schichtwachstum, Grenzflächenreaktion und Elektronische Struktur von ultradünnen 3d-Übergangsmetalloxid/Metall-Schichtsystemen — •M. Nagel, L. Zhang und T. Chassé — Institut für Physikalische und Theoretische Chemie, Universität Tübingen, Auf der Morgenstelle 8, D-72076 Tübingen

Ultradünne Schichten von Mn auf NiO(100) und Ni auf MnO(100)-Einkristalloberflächen (nominelle Schichtdicken <10nm) wurden in-situ mittels Photoemissionsspektroskopie schichtdickenabhängig charakterisiert. Die Auswertung der O1s-, Mn2p- und Ni2p-Rumpfelektronenspektren ergab Hinweise auf ein Inselwachstum und die partielle Oxidation des Metalls an der Grenzfläche bei den gewählten Präparationsbedingungen. Außerdem wurden ultradünne, pseudomorphe MnO- und NiO-Schichten auf Ag(100)-Einkristalloberflächen präpariert (analog zu [1,2]) und mit XPS sowie LEED in-situ analysiert. Bei der Präparation der MnO-Schichten wurden ergänzend Mn3s-Spektren zur Überprüfung des Oxidationszustandes herangezogen. Nach Aufdampfen einer Deckschicht aus Sb wurden die Proben ex-situ mit XES und XAS in Fluoreszenzdetektion charakterisiert. Die O K_α, Mn $L_{2,3}$ und Ni $L_{2,3}$ Röntgenabsorptions- und Fluoreszenzspektren der Schichtsysteme sowie entsprechender Volumen-Referenzproben wurden ausgewertet.

Im direkten Vergleich der ultradünnen Schichten zu den Referenzproben wurden Veränderungen in der elektronischen Struktur durch die verringerte Dimensionalität bzw. das pseudomorphe Wachstum beobachtet.

[1] F. Müller et al., Surf. Sci. 520, 158 (2002)

[2] S.A. Krasnikov et al., Thin Solid Films 428, 201 (2003)

O 15.30 Fr 17:00 Poster TU D

MOVPE growth analysed by in-situ SPM — •Raimund Kremzow, Bert Rähmer, Markus Breusing, Markus Pristovsek, and Wolfgang Richter — Technische Universität Berlin, IFP, Sekr. PN 6-1 Hardenbergstr. 36, 10623 Berlin

To get insight into the formation of nanostructures, an *in-situ* analysis of the sample morphology during the growth is highly desirable. Especially for the most common technique epitaxial method, (**m**etal**o**rganic **v**apour **p**hase **e**pitaxy – MOVPE). At present no tool exists which can measure the surface topography in real time and real space with high spatial resolution. We developed a specially designed SPM to deal with the limited space and high temperatures in the MOVPE reactor (caused by the thermal conductivity of the carrier gas). In addition, vibrational disturbances introduced by the pumping system and gas-flow had to be minimized. Another problem arises by the need not to disturb the actual layer growth. Therefore, the tip has to be longer than 2 cm in order to bridge the distance between liner tube and susceptor. The set-up we present, continuosly tolerates sample and gas phase temperatures up to 550°C without degradation of the piezo elements.

O 15.31 Fr 17:00 Poster TU D

Fabrication of well-defined nickel films on self-assembled monolayers — •Yian Tai, Andrey Shaporenko, Wolfgang Eck, Michael Grunze, and Michael Zharnikov — Angewandte Physikalische Chemie, Universität Heidelberg, Im Neuenheimer Feld 253, 69120 Heidelberg, Germany

Self-assembled monolayers (SAMs) suit well as model organic surfaces for metal evaporation experiments. In addition, the fabrication of metal wires on SAM surface is an important issue for future molecular electronics. The major difficulty in fabricating well-defined metallic films on the SAM surface is the penetration of metal atoms into the SAM and to the SAM-substrate interface. Taking nickel as a test adsorbate, we showed that this process can be partly suppressed through the fictionalization of SAMs with a reactive tail group. The full suppression has been achieved by a combination of the SAM fictionalization and electron-induced cross-linking of the molecular layer - a well-defined and stable nickel film on the SAM support could be fabricated. In addition, several interesting effects were observed including a non-homogeneous irradiation-induced cross-linking within a SAM and a drastic decrease in molecular tilt of the SAM constituents at the initial stage of the Ni deposition on thiol-terminated aromatic SAMs. The latter effect was attributed to the formation of Ni-thiol complexes at the SAM-ambient interface.

O 15.32 Fr 17:00 Poster TU D

Spectroscopy and microscopy studies for the development of lithography with a monomolecular resist — •Michael Zharnikov[1], Andrey Shaporenko[1], Anne Paul[1], Armin Gölzhäuser[2], and Andreas Scholl[3] — [1]Angewandte Physikalische Chemie, Universität Heidelberg, Im Neuenheimer Feld 253, 69120 Heidelberg, Germany — [2]Physik Supramolekularer Systeme, Universität Bielefeld, Universitätsstr. 25, 33615 Bielefeld, Germany — [3]Advanced Light Source, Lawrence Berkeley National Laboratory, CA 94720, USA

Soft X-ray absorption microscopy was applied to image and characterize molecular patterns produced by electron irradiation of aliphatic and aromatic thiol-derived self-assembled monolayers (SAMs) on Au substrates. The measurements were performed at all relevant absorption edges. The fabricated patterns could be clearly imaged with a lateral resolution better than 150 nm, which, e.g., allowed to distinguish a fine structure of 1 μm features. The X-ray absorption microspectra derived from different areas of the SAM patterns provided specific chemical information on pristine and irradiated areas, and unexpected features in these patterns. The quality of the microspectra is comparable with that of the analogous X-ray absorption spectra acquired with a standard equipment from homogeneous SAMs. In particular, a chemical transformation of the functional tail groups within the irradiated areas of the patterned aromatic SAMs could be directly monitored.

O 15.33 Fr 17:00 Poster TU D

Ultra-thin hexaphenylene films grown on Au(111) and Au(433) — •Stefan Müllegger, Axel Stupnik, Manfred Leisch, and Adolf Winkler — Institute of Solid State Physics, Graz University of Technology, Austria.

The physical properties of ultra-thin films of organic semiconducting materials are to a great extent determined by their structure and morphology. This is important for both fundamental and applied research (e.g. organic thin film transistors, organic light emitting devices). We present experimental investigations on ultra-thin films of para-hexaphenylene (6P) grown by an organic molecular beam epitaxy (OMBE) technique on single crystalline Au(111) and vicinal Au(433) surfaces under ultra-high vacuum conditions. Founded on a variety of surface analytical techniques, e.g. low energy electron diffraction (LEED), thermal desorption spectroscopy (TDS), x-ray photoelectron spectroscopy (XPS) and scanning tunnelling microscopy (STM), several aspects are discussed, concerning the development of a highly regular structure of the first and second 6P monomolecular layer as well as the kinetics of adsorption and growth of several nm thick 6P films. Although 6P is considered chemically rather stable, experimental evidence for a strong dissociative behaviour of 6P adsorbed on the Au(111) surface at elevated temperatures is presented.

O 15.34 Fr 17:00 Poster TU D

Stereochemistry of 2,3-butanediol adsorbed on Si(001) surfaces from *first-principles* calculations — •Kaori Seino, Wolf G. Schmidt, and Friedhelm Bechstedt — Institut für Festkörpertheorie und -optik, Friedrich-Schiller-Universität Jena, Max-Wien-Platz 1, 07743 Jena, Germany

The formation of organic thin films on semiconductors allows for adding biological and chemical functionality to microelectronics. Therefore the microscopic details and electronic properties of the interfaces formed by the adsorption of organic molecules on inorganic substrates have become topics of intense research. Here we present results of *first-principles* calculations on the adsorption of 2,3-butanediol on Si(001) surfaces based on density-functional theory in generalized gradient approximation (DFT-GGA). 2,3-butanediol is one of the simplest diol molecules and thus a suitable model system, yet it has found interest in the context of forming chiral surfaces [1]. From our calculations we find that the effects of conformation, well-known to influence the stability of gas-phase molecules, are also important for the interface energetics. The electronic properties for the most relevant bonding configurations are discussed.

[1] J. W. Kim *et al.*, Surf. Sci. **559**, 179 (2004).

O 15.35 Fr 17:00 Poster TU D

Einfluss des Substrates auf die optischen Eigenschaften von HBC-Moleküllagen — Roman Forker[1], Robert Nitsche[1], •Thomas Dienel[1], Klaus Müllen[2], Karl Leo[1] und Torsten Fritz[1] — [1]Institut für Angewandte Photophysik, TU Dresden, Germany — [2]MPI für Polymerforschung, Ackermannweg 10, 55128 Mainz, Germany

Mit Hilfe der Differentiellen Reflexionsspektroskopie (DRS) wurden die optischen Konstanten von Hexa-peri-benzocoronen (HBC) in Abhängigkeit von der Schichtdicke *in situ* auf verschiedenen Substraten ermittelt. Der Messaufbau ermöglicht es, während des Schichtwachstums die Veränderung des optischen Spektrums von typischen Monomerstrukturen hin zu Kristallstrukturen zu beobachten. Dabei zeigt HBC auf Glimmer für Submonolagen ein ähnliches spektrales Verhalten wie in Lösung, während es auf HOPG und Au(111) stark verbreiterte Monomerspektren aufweist. Frühere STM-Aufnahmen [1] lassen eine Verringerung der Molekülsymmetrie gegenüber dem freien HBC-Molekül vermuten, und es wird der Frage nachgegangen, ob dies zu zusätzlichen Peaks im ε_2-Spektrum führt.
[1] T. Schmitz-Hübsch et al., Surf. Sci. **445**, 358 (2000).

O 15.36 Fr 17:00 Poster TU D

Growth of thin polymer films: Monte Carlo simulations and experiments — •Christian Vree[1], Johanna Röder[2], Hans-Ulrich Krebs[2], and S. G. Mayr[1] — [1]I. Physikalisches Institut, Universität Göttingen — [2]Institut für Materialphysik, Universität Göttingen, Friedrich-Hund-Platz 1, 37077 Göttingen

Vapour deposition of thin polymer films was studied by Monte Carlo (MC) simulations and compared with experiments. In the MC simulations single chain molecules are deposited randomly on a lattice, on which they diffuse with the kinetic of the Reptation model. The dependence of roughness and morphology of the surface on film thickness, energy of deposited particles, relaxation time and chain length are investigated. Generally we observe a strong roughening, which starts abruptly at a critical thickness. In the experiment thin PMMA films were produced on a Si substrate using PLD and spin coating at room temperature. The film surfaces were characterized by atomic force microscopy and scanning electron microscopy.

Differences and similarities of experiment and modelling as well as their possible reasons are discussed.

O 15.37 Fr 17:00 Poster TU D

Influence of the Molecular Structure on the Interface Formation between Magnesium and Organic Semiconductors — •Gianina Gavrila[1], Mihaela Gorgoi[1], Walter Braun[2], and Dietrich R.T. Zahn[1] — [1]Institut für Physik, Technische Universität Chemnitz, D-09107, Chemnitz, Germany — [2]BESSY GmbH, Albert-Einstein-Straße 15, D-12489 Berlin, Germany

Magnesium is often used in organic devices as a low work function metal contact. On the other hand it is a highly reactive metal. Its reactivity may also depend of the detailed structure of organic molecules involved. Here, 15 nm thick films of perylene derivatives, i.e. 3,4,9,10-perylenetetracarboxylic dianhydride -PTCDA, 3,4,9,10-perylenetetracarboxylic diimide-PTCDI and dimethyl-3,4,9,10-perylenetetracarboxylic diimide-DiMe-PTCDI were deposited onto sulpfur passivated GaAs substrates. A detailed study of the interface formation between these materials and Mg using high resolution photoemission spectroscopy is presented. The differences observed in the evolution of C1s, O1s, N1s and Mg2p core levels and valence band spectra as a function of Mg thickness differences are related to the distinct molecular end groups and with the degree to which the metal atoms diffuse into the layer.

O 15.38 Fr 17:00 Poster TU D

Selbstorganisierte Monolagen durch redox-aktives Bis(diphenyl-phosphan)ferrocen: Untersuchungen mit optischer Frequenz-verdopplung — •B. Krohn[1], T. Auch[2], T. Weidner[1], U. Siemeling[2], and F. Träger[1] — [1]Institut für Physik, Universität Kassel, Heinrich-Plett-Str.40, 34132 Kassel — [2]Institut für Chemie, Universität Kassel, Heinrich-Plett-Str.40, 34132 Kassel

Thiol- und Sulfidderivate sind heute die am besten untersuchten und vielversprechendsten Kandidaten für selbstorganisierte Monolagen auf Goldoberflächen.

Doch auch Phosphane zeigen vielfältige Wechselwirkungen mit Gold. Einer der interessantesten Kandidaten unter ihnen ist das 1,1'-Bis(diphenylphosphan)ferrocen (DPPF). Es spielt wegen seiner katalytischen Eigenschaften in der chemischen Synthese eine übergeordnete Rolle. Während seine vielseitige Komplexchemie im Hinblick auf atomares Gold bereits gründlich untersucht ist, wird das Grenzflächenverhalten von DPPF hier erstmalig beschrieben.

Wir haben die Adsorptionsdynamik auf Gold mit optischer Frequenzverdopplung in situ und in Echtzeit verfolgt. Es zeigt sich, dass DPPF einen hervorragenden Baustein zur Präparation redox-aktiver monomolekularer Schichten auf Goldoberflächen darstellt.

O 15.39 Fr 17:00 Poster TU D

Energy and time resolved coherent x-ray reflectivity from a smooth polymer film — •Gudrun Gleber, Tobias Panzner, and Ullrich Pietsch — Institut für Physik, Universität Potsdam, Am Neuen Palais 10, D-14415 Posdam

Since recent years, x-ray-photon-correlation-spectroscopy is used for the investigation of time depending processes in thin films. Up to now these experiments are performed using single wavelengths.

Recently we have shown that a pink beam provited by the white beam beamline at Bessy II can exploited for coherence experiments [1]. Here we present, for the first time, time resolved reflectivity measurements from thin polymer films using white synchrotron radiation. The advantage of this approach is the fact, that one can measure simultaneous the time correlation at different values of the momentum transfer.

In particular we have investigated the melting of a polymer film on a silicon substrate as a first example for this new kind of measurements. In detail we will show the extracted autocorrelation functions at temperatures below and above the glass temperature of the polymer film.

[1] W. Leitenberger et.al. Physica B 2004

O 15.40 Fr 17:00 Poster TU D

A multi-parameter Ising model for the adsorption of molecules on structured surfaces — •Carsten Olbrich[1], Klaus Morawetz[1], Sibylle Gemming[1,2], Reinhard Scholz[1], Michael Schreiber[1], Regina Ermrich[2], and Gotthard Seifert[2] — [1]Institut für Physik, Technische Universität, D-09107 Chemnitz — [2]Institut für Physikalische Chemie, Technische Universität, D-01062 Dresden

Several modifications of the standard two-parameter Ising model are necessary for the mesoscopic modelling of a realistic adsorbate ensemble on a non-ideal substrate. Depending on the shape of the molecule, the nearest-neighbour coupling exhibits a directionality, and also additional coupling terms with next nearest neighbours are taken into account. Structured or defective surfaces are modelled by local modifications of the magnetisation term. Several sets of coupling parameters were derived from first-principles calculations on PTCDA monomer, dimer, and adsorbate systems. The adsorbate distribution on the surface was investigated by Metropolis-Monte-Carlo simulations and cluster statistics employing the Hoshen-Kopelman cluster recognition algorithm. It was observed that surfacedefects like steps influence the pattern formation mainly close to the critical temperature of the order-disorder transition. It could be shown that all adsorbate-adsorbate interactions are connected by a straightforward scaling in the critical temperature, whereas the adsorbate-substrate interaction is of a more complicated nature, especially in the presence of surface defects.

O 15.41 Fr 17:00 Poster TU D

In-situ X-ray Diffraction study of organic-organic heterostructures of Diindenoperylene and copper-hexadecafluorophthalocyanine — •Esther Barrena[1], Dimas García de Oteyza[1], J. Oriol Ossó[2], Stefan Sellner[1], and Helmut Dosch[1,3] — [1]Max-Planck-Institut für Metallforschung, Heisenbergstr.3, 70569 Stuttgart, Germany — [2]Institut de Ciència de Materials de Barcelona CSIC, 08190 Bellaterra, Spain — [3]Institut für Theoretische und Angewandte Physik, Universität Stuttgart, 70550 Stuttgart, Germany

Many organic devices like Light-Emitting Diodes (OLEDs), solar cells or ambipolar transistors are based on p-n junctions of organic semiconductors. Here we present an in-situ X-ray diffraction study of the structure of bilayers of Diindenoperylene (DIP) and copper-hexadecafluorophthalocyanine (F16PcCu), p-type and n-type semiconductors, respectively. The molecular films have been grown at different temperatures on silicon oxide by Organic Molecular Beam Deposition. We show that DIP on F16PcCu grows in the Stransky-Krastanov growth mode at 120°C. Interestingly, a change in the F16CuPc structure at the organic-organic interface is induced. At 25°C and -10°C, DIP molecules form a well ordered film and no structural rearrangement of F16PcCu is observed. For bilayers grown in the inverse order, i.e F16CuPc on DIP, changes on the F16CuPc structure are observed as well. Complementary studies by AFM support the results.

O 15.42 Fr 17:00 Poster TU D

Laser induced local decomposition of octadecylsiloxane monolayers: Patterning in an ultra-high vacuum environment — •Rafael Bautista Mester, Thorsten Balgar, Nils Hartmann und Eckart Hasselbrink — Universität Duisburg-Essen, Campus Essen, Fachbereich Chemie, Universitätsstr. 5, 45141 Essen

A procedure for direct patterning of octadecylsiloxane (ODS) monolayers has been developed. Silicon substrates were coated with ODS in a millimolar solution of octadecyltrichlorosilane [1]. Subsequently, patterning was carried out at ambient conditions using a highly focused laser beam of an argon ion laser operated at 514 nm [2]. In order to investigate the specific role of oxygen and water in the overall patterning process additional experiments were carried out at well-defined conditions in an ultra-high vacuum environment. Similar to the results at ambient conditions here structures with lateral dimensions well below the laser spot diameter can be prepared. A general mechanism of the patterning process is discussed.

[1] Th. Balgar, R. Bautista, N. Hartmann and E. Hasselbrink, Surf. Sci. 532-535 (2003) 963.

[2] N. Hartmann, Th. Balgar, R. Bautista, S. Franzka and E. Hasselbrink, Proc. SPIE 5223 (2003) 9.

O 15.43 Fr 17:00 Poster TU D

Combined Normal and Torsional NC-AFM Measurements: PTCDA on KBr(001) — •Tobias Kunstmann, Andreas Schlarb, and Rolf Möller — Universität Duisburg-Essen, D-45141 Essen, Germany

Dissipative lateral forces provide the main contribution to friction. To measure these forces the tip has to move parallel to the surfaces. This can be achieved either by using the "q-plus sensor"[1], or torsional modes of a cantilever [2]. The normal and torsional modes of a commercially available cantilever have been excited simultaneously. For our measurements we have used the frequency shift (df) of the normal mode to control the tip sample distance. Additionally the energy dissipated in the normal mode has been recorded. The frequency shift and the damping of the lateral oscillation were measured independently providing the conservative as well as the dissipative lateral forces. The experiments have been performed on PTCDA on a KBr(001) surface. While the dissipation in normal mode does not show a difference between plain KBr and PTCDA-crystallites, the dissipation for the torsional mode shows a significant increase on top of the PTCDA islands.

This work was funded by the SFB616 "Energy dissipation at surfaces" of the Deutsche Forschungsgemeinschaft.

[1] F.J.Giessibl et al., Proc. Nat. Acad of Sci. US 99 (19), 12006 (2002)

[2] O. Pfeiffer et al., Phys. Rev. B 65 (16), 161403 (2002)

O 15.44 Fr 17:00 Poster TU D

NMR and XAFS Investigation of the Structure of Mo(allyl)4 Followed by Wet Chemical Deposition of the Complex on a Thin Al2O3 Film and Subsequent Characterisation Using XPS — •Karifala Dumbuya[1], Sven Schroeder[2], Norbert Weiher[2], Klaus Christmann[1], and Tal Perry[1] — [1]Free University Berlin, Institute of Chemistry, Department of Physical and Theoretical Chemistry, Takustrasse 3, 14195 Berlin — [2]University of Manchester, School of Chemical Engineering and School of Chemistry, PO Box 88 Sackville Street, Manchester M 60 1 QD, UK

We report the synthesis and structural ellucidation of Mo(C3H5)4 using solid and liquid state NMR (13C, 1H) and XAFS of the complex in solution. The NMR results agree remarkably well with previous work with the 1H showing five resonances (four doublets and a multiplet) indicating five different protons. The 13C also revealed three different carbons, suggesting that all four allyl groups are equivalent. To our knowledge, this is the first attempt at soild state NMR study on this complex. XAFS investigation of the Mo k-edge revealed a cordination number of 3.6 for molybdenum in the first cordination shell, i.e., an average of 11 C-atoms. The average Mo-C distance was 2.35 Å, a value which compares well with Mo-C distances in related molybdenum complexes and supports the case for a symmetrical pi-allyl system. Depostion of the complex from a solution of pentane on a freshly prepared Al2O3 surface in ultra high Vacuum with the help of a specially designed transfer cell proved very successful, albeit significant silicon contamination. Investigation of the contaminant is in progress.

O 15.45 Fr 17:00 Poster TU D

Surface Structures and Atomic Details of CeO$_2$(111) revealed by Dynamic Force Microscopy — •S. Gritschneder[1], Y. Namai[2], Y. Iwasawa[2], and M. Reichling[1] — [1]Fachbereich Physik, Universität Osnabrück, Barbarastraße 7, 49076 Osnabrück, Germany — [2]Department of Chemistry, The University of Tokyo, 7-3-1 Hongo, Bunkyo-ku, Tokyo 113-0033, Japan

Ceriumdioxide is a catalytically active material with unique properties that allow it to store and release oxygen. It is highly interesting to analyse this catalytic surface on the atomic level to gain an in-depth understanding of the involved chemical processes and help to establish structure-function relationships for catalysis. In this contribution we present highly resolved images and atomic details of surface features on CeO$_2$(111) like terrace structures, step edges, kinks and hexagonally shaped pits that are naturally formed during surface preparation by sputtering and annealing cycles. We find that such structures can well be imaged with atomic resolution and exhibit a morphological characteristics that is in details significantly different from that of cleaved CaF$_2$(111), a surface with exactly the same crystallographic structure and a very similar lattice constant and ionic radii. We demonstrate that the non-contact, constant-height mode is the preferable mode of operation for dynamic force microscopy imaging at room temperature as it allows maximum resolution and undesired regulation artefacts can be minimized by carefully choosing scanning parameters, like detuning, scanning speed, and the gain of the distance regulation loop.

O 15.46 Fr 17:00 Poster TU D

Investigation of the La$_{0.7}$Sr$_{0.3}$MnO$_3$/SrTiO$_3$(100)-interface by X-ray photoelectron spectroscopy under optical excitation — •Elke Beyreuther[1], Stefan Grafström[1], Christian Thiele[2], Kathrin Dörr[2], and Lukas Eng[1] — [1]Institut für Angewandte Photophysik, Technische Universität Dresden, D-01062 Dresden — [2]IFW Dresden, Postfach 270116, D-01171 Dresden

The functional properties (conductivity, spin polarisation) of layered perovskite structures are crucially influenced by the electronic state distribution at internal interfaces.

The shift of an X-ray photoelectron spectrum under simultaneous optical excitation in the ultraviolet and visible range is equivalent to a surface photovoltage (SPV) and hence provides information about electronic surface and interface states, barrier heights and relaxation times. So far, semiconductor surfaces as well as the interface between organic films and semiconducting or metallic substrates have been characterized succesfully by the technique [1].

Here, we report on SPV measurements on epitaxially grown 15 nm thick La$_{0.7}$Sr$_{0.3}$MnO$_3$ layers on undoped and Nb-doped SrTiO$_3$(100) substrates. The plot of the SPV versus the excitation wavelength reflects the absorption characteristics of the substrate and reveals a continuous distribution of interface states in the sub-bandgap range. The interpretation of the results within the Schottky theory of classical metal-semiconductor contacts is discussed critically.

[1] S. Teich *et al.*, Surf. Sci. **552**, 77-84 (2004)

O 15.47 Fr 17:00 Poster TU D

Growth and electronic structure of epitaxial $Ba_{0.7}Sr_{0.3}O$ layers on the Si(001) surface — •Anddreas Gerdes, Jan Zachariae, and Herbert Pfnür — Institut für Festkörperphysik, Universität Hannover, Appelstr. 2, 30167 Hannover

We investigated the growth conditions, crystalline quality and stoichiometry of the medium k ($\epsilon_r \approx 30$) $Ba_{0.7}Sr_{0.3}O$ films using high resolution LEED, UPS, XPS and EELS. Lattice matched $Ba_{0.7}Sr_{0.3}O$ layers were grown on a intermediate layer on the Si(001) substrate in UHV by evaporation of the metals in an ambient oxygen pressure. The quality of oxide layers depends on two conditions: the kind of the intermediate layer and the accurate oxygen dose, which was determined by mass accumulation on a quartz crystal micro balance. A correct fraction of Ba and Sr in the mixed oxide layers leads to well ordered and lattice matched oxide films from a few monolayers up to 20 nm and more. To obtain monocrystalline $Ba_{0.7}Sr_{0.3}O$ layers, although of different quality, it is necessary to start the growth on one of the three following types of intermediate layers: strontium silicide layers $\Theta \leq 1$ ML grown at $T \geq 750\,°\mathrm{C}$, strontium metal layers $\Theta > 1$ ML grown at $T \leq 650\,°\mathrm{C}$ and the silicate layers (1 ML of Sr_2SiO_4). The electronic structure, surface roughness and interface oxidation for the growth on different intermediate layers will be discussed.First results of the growth of $Ba_{0.7}Sr_{0.3}O$ on vicinal Si(001) surfaces to generate a stepped insulator surface and the formation mechanism of surface F-centers will also be presented.

O 15.48 Fr 17:00 Poster TU D

Charged and non-charged surface defects on NiO(001) investigated by AFM — •Uwe Kaiser, Nico Plock, Alexander Schwarz, and Roland Wiesendanger — Institut für Angewandte Physik, Universität Hamburg, Jungiusstr. 11, 20355 Hamburg

Surface defects of transition-metal oxides like NiO are important for their catalytic behavior as they strongly enhance the reactivity of the surface. In this study, we investigated the (001)-surface of NiO under UHV-conditions with our home-built atomic force microscope. Typical AFM-images show flat terraces of monatomic height with widths of some ten nanometers. The image quality strongly depends on the tip condition, which could be improved by repeatedly touching the surface with the tip. With such tips, it was possible to detect extended vacancy-islands and point defects down to the atomic scale. The circumferences of some of the vacancies appear elevated, while others do not show this specific feature. In some cases, very faint elevated circular contrasts on terraces can be found without the presence of a vacancy. As ionic crystals can trap charges like electrons in positively charged vacancy sites, these different contrasts can be interpreted as differently charged vacancies at or just below the surface.

O 15.49 Fr 17:00 Poster TU D

Surface and Interface Structures of $ZrO_2(111)$ Films on Pt(111) — •K. Meinel[1], A. Eichler[2], K.-M. Schindler[1], H. Neddermeyer[1], and W. Widdra[1] — [1]Martin-Luther-Universität Halle-Wittenberg, FB Physik, D-06099 Halle, Germany — [2]Institut für Materialphysik und Center for Computational Material Science, Universität Wien, Sensengasse 8/12, A-1090 Wien, Austria

ZrO_2 films are prepared on Pt(111) by reactive deposition of Zr in an O_2 atmosphere followed by post-annealing and characterized by STM, LEED and DFT calculations. After deposition, the films display a slightly rotated $p(1 \times 1)$ structure. Post-annealing of submonolayer films yields ZrO_2 films having a slightly compressed (4×4) structure, which is commensurate to a (5×5) structure of the Pt(111) interface. Post-annealing of thicker films yields a (2×2) structure, which is slightly expanded and commensurate to a $(\sqrt{7} \times \sqrt{7})$ structure of the Pt(111) interface. Continuing the annealing induces the formation of domains possessing a (1×1) structure rotated by $\pm 6.6°$. These domains are energetically favored and grow at the expense of the (2×2) areas. With the film rotation, a $(3\sqrt{3} \times 3\sqrt{3})$ film structure develops, which is slightly compresssed and commensurate to a rotated $(\sqrt{19} \times \sqrt{19})R \pm 36.6°$ structure of the Pt(111) interface. High temperature annealing ($T > 1200$ K) finally yields incommensurate structures of expected $Zr_xO_yPt_z$ phases.

O 15.50 Fr 17:00 Poster TU D

Thick Titanium Oxide Films by Unfiltered Arc Deposition — •Peter Drechsler and Roger Thull — Abteilung für Funktionswerkstoffe der Medizin und Zahnheilkunde, Universitätsklinikum Würzburg, Pleicherwall 2, 97070 Würzburg

Thick titanium oxide (Rutile) films have actractive properties like good blood compatibility and good corrosion resistance which are very suitable for medical implants. A sufficient thickness supplies the essential wear resistance.

The presented titanium oxide films are deposited by means of unfiltered arc sputtering technique on polycrystalline titanium and steel surfaces. The film thickness is 3–6 microns depending on the deposition time with a deposition rate of 4 microns/hour. The substrate temperature was varied from room temperature to 870 K. The ratio of the anatase to rutile phases depends on the subrate temperature as XRD measurements revealed. Above 670 K no anatase phase could be found. The polycrystalline rutile films grew predominately in (110)-direction.

The optical band gap of the rutile films was measured by means of UV-VIS spectroscopy. The band gap was found at 3.00 ± 0.02 eV with low variation with the film thickness.

O 15.51 Fr 17:00 Poster TU D

Applications of High Speed Scanning Capacitance Spectroscopy for the analysis of semiconductor microdevices — •Martin von Sprekelsen and Roland Wiesendanger — University of Hamburg, Institute of Applied Physics and Microstructure Research Center, Jungiusstrasse 11, D-20355 Hamburg, Germany

High spatial resolution down to the nanometer scale becomes essential for analytical tools for semiconductor devices. On the other hand, in the semiconductor industry, scanning capacitance microscopy (SCM) is an established analytical method to obtain 2D-dopant profiles of charge carrier concentrations; these profiles are usually taken at a constant bias voltage (Vbias). However the spatial resolution of SCM is limited by unavoidable side effects such as mobile surface charges or the strong influence of Vbias on the SCM profiles. To overcome these restrictions, we develop Highspeed Scanning Capacitance Spectroscopy (HSSCS) which is performed by modulating the Vbias voltage at a frequency in the kHz-range. The modulated electric field virtually traps mobile surface charges. Furthermore, the highspeed method allows us to measure capacitance spectra for Vbias, by which we can analytically get rid of the infulence of Vbias.

We present HSSCS dopant profiles on Si-semiconductor samples of ultra-shallow junctions with high resolution down to 10 nm. Further results of HSSCS on III-V-semiconductors samples are also discussed.

O 15.52 Fr 17:00 Poster TU D

Influence on alkali dopants on V2O5. DFT cluster model studies. — •Malgorzata Witko and Robert Grybos — Institute of Catalysis and Surface Chemistry, PAS, ul. Niezapominajek 8, 30 239 Kraków, Poland

Selectivity to partially oxidized products in oxidative dehydrogenation (ODH) depends on basicity of the surface (nucleofilicity of oxygen atoms). From the experiment it is known that alkali metal dopants change the basicity of the surface and thus influence the selectivity. To understand the role of alkali additives on the behavior of the (010)V2O5 surface cluster DFT calculations are carried out. Alkali metal is approach to the surface and its position is optimized. Changes in electronic structures for systems without and with alkali are discussed in terms of electronic structure, electrostatic potentials and total energy of the systems. It is found that alkali adsorbs on the surface in the "hole" site between four vanadyl oxygen atoms sticking out of the surface. Only slightly less favored site is the "hole" between four bridging oxygen atoms. Alkali metal transfers an electron to the empty d-band of vanadium ions leading to its reduction. Through a polarization effect the negative charge accumulates on O atoms increasing their nucleophilicity, however this influence is very short-range. As a result, the oxygen atoms affected by dopant are at the same time blocked by them. Blocking of the most active sites may be the main reason behind increased selectivity of doped catalyst.

O 15.53 Fr 17:00 Poster TU D

Effect of support and additives on properties of molybdena-based catalysts. — •Renata Tokarz-Sobieraj and Malgorzata Witko — Institute of Catalysis and Surface Chemistry, PAS, ul. Niezapominajek 8, 30 239 Kraków, Poland

Molybdenum oxide-based catalysts are active and selective in many reactions of very different types e.g. selective oxidation, oxidative dehydrogenation. The catalytic properties of such catalysts strongly depend on acid-base properties of catalysts surfaces, which determine the strength of surface-substrate interactions and facilitate the desorption of products from the surface. Experiment shows that acid-base properties of an oxide catalyst can be controlled by the introduction of additives or usage of different supports. In the present work, the effect of additives (K, Ni, Cr, Pt) and effect of the support (SiO2, Al2O3, TiO2, MgO) on the electronic and geometric structures is discussed by means of quantum chemical calculations based on the density functional theory (DFT), using cluster model. Theoretical data shows that substitution of molybdenum atom(s) in the cluster by additive atoms or atoms from different supports changes the local electronic state and, what follows, the local reactivity of different surface oxygen sites (Mo=O and Mo-O-X) that are present at the catalyst surface. The results of calculations are compared with the experimental findings.

O 15.54 Fr 17:00 Poster TU D

Simulations of Analogue Control Circuits for the Dynamic Scanning Force Microscope — •Rebecca Kastebo and Michael Reichling — Fachbereich Physik, Osnabrück Universität, Barbarastr.7, 49069 Osnabrück

We study the behaviour of an analogue control circuit presently used in our dynamic scanning force microscope (SFM) by performing simulations of the circuit in the framework of a SPICE program. We devote our simulations to the separation regulator circuit which is responsible for controlling the distance between the cantilever and the sample. In detail, we investigate the response time and the stability conditions in order to avoid oscillations in the circuit, which may cause damage to both, the cantilever and the sample. We compare the results of our simulation to tests performed on the physical circuit of the SFM. It is the aim to optimise the circuits and control parameters depending on the experimental conditions, i.e. the sample and the imaging goal.

O 15.55 Fr 17:00 Poster TU D

Testing SFM-Cantilevers in the Ultra-High Vacuum — •Heiner Lindemann, Lutz Tröger, Sebastian Gritschneder, and Michael Reichling — Fachbereich Physik, Universität Osnabrück, Barbarastraße 7, D-49076 Osnabrück

For taking high-resolution images with a dynamic scanning force microscope (SFM) operated in the so-called non-contact mode, cantilevers with a high Q-factor (about 100.000) are required, i.e. the response function should exhibit a very narrow peak. When detecting the oscillation with a light source operating in the infrared ($\lambda \sim 800$nm or higher), it is essential to use reflex-coated cantilevers as in this wavelength region the material of the cantilever (silicon) is nearly transparent. The reflex-coating, however, decreases the effective Q of the cantilever.
To determine the Q-factor before installing the cantilever into the SFM, cantilevers are tested in a separate ultra-high vacuum (UHV). We designed a setup where cantilevers of different SFM types can be fixed to measure the response function. We describe the design of the test station including a laser light source, a four-quadrants-photodiode and electronics to detect the oscillation of the cantilever that is exited by a piezo ceramic and present testing results obtained with various types of cantilevers.

O 15.56 Fr 17:00 Poster TU D

Detailed analysis of the response characteristic of a dynamic scanning force microscopy feedback control system — •Frank Ostendorf, Sabine Hirth, and Michael Reichling — Fachbereich Physik, Universität Osnabrück, Barbarastr. 7, 49076 Osnabrück

To obtain high resolution dynamic scanning force microscopy (SFM) images, the understanding and optimisation of the feedback control system is very important. Therefore, we analysed in detail the response characteristic of our electronic circuits. A typical feedback control system for dynamic SFM consist of three independent loops: amplitude control, demodulation control, and distance control. These three loops were analysed by means of a measurement simulation and under realistic imaging conditions. By optimising various components of the feedback control system, we enhance the signal-to-noise-ratio and improve SFM imaging stability.

O 15.57 Fr 17:00 Poster TU D

Development of a high-resolution SFM for use in a UHV cryogenic temperature environment — •Lutz Tröger und Michael Reichling — Universität Osnabrück, Barbarastr. 7, 49076 Osnabrück

We describe the development of a high-resolution SFM for use in a UHV cryogenic temperature environment. The design concept aims at highest resolution studies and is optimised for atomic precision force spectroscopy. The microscope utilises a laser interferometer for cantilever oscillation detection and an integrated eddy current damping stage to reduce mechanical noise. Additionally the commercial LHe/LN$_2$-bath-cryostat providing the cooling is equipped with a second stage of external kinematic vibration damping. We demonstrate the capability of the detection and scanning system and show first test measurements concerning mechanical stability and functionality.

O 15.58 Fr 17:00 Poster TU D

Lokal aufgelöste berührungslose Leitfähigkeitsmessungen (Wirbelstrommikroskopie) — •Tino Roll, Martin Görlich und Marika Schleberger — Universität Duisburg-Essen, Fachbereich Physik, 45117 Essen

Bei der Wirbelstrommikroskopie wird ein Rasterkraftmikroskop mit einem magnetischen AFM-Cantilever im non-contact-Modus betrieben. Dessen Oszillation führt zu Wirbelströmen in leitenden Materialien. Aufgrund dieser Wirbelströme kommt es zu einer zusätzlichen Wechselwirkung zwischen Spitze und Probe. Die Dämpfung der Cantilever-Oszillation dient als Messgröße für die mikroskopische Leitfähigkeit der Probe, das heißt Flächen konstanter Dämpfung entsprechen Flächen konstanter Leitfähigkeit. Ebenso ist es möglich, magnetische Domänen mit Hilfe leitender oszillierender AFM-Spitzen abzubilden. Experimentelle Daten zeigen, dass die Wirbelstrommikroskopie eine geeignete Methode zur Untersuchung der Leitfähigkeit ohne Kontakt zur Oberfläche ist.

O 15.59 Fr 17:00 Poster TU D

Construction of an Atomic Force Microscope combined with a Field Ion Microscope — •Daniel Braun, André Schirmeisen, Hendrik Hölscher, and Harald Fuchs — Physikalisches Institut, WWU Münster, Wilhelm-Klemm-Str. 10, 48149 Münster

While the atomic force microscope (AFM) is capable of resolving surfaces with atomic resolution, the exact configuration of the tip is entirely unknown. But it is necessary to know the exact position and identity of the tip atoms to understand the contrast mechanisms in atomic force microscopy. A method that allows to determine the position of the tip atoms with atomic precision is the field ion microscope (FIM).

We build an AFM according to a design previously published [1] for operation at low temperatures under an ultra high vacuum (UHV) conditions. The construction of the microscope body features a very high mechanical stability that makes an external damping mechanism unnecessary. The original design uses a silicon cantilever as the force sensor; its bending is detected by an optical interferometer. However, it is very difficult to use conventional silicon tips in a FIM. Therefore we intend to use a tuning fork [2], which allows us to use an appropriate material, e.g. tungsten, as the tip material of the force sensor. Our goal is to investigate how the contrast mechanism in AFM is influenced by the exact geometry of the last atoms of the tip.

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

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

O 15.60 Fr 17:00 Poster TU D

An approach on near-field Raman spectroscopy using the tetrahedral SNOM tip — •Stefan Klein[1], Ulrich Fischer[1], Daniel Molenda[1], Harald Fuchs[1], and Michael Hietschold[2] — [1]Physikalisches Institut, Westfälische-Wilhelms-Universität Münster, Wilhelm-Klemm-Str. 10, D-48149 Münster — [2]Institut für Physik, TU Chemnitz, D-09107 Chemnitz

The effect of field enhancement at nanoscale metallic structures is critical to optical phenomena such as surface-enhanced Raman scattering (SERS). Assemblies of coupled metal nanoparticles attracted high interest as SERS active systems supporting so called hot-spots of the electric field. Most recently tip-enhanced Raman scattering (TERS), where a metallic tip is situated near a smooth surface covered by Raman active species has been reported. The experimental results show, that only a small amount of molecules in the near-field of the laser irradiated tip-apex contributes to an observed characteristic Raman spectrum. The tip acts in these experiments similar to a single particle supporting a single hot-spot, which enhances the incident electric field. Different experimental approaches on TERS have been realized using metal coated AFM cantilevers or STM tips. Here we present an approach on near-field Raman spectroscopy using the tetrahedral SNOM tip to investigate molecular monolayers on gold films.

O 15.61 Fr 17:00 Poster TU D

Accuracy and Resolution Limits of Kelvin Probe Force Microscopy — •Christian Loppacher, Ulrich Zerweck, Tobias Otto, Stefan Grafström, and Lukas Eng — Institut für Angewandte Photophysik, Technische Universität Dresden, D-01062 Dresden

Kelvin probe force microscopy is a scanning probe technique capable of mapping the local surface potential or workfunction on various surfaces with high spatial resolution. This technique can be realized on the basis of either an amplitude-sensitive method or a frequency modulation method, which are sensitive to the electrostatic force and its gradient, respectively. We present a detailed experimental and theoretical study of the accuracy and resolution provided by the two methods, including a novel setup for the frequency modulation technique. Au(111) with a submonolayer coverage of KCl serves as a test sample exhibiting extended sharply bounded areas that differ in workfunction by an amount well known from ultraviolet photoelectron spectroscopy. The experimental results are compared with the predictions of a numerical simulation based on a realistic model for the tip-sample geometry. Good agreement is found. The experimental analysis allows us to specify the lateral, vertical and potential resolution that can be achieved with the two methods for a given tip size. Our work clearly proves that the frequency modulation method is preferable in most applications because it (i) provides much higher lateral resolution, (ii) yields quantitative surface potential values on areas larger than the tip radius, and (iii) is little affected by variations of the tip-sample distance during topographic imaging.

O 15.62 Fr 17:00 Poster TU D

Accuracy and Resolution Limits of Kelvin Probe Force Microscopy — •Christian Loppacher, Ulrich Zerweck, Tobias Otto, Stefan Grafström, and Lukas Eng — Institut für Angewandte Photophysik, Technische Universität Dresden, D-01062 Dresden

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O 15.63 Fr 17:00 Poster TU D

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O 15.64 Fr 17:00 Poster TU D

Formation of Ag islands on Ag(111) using atomic force microscopy in the dynamic mode — Michaela Zeyer-Düsterer, •Rene Schmidt, Alexander Schwarz, and Roland Wiesendanger — Institut für Angewandte Physik, Universität Hamburg, Jungiusstr. 11, 20355 Hamburg

Ag vacancy and adatom islands on Ag(111) have been frequently regarded as a test system to study the growth and dynamics of 2D-nanostructures. Conventionally, such structures are created by argon ion bombardment and subsequent heating. However, in this study we utilized atomic force microscopy in the dynamic mode to create and image vacancy and adatom islands on flat Ag(111) terraces. Their formation occurs when the tip enters the repulsive interaction regime. Non-invasive stable imaging on the resulting structures is possible in the non-contact attractive regime. The application of local force spectroscopy enables to examine the growth mechanism in more detail. Particularly, the influence of external parameters like the applied repulsive force and the oscillation amplitude on the island size are evaluated.

O 15.65 Fr 17:00 Poster TU D

Surface investigations of single junction thermal converters in the infrared spectral range — •Viktor Schlosser[1], Gernot Heine[2], M. Garcocz[2], W. Waldmann[2], and Gerhard Klinger[3] — [1]Institut für Materialphysik, Universität Wien — [2]Bundesamt für Eich- und Vermessungswesen, Wien — [3]Institut für Meteorologie und Geophysik, Universität Wien

The ac-dc transfer standard is one of the basic electrical standards, by which the ac voltage and ac current are deduced from their dc counterparts. A well established method is the comparison of electrical power between ac- and dc- voltage by converting the power to force or heat. Converters may be recognised as reference standard and the system is called "ac-dc transfer standard". Differences in the signal between ac- and dc- power generation depend on frequency and waveform. In the low frequency regime the thermal ripple dominates the error introduced by the thermal converter. Thermocouple measurements of the bulk temperature of a bead of a single junction thermal converter suggest that a significant thermal ripple exists only at frequencies below 20Hz. A scanning infrared radiation imaging set up was used to investigate the bead's surface. By this method frequency dependent temperature modulations were observed up to frequencies of 200Hz. The experimental method will be presented and the results will be discussed.

O 15.66 Fr 17:00 Poster TU D

Stack-type vibration decoupling for scanning probe applications — •F. Müller[1], A.-D. Müller[1], D. Billep[2], St. Kurth[3], A. Shaporin[2], M. Hietschold[1], and W. Dötzel[2] — [1]Chemnitz University of Technology, Institute of Physics, Solid Surfaces Analysis Group, 09107 Chemnitz — [2]Chemnitz University of Technology, Faculty of Electricl Engineering and Information Technology, Microsystems and Device Technology Group, 09107 Chemnitz — [3]Fraunhofer IZM, Micro Devices and Equipment, Reichenhainer Strasse 88, 09126 Chemnitz

In Scanning Tunneling Microscopy (STM), a stack of mechanically coupled metal plates is commonly used as vibration isolation to obtain atomically resolved images. In this work, the transmission of mechanical vibrations through this stack is studied in dependence on its geometrical dimensions and material properties [1, 2]. A phase sensitive correlation analysis between a defined mechanical excitation and the resulting movement of different plates in vertical and lateral directions allows to quantify the efficiency of the vibration damping in a frequency range till 200 Hz. From the characteristics obtained at the example of the Pocket STM, the typical frequency response function (FRF) of the stack is obtained. For optimization purposes, a finite element model of the device was used. Modal and transient analysis of the device were performed for various combinations of geometrical parameters and material properties. Modelling results show satisfactory similarities with the measurements taken at the STM stack.
[1] S.I. Park, C.F. Quate, Rev. Sci. Instrum. 58, 2004-2009 (1987). [2] D.W. Pohl, IBM J. Res. Develop. 30 (4), 417-427 (1986).

O 15.67 Fr 17:00 Poster TU D

Tribological properties of amorphous and crystalline antimony nanoparticles studied by SFM and TEM — •Claudia Ritter[1], Udo D. Schwarz[2], Bert Stegemann[1,3], Markus Heyde[1,4], and Klaus Rademann[1] — [1]Humboldt-Universität zu Berlin, Institute of Chemistry, Brook-Taylor-Str. 2, D-12489 Berlin, Germany — [2]Department of Mechanical Engineering, Yale University, P.O. Box 208284, New Haven, CT 06520-8284, USA — [3]Federal Institute of Materials Research and Testing (BAM), D-12200 Berlin, Germany — [4]Fritz-Haber-Institute of the Max-Planck-Society, Faradayweg 4-6, D-14195 Berlin, Germany

The fundamentals of friction, in particular, the interplay between friction, adhesion, true contact area and crystalline structure at the interface, are still insufficiently understood. In this investigation, antimony nanoparticles grown on HOPG and MoS$_2$ were used as a model system. The morphology of the nanoparticles was characterized by SFM, SEM and TEM. Thus, both the interface structure and the real contact area were accurately determined. The TEM study revealed a size dependent amorphous-polycrystalline phase transition. Controlled translation of the particles was induced by the action of the oscillating tip in dynamic mode SFM. During manipulation, the power dissipated due to tip-sample interactions was recorded. Particles with contact areas below 10000 nm^2 were much easier to move compared to their larger counterparts. We suggest that structural lubricity might be the reason for the low dissipation in the small amorphous particles, while elastic multistabilities might dominate energy dissipation in the larger polycrystalline particles.

O 15.68 Fr 17:00 Poster TU D

Abbildung biologischer Proben mit dem CE-Modus in derRasterkraftmikroskpie — •Jens Falter, Jan-Erik Schmutz, Daniel Ebeling, Marcus Schäfer und Hendrik Hölscher — Center for NanoTechnology (CeNTech) und Physikalisches Institutder Universität Münster, Gievenbecker Weg 11, 48149 Münster

Die dynamische Rasterkraftmikroskopie ermöglicht neue Einblicke und Erkenntnisse in die Oberflächenphysik. Die Wechselwirkungen an Oberflächen können mit der dynamischen Kraft-Spektroskopie ausgemessen werden. Bei tiefen Temperaturen im Hochvakuum ist dies sogar mit dreidimensionaler Auflösung möglich [1]. Aufgrund verschiedener experimenteller Probleme war diese Methode aber auf das Vakuum beschränkt. Um dynamische Rasterkraftspektroskopie auch an Luft und in Flüssigkeiten zu ermöglichen, haben wir den sogenannten CE-Modus implementiert. Mit dieser Technik ist die Rekonstruktion der Spitzen-Proben-Wecheselwirkung ebenfalls möglich [2]. Wir haben die Möglichkeiten dieses Ansatzes insbesondere für biologische Proben untersucht. Im Vordergrund stehen dabei Messungen in Flüssigkeiten, dem natürlichen Medium für biologische Proben.

[1] H. Hölscher, S. M. Langkat, A. Schwarz, R. Wiesendanger, Appl. Phys. Lett. **81**, 4428 (2002)

[2] H. Hölscher, B. Gotsmann, A. Schirmeisen, Phys. Rev. B **68**, 153401 (2003)

O 15.69 Fr 17:00 Poster TU D

Adhesion forces studied with colloid probe atomic force microscopy — •Bert Stegemann, Henrik Backhaus, Heinz Kloss, and Erich Santner — Bundesanstalt für Materialforschung, BAM - VIII.1 Tribologie und Verschleißschutz, Unter den Eichen 44-46, D-12205 Berlin

Adhesion is of fundamental importance for the tribological behavior, e.g., in nanomechanical devices. A promising approach to determine interfacial adhesion at sub-micron scale is to measure pull-off forces with an atomic force microscope (AFM). As adhesion depends on numerous factors, such as contact area, environment and dynamics, there is still a lack of reliable quantitative data. Here, we report on a systematic analysis of AFM pull-off forces for well-defined systems under ultrahigh vacuum conditions. Interaction geometry is controlled by means of colloid AFM probes, i.e., microspheres attached at the end of bare AFM cantilevers. Clean sample surfaces of a wide range of single crystal metals and compound materials were prepared by subsequent Ar ion sputtering and annealing as affirmed by surface analytical techniques. The influence of experimental parameters, like applied load, contact time and contact area on the pull-off forces is discussed. The results obtained are compared with predictions from theoretical models and correlated with macroscopic mechanical properties of the materials.

O 15.70 Fr 17:00 Poster TU D

Optical properties of silver cluster ensembles — •Hadj Mohamed Benia, Niklas Nilius, and Hans-Joachim Freund — Fritz-Haber-Institut der Max-Planck-Gesellschaft, Faradayweg 4-6, 14195 Berlin

By means of photon emission spectroscopy with an STM, we have studied the electromagnetic coupling in silver cluster ensembles. The ensembles were prepared by two techniques: (i) atom deposition on a thin alumina film in UHV and (ii) deposition of size-selected silver colloids, prepared by a reverse micelle technique, on gold and HOPG substrates. Silver on alumina grows with a very low cluster density. The corresponding cluster ensemble shows one plasmon resonance, indicative for weak cluster-cluster coupling. In contrast, measurements on dense colloidal cluster arrays reveal two plasmon peaks, shifted to higher and lower energies with respect to the one observed for alumina-supported Ag clusters. The presence of two resonance peaks is explained by considerable electromagnetic coupling in the cluster ensemble.

O 15.71 Fr 17:00 Poster TU D

Charge Carrier Dynamics at Silicon surfaces: A Time-Resolved Photoemission Study with Combined Laser and Synchrotron Radiation. — •Tatjana Giessel[1], David Bröcker[1], Helena Prima Garcia[1], Ramona Weber[1], Martin Weinelt[1,2], and Wolf Widdra[3] — [1]Max-Born-Institut, Berlin, Germany — [2]Freie Universität, Berlin, Germany — [3]Martin Luther Universität, Halle, Germany

Charge carrier dynamics at the Si(100) surface and for thin oxide layers on Si(100) have been studied by probing the time-dependent surface photovoltage (SPV). Electron-hole pairs are excited in the near-surface region by femtosecond lasers pulses and the subsequent dynamics of charge carrier recombination is determined by time-resolved Si 2p core-level photoemission using synchrotron radiation. For laser fluences up to $60\mu J/cm^2$ the observed non-exponential decay of the SPV can be described within a model based on thermionic emission. For higher laser fluences up to $60mJ/cm^2$ an oscillation of the SPV in time is observed. A fast drop of the SPV within 100 ps is followed by a slow increase reaching its maximum at several 100 nanoseconds. An even slower decay in the microsecond range then restores the primary SPV. The decay time of the initial fast drop of the SPV decreases with increasing sample temperature, which suggests a phonon mediated charge-carrier recombination-process. The subsequent SPV dynamics on the time scale of hundreds of nanoseconds to microseconds are assigned to diffusion-limited processes.

O 15.72 Fr 17:00 Poster TU D

Electron-electron correlations at the LiF(100) surface probed via (e,2e) spectroscopy — •Frank O. Schumann, Jamal Berakdar, and Jürgen Kirschner — MPI f. Mikrostrukturphysik, Weinberg 2, 06120 Halle

Electronic correlations manifest themselves in many-body effects like superconductivity and magnetism. Due to the Coulomb and exchange interaction two electrons tend to avoid each other leading to an exchange-correlation hole. We studied the correlation between two electrons by probing the emission of electron pairs from a LiF(100) surface upon excitation with 32 eV primary electrons. The set-up consists of a channelplate, followed by a central collector and a pulsed electron gun. The energy of the electrons follows from their flight times. We find correlation in energy and k-space of an electron pair, where one electron originates from the top of the valence band. We selected the energies of the ejected electron pair to be E_1=9 eV and E_2=8 eV, respectively. Mapping the correlation as a function of the in-plane momentum of the second electron results in the observation of a zone of reduced intensity. The extension of this exchange-correlation hole is $\sim$1 Å^{-1} which is in the range of theoretical predictions on double photoemission. Another experimental fact is the sensitivity of the correlation hole to decoherence effects, an aspect which is largely unexplored theoretically. Increasing the impinging electron energy to 33.7 eV allows for inelastic scattering of the electron pair. This opens up a decoherence channel and the correlation hole vanishes. Varying the primary energy is therefore a tool for tuning on or off decoherence effects.

O 15.73 Fr 17:00 Poster TU D

Electron coincidence spectroscopy on Xe/Cu(111) — •Carsten Winkler and Jürgen Kirschner — MPI f. Mikrostrukturphysik, Weinberg 2, D-06120 Halle

Correlation between electrons is a fundamental characteristics of systems containing many electrons. In the present experiments, electron coincidence spectroscopy (e,2e) has been carried out in order to study energy distributions of correlated electrons ejected from condensed Xe films. The films have been prepared by dosing 20 L of Xe onto a Cu(111) single crystal surface that was cooled down by ℓHe to a temperature of $T_p \simeq 50$ K. The incoming (primary) electrons are generated by a pulsed electrom source with a kinetic energy in the range of 20 eV $\leq E_p \leq$ 35 eV. The scattered (secondary) coincidend electrons, on the other hand, are detected by using two reflection time-of-flight (TOF) spectrometers. With that, the kinetic energies E_1 and E_2 of the corresponding coincident electrons can be calculated from its flight time from sample the to the detector.

As a first step, TOF spectra were taken for Xe adsorbed on Cu(111) at energies of $E_p = 20$ eV and $E_p = 25$ eV. Compared to the corresponding data of metals like Cu or Co, these measurements show rather high coincidence count rates. The data generally show a distinct feature in the region $(E_1 + E_2) = E_p - W$ with $E_1 = E_2$. Here, W is the work function that was determined to be $W \simeq 8$ eV. These promising results of the very first (e,2e)-coincidence studies on solid Xe are an encouragement for further systematic investigations, namely varying the Xe film thickness. (2004)

O 15.74 Fr 17:00 Poster TU D

Manipulation of ultrafast surface processes using fs-pulse shaping — •Felix Steeb, Marlies Wessendorf, Jörg Lange, Alexander Mönnich, Stefan Mathias, Martin Aeschlimann, and Michael Bauer — FB Physik, TU Kaiserslautern, Erwin-Schrödinger-Str. 46, 67663 Kaiserslautern

In recent years, coherent control of ultrafast processes in the gas phase [1] or in the liquid phase [2] by means of adaptive femtosecond pulse shaping has been demonstrated.

In this paper, we present first attempts to employ the pulse shaping technique to the manipulation of ultrafast surface processes, such as surface chemical reactions.

For the Two-Photon-Photoemission (2PPE) yield from the occupied shockley surface state of a Cu(111) surface, we find a complex dependence on the spectral phase of the exciting pulse, modulated by a programmable 640-stripe liquid crystal spatial light modulator incorporated into a conventional 4f-setup. Resonance enhanced excitation induced by an unoccupied adsorbate state, e.g. Cs/Cu(111), modifies this dependence. Model calculations within the framework of the Liouville-von-Neumann equitations can qualitatively reproduce the experimental data. Future prospects, e.g. possible schemes to control a surface chemical reaction using pulse-shaping techniques and other potential applications are discussed.

[1] - A. Assion et al.: Science 282, 919 (1998)

[2] - T. Brixner et al: Nature 414, 57 (2001)

O 15.75 Fr 17:00 Poster TU D

Limitations in the use of a 2D hemispherical energy analyser for PES in combination with a low-repetitive ultrashort photon source — •S. Mathias[1], O. Heinz[2], S. Passlack[1], D. Mittnacht[1], V. Temnov[2], M. Bauer[1], D. von der Linde[2], and M. Aeschlimann[1] — [1]FB Physik, TU Kaiserslautern, 67663 Kaiserslautern — [2]Institut für experimentelle Physik, Uni Duisburg Essen, 45117 Essen

One of the main advantages of hemispherical electron analysers equipped with a 2D detector is their high efficiency due to the parallel detection scheme with respect to energy and momentum. It makes these systems highly preferable for specific applications e.g. for the use with low-repetitive photon sources such as laser-based femtosecond UV-sources. In this study a 2D analyser has been used for 2 Photon Photoemission spectroscopy from an occupied surface state of Cu(111) using a 1 kHz laser amplifier system. For comparison, corresponding data have also been recorded using a ToF electron analyzer and a high repetitive (80 MHz) Ti:Sapphire laser. Particular focus has been set on the spectral broadening due to space charge effects which become apparent at sufficient high pulse intensities from the 1 kHz amplifier. The experimental data are compared with numerical simulations which support the relevance of space charge effects. Our results show that the 2D analyzer scheme is suitable for high-resolution angular-resolved electron spectroscopy in combination with low repetitive laser sources and may in the future be used complementary to conventional ToF-detectors.

O 15.76 Fr 17:00 Poster TU D

New measurements on the Casimir-van der Waals potential — •Lodewijk Arntzen — Physikalisches Institut, Heidelberg University, 69120 Heidelberg

We recently measured quantum reflection of cold helium atoms from a purely attractive potential. The interaction could be identified as originating from the Casimir force between a single atom and semi-conducting surface. We are now specifically investigating the temperature behavior of the Casimir-van der Waals potential. Within the incident energy range between μeV and neV, the surface temperature is varied from 300 K to 1200 K. These new measurements show that the quantum reflected intensities decrease sharply and reproducibly with increasing temperature. We will present different mechanisms that may account for this observation. In addition the Debye-Waller effect, the temperature dependence of the electric permittivity and magnetic effects will be adressed.

O 15.77 Fr 17:00 Poster TU D

Force microscopy analysis of etch pits for crystal defect assignment — •Christian Motzer und Michael Reichling — Fachbereich Physik, Universität Osnabrück, Barbarastr. 7, 49069 Osnabrück

Ex-situ scanning force microscopy analysis of etched (111) CaF_2 cleavage plates were carried out to study crystal defects. Etch figures are well known to be related to certain crystal defects and were studied by several microscopy methods to determine the etch pit density (EPD) which relate to the dislocation density in a crystal. Force microscopy enables us to investigate in detail the etch figures and reveal more than the occurance of dislocation etch pits. We found several types of etch pits which relate to different kinds of defects. Point bottom etch pits and flat pits are discussed in relation to their crystal defect origins. Segregation connected with dislocations alter the kinetic during dissolution and hence change the appearance of etch pits, e.g. etch pits appear with multiple inner walls.

O 15.78 Fr 17:00 Poster TU D

A setup for grazing incidence x-ray scattering measurements at the SAW2 beamline of DELTA — •Christof Krywka[1], Michael Paulus[1], Christian Sternemann[1], Michael Volmer[1], Oliver H. Seeck[2], and Metin Tolan[1] — [1]Experimentelle Physik I, DELTA, Universität Dortmund, Maria-Goeppert-Mayer Strasse 2, 44221 Dortmund, Germany — [2]HASYLAB am DESY, Notkestraße 85, 22603 Hamburg

We report on an experimental setup installed at the SAW2 (Superconducting Asymmetric Wiggler) beamline of the Dortmund Electron Accelerator DELTA that allows grazing incidence small angle scattering (GISAXS) experiments on liquid surfaces. GISAXS is a unique technique to probe surface and near-surface structures of soft materials. The setup was designed for photon energies between 8 and 15keV using a six circle diffractometer in combination with a focussing mirror. First GID experiments have already been succesfully performed on water and aqueous NaJ solution as well as on polypropylenglycol (PPG) samples.

O 15.79 Fr 17:00 Poster TU D

Time-Resolved Reflection High-Energy Electron Diffraction – Pump-Probe Experiments on Clean and Bi-covered Si Surfaces — •A. Janzen, B. Krenzer, and M. Horn-von Hoegen — Universität Duisburg-Essen, Institut für Experimentelle Physik, 45117 Essen

Time-resolved Reflection High-Energy Electron Diffraction opens a new pathway to investigate the structural dynamics at surfaces subsequent to an intense electronic excitation by a fs-laser pulse. By variation of the time delay between a fs-laser-pump pulse and a ps-electron-probe pulse the transient state of the surface under examination can be determined. The construction of a laser-driven electron gun providing picosecond electron pulses and the setup of an electron diffraction apparatus has already been successfully accomplished.

We are now conducting studies of ultrafast heating phenomena after laser excitation of clean Si surfaces and thick Bi-films epitaxially grown on Si. The last step in the chain of processes following the excitation is the transient heating of the lattice, leading to a drop in the diffraction spot intensity (*Debye-Waller effect*). Since Bi has a much lower Debye temperature than Si, $\Theta_{D,Bi} = 119$ K compared to $\Theta_{D,Si} = 652$ K, the Debye-Waller effect is much more pronounced on Bi surfaces than on Si surfaces. First results of the pump-probe experiments and a discussion of the encountered problems will be presented.

O 15.80 Fr 17:00 Poster TU D

Contrast mechanisms in imaging spectroscopy using the *nano*ESCA — •S. Schmidt[1], F. Forster[2], F. Reinert[2], M. Escher[3], N. Weber[3], M. Merkel[3], D. Funnemann[4], B. Krömker[4], Ch. Ziethen[5], P. Bernhard[5], H.-J. Elmers[5], G. Schönhense[5], and S. Hüfner[1] — [1]Universität des Saarlandes, D-66041 Saarbrücken — [2]Universität Würzburg, D-97074 Würzburg — [3]Focus GmbH, D-65510 Hünstetten — [4]OmicronNanoTechnology GmbH, D-65232 Taunusstein — [5]Universität Mainz, D-55128 Mainz

We present the results obtained during synchrotron measurements using the *nano*ESCA prototype for imaging XPS to demonstrate its imaging capabilities of elemental, chemical, magnetic and orientational contrast in prototypical samples with a spatial resolution better than 120 nm, an energy resolution of $\Delta E \leq 110$ meV and the ability to image electrons with kinetic energies up to 1.6 keV [1]. We demonstrate the extension of the standard applications of imaging ESCA systems to the use of MCD and MLDAD contrast in the Fe 2p XPS core-level spectra to map ferromagnetic domains. We also show how the *nanoESCA* setup can be used to distinguish between different grain orientations in poly-crystalline materials by measuring the electronic structure of single grains [2].

[1] M. Escher *et al.*, J. Phys.: Condens. Matter, in print.

[2] M. Escher *et. al*, J. Electron Spectrosc. Relat. Phenom., in print

O 15.81 Fr 17:00 Poster TU D

A multichannel detection photoemission experiment — •Michael Helle, Martin Marczynski, Matthias Kalläne, Sönke Harm, Kai Rossnagel, and Lutz Kipp — Institut für Experimentelle und Angewandte Physik, Universität Kiel, D-24098, Germany

It is possible to reduce the data collection times of angle-resolved photoelectron spectroscopy (ARPES) by means of parallel detection of electron energy and angle by at least a factor of ten. Parallel detection is implemented by equipping a hemispherical analyzer which is rotatable about the sample in ultrahigh vacuum with a position and time sensitive microchannel plate detector with delay-line readout (DLD: delay-line detector).
The construction and the characterization of a home-built hemispherical analyzer with DLD from the Roentdek company will be presented. First measurements of the layered transition metal dichalcogenide $TiTe_2$ before and after adsorption of potassium will be shown.
This work was supported by the BMBF proj. no. 05 KS1 FKB.

O 15.82 Fr 17:00 Poster TU D

Scaling laws of the angular emission distribution of laser ablated plasma pulses from monoatimic and binary targets in a mass range from 27 to 184 — •Shailendra Nath Srivastava and Klaus Rohr — Technical University of Kaiserslautern, D 67663 Kaiserslautern, Germany

In the present experiment we have investigated emission characteristics of laser produced plasma pulses quantitatively and over a wide mass range. Targets have been monoatomic Al, Ti, Cu, Mo, W and compounds of these with different stoichiometric ratios. Thereby the (average) mass covers a range from 27 to 184. The following major results are observed: (1) The emission cones of all species steepen continuously as a function of the (average) atomic mass. Thereby, for the first time, the widths can be well described by a general scaling law namely k/A + c. Here k and c systematically depend on the size of the ablation area. (2) The measured widths of the compound systems agree with averaged data of its single pure component if the corresponding stoichiometric ratios of the pure targets are used. This suggests that stoichiometry is essentially conserved. (3) All emission shapes can be fitted uniquely by Gauß-functions which reflects the dominating effect of the spatial shape of the laser pulse on the shape of the emission distribution. The result are essential for practical applications, they allows quite simply predictions of emission distributions of monoatomic species hardly to measure otherwise (e.g. gases) and of compound systems of arbitrary compositions.

O 15.83 Fr 17:00 Poster TU D

UHV compatible high-pressure reaction cell for in-situ IR and kinetic studies of single model catalysts — •Thomas Häring, Thomas Diemant, Zhong Zhao, Hubert Rauscher, and R. J. Behm — Abt. Oberflächemchemie und Katalyse, Universität Ulm, 89069 Ulm

We have designed and constructed a high pressure reaction cell for in-situ IR (PEM-IRAS) and kinetic measurements at pressures up to 100 mbar. The cell is attached to a UHV system equipped with standard facilities for sample preparation and characterization. The small volume of the cell and the low leak rate over the differentially pumped seal allows to follow reactions under batch conditions for several hours; well-defined gas flow rates can be established by calibrated capillaries. We present details of the setup of the reaction cell and discuss the performance of the system.

O 15.84 Fr 17:00 Poster TU D

Advances in nanofocusing with reflective photon sieves — •Jan Bartussek, Jens Buck, Matthias Kalläne, Sönke Harm, Kai Rossnagel, and Lutz Kipp — Institut für Experimentelle und Angewandte Physik, Universität Kiel, D-24098 Kiel

Photon sieves are a new type of diffraction optics for focusing synchrotron radiation to submicrometer dimensions. They appear especially promising for future angle and spatially resolved photoemission experiments at the VUV-FEL at HASYLAB, because side lobes in the intensity pattern in the focal plane can be suppressed almost completely by applying smooth window functions. In addition, by separating zero from first order light the background can be reduced significantly. Using a knife edge scanner we measured focal spots for photon sieves optimized for a photon energy of 100 eV. Experiments were carried out at beamline BW3 at HASYLAB. The results are discussed in the context of numerical simulations. Work is supported by BMBF proj. no. 05 KS1 FK1.

O 16 Hauptvortrag Himpsel

Zeit: Samstag 09:00–09:45 Raum: TU EB301

Hauptvortrag

O 16.1 Sa 09:00 TU EB301

Low-dimensional electrons at silicon surfaces — •Franz J. Himpsel — Physics Dept., University of Wisconsin Madison, 1150 University Ave., Madison, WI 53706, USA

It has become possible to create a class of low-dimensional chain structures on silicon surfaces that are metallic [1,2]. Electrons near the Fermi level are de-coupled from the substrate because their energy lies in the band gap. The metal atoms, however, are rigidly tied to the silicon lattice in substitutional positions according to x-ray diffraction [3] and first principles band calculations [4]. The dimensionality can be controlled by using stepped surfaces with adjustable step spacing. Ratios of the intrachain coupling to the inter-chain coupling between 10:1 and more than 70:1 have been achieved. In addition, the band filling can be varied, including fractional fillings, such as 8/3 of an electron per chain atom [2]. That creates an opportunity to systematically search the parameter space for exotic states predicted for one-dimensional electrons, such as a collective excitation where spin and charge separate. This wide-open territory of low-dimensional structures is explored in real and reciprocal space by scanning tunneling microscopy and angle-resolved photoemission.

[1] Himpsel et al., J. Phys. Condens. Matter 13, 11097 (2001). [2] Crain et al., Phys Rev. Lett. 90, 176805 (2003) and Phys. Rev. B 69, 125409 (2004). [3] Robinson et al., Phys. Rev. Lett. 88, 096104 (2002). [4] Sanchez-Portal et al., Phys. Rev. B 65, 081401 (2002) and Phys. Rev. Lett. 93, 146803 (2004); Erwin, Phys. Rev. Lett. 91, 206101 (2003).

O 17 Hauptvortrag Stampfl

Zeit: Samstag 09:45–10:30 Raum: TU EB301

Hauptvortrag

O 17.1 Sa 09:45 TU EB301

Order-disorder Surface Phase Transitions from First-principles — •Catherine Stampfl[1], M. Borg[2], A. Mikkelsen[2], J. Gustafson[2], E. Lundgren[2], M. Scheffler[3], and J.N. Andersen[2] — [1]School of Physics, The University of Sydney, Australia — [2]Department of Synchrotron Radiation Research, Institute of Physics. Lund University, Sweden — [3]Fritz-Haber-Institut der Max-Planck-Gesellschaft, Faradayweg 4-6, Berlin-Dahlem, Germany

One of the most important goals of theoretical surface science is to achieve an ab initio atomistic description that can predict phenomena and properties occurring on macroscopic length and long time scales [1]. Clearly, knowledge of the surface structure and composition are crucial ingredients for such a description. This talk will discuss through the example of Na-Al surface alloys, state-of-the-art first-princples based theoretical methodology and concepts which allow an accurate and fast predictive description of equilibrium surface structures and phase transitions as a function of temperature and stoichiometry [2]. The system is described using a lattice-gas Hamiltonian (LGH), together with Monte Carlo (MC) simulations. In addition to standard MC, the new MC algorithm of Wang and Landau [3] is employed in which the density of (configurational) states are explicity obtained. From this the thermodynamic quantities such as the free energy and entropy are directly determined.
[1] K. Reuter, C. Stampfl and M. Scheffler, Handbook of Materials Modeling, Volume 1, Fundamental Models and Methods, Sidney Yip (Ed).
[2] M. Borg, et al. to be published.
[3] F. Wang and D.P. Landau, Phys. Rev. Lett. 86, 2050 (2001).

O 18 Adsorption an Oberflächen II

Zeit: Samstag 10:45–13:00 Raum: TU EB301

O 18.1 Sa 10:45 TU EB301

Experimental determination of surface stress of H/Si(001) — •Peter Kury[1], Jan van Heys[2], Eckhard Pehlke[2], and Michael Horn-von Hoegen[1] — [1]Institut für Laser- und Plasmaphysik, Universität Duisburg-Essen, 45141 Essen — [2]Institut für Theoretische Physik und Astrophysik, Universität Kiel, 24098 Kiel

The adsorption of hydrogen on Si(100) is one of the most profoundly investigated model systems for the study of reaction dynamics on semiconductor surfaces. The interest in this system, however, is not only motivated by fundamental questions regarding the chemisorption dynamics, but also by the technologically relevant epitaxial growth by means of chemical vapor deposition using silanes. Surface stress is an important surface property, intimately linked to the electronic structure of the surface, which is known to provide the driving force for structure formation on mesoscopic length scales, e.g. in case of the clean Si(100) surface. In the system H/Si(100), however, the role of surface stress is yet unknown. We present stress data for this system as a function of hydrogen coverage measured by SSIOD (surface stress induced optical deflection [1]) and compare to the theoretical surface stress tensor for various partially hydrogen-covered Si(100) surfaces predicted by density-functional total-energy calculations. [1] P. Kury et al., Rev. Sci. Instrum., in press.

O 18.2 Sa 11:00 TU EB301

Structure and Stability of the H / Ir (100) Adsorbate System — •Lutz Hammer, Daniel Lerch, Andreas Schmidt, Andreas Klein, Stefan Müller und Klaus Heinz — Festkörperphysik, Universität Erlangen-Nürnberg, Staudtstr.7, D-91058 Erlangen

The structure and energetics of hydrogen adsorption on the $Ir(100) - 1 \times 1$ and -5×1 surface phases were studied by LEED, STM and first-principles calculations. For the metastable $Ir(100) - 1 \times 1$ surface ab-initio DFT calculations surprisingly find the bridge site as the energetically stable adsorption site for all H-coverage values considered. A LEED structure analysis performed for this system confirms both this adsorption site and the substrate multilayer relaxation predicted by DFT. For the $5 \times 1 - hex$-phase, the reconstructed ground state of $Ir(100)$, again an excellent agreement between the geometrical results of LEED and DFT was achieved. For this phase the heat of adsorption for the bridge and hollow site is degenerate and about 0.2 eV less than for the 1×1-phase. The heat of adsorption values computed for other sites point towards a one-dimensional diffusion of hydrogen on the quasi-hexagonal surface. The structural modifications induced by H can be regarded as a precursor state for the lifting of the reconstruction. As the hydrogen induced $5 \times 1 - hex \rightarrow 1 \times 1$ deconstruction is kinetically hindered, a new 1×1-like phase ($5 \times 1 - H$) is formed instead. The bridge site is again the favoured adsorption site, with a heat of adsorption equivalent to that of the 1×1-phase. Again the structural parameters revealed from LEED and DFT agree in all details.

O 18.3 Sa 11:15 TU EB301

Einfluss von Oberflächenverunreinigungen auf die Speicherung von Wasserstoff in Form von Metallhydriden — •Mark Schülke[1], Hubert Paulus[2], Karl-Heinz Müller[1,2] und Martin Lammers[2] — [1]Hochschule für Technik und Wirtschaft Südwestfalen — [2]Institut für Technologie- und Wissenstransfer an der Hochschulabteilung Soest

Die Wasserstoffspeicherung in Metallhydriden ist auf Grund der hohen Sicherheit und der hohen volumenbezogenen Speicherdichte eine viel versprechende Alternative zu den herkömmlichen Speicherformen. Das H-Absorptionsvermögen von Metallhydriden hängt in hohem Maße von Oberflächenkontaminationen ab. Im Rahmen der Untersuchungen an verschiedenen AB_2-Legierungen auf Ti-Zr-Basis wurden Oberflächenkontaminationen durch definierte Präparationsschritte eingestellt und deren Einfluss auf die H-Absorption untersucht. Hierzu wurden die Oberflächen mit AES, XPS und SNMS charakterisiert und Beladungsexperimente in einer KDI-Anlage durchgeführt. Die Untersuchungen zeigen, wie sich Variationen in den Legierungszusammensetzungen auf das Kontaminationsverhalten auswirken. So besitzen die Legierungen auch nach mehrwöchiger Lagerung an Luft nur eine wenige Atomlagen dicke Kontaminationsschicht, die durch Sputtern bzw. durch Aktivierungsprozesse (Tempern in H-Atmosphäre) entfernt werden kann. Nach wenigen Aktivierungszyklen besitzen sie wieder ihre volle Kapazität. Ziel der Untersuchungen ist/war es, am Beispiel ausgesuchter Metalllegierungen den Einfluss von Verunreinigungen in der Gasphase und im Material auf wichtige Prozesse bei der H-Absorption zu untersuchen.

O 18.4 Sa 11:30 TU EB301

H on Pt(110): Atypical chemisorption site at low coverages, typical at high covarages? — •Rinaldo Zucca and Josef Redinger — Center f. Computational Materials Science, Vienna University of Technology, Getreidemarkt 9/134, A-1060 Vienna, Austria

A recent analysis of an hydrogen-modified Pt(110) surface with quantitative LEED and DFT calculations established a strong dependence of (1x2) missing row surface Pt lattice relaxations on the H atom coverage. Contrary to former assignments, both experiment and DFT calculations agree that at low coverages (β_2-state) H occupies adsorption sites above the outermost close-packed rows. A careful theoretical study of possible sites and trajectories revealed the short-bridge site on the outermost row, and not the fcc pseudo-threefold site at the (111) microfacets of the missing row surface's deep troughs as the preferred chemisorption site. Possible adsorption sites and adsorbate structures at higher coverages, such as found in the β_1-state, are presently under investigation.

O 18.5 Sa 11:45 TU EB301

Analyzing the order-disorder transition in hydrogen adsorption on Pd(111) with a first-principles lattice gas hamiltonian approach — •Cesar Lazo[1], Karsten Reuter[2], Volker Blum[2], Frerich Keil[1], and Matthias Scheffler[2] — [1]TU Hamburg-Harburg, Eissendorfer Str. 38, D-21071 Hamburg — [2]Fritz-Haber-Institut, Faradayweg 4-6, D-14195 Berlin

The interaction of hydrogen with Pd surfaces is of particular interest in many industrial reactions, including hydrogenation and fuel cell technologies. We set out to study the mesoscopic ordering behavior of hydrogen on Pd(111) from first-principles by parametrizing a lattice gas Hamiltonian (LGH) with density-functional theory (DFT) data. The subtle energy differences involved in the hydrogen bonding make this a critical test case, and we discuss the present methodological limitations with respect to basis set, exchange-correlation functional, and LGH expansion. Using our LGH model we then carry out Monte Carlo simulations in order to obtain the (T, p)-phase diagram, as well as the configurational energy density of states (DOS) using the Wang-Landau algorithm. With this DOS we calculate the configurational entropy and can correlate it with the experimentally observed low critical temperatures for the order-disorder transition in the H/Pd(111) system.

O 18.6 Sa 12:00 TU EB301

PM-IRAS and XPS studies of methanol oxidation on Pd model catalysts — •Marta Borasio, Oscar Rodríguez de la Fuente, Günther Rupprechter, and Hans-Joachim Freund — Fritz-Haber-Institut, Faradayweg 4-6, 14195 Berlin

Methanol decomposition and oxidation on Pd(111) and Al_2O_3 supported Pd nanoparticles were studied by Polarization-Modulation Infrared Reflection Absorption Spectroscopy (PM-IRAS) and X-ray Photoelectron Spectroscopy (XPS) from ultrahigh vacuum (UHV) to 15 mbar, at temperatures up to 450 K. Under high pressure these processes were also followed by gas chromatography (GC).

Methanol decomposition proceeds via dehydrogenation to CO and hydrogen or via methanolic C-O bond scission producing carbonaceous species (CH_x or C), which deactivate the catalyst. The kinetics of the evolution of these species and their preferred binding sites were analyzed. During methanol oxidation at mbar pressure surface species (CO, CH_xO) and products (CO_2, H_2O, CH_2O) were detected by PM-IRAS and GC, respectively, with XPS being utilized for pre- and post-reaction surface analysis.

O 18.7 Sa 12:15 TU EB301

Adsorbate induced surface stress for $(2 \times 1)O$ on Cu(110) measured with an STM — •Christian Bombis, Marina Moiseeva, and Harald Ibach — Institut für Schichten und Grenzflächen ISG 3, Forschungszentrum Jülich GmbH, 52425 Jülich

The formation of the so-called (2×1) oxygen stripe phase on Cu(110) is imaged in situ with an STM and simultaneously a quantitative determination of the induced surface stress is accomplished. For this intention the bending bar technique is utilized with the bending measured by the STM. Due to the anisotropy of the Cu(110) surface, two experiments, one with the $[1\bar{1}0]$-direction and a second with the [001]-direction along the bar have to be carried out for a quantitative analysis of the induced surface stress. From the two experiments we calculate the induced surface stress. We find that the difference $\Delta\tau$ of the surface stresses of the $(2 \times 1)O$ phase on Cu(110) and the clean Cu(110) surface is compressive for both directions, in accordance with the adsorption of oxygen on other surfaces. The stress depends significantly on the coverage. Orthogonal to the oxygen stripes ($[1\bar{1}0]$-direction) the data can be fitted to $\Delta\tau_{[1\bar{1}0]} \approx (-0,24 - 1,7 \times e^{-2,5\times\theta_s})Nm^{-1}$ and parallel to the stripes ([001]-direction) to $\Delta\tau_{[001]} \approx (-0,37 - 2,65 \times e^{-2,52\times\theta_s})Nm^{-1}$.

O 18.8 Sa 12:30 TU EB301

When Seeing is Not Believing: The case of O on Ag(111) — •Angelos Michaelides, Karsten Reuter, and Matthias Scheffler — Fritz-Haber-Institut, Faradayweg 4-6, D-14195, Berlin

A number of recent studies indicate that, under the oxygen rich conditions of oxidation catalysis, some transition metal catalysts are covered in thin oxide overlayers. Moreover, it has been suggested that such 'surface-oxide' layers are catalytically active, and that this role is not performed by the pure metal surfaces as was traditionally assumed. This contemporary picture can be traced back to Ag catalysis, where over 30 years ago it was suggested that the top layer of Ag(111) reconstructed to an epitaxial Ag_2O overlayer upon exposure to oxygen. Extensive experimental work, including scanning tunnelling microscopy studies in which the oxide was apparently imaged with atomic resolution [1], and density functional theory calculations [2,3] largely confirmed this interpretation. However, subsequent density functional theory results, presented here, augmented with thermodynamic calculations, indicate that previous conclusions are significantly incomplete and that the structure of this original surface-oxide must be reconsidered.

[1] C. Carlisle *et al.*, Phys. Rev. Lett. **84**, 3899 (2000).
[2] A. Michaelides, M.-L. Bocquet, P. Sautet, A. Alavi, and D.A. King, Chem. Phys. Lett. **367**, 344 (2003).
[3] W.X. Li, C. Stampfl, and M. Scheffler, Phys. Rev. Lett. **90**, 256102 (2003).

O 18.9 Sa 12:45 TU EB301

High pressure STM for atomic resolution studies of surface reactions under realistic conditions — •A. Männig, H. Hoster, H. Rauscher, and R. J. Behm — Abt. Oberflächenchemie und Katalyse, Universität Ulm, D-89096 Ulm

We describe the design and the performance of a high pressure video STM (HP-STM), which allows the atomically resolved analysis of adsorption processes and reactions in a pressure range from ultra high vacuum (10^{-10} mbar) up to atmospheric pressure (1000 mbar). The HP-STM was designed to investigate catalytic reactions under steady state conditions over the so called 'pressure gap'. The high pressure cell with a volume of about 2.5 liters is attached to a UHV preparation / analysis chamber. First atomic resolution results on the oxygen adsorption, e.g. on pure and modified Ru(0001) surfaces are presented.

O 19 Nanostrukturen II

Zeit: Samstag 10:45–13:00 Raum: TU EB420

O 19.1 Sa 10:45 TU EB420

First Principles Simulations of Ice Nucleation at Metal Surfaces — •Angelos Michaelides and Matthias Scheffler — Fritz-Haber-Institut, Faradayweg 4-6, D-14195, Berlin

Ice nucleation at solid surfaces is of relevance to countless scientific and technological processes. In particular the nucleation of ice nano-crystals on metal surfaces is often a key first step in cloud formation and corrosion [1]. Yet unfortunately this remains one of the most poorly understood natural phenomena; severely lacking in atomic level understanding. Here, we discuss detailed density functional theory studies aimed at putting our understanding of ice nucleation at metals on a much firmer footing. Specifically the properties of H_2O hexamers - the smallest 'building blocks' of ice - adsorbed on a number of close-packed transition metal surfaces have been examined. We find that the competing influences of substrate reactivity and hexamer-substrate epitaxial mismatch conspire to yield a rich variety of (novel) hexameric ice structures, some of which have been observed by recent scanning tunnelling microscopy experiments [2].

[1] H.R. Pruppacher and J.D. Klett, *Microphysics of Clouds and Precipitation*, (Kluwer, Dordrecht, 2003)
[2] K. Morgenstern, *et al.*, (To be published).

O 19.2 Sa 11:00 TU EB420

Theoretical analysis of quantum-size effects of Pb(100) films – the role of symmetry and implications for "elctronic growth" — •Dengke Yu and Matthias Scheffler — Fritz Haber Institut, Berlin

We performed detailed density-functional theory studies of lead films as function of thickness. In particular we will discuss in this talk the total energies, bandstructures, workfunctions, and surface relaxations. The results for Pb(100) exhibit noticeable oscillation with thickness which are ruled by quantum well states of different character. Their interplay gives rise to an interesting behavior that goes beyond the standard free-electron description of quantum-size effect. Consequences for "elctronic growth", i.e. for an enhanced stability of certain film thicknesses are discussed. We also compare our finding in Pb(100) with other lead surface orientations.

O 19.3 Sa 11:15 TU EB420

Ab initio study of vicinal surfaces: electronic confinement, magnetic wires and adsorbate interactions — •A.L. Klavsyuk[1], V.S. Stepanyuk[1], W. Hergert[2], and P. Bruno[1] — [1]Max-Planck-Institut für Mikrostrukturphysik, Weinberg 2, 06120 Halle, Germany — [2]Fachbereich Physik, Martin-Luther-Universität, Halle-Wittenberg, Friedemann-Bach-Platz 6, D-06099 Halle, Germany

Electronic structure of Cu(554) is studied using the density functional theory and the SKKR Green's function method. The band dispersion is presented. We compare our results for Cu(554) and Cu(111). The confinement of surface-state electrons near steps is discussed. The short and long-range electronic interactions between magnetic adatoms near steps and on the terrace are calculated. The effect of the electronic confinement on the adsorbate-adsorbate interaction is demonstrated. We study the influence of the decoration of step edges with Fe monoatomic rows on the behavior of surface-state electrons confined between regularly arranged steps. Confinement of unoccupied states in monoatomic chains is discussed. The atomic relaxations near steps on Cu(554) and Fe/Cu(554) are determined performing atomic-scale simulations with the ab initio based interatomic potentials.

O 19.4 Sa 11:30 TU EB420

Talbot effect on 2D colloidal crystals — •Manuel Gonçalves and Othmar Marti — University of Ulm - Dept. of Experimental Physics, Albert-Einstein-Allee 11, D-89069 Ulm, Germany

The Talbot effect occurs when a two-dimensional periodic structure is illuminated by a planar wavefront. The standard theoretical explanation of this effect is based on Fresnel diffraction and on the paraxial approximation. The assumptions used for the Fresnel diffraction and the paraxial approximation do not apply for structures with lattice constants comparable to the wavelength. Colloidal crystals of spheres with a diameter of few micrometers have been produced. The 2D crystals, under planar illumination of laser light, produce self-images. The distance between the crystal and the self-image depends on the symmetry of the lattice, on the wavelength and on the lattice constant. The experimental results have been compared with simulations based on the diffraction at an array of small apertures, using Rayleigh-Sommerfeld diffraction integrals without any approximations. The experimental data shows that colloidal crystals can be used as Talbot illuminators for distances of several tenths of μm.

O 19.5 Sa 11:45 TU EB420

Ioneninduzierte Defektstrukturen auf Oberflächen — •Thorsten Peters[1], Henning Lebius[2] und Marika Schleberger[1] — [1]Universität Duisburg-Essen, Fachbereich Physik, 45117 Essen — [2]CIRIL GANIL, rue Claude Bloch, BP 5133, 14070 Caen, Cedex 5, France

Hochgeladene Ionen bieten die Möglichkeit, nicht nur über ihre kinetische, sondern auch über ihre potentielle Energie sehr hohe Energiedichten auf Oberflächen zu erzielen (bis zu $10^{14} W/cm^2$) und dort bleibende Defekte zu verursachen. Wir haben untersucht, inwiefern das Einbringen hoher potentieller Energien auf Isolator- ($SrTiO_3$, TiO_2, SiO_2 und Al_2O_3) und Halbleiteroberflächen (Si) zu Defekten in der Oberflächenmorphologie führt. Bestrahlt wurden die Proben mit $^{36}S^{15+}$-, $^{208}Pb^{23+}$-, $^{129}Xe^{15+}$ und $^{129}Xe^{29+}$- Ionen mit Energien zwischen 270 keV und 410 MeV. Untersucht wurde jeweils die Oberflchenbeschaffenheit mittels Rasterkraftmikroskopie, sowohl an Luft als auch *in situ* direkt nach Präparation und Bestrahlung. Es konnte gezeigt werden, dass sich nur für bestimmte Projektil-Oberflächen-Kombinationen einzelne Defekte auf den Oberflächen in Form von hügelartigen Erhebungen ausbilden. Der quantitative Zusammenhang zwischen dem Ladungszustand der Projektile und der Anzahl, Form und Abmessungen der Defekte soll in zukünftigen Experimenten näher untersucht werden.

O 19.6 Sa 12:00 TU EB420

Grazing incidence Ar^+ ion induced creation and azimuth dependent evolution of nanogrooves on Cu(001) — •Herbert Wormeester, Michael Ovsyanko, Geogiana Stoian, and Bene Poelsema — MESA+ Institute for Nanotechnology, University of Twente, Enschede, The Netherlands

Grazing incidence 800 eV Ar^+ sputtering on a Cu(001) surface leads to the formation of nanogrooves in which only 3 layers are involved. With high resolution LEED we found that initially the distance between the nanogrooves L depends linearly on the sputter time: $L=L_0+St$. Both the initial average distance L_0 and a separation rate S depends on temperature. For sputtering along the [110] and [100] azimuths, a similar L_0 is found while a higher slope is observed along [100]. For increased sputter time, L clearly saturates for sputtering along the [100]. Annealing experiments of initially created grooves show a similar separation rate S, indicating that this behaviour does not originate from the ion sputtering. The temporal evolution and observed saturation of the distance between the nanogrooves along both the [100] and [110] azimuth will be discussed.

O 19.7 Sa 12:15 TU EB420

Pattern defects and their effect on roughness in ion bombardement induced ripple formation — •Henri Hansen, Alex Redinger, Georgiana Stoian, Sebastian Messlinger, and Thomas Michely — I.Physikalisches Institut. RWTH Aachen. 52056 Aachen

Pattern formation by 5 keV Ar^+ ion bombardement at an angle of 83° with respect to the surface normal was studied in the temperature range from 250 K to 720 K.

The nature and density of defects in the ensuing ripple patterns was quantitatively analysed and correlated with the surface morphological evolution. For fixed fluence of 20 MLE a sudden increase in normalized defect density above 450 K is attributed to the onset of step edge diffusion, which tends to align ripple crests along $\langle 110 \rangle$-direction, whereas ion beam forces the ripple crests to orient along the $\langle \bar{1}\bar{1}2 \rangle$-direction. Defects in the pattern are spots of high local roughness and thus contribute significantly to the increase of pattern roughness above 450 K.

O 19.8 Sa 12:30 TU EB420

Multicomponent nanowires formed by nano shadow masks based on delamination — •Rainer Adelung, Mady Elbahri, Shiva Kumar Rudra, Abhijit Biswas, and Rainer Kunz — Lehrstuhl für Materialverbunde, Technische Fakultät der Universität Kiel, Kaiserstrasse 2, 24143 Kiel, Germany

Simple ways to realize aligned nanostructures are still of interest, as conventional sub 100nm photolithography is not handy with respect to different materials or everyday lab use. Recently, we could show that directed fracture in thin films can be used to fabricate various nanowire structures [1]. But limits of the approach are for example the fabrication nanowires of two different materials in a distance of a few nanometer. Many deficiency like this can be overcome, by being more destructive and going beyond thin film fracture. Adding delamination at the crack sides produces nanoscale shadow masks that create a workspace, allowing to deposit material for multicomponent nanowires, or removing material to trench nanochannels. Various examples of nanostructures will be shown and their application for e.g. sensors or as templates for biological samples will be discussed.

[1] R. Adelung et al., Nature Materials 3, 375, (2004)

O 19.9 Sa 12:45 TU EB420

STM-based nanolithography of diamond-like carbon films — •Thomas Mühl — IFW Dresden, Helmholtzstr. 20, D-01069 Dresden

The spatially localized emission current of a scanning tunneling microscope tip leads to a local graphitization of diamond-like carbon thin films. Using this technique, lines and dots smaller than 10 nm in size can be written. Time resolved studies of the nanostructure growth under the STM tip will be presented, as well as time resolved graphitization of macroscopic areas of metal-contacted diamond-like carbon films induced by high current densities. Due to the widely different properties of diamond-like and graphite-like carbon, there are a lot of possible applications for such graphite nanostructures on diamond-like films. In addition, metal nanowires and nanodots can be produced by shadow (shallow angle) deposition on these carbon nanostructures.

O 20 Organische Dünnschichten II

Zeit: Samstag 10:45–13:00 Raum: TU EB202

O 20.1 Sa 10:45 TU EB202

Interface Formation of Phthalocyanines with Hydrogen Passivated Si(111) — •Mihaela Gorgoi and Dietrich R.T. Zahn — Institut für Physik, Technische Universität Chemnitz, D-09107 Chemnitz, Deutschland

Hybrid devices such as organic light emitting diodes, solar cells or thin film transistors, based on phthalocyanine (Pcs) materials and silicon receive special attention nowadays. Therefore the knowledge of the Pc/Si interface electronic properties is required. This work studies the interface formation between the organic semiconductors, namely copper phthalocyanine ($CuPc$) and perfluorinated copper phthalocyanines (F_4CuPc,$F_{16}CuPc$), and hydrogen passivated Si(111) using photoemission and inverse photoemission spectroscopy. With these techniques the energy level alignment of the highest occupied and lowest unoccupied molecular orbitals (HOMO and LUMO) with the valence band maximum (VBM) and the conduction band minimum (CBM) of Si are determined. The HOMO and LUMO for the three materials reveal dissimilar trends in the direction of energy shifts as a function of Pcs thickness. While for $CuPc$ the shift is towards higher binding energy with increasing film thickness, for $F_{16}CuPc$ both HOMO and LUMO are shifting towards lower binding energy. The energy shifts are proposed to originate from changes in molecular orientation and the direction of the shifts to arise from the degree of fluorination.

O 20.2 Sa 11:00 TU EB202

A simple model system for silicon/organic interfaces: Si(111)-CH_3 — •Ralf Hunger[1], Rainer Fritsche[1], Bengt Jaeckel[1], Taek Lim[1], Lauren J. Webb[2], Nathan S. Lewis[2], and Wolfram Jaegermann[1] — [1]Darmstadt University of Technology, Surface Science Division, Department of Materials Science, Petersenstr. 23, 64287 Darmstadt — [2]California Institute of Technology, Division of Chemistry and Chemical Engineering, Pasadena, CA 91125

Conceptually, methyl-terminated silicon (111), Si(111)-CH_3, is one of the simplest possible silicon-organic interface structures. The Si(111)-CH_3 structure may serve as a reference system for more complex silicon/organic interfaces. It has the inherent advantage that the silicon surface is chemically and electronically passivated by the methyl-termination.

Employing high resolution synchrotron and ultraviolet photoelectron spectroscopy and low energy electron diffraction, we have analyzed the properties of Si(111)-CH_3 surfaces that were prepared in a wet chemical two-step chlorination/alkylation process. The investigations show that well-defined surfaces with high chemical stability and near ideal electronic passivation could be obtained. A (1x1) surface structure, a well-defined carbon 1s core level emission, and in the Si2p line a distinct surface core level shift of the carbon-bonded surface silicon atoms are found. According to these results, methyl-terminated Si(111) appears as suitable template for the preparation of silicon/organic hybrid device structures.

O 20.3 Sa 11:15 TU EB202

Growth of Alkylsiloxane monolayers on patterned silicon substrates — •Thorsten Balgar, Nils Hartmann, Steffen Franzka, and Eckart Hasselbrink — Universität Duisburg-Essen, Campus Essen, Fachbereich Chemie, Universitätsstr. 5, 45141 Essen

We present a laser direct writing technique for patterning of silicon substrates on the submicrometer scale. The patterned substrates are used for selective coating in a millimolar solution of Octadecyltrichlorosilane (OTS) [1]. The OTS molecules build up an alkylsiloxane monolayer via self-assembling in well defined surface areas [2][3]. Three different approaches were developed to create structured organic monolayers with lateral features ranging from several microns down to 120 nm.

[1] Th. Balgar, R. Bautista, N. Hartmann and E. Hasselbrink, Surf. Sci. 532-535 (2003) 963

[2] N. Hartmann, Th. Balgar, R. Bautista, S. Franzka and E. Hasselbrink, Proc. SPIE 5223 (2003) 9, Physical Chemistry of Interfaces and Nanomaterials II

[3] Th. Balgar, S. Franzka, N. Hartmann and E. Hasselbrink, Langmuir 20 (2004) 3525

O 20.4 Sa 11:30 TU EB202

Submicron chemical patterning of silicon substrates by laser direct writing: A simple photothermochemical model — •Nils Hartmann, Thorsten Balgar, Steffen Franzka, and Eckart Hasselbrink — Universität Duisburg-Essen, Campus Essen, Fachbereich Chemie, Universitätsstr. 5, 45141 Essen

Recently laser direct writing has been shown to provide a versatile means for the preparation of laterally structured alkylsiloxane monolayers on silicon substrates [1,2]. Respective procedures either are based on the preparation of suitable templates or on direct patterning of coated substrates. A common feature of all these procedures is the capability to create patterns with lateral dimensions which are significantly below the diffraction-limited laser spot diameter. At a $1/e^2$ laser spot diameter of 2.5 microns, for example, well-confined lines with a width down to 120 nanometers have been prepared. Here we present a simple model, which considers the laser-assisted local annealing of the substrate and the strongly temperature dependent kinetics of the initiated chemical processes. The model allows to reproduce the experimentally observed dependence of the line width on the incident laser power and the writing speed and provides a simple explanation for the unexpectedly high resolution capability of the patterning technique.

[1] Th. Balgar, S. Franzka, N. Hartmann and E. Hasselbrink, Langmuir 2004, 20, 3525.

[2] N. Hartmann, Th. Balgar, R. Bautista, D. Dahlhaus, S. Franzka and E. Hasselbrink, Proc. SPIE 2003, 5223, 9.

O 20.5 Sa 11:45 TU EB202

Engineering of GaAs (100) surface with 4'-substituted aromatic self-assembled monolayers — •Michael Zharnikov[1], Andrey Shaporenko[1], Adlkofer Klaus[2], Avi Ulman[3], Michael Grunze[1], and Motomu Tanaka[2] — [1]Angewandte Physikalische Chemie, Universität Heidelberg, Im Neuenheimer Feld 253, D-69120 Heidelberg, Germany — [2]Lehrstuhl für Biophysik E22, Technische Universität München, James-Franck-Strasse, D-85748, Garching, Germany — [3]Department of Chemical Engineering, Polytechnic University, Brooklyn 11201, New York, USA

High-resolution x-ray photoelectron spectroscopy and near edge x-ray absorption fine structure spectroscopy were applied to characterize GaAs (100) surface engineered by self-assembled monolayers (SAMs) of 4'-substituted aromatic molecules: 4'-methyl-4-mercaptobiphenyl (CH_3-BPT) and 4'-hydroxy-4-mercaptobiphenyl (OH-BPT). These molecules were found to form ordered and densely packed SAMs on GaAs, which were able to protect the substrate from degradation under ambient conditions. The molecular attachment in the SAMs occurs over As-thiolate bond while the intact aromatic backbones have an upright orientation with average tilt angles of 31.0° and 37.2° for CH_3-BPT and OH-BPT films, respectively. The difference in the tilt angle is attributed to a higher (by 7-10%) packing density of the former SAM, suggesting that the character of 4'-substitution affects the SAM quality in the case of GaAs substrate.

O 20.6 Sa 12:00 TU EB202

In-Situ study of the first stages of F16CuPc growth on SiO2 — •Dimas Garcia de Oteyza [1], Esther Barrena[1], Oriol Ossó[2], Stefan Sellner[1], and Helmut Dosch[1,3] — [1]Max Planck Institut für Metallforschung, Stuttgart — [2]Institut de Ciència de Materials de Barcelona, CSIC — [3]Institut für Theoretische und Angewandte Physik, Universität Stuttgart

We have studied the first stages of F16CuPc growth on SiO2 by AFM and in-situ X-ray measurements. For thicker films they form a well ordered layered structure, with layers of virtually upright standing molecules and a spacing of 14.3 Å. At low coverage, both techniques coincide in the observation of striking structural changes on the first layers. The layer heights found for the first, second and third layers are 12.5 Å, 15 Å and 21 Å respectively. Besides, both the size and the aspect ratio of the elongated crystallites increase in the subsequent layers. From the X-ray data an additional layer at the interface with the SiO2 is obtained. This layer has a saturation thickness of around 6.5 Å and it shows a periodicity in the surface plane of 15 Å, which corresponds to the molecular size along one of its sides. The electronic density of this interfacial layer is about half of the electronic density of the thicker films. The growth behaviour of the first 3 layers has been characterized by both techniques. AFM and in-situ X-ray diffraction show a very good agreement.

O 20.7 Sa 12:15 TU EB202

Strongly Enhanced Thermal Stability of Crystalline Organic Thin Films Induced by Aluminum Oxide Capping Layers — •S. Sellner[1,2], A. Gerlach[3], F. Schreiber[3], M. Kelsch[1], N. Kasper[1], H. Dosch[1,2], S. Meyer[4], J. Pflaum[4], M. Fischer[5], and B. Gompf[5] — [1]Max-Planck-Institut für Metallforschung, Stuttgart, Germany — [2]Institut für Theoretische und Angewandte Physik, Universität Stuttgart, Germany — [3]Physical and Theoretical Chemistry Laboratory, Oxford University, UK — [4]III. Physikalisches Institut, Universität Stuttgart, Germany — [5]I. Physikalisches Institut, Universität Stuttgart, Germany

We show that the thermal stability of organic semiconductor thin films can be strongly enhanced by capping with an aluminum oxide layer. By thermal desorption spectroscopy and *in-situ* X-ray diffraction we demonstrat that organic films do not only stay on the substrate, but even remain crystalline up to 270°C above their desorption point for uncapped films [1]. Different parameters contributing to the stability enhancement and eventual breakdown of the crystalline order of the organic film at elevated temperatures were identified. We argue that this very efficient enhancement of the thermal stability compared to uncapped and also to metal-capped organic layers is related to the low mobility of aluminum oxide and the structurally well-defined as-grown interfaces exhibiting limited interdiffusion. Possible mechanisms for the eventual breakdown at high temperatures will be discussed.

[1] Sellner et al., Adv. Mat. 16 (2004), p. 1750

O 20.8 Sa 12:30 TU EB202

Transport in capped organic thin film transistors at elevated temperatures — •S. Meyer[1], J. Wrachtrup[1], J. Pflaum[1], S. Sellner[2], G. Ulbricht[2], A. Gerlach[3], F. Schreiber[3], M. Fischer[4], and B. Gompf[4] — [1]III. Physikalisches Institut, Universität Stuttgart — [2]Max-Planck-Institut für Metallforschung, Stuttgart — [3]Physical and Theoretical Chemistry Laboratory, Oxford University, UK — [4]I. Physikalisches Institut, Universität Stuttgart

The thermal stability of the organic semiconducting layer is of crucial importance for the device performance in organic electronics. To address this problem we have performed comparative studies on organic thin film transistors (OTFTs) utilizing pentacene thin films with and without capping layer. The latter is realized by a 50nm thick sputter layer of aluminum oxide. On pentacene TFTs a field-effect is demonstrated up to temperatures of 250°C which is about 170°C above the desorption point of uncapped pentacene films on SiO_2. From the TFTs characteristics a complex behavior of the temperature dependent hole mobility and threshold voltage can be deduced, indicating that the device operation at these elevated temperatures is predominantly limited by the transistor structure, i.e. metal-diffusion at the contacts, and not by the organic material. Detailed studies by thermal desorption spectroscopy and X-ray diffraction on capped pentacene and diindenoperylene thin films show that the organic layer remains crystalline far above the breakdown temperature of the TFTs as a function of heating rate, thickness and stoichiometry of the AlOx. capping layer [1].

[1] Sellner et al., Adv. Mat. **16** (2004) 1750

O 20.9 Sa 12:45 TU EB202

Post-functionalization of self-assembled alkylsiloxane monolayers for gold colloid adsorption — •Daniel Dahlhaus, Steffen Franzka, Nils Hartmann, and Eckart Hasselbrink — Universität Duisburg-Essen, Campus Essen, Fachbereich Chemie, Universitätsstr. 5, 45141 Essen

Self-assembled monolayers (SAMs) are widely recognized for their use in a range of technological applications, including optoelectronic devices and biological sensors. Depending on the detailed application SAMs with varying terminal groups are required. Of particular interest for the adsorption of gold nanoparticles are SAMs exposing amino and thiol groups. In our experiments we first prepared octadecylsiloxane (ODS) monolayers by immersion of freshly cleaned silicon oxide substrates in a millimolar solution of octadecyltrichlorosilane [1]. For characterization contact angle measurements and atomic force microscopy were used. A chemical functionalization of the ODS monolayers has then been achieved by free-radical bromination using visible light. Subsequently, the bromine groups can be replaced by other functional groups such as amines and thiols [2]. Preliminary results indicate the adsorption of gold colloids on these functionalized ODS monolayers.

[1] N. Hartmann, T. Balgar, R. Bautista, E. Hasselbrink, Surf. Sci., 532-535 (2003) 963.

[2] N. Balachander, C.N. Sukenik, Langmuir, 6 (1990) 1621.

O 21 Elektronische Struktur II

Zeit: Samstag 10:45–13:00 Raum: TU EB107

O 21.1 Sa 10:45 TU EB107

Contribution of electron-magnon scattering to the lifetimes of lanthanide-metal surface states studied by scanning tunneling spectroscopy — •Daniel Wegner, Andreas Bauer, and Günter Kaindl — Institut für Experimentalphysik, Freie Universität Berlin, Arnimallee 14, D-14195 Berlin-Dahlem

While electron dynamics at surfaces of noble metals is well understood by now, we still have a rather poor knowledge of electron dynamics at transition-metal surfaces, in particular for magnetic systems where electron-magnon scattering has to be taken into account. A better understanding would be of particular importance for spin electronics.

We have systematically studied lifetime broadening of exchange-split (0001)-surface states for all trivalent lanthanide metals by low-temperature scanning tunneling spectroscopy (STS) at 10 K. Since those states are highly spin-polarized, they allow for a separate analysis of majority (spin-up) and minority (spin-down) states. The results give evidence for strong electron-magnon scattering of the minority states, while for the majority states, electron-electron and electron-phonon scattering seem to be dominant.

O 21.2 Sa 11:00 TU EB107

Surface state scattering by atomic–scale clusters on noble metals — •S. Lounis, Ph. Mavropoulos, S. Blügel, and P. H. Dederichs — Institut für Festkörperforschung, Forschungszentrum Jülich, D-52425 Jülich, Germany

When surface state electrons scatter at perturbations, such as magnetic or nonmagnetic adatoms or clusters on surfaces, an electronic resonance can develop at the bottom of the surface state band for both spin channels. In the case of adatoms, these states have been found very recently in scanning tunneling spectroscopy experiments of the group of R. Berndt (University of Kiel). Motivated by these experiments, we carried out a systematic theoretical investigation of the electronic structure of these surface states in the presence of magnetic and non-magnetic 3d atoms on Cu(111) and Ag(111) surfaces. The calculations are performed using the full-potential scalar–relativistic Korringa-Kohn-Rostoker Green–function method extended to treat noncollinear magnetic nanostructures on surfaces.

We extended this investigation to dimers and trimers, and investigate how the resonance state depends on cluster size and complexity of the magnetic configuration.

–Work supported by the DFG Schwerpunktsprogramm “Clusters on Surfaces” (SPP 1153).

O 21.3 Sa 11:15 TU EB107

Spin Filtering at a Ferromagnetic-Paramagnetic Interface Observed by Spin-Polarized Standing Waves — •Jörg Schäfer[1], Markus Hoinkis[1], Eli Rotenberg[2], and Ralph Claessen[1] — [1]Institut für Physik, Universität Augsburg — [2]Advanced Light Source, Berkeley, USA

For thin Fe films the spin-selective transmission of electrons near the Fermi level across a ferromagnetic-paramagnetic interface is investigated. The majority and minority Fermi surface sheets of the Fe film are probed for standing wave formation by angle-resolved photoemission. Knowledge of the exchange-split Fermi surface from density functional calculations allows straightforward assignment of the spin character. Reflection at the interface is expected to lead to quantum well states. However, using a W(110) substrate, these are observed only for majority states, which is attributed to a strongly spin-dependent transmission through the Fe/W interface. This can be traced back to the Fermi surface topologies of the connecting solids, and the choice of the Fe/W-interface for this reason produces a particularly strong effect.

O 21.4 Sa 11:30 TU EB107

Role of the spin in quasiparticle interference — •Ph. Hofmann[1], J. I. Pascual[2,3], G. Bihlmayer[4], Yu. M. Koroteev[5,6], H.-P. Rust[3], G. Ceballos[3], M. Hansmann[3], K. Horn[3], E.V. Chulkov[5], S. Blügel[4], and P.M. Echenique[5] — [1]Institute for Storage Ring Facilities, University of Aarhus, Denmark — [2]Institut für Experimentalphysik, Freie Universität Berlin — [3]Fritz-Haber-Institut der MPG, Berlin — [4]Institut für Festkörperforschung, Forschungszentrum Jülich — [5]Donostia International Physics Center (DIPC), Basque Country, Spain — [6]Institute of Strength Physics and Materials Science, Tomsk, Russia

Defects on metal surfaces are screened by the surrounding electron gas, leading to the formation of standing electron waves or, more correctly, quasiparticle interference patterns. These patterns can be observed by scanning tunneling microscopy, either for a very small tunneling voltage or in conductance images. A Fourier transformation of conductance images can therefore give valuable information about the electronic structure and Fermi surface of quasi two-dimensional systems. Here we show that even in non-magnetic systems the spin of the quasiparticles can have a profound effect on the interference patterns. On Bi(110), where the surface state bands are not spin-degenerate, the patterns are not related to the dispersion of the electronic states in a simple way. In fact, the features which are expected for the spin-independent situation are absent and the observed interference patterns can only be interpreted by taking spin-conserving scattering events into account.

O 21.5 Sa 11:45 TU EB107

k-dependent electronic structure of NiMnSb single-crystal surfaces — •Juliet Correa, Christian Eibl, Jürgen Braun, Georgi Rangelov, and Markus Donath — Physikalisches Institut, Westfälische Wilhelms-Universität Münster, Wilhelm-Klemm-Str. 10, 48149 Münster

The half-Heusler alloy NiMnSb is believed to be a half-metallic ferromagnet with 100% spin polarization at the Fermi level. This property makes it an interesting material for spintronic applications. Detailed understanding of the band structure of NiMnSb, not only in the bulk but also at surfaces and interfaces, is essential to developing spintronic applications. To date, however, the only data available are of the density of states, specifically from polycrystalline samples. We present angle-resolved photoemission results from a carefully prepared and surface-characterized NiMnSb(100) single crystal. We observed clear energy dispersion of occupied bulk states as a function of the wave vector parallel to the surface. Our results are discussed along with band structure calculations.

O 21.6 Sa 12:00 TU EB107

Electronic structure of NiO thin films on Ag(001) — •Markus Däne[1], Diemo Ködderitzsch[1], Wolfram Hergert[1], Arthur Ernst[2], Walter M. Temmerman[3], Zdzislawa Szotek[3], Christian Hagendorf[1], Henning Neddermeyer[1], and Wolf Widdra[1] — [1]Fachbereich Physik, Martin Luther Universität Halle-Wittenberg, Friedemann-Bach-Platz 6, 06108 Halle, Germany — [2]Max Planck Institute of Microstructure Physics, 06120 Halle, Germany — [3]Daresbury Laboratory, Daresbury, Warrington WA4 4AD, United Kingdom

In this work we apply the self-interaction corrected LSDA formalism, as implemented in the TB-LMTO-ASA method, to study the electronic and magnetic structure of thin transition metal oxide (TMO) films on metallic substrates. Here the properties of NiO thin films (up to 5 layers) on the Ag(001) surface are investigated. Relaxations at the Ag oxide interface are taken into account. The gap formation of the oxide thin film depending on film thickness and magnetic structure is studied. The influence of the metallic substrate is revealed by comparison with freestanding NiO films. The results can be compared to experimental data obtained by scanning tunneling microscopy and spectroscopy (STM/STS) for one to three layer thick NiO islands on Ag(001). The variation of the normalized differential conductance is discussed with respect to the calculated local density of states.

O 21.7 Sa 12:15 TU EB107

The Si(111)-(7×7) surface: a correlated electronic Hubbard system? — •Richard Schillinger, C. Bromberger, H. J. Jänsch, H. Kleine, O. Kühlert, C. Weindel, and D. Fick — Philipps-Universität, Fachbereich Physik and Zentrum für Materialwissenschaften 35032 Marburg, Germany

Li adsorption at extremely low coverages (10^{-3} ML and below) on the metallic Si(111)(7×7) surface has been studied by β-NMR experiments (measurement of T_1-times). Instead of increasing linearly with sample temperature, as expected for a metallic system, the relaxation rates $\alpha = 1/T_1$ are quite surprisingly constant in between 50 K and 300 K and rise considerably above. This temperature dependence points to an extremely localized and thus narrow band (width below 5 meV) which pins the Fermi energy. It is energetically located within an approximately 600 meV wide gap in between a lower filled and an upper empty Hubbard band. Due to its extremely narrow width it cannot be detected in photo emission experiments. In Dynamic Mean Field Theory (DMFT) based on Hubbard Hamiltonians [1,2] this kind of density of states is typical for correlated electron systems being close to a Hubbard metal-insulator transition.

[1] G. Kotliar and G. Vollard, Physics Today, March 2004

[2] Pou et al., Phys. Rev. Lett. **63** 4309 (2000)

O 21.8 Sa 12:30 TU EB107

Continuous tuning of electronic correlations by alkali adsorption on layered 1*T*-TaS$_2$ — •Kai Rossnagel[1,2], Eli Rotenberg[2], H. Koh[2], N.V. Smith[2], and L. Kipp[1] — [1]Institut für Experimentelle und Angewandte Physik, Universität Kiel, D–24098 Kiel, Germany — [2]Advanced Light Source, Lawrence Berkeley National Laboratory, Berkeley, CA 94720, USA

Angle-resolved photoemission spectroscopy shows that a Mott-Hubbard type metal-insulator transition occurs at the Rb adsorbed surface of the layered charge-density-wave compound 1*T*-TaS$_2$. The transition is driven by adsorption induced modifications of the charge-density wave and of the interlayer coupling, leading to an increase of the on-site Coulomb correlation energy and a narrowing of the Ta 5*d* band perpendicular to the layers, respectively. The continuous rearrangement of spectral weight is measured live during the deposition process.

The experiments were carried out at the *Electronic Structure Factory* at beamline 7 of the Advanced Light Source in Berkeley. Work at the University of Kiel is supported by DFG Forschergruppe FOR 353. K.R. gratefully acknowledges support by the Alexander von Humboldt Foundation.

O 21.9 Sa 12:45 TU EB107

Surface-state localization at adatoms — J. Kröger, L. Limot, E. Pehlke, and •R. Berndt — Institut für Experimentelle und Angewandte Physik, Institut für Theoretische und Astrophysik, Christian-Albrechts-Universität zu Kiel, D-24098 Kiel

Low-temperature scanning tunneling spectroscopy of magnetic and non-magnetic metal atoms on Ag(111) and on Cu(111) surfaces reveals the existence of a common electronic resonance at an energy below the binding energies of the surface states. Using an extended Newns-Anderson model, we assign this resonance to an adsorbate-induced bound state, split off from the bottom of the surface-state band, and broadened by the interaction with bulk states. A lineshape analysis of the bound state indicates that native adatoms decrease the surface-state lifetime, while a cobalt adatom causes no significant change.

O 22 Rastersondentechniken I

Zeit: Samstag 10:45–13:00 Raum: TU EB407

O 22.1 Sa 10:45 TU EB407

Long-range energy dissipation in non-contact AFM — •Domenique Weiner[1,2], André Schirmeisen[1,2], and Harald Fuchs[1,2] — [1]Physikalisches Institut, Westfälische Wilhelms-Universität Münster, Wilhelm-Klemm-Str. 10, 48149 Münster — [2]CeNTech, Center for Nanotechnology, Gievenbecker Weg 11, 48149 Münster

The dissipated energy between tip and sample of an AFM driven in the non-contact mode is the subject of current research. The long-range dissipation and its underlying mechanisms are not well understood [1]. The dependence of the dissipation on the oscillation amplitude and the temperature can give a better insight in this effect. We are using a UHV-VT-AFM (Omicron), which enables us to get the frequency shift and the damping signal as a function of the distance between tip and sample. From these values it is possible to calculate the conservative forces and the dissipation. We apply a voltage between tip and sample to measure the electrical dissipation. We are using commercial silicon cantilevers covered with a PtIr-layer, which is about 30 nm thick to guarantee a metallic contact. The investigated Au (111) surface is sputtered and annealed under ultra-high vacuum conditions. This single crystal shows a dissipation signal, which roughly depends on the distance by the power law 1/zn where n=3.5 at RT, which is comparable to other investigations [2,3]. In particular we focus on the temperature dependence of the non-contact friction in order to understand the origin of the dissipation, which might be linked to van der Waals friction [1] or electrical dissipation [4].[1] Volokitin et al., PRL 91, 2003, [2] Gotsmann et al., PRL 86, 2001, [3] Stipe et al., PRL 87, 2001, [4] Denk et al., APL 59, 1991

O 22.2 Sa 11:00 TU EB407

Force-Distance studies by Atomic Force Microscopy using a Double Tuning Fork Sensor at Low Temperature — •Markus Heyde, Maria Kulawik, Hans-Peter Rust, and Hans-Joachim Freund — Fritz-Haber-Institute of the Max-Planck-Society, Faradayweg 4-6, D-14195 Berlin, Germany

A double quartz tuning fork sensor for low temperature ultrahigh vacuum atomic force and scanning tunneling microscopy [1] has been developed. The noise performance of the force sensor as well as the tip preperation is important for optimizing the resolution in the non-contact mode of an atomic force microscope. The features of the new sensor are discussed and compared to previous designs. A set of frequency shift versus distance curves measured at low temperature will be presented. Force and energy versus distance has been calculated from frequency versus distance data [2] . Recent measurements performed on Ag(100) and a thin Al$_2$O$_3$ film on NiAl(110) will be shown.

[1] M. Heyde *et al.*, Rev. Sci. Instrum. 75, 2446 (2004).

[2] J. E. Sader and S. P. Jarvis, Appl. Phys. Lett., 84, 1801 (2004).

O 22.3 Sa 11:15 TU EB407

Thermal atomic force microscopy in vacuum — •Martin Hinz[1], Bernd Gotsmann[2], Mark A. Lantz[2], Urs Dürig[2], Johannes Windeln[2], and Othmar Marti[1] — [1]Department of Experimental Physics, University of Ulm, 89069 Ulm, Germany — [2]IBM Research GmbH, Säumerstrasse 4, 8803 Rüschlikon,Switzerland

In conventional atomic force microscopy (AFM) studies a sharp tip located on the end of a cantilever beam is used to image the topography of a sample surface. Variations on this technique have also been developed to probe a variety of other surface properties on the nm-scale, such as mechanical, tribological , magnetic and electrical properties. In this study, purpose-designed heatable cantilevers are used to perform heat transfer measurements of point contacts. An AFM is operated at high vacuum (10^{-6} mbar) where the heat conduction through air is suppressed and the heat flow from the tip to the sample can be measured. The corresponding thermal tip sample contact resistance is measured on different samples such as silicon and thin polymer films. Finally, thermal imaging of a two phase sample system will be presented.

O 22.4 Sa 11:30 TU EB407

Capacitive force detection in dynamic mode Atomic Force Microscopy — •A.-D. Müller, F. Müller, T.D. Long, and M. Hietschold — Chemnitz University of Technology, Institute of Physics, Solid Surfaces Analysis Group, 09107 Chemnitz

Non-optical methods for the deflection detection of a cantilever beam have many advantages concerning the adjustion and applicability to multi-cantilever applications. The capacitive detection based on a second electrode placed behind the cantilever beam has never achieved to get in use, because its sensitivity was estimated to be too low. This contribution restarts the considerations about the capacitive detection of the cantilever deflection for dynamic mode applications with stiff cantilever beams. Distance dependent curves of the force derivative detected capacitively allow to estimate and compare the method with other detection mechanisms.

O 22.5 Sa 11:45 TU EB407

Scanning Ion Conductance Microscopy — •Tilman E. Schäffer, Pia Heidenreich, Matthias Böcker und Harald Fuchs — Physikalisches Institut and Center for Nanotechnology (CeNTech), Universität Münster, Gievenbecker Weg 11, 48149 Münster

We built a scanning ion conductance microscope (SICM) with shear-force distance control. In a SICM, a tapered micropipette with an opening diameter of less than 100 nm is filled with electrolyte and acts as local ion conductance probe while being scanned over a sample surface. To obtain a meaningful interpretation of the measured ion conductance, we keep the pipette-sample distance constant by implementing a complementary shear-force distance control that works under liquid. The vibration amplitude of the pipette we detect optically with the help of a laser beam that we focus onto the thin end of the pipette. In this way, we simultaneously measure two complementary surface properties: topography and ion conductance. We imaged different samples such as CDs, nanogrids and cells, all in liquid. The imaging force was low enough to allow damage-free imaging, even on soft samples.

O 22.6 Sa 12:00 TU EB407

Quantitative Measurement of Tip-Sample Forces by Dynamic Force Microscopy in Ambient Conditions — •Hendrik Hölscher[1], Jan-Erik Schmutz[1], Boris Anzcykowski[2], Marcus Schäfer[1], and Harald Fuchs[1] — [1]Center for NanoTechnology (CeNTech), University of Münster, Gievenbecker Weg 11, 48149 Münster — [2]nanoAnalytics GmbH, Gievenbecker Weg 11, 48149 Münster

Dynamic force spectroscopy (DFS) applied in vacuum is a powerful tool to measure conservative as well as dissipative tip-sample interactions with atomic resolution. In contrast to the often applied measurement of force-vs-distance curves measured in contact-mode dynamic force spectroscopy has the advantage that the full range of tip-sample forces can be continuously detected without hysteresis effects caused by the so-called jump-to-contact of the tip towards the sample surface. Despite of the great capabilities of quantitative dynamic force spectroscopy this technique has not been applied in air or liquids up to now. Nonetheless, a recently introduced algorithm [1] now allows the reconstruction of the tip-sample interactions using the so-called constant excitation mode (CE-mode). Since this mode works in air and liquids dynamic force spectroscopy can also be applied in ambient conditions. We present first experimental applications of this approach for different types of samples.

[1] H. Hölscher, B. Gotsmann, A. Schirmeisen, Phys. Rev. B **68**, 153401 (2003)

O 22.7 Sa 12:15 TU EB407

Cantilever Sensors for Biomolecular Recognition — •Martin Bammerlin and Urs Hubler — Concentris GmbH, Davidsbodenstrasse 63, CH-4056 Basel, Switzerland

Chemically functionalized cantilevers hold a big promise for a multitude of novel sensor applications. We have designed a new cantilever sensor platform taking advantage of the high detection sensitivity for chemical substances and label-free recognition of biomolecules such as DNA or proteins. The "Cantisens Research"system features an integrated two-stage temperature control and a programmable liquid handling system for experiments under stable and controlled conditions. Up to eight surface interaction signals can be measured simultaneously, allowing multiplexed assays and the use of reference channels to cancel out unspecific bindings. In the first part, an overview of the most prominent aspects of the instument design and features will be given. The second part will focus on recent measurement results in the field of biomolecular recognition.

O 22.8 Sa 12:30 TU EB407

FM demodulated Kelvin probe force microscopy for surface photovoltage tracking — •Ulrich Zerweck, Christian Loppacher, Sebastian Teich, Tobias Otto, Elke Beyreuther, Stefan Grafström, and Lukas M. Eng — Institut für Angewandte Photophysik, Technische Universität Dresden, D-01062 Dresden

The surface photovoltage (SPV) of a structured semiconductor surface is deduced via detection of the contact potential difference measured with Kelvin probe force microscopy (KPFM). The experimental setup is based on a quantitative KPFM method complemented with modulated laser illumination in order to measure SPV. In contrast to similar studies based on scanning tunnelling microscopy, KPFM offers the advantage that there is virtually no DC field between tip and sample and, therefore, the SPV is not affected by the presence of the tip.

O 22.9 Sa 12:45 TU EB407

Measurement of the near-field distribution of a wave guide with sub-wavelength aperture on a macroscopic scale — •Oliver Schimek, Georgios Ctistis, Jens J. Paggel, and Paul Fumagalli — Institut für Experimentalphysik, Freie Universität Berlin, 14195 Berlin

The optical near-field is a very useful and interesting experimental tool, which in scalar diffraction theory is well known and widely understood. Scalar diffraction theory however does not include polarization. Very little is known about polarization in the near-field. Also no direct measurement of the field distribution has been presented yet. On the other hand, theoreticians presented a large amount of calculations describing the near-field for a better understanding of the gained experimental results in scanning near-field optical microscopy. We present here our results on the measurements of the near-field of microwaves directed through a wave guide and a sub-wavelength aperture. We used a standard klystron with a wavelength of 3.3 cm and an aluminium tube as wave guide as well as differently shaped apertures. We measured the field intensity in two polarisation directions, its dependence from aperture size, and distance from the aperture. These results are compared with theoretical predictions.

O 23 Hauptvortrag Echenique

Zeit: Samstag 14:00–14:45 Raum: TU EB301

Hauptvortrag

O 23.1 Sa 14:00 TU EB301

Electron dynamics at surfaces — •Pedro M. Echenique — Departamento de Física de Materiales UPV/EHU, and "Unidad Física de Materiales"(CSIC-UPV/EHU), Apartado 1072, 20080 San Sebastián, Spain; Donostia Interacional Physics Center, Po Manuel de Lardizabal 3, 20018 San Sebastián, Spain

An overview of recent theoretial and experimental investigations of electron dynamics in surface and image-potential states at metal surfaces as well as some results for bulk materials are presented. The relevance of a quasiparticle concept in this relation is disscussed. Some detailes of our theoretical threatment of a many-body theory beyond a free-electron description is reported. Thus, the different chanells for quasipartice decay such as the electronic intra- and inter-band transitions and the electron-phonon scattering are addressed.

O 24 Teilchen und Cluster I

Zeit: Samstag 15:00–17:00 Raum: TU EB301

O 24.1 Sa 15:00 TU EB301

Depostion magischer Silizium Cluster — •Felix von Gynz-Rekowski, Dong Chan Lim, Tim Fischer, Nils Bertram, Rainer Dietsche, Ignacio Lopez, Young Dok Kim und Gerd Ganteför — Universität Konstanz, 78457 Konstanz

Seit der Entdeckung des „supermagischen“ Clusters C$_{60}$[1] hat sich die Frage, ob es möglich ist, aus stabilen Clustern neue Festkörper zu synthetisieren, zu einem spannenden Forschungsgebiet entwickelt.

Dieser Fragestellung nachgehend wurden die „magischen“ Silizum Cluster Si$_4$[2] & Si$_7$ massenselektiert und weich ($E_{\text{KIN}} \leq 0{,}3$ eV/Atom) auf Graphit (HOPG), armophem Kohlenstoff und Silbereinkristaloberflächen deponiert und mittels XPS, UPS, STM, Auger, LEED und HREELS untersucht. Die Resultate wurden mit denen der „nichtmagischen“ Vertreter Si$_8$ & Si$_9$ und des Silizium Monomeres verglichen.

Unsere Ergebnisse deuten darauf hin, dass magische Silizium Cluster nicht zu größeren Siliziumaggregaten verschmelzen, keine starke chemische Wechselwirkung mit dem Substrat haben und gegenüber Sauerstoff inert scheinen[3], im Gegensatz zu deponierten Silizium Monomeren, die zur Oxidation neigen und auf amorphem Kohlenstoff carbidisieren.

[1] H. W. Kroto, J. R. Heath, S. C. O'Brien, R. F. Curl und R. E. Smalley, Nature 318, 162 (1985)
[2] M. Grass, D. Fischer, M. Mathes, G. Ganteför und P. Nielaba, Appl. Phys. Lett. 81, 3810 (2002)
[3] M. Mathes, M. Grass, Y.D. Kim und G. Ganteför, Surf. Sci. 552, L58, (2004)

O 24.2 Sa 15:15 TU EB301

Elektronische Charakterisierung von Si-Nanopartikeln aus der Gasphase unter Einwirkung uniaxialer Kräfte — •Ingo Plümel[1,2], Hartmut Wiggers[2] und Axel Lorke[1] — [1]Laboratorium für Festkörperphysik, UniversitätDuisburg–Essen, Lotharstraße 1, 47048 Duisburg — [2]Institut für Verbrennung und Gasdynamik,Universität Duisburg–Essen, Lotharstraße 1, 47048 Duisburg

Das Kompaktierungsverhalten von nano- und mikrokristallinem Silizium-Pulver wurde unter Einwirkung einer uniaxialen Kraft im Bereich von 37MPa bis 750MPa durch DC-Messungen und Impedanzspektroskopie im Frequenzbereich von 10Hz bis 10MHz charakterisiert.

Die Leitfähigkeit und Impedanz werden durch druckabhängige Umordnungsprozesse innerhalb des Pulvers und durch Deformation der Partikel- und Elektrodengrenzflächen bestimmt. Zeitabhängige Leitfähigkeitsmessungen bei konstanter Kraft zeigen drei Bereiche, die jeweils von unterschiedlichen Effekten dominiert werden.

Untersuchungen des Verhaltens mit Impedanzspektroskopie ermöglichen eine genauere Charakterisierung der ablaufenden Relaxationsprozesse. Die verschiedenen Beiträge zur Gesamtimpedanz lassen sich mittels Entwicklung und Anpassung eines Ersatzschaltbildes auflösen. Durch Auswertung der zeitlichen Änderung der separierten Kapazitätsbeiträge kann das Pulver mit Hilfe eines Effektiv-Medium-Modells charakterisiert werden.

Zwischen Probenleitfähigkeit und äußerer Kraft zeigt sich beim Nanopulver ein exponentieller Zusammenhang, während beim Mikropulver ein Potenzgesetz gilt.

O 24.3 Sa 15:30 TU EB301

Colorimetric properties of titanium group nitride nanoparticles and their optimization — •A. Reinholdt[1], R. Pecenka[1], Th. E. Weirich[2], and U. Kreibig[1] — [1]I. Phys. Inst. 1A der RWTH Aachen, Postfach, 52056 Aachen — [2]GFE der RWTH Aachen, Ahornstr. 55, 52074 Aachen

If long-term stable color pigments are needed, inorganic materials have advantages against organic dyes, which may disintegrate in time or by irradiation of UV light. The richness of colors is high if the colorants are nanoparticles because of selective extinction effects (e.g. Mie resonances). Beside other materials, the nitrides of the titanium group turned out to be well suited for this application due to the Drude-like contibutions to their dielectric functions [1,2].

In this presentation, results of the colorimetric investigation of embedded TiN and ZrN nanoparticles are shown. Experimental data and simulations based upon extensions of Mie's theory are presented, both displaying the dependency of the chromaticity coordinates on the concentration, sample thickness and the embedding material. We will discuss the applicability of these nanoparticles as color pigments and the possibilities of color optimization. All data will be presented in the CIE 1976 ($L^*a^*b^*$) color space system.

[1] A. Reinholdt *et al.*: Appl. Phys. B **77**, 681-686 (2003)
[2] A. Reinholdt *et al.*: Eur. Phys. J. D **31**, 69-76 (2004)

O 24.4 Sa 15:45 TU EB301

Photochrome Silbernanopartikel in TiO$_2$ — •Alexander N. Sprafke[1], Christian Dahmen[1], Gero von Plessen[1], Matthias Wuttig[1], John Okumu[2] und Martina Luysberg[3] — [1]I. Physikalisches Institut (IA), RWTH Aachen, D-52056 Aachen — [2]Department of Physics, Kenyatta University, P. O. Box 43844, Nairobi-Kenya — [3]IFF/ Forschungszentrum Jülich, D-52428 Jülich

Die besondere Eigenschaft photochromer Materialien ist die reversible Änderung ihrer optischen Eigenschaften nach Bestrahlung mit Licht. In dieser Arbeit werden dünne Schichten bestehend aus Titandioxid und Silbernanopartikeln vorgestellt, die Mehrfarbenphotochromismus aufweisen. Durch dc-Magnetronsputtern und nachfolgende thermische Behandlung werden 60 nm dicke TiO$_2$-Filme mit eingebetteten Silbernanopartikeln, die eine breite Größen- und Formverteilung aufweisen, hergestellt. Durch Lasereinstrahlung lassen sich die optischen Eigenschaften dieses Systems derart manipulieren, dass die bestrahlte Stelle die Farbe des Laserlichtes annimmt. Dieser Effekt beruht auf der Veränderung der Plasmonenresonanz der Partikel als Folge der Bestrahlung. Wir deuten diese Änderung als Ergebnis lichtinduzierter Elektronenemission aus den Partikeln. Die beobachteten Effekte sind nicht auf sputterdeponierte Ag-TiO$_2$-Nanokompositfilme beschränkt, sondern treten auch in 2 nm großen Ag-Clustern, die mit einer Clusterstrahlanlage hergestellt wurden, auf.

O 24.5 Sa 16:00 TU EB301

Efficient oxydation and Reduction of Ag nanoparticles — •Dong Chan Lim, Ignacio Lopez-Salido, Felix v. Gynz-Rekowski, and Young Dok Kim — Department of Physics, University of Konstanz, D.78457, Konstanz, Germany

Ag nanoparticles on SiO2/Si surfaces synthesized using Tollens reagents and subsequent acid-etching were studied using X-ray Photoelectron Spectroscopy (XPS) and Scanning Tunnelling Microscopy (STM). Ag nanoparticles smaller than 4-5nanometers show positive chemical shifts of the Ag 3d states with respect to the bulk values, in agreement with previous studies on Ag nanoparticles on titania and alumina. Ag nanoparticles smaller than 2-3 nanometers undergo reversible oxidation and reduction by reacting with H2O2/H2O and subsequent heating under vacuum to 150 °C, which were not found for the bulk counterparts, demonstrating unique chemical properties of nanoparticles compared to the bulk counterparts.

O 24.6 Sa 16:15 TU EB301

Tunneling Spectroscopy of large deposited silver clusters on Germanium (001) — •K.-L. Jonas, F. Geisler, J. Bansmann, V. v. Oeynhausen, and K.-H. Meiwes-Broer — Institut für Physik, Universität Rostock, Universitätsplatz 3, 18051 Rostock

Silver clusters of several nanometer sizes are produced by continuous arc discharge in a hollow cathode design and deposited onto germanium (001). The cluster source is directly attached to a UHV-chamber and provides a high cluster flux of about $6\cdot10^8/cm^2s$. Low temperature tunneling spectroscopy is used to analyse the density of states and the transport via the cluster/interface system, respectively. The clusters are sufficiently fixed at their positions due to the significant silver-germanium interaction when observed by tunneling at over wide parameter range. Transport under the probing tip - known for weakly interacting systems - is suppressed. The spectra observed contain several structures as a dip-like conductance drop to finite but non-zero values at the Fermi level. The dip is discussed in terms of an underlying Schottky contact. Following this idea, the non-zero conductance indicates leak channels in the interface region via silver- germanium bonds. Further, distinct conductance maxima are found. These maxima positions are discussed with respect to one-dimensional quantization of electronic states.

O 24.7 Sa 16:30 TU EB301

Silver Nanowires — •Dieter Wagner[1], Andreas Graff[2], Harald Ditlbacher[3], and Uwe Kreibig[1] — [1]I. Physikalisches Institut 1A, RWTH Aachen, 52056 Aachen — [2]MPI für Mikrostrukturphysik, 06120 Halle — [3]Karl-Franzens-Universität Graz/Austria

Free silver nanowires were produced in an aqueous electrolyte by a novel chemical reaction. The diameters are about 27 nm, the lengths range up to more than 70 μm. (!) Their structure was found by TEM analysis (SAED) and HRTEM to consist of five monocrystalline rods of triangular cross section. [1]

Here we present the results of two optical experiments on these nanowires. In the first experiment the polarisation dependency of scattered visible light of one single wire in the spectral region of the plasmon resonance was confirmed by using Zsigmondy darkfield microscopy. Only if the incident electrical field has a component perpendicular to the wire axis, a spectrally selective plasmon polariton is excited. By the second experiment the applicability of the wires as plasmon wave guides was demonstrated. Exciting the plasmon polariton locally at one tip of the wire the decrease of its intensity along the wire axis could be registrated by nearfield fluorescence exitation of a dye embedded in the surrounding PMMA medium. As a result, the propagation length is larger than 10 μm.

[1] A. Graff, D. Wagner , H. Ditlbacher and U. Kreibig, Silver Nanowires, European Physical Journal (EPJ) D, to appear.

O 24.8 Sa 16:45 TU EB301

The lateral Photoemission Distribution from a defined Cluster/Substrate System as probed by PEEM — •Michael Bauer, Carsten Wiemann, Martin Rohmer, Michael Munzinger, and Martin Aeschlimann — Fachbereich Physik, TU Kaiserslautern, 67663 Kaiserslautern

We used 2 Photon Photoemission Electron Microscopy (PEEM) to investigate the lateral distribution of the nonlinear photoemission yield from a defined and homogeneous system of silver clusters supported by a HOPG substrate. The PEEM images show very bright and well separated spots at the surface responsible for the dominant yield of a lateral integrating photoemission experiment. Furthermore, we find that the 2PPE signal for the latter case is strongly inhomogeneous broadened. A spectroscopy mode of the PEEM enables us to focus on the homogeneous contribution from a single emitter related to single electron excitations as well as collective (plasmon) excitations. In this way we are able to show that the emitter source is either a small silver particle or a number of strongly coupled silver particles.

O 25 Zeitaufgelöste Spektroskopie II

Zeit: Samstag 15:00–17:00 Raum: TU EB420

O 25.1 Sa 15:00 TU EB420

Anregungs- und Relaxationsdynamik von Elektronen in laserbestrahlten Metallen — •Bärbel Rethfeld[1] und Andreas Kaiser[2] — [1]Institut für Laser- und Plasmaphysik, Universität Duisburg–Essen, D-45117 Essen — [2]Institut fuer Physik, Humboldt-Universität Berlin, 12489 Berlin

Mittels eines ultrakurzen Laserpulses kann das freie Elektronengas in Metallen stark im thermodynamischen Gleichgewicht gestört werden. Durch Elektron–Elektron Stöße thermalisiert das Elektronengas zu einem Gleichgewicht höherer Temperatur; gleichzeitig wird durch Elektron–Phonon Stöße Energie an das Gitter abgeben. Diese elementaren Stoßprozesse werden in einer zeit- und energieaufgelösten Beschreibung durch Boltzmann'sche Stoßintegrale im Detail berücksichtigt, wodurch wir explizit die Verteilungsfunktion der Elektronen und Phononen während und nach der Bestrahlung berechnen können. Die Ergebnisse zeigen, dass durch eine nicht abgeschlossene Thermalisierung des Elektronengases der Energietransfer an das Gitter verlangsamt werden kann. Es werden Relaxations- und Thermalisierungszeiten für das freie Elektronengas in Aluminium ermittelt.

O 25.2 Sa 15:15 TU EB420

Time Resolved Nonlinear Magneto-Optical Spectroscopy at Gd(0001) Surface: Ultrafast Lattice and Spin Dynamics — •Ilie Radu, Alexey Melnikov, Uwe Bovensiepen, Kai Starke, Eckart Matthias, and Martin Wolf — Freie Universität Berlin, Fachbereich Physik, Arnimmalle 14, 14195 Berlin

Pump-probe second harmonic generation (SHG) measurements performed on ferromagnetic Gd(0001) surfaces revealed the existence of a coupled coherent phonon-magnon mode at frequency of 3 THz [1]. This is reflected in oscillatory contributions in the transient SHG signal for the electron, phonon and spin subsystems. Here, we present the strong wavelength dependence of incoherent and coherent components of the time-resolved SHG response following the excitation with 35 fs laser pulses within 740-860 nm wavelength range. The SHG process at Gd surfaces evolves resonantly enhanced via the unoccupied surface state component which implies a high spectral sensitivity. With increasing photon energy we observe an increase in the incoherent contribution and a decrease in the coherent part of the excitation. This is ascribed to a population build-up in the unoccupied spin down surface state which increases with hν, while the depopulation of the occupied component, occurring simultaneously, varies just weakly with photon energy.

This project is funded by DFG through SPP 1133.

[1] A. Melnikov et al.; Phys. Rev. Lett. 91, 227403 (2003)

O 25.3 Sa 15:30 TU EB420

Spin-dependent electron dynamics in front of an ultrathin iron film — •Anke Schmidt[1], Martin Pickel[2], Martin Wiemhöfer[2], Markus Donath[2], and Martin Weinelt[3] — [1]Lehrstuhl für Festkörperphysik, Staudtstraße 7, 91058 Erlangen — [2]Physikalisches Institut, Universität Münster, Wilhelm-Klemm-Straße 10, 48149 Münster — [3]Max-Born-Institut, Max-Born-Straße 2A, 12489 Berlin

Ultrafast demagnetisation of ferromagnetic thin films upon laser excitation is a phenomenon not yet fully understood. It is still controversial which processes lead to the loss of total magnetic moment. Two-photon photoemission (2PPE) provides a powerful tool for the investigation of electron dynamics and the identification of scattering processes at surfaces [1].

We have studied the energetics and dynamics of exchange-split image-potential states on ultrathin iron films on Cu(100) with time-, energy-, and spin-resolved bichromatic 2PPE. We are able to observe the exchange splitting of the first and the second image-potential state directly. In time- and spin-resolved measurements, spin-dependent lifetimes were found. A linewidth analysis of the energy-resolved 2PPE-spectra shows spin-dependent dephasing, which indicates a spin-dependent elastic scattering process.

[1] K. Boger, M. Weinelt and Th. Fauster, Phys. Rev. Lett. **92**, 126803 (2004)

O 25.4 Sa 15:45 TU EB420

Electron dynamics in thin Ag-films on Si(100) — •Claudia Kennerknecht[1], Sven Schramm[1], Walter Pfeiffer[1], Olaf Weisse[2], and Eckart Hasselbrink[2] — [1]Physikalisches Institut, Universität Würzburg, Am Hubland, 97070 Würzburg — [2]Fachbereich Chemie, Universität Duisburg-Essen, Universitätstr. 5, 45117 Essen, Germany

The properties of Ag-films of few nanometers thickness differ substantially from bulk materials. So called quantum well states appear because of the confinement in one dimension [1]. In addition, thin films show unexpected catalytic bevior. Using time-resolved multiphoton photoemission spectroscopy we gain information about the transient electron distribution of our sample. The spectra reveal the internal thermalization and cooling of the electron gas.

Measurements on thin Ag-films on n-doped Si(100) show a wavelength dependence which can be explained by different absorption in the Ag-film and the Si substrate. Time-resolved measurements reveal larger relaxation times compared to measurements on thin Ag-films on MgO(100) and single crystals [2]. We attribute this influence of the substrate to carrier injection from the photoexcited Si.

[1] Matsuda et al, Phys. Rev. B 65 (2002)

[2] Aeschlimann et al, Appl. Phys. A 71 (2000)

O 25.5 Sa 16:00 TU EB420

Ultrafast dynamics of the exchange split surface state of Gd(0001)/W(110) — •Martin Lisowski, Panagiotis Loukakos, Uwe Bovensiepen und Martin Wolf — Freie Universität Berlin, Fachbereich Physik, Arnimallee 14, 14195 Berlin

Gadolinium is a model system for ferromagnetic materials where the exchange interaction of localized magnetic moments is mediated via spin-polarization of the conduction band electrons (RKKY interaction). An interesting question is, whether it is possible to demagnetize such a ferromagnet on a femto-second time scale by disturbing the conduction band electrons. We use time resolved photoelectron spectroscopy to investigate the dynamics of the Gd(0001)/W(110) surface upon excitation with an optical pump pulse. The use of a probe photon energy above the work function of Gd allows us to directly measure the transient electron temperature as well as the occupied and unoccupied part of the exchange split surface state, which serves as a probe for magnetism. We observe a sub pico-second reduction of the SS binding energy. Comparison with a two-temperature model simulation shows that the decrease in binding energy is initially faster than the increase in lattice temperature, excluding a simple lattice heating effect as explanation. A damped oscillation of 2.8 THz frequency and 1 ps damping time is superimposed on the binding energy shift and is attributed to a coherent LO phonon-magnon mode.

O 25.6 Sa 16:15 TU EB420

Momentum-dependent dynamics of buried interface states in Ar/Cu(100) — •M. Rohleder, W. Berthold, J. Güdde und U. Höfer — Fachbereich Physik und Zentrum für Materialwissenschaften, Philipps-Universität Marburg, D-35032 Marburg

The electronic properties of interfaces play a fundamental role in both basic and applied research. In particular, the dynamics of electrons located at solid-solid interfaces is a key to many technological applications. Only recently, we have demonstrated the existence of buried interface states in the Ar/Cu(100) system and investigated the transient decay of these image-like states by means of time-resolved two-photon photoemission [1]. In this study, we focus on momentum-dependent relaxation processes in the nearly-free-electron bands. The experiments were performed by using a hemispherical analyzer equipped with a 2d detector, allowing for single-shot $E(k)$ measurements. The parabolic dispersion could be mapped for the first $n' = 1$ interface state. Its effective mass is only 0.6 m_e as a consequence of the highly corrugated potential inside the Ar layer. For finite parallel momenta we found an increase of the decay rate proportional to the kinetic energy of parallel motion, $\Gamma = \hbar/\tau = 6.3$ meV $+ 0.012\ E_{\|}$. Our results infer that the situation is similar to the image-potential states of clean Cu(100) [2] where inelastic interactions with metal electrons lead to interband decay into the bulk and intraband scattering inside the bands.

[1] M. Rohleder *et al.*, submitted to Phys. Rev. Lett.
[2] W. Berthold *et al.*, Phys. Rev. Lett. **88**, 056805 (2002).

O 25.7 Sa 16:30 TU EB420

How much does the surface projected band structure influence ultra fast charge transfer at a surface?
The case of Ar adsorbed on Cu(111) and Cu(100) — •Alexander Föhlisch, Sethuraman Vijayalakshmi, Franz Hennies, Annette Pietzsch, Mitsuru Nagasono, and Wilfried Wurth — Universität Hamburg, Institut für Experimentalphysik, Luruper Chaussee 149, D-22761 Hamburg

Surfaces and interfaces determine many properties of matter. Next to the geometric structure of the surface the surface projected bulk band structure and surface states and resonances play an important role. Even the difference of the surface electronic structure of different crystal faces has consequences for the charge transfer dynamics at these surfaces. Charge transfer at the Cu(100) and Cu(111) surfaces has drawn considerable attention from experiment and theory [1,2,3], due to the difference of their surface projected band gap. Using core hole clock spectroscopy we have shown in previous work that ultra fast charge transfer varies significantly for different metal surfaces [4].

In this contribution we show that charge transfer of the 4s electron of core-excited $2p_{3/2}^{-1}4s^1$ Ar adsorbed on the Cu(100) surface is a factor of two faster than on the Cu(111) surface.

This work was supported by the DFG SPP 1093.

[1] M. Bauer et al., Phys. Rev. B **60**, 5016 (1999)
[2] A.G. Borisov et al., Phys. Rev. Lett. **86**, 488 (2001)
[3] J. P. Gauyacq and A. G. Borisov, Phys. Rev. B **69**, 235408 (2004)
[4] A. Föhlisch et al., Chem. Phys. **289**, 107 (2003)

O 25.8 Sa 16:45 TU EB420

Scattering by Co adatoms between image-potential bands on Cu(001) — •Klaus Boger[1], Martin Weinelt[2], and Thomas Fauster[1] — [1]Lehrstuhl für Festkörperphysik, Universität Erlangen-Nürnberg, Staudtstr. 7, 91058 Erlangen — [2]Max-Born-Institut, Max-Born-Straße 2A, 12489 Berlin

The increasing resolution and sensitivity of photoelectron spectroscopy reveals more and more details about the influence of defects. By means of time- and angle-resolved two-photon photoemission the various scattering processes induced by adsorbate atoms can be studied [1]. We now have examined the dynamics of electrons in image-potential states on the Cu(001) surface covered by statistically distributed Co adatoms. Even at low coverages of about 0.6% of a monolayer strong scattering from higher image-potential bands into the first one is observed. From the measured data the transfer of energy and parallel momentum at these scattering processes can be determined.

[1] K. Boger, M. Weinelt, and Th. Fauster, Phys. Rev. Lett. **92** (2004) 126803

O 26 Oxide und Isolatoren I

Zeit: Samstag 15:00–17:00 Raum: TU EB202

O 26.1 Sa 15:00 TU EB202

Jahn-Teller stabilization of a "polar" metal oxide surface: Fe_3O_4(001) — •Rossitza Pentcheva, Wolfgang Moritz, and Matthias Scheffler — Section Crystallography, Dept. of Earth and Environmental Sciences, LMU München

We present a systematic investigation of the composition, structure and properties of the Fe_3O_4(001)-surface based on density-functional theory (DFT). Using *ab initio atomistic thermodynamics* [1] we predict that a "polar" termination is the lowest energy configuration over the entire range of accessible oxygen pressures. The stabilization of the surface involves a fundamentally different mechanism, which has not been considered so far: While most of the previous studies proposed an ordering of surface vacancies as the origin of the experimentally observed $(\sqrt{2} \times \sqrt{2})R45°$-reconstruction, here it is explained as a Jahn-Teller distortion of the surface atoms forming a *wave-like* pattern along the [110]-direction. Both x-ray diffraction (XRD) [2] and low energy electron diffraction (LEED-I/V) analyses support the theoretically predicted model. Calculated STM images and surface core level shifts are compared to available experimental data. The predicted halfmetal-to-metal transition from bulk to the surface is relevant in view of future applications (*e.g.* in spintronic devices). [1] K. Reuter and M. Scheffler, Phys. Rev. B 65, 035406, (2002). [2] R. Pentcheva, F. Wendler, N. Jedrecy, H.L. Meyerheim, W. Moritz, and M. Scheffler, submitted to Phys. Rev. Lett.

O 26.2 Sa 15:15 TU EB202

Theoretical Study of the Fe_3O_4(111) Surface Structure and Physical Properties — •Aleksey Kuznetsov, Martin Friák, and Matthias Scheffler — Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, Germany

The Fe_3O_4(111) surface has been studied intensively since several years due to its potential application in spintronics (Yu. S. Dedkov et al., Phys. Rev. B 65 (2002) 064417). The unreconstructed surface can expose six possible terminations, but only three of them have been clearly resolved experimentally (e.g. N. Berdunov et al., Phys. Rev. B 70 (2004) 085404). Moreover, self-consistent band structure calculations of the Fe_3O_4(111) surface are still lacking.

We present the results for the different surface terminations, in particular addressing the stability, electronic structures, and magnetic properties. Employing ab initio atomistic thermodynamics we identified the most stable surface termination. All calculations were performed using density-functional theory together with the all-electron full-potential linearized augmented plane-wave method as implemented in the WIEN2k code.

O 26.3 Sa 15:30 TU EB202

DFT-Rechnungen zur Adsorption und Dissoziation von Wasser auf Fe3O4(111) — •Wolfgang Ranke[1], Maria E. Grillo[2] und Carsten Menke[2] — [1]Fritz-Haber-Institut der MPG, Faradayweg 4-6, 14195 Berlin — [2]Accelrys GmbH, Inselkammerstr. 1, 82008 Unterhaching

Die Fe3O4(111)-Oberfläche ist regulär mit 1/4 ML Eisen über einer vollen Sauerstofflage terminiert. Die anfängliche Adsorption von Wasser verläuft ungewöhnlich, nämlich dissoziativ [1,2] und ohne Aktivierungsschwelle [1]. DFT-Rechnungen zeigen, dass die Dissoziation über einen molekular auf Fe gebundenen Zwischenzustand erfolgt. Die OH-Gruppe bleibt auf diesem Platz während das abgespaltene H-Atom über zwei konkurrierende Wege zum übernächsten O-Platz gelangt, wo es eine strukturell unterschiedliche zweite OH-Gruppe bildet, in voller Übereinstimmung mit IRAS-Messungen [2]. Nach Sättigung dieser gamma-Spezies adsorbiert weiteres Wasser (beta-Spezies) molekular über Wasserstoffbrücken zu den beiden OH-Gruppen. Deren Bindungen zum Substrat bleiben erhalten sodass die gebildeten Aggregate nicht einem konventionellen Wasser-Dimer entsprechen. Die mögliche Rolle einer solchen Anordnung für die Aktivierung von Wasser in katalytischen Prozessen wird diskutiert. [1] Y. Joseph et. al., J. Phys. Chem. B 104 (2000) 3224. [2] U. Leist et al., Phys. Chem. Chem. Phys. 5 (2003) 2435.

O 26.4 Sa 15:45 TU EB202

Interaction of atomic hydrogen with FeO(111), Fe3O4(111) and alpha-Fe2O3(0001-biphase) surfaces — •Wolfgang Ranke[1], Weixin Huang[2], and Robert Schlögl[1] — [1]Fritz-Haber-Institut der MPG, Faradayweg 4-6, 14195 Berlin — [2]Now at: Dept of Chem. Phys., Univ. of Science and Technology of China, Hefei 230026, P.R.China

Hematite Fe2O3 is used as catalyst in the dehydrogenation of ethylbenzene to styrene. The formed hydrogen reduces the oxide but little is known about the the mechanism. Therefore, the interaction with molecular and atomic hydrogen and its desorption was studied on epitaxial iron oxide films of different phases using LEED, XPS and TDS. Room temperature exposure to atomic H causes partial disordering. Both OH groups and reduced (but not yet metallic) iron appear in XPS. FeO domains react very quickly and TDS shows only water desorption explaining the observed reduction. Fe2O3 domains react more slowly. Even at RT, Fe3O4 domains are formed. TDS shows desorption of both H2O and H2. Upon flashing, reduced iron and OH remain but the oxide reorders and separates into Fe2O3 and Fe3O4. Oxidation restores the original surface. The implications for the behavior of the catalyst will be discussed.

O 26.5 Sa 16:00 TU EB202

Pt surface structure in presence of an oxygen atmosphere — •Timo Jacob and Matthias Scheffler — Fritz-Haber-Institut der MPG, Berlin, Germany

Nowadays Platinum is used to catalyze a whole variety of different reactions. Expecially for electrocatalytic processes (such as in fuel cells) Pt is still one of the most sufficient materials providing a high rate for oxygen reduction at the cathode. However, this reaction occurs in a multi-component environment and under conditions of finite temperature, pressure, and electrode potential ($p = 1\,\mathrm{bar}$, $T = 80 - 100\,\mathrm{C}$, $\phi \neq 0\,\mathrm{V}$). Thus, the model of an pure and perfect Pt(111) surface, which is often used to study this reaction, is clearly incomplete.

Therefore, to study the cathode reaction mechanism our first investigations aim on the realistic Pt(111) surface structure, which then will be the basis of further studies. Using density functional theory (DFT) in combination with a modified *ab inito* atomistic thermodynamics (capable to treat the electrode potential), we started with the $V = 0$ case and calculated the corresponding p/T-phase diagram, which led to interesting surface-oxide structures.

O 26.6 Sa 16:15 TU EB202

A Combined In-situ SXRD and HRCLS study of the Oxidation of Ag(111) — •Alexander Reicho[1], Andreas Stierle[1], Ioan Costina[1], Helmut Dosch[1], Edvin Lundgren[2], Johan Gustafson[2], and Jesper Andersen[2] — [1]Max-Planck-Institute for Metals Research, Heisenbergstr. 3, 70569 Stuttgart, Germany — [2]Department of Synchrotron Radiation Research, Lund University, Box 118, S-22100, Sweden

Silver is used as catalyst for the epoxidation of ethylene and during the partial oxidation of methanol to formaldehyde. The formation of an oxygen induced p(4x4) reconstruction of the Ag(111) surface was reported, which was made responsible for the catalytic activity of Ag. We will present an in-situ surface x-ray diffraction study on the interaction of oxygen with the Ag(111) surface from UHV up to 2 bar, which will shed new light on the previously proposed structural model of the p(4x4) reconstruction and the stability diagram of the Ag(111)/O-system, which can be compared with theoretical studies. In addition High Resolution Core Level Spectroscopy was applied to get information about the binding geometry of the oxygen atoms. In the presentation several structural models of the p(4x4) reconstruction will be discussed.

O 26.7 Sa 16:30 TU EB202

In-situ investigations of Ga_2O_3 stability on the CoGa(100) surface — •Alina Vlad[1], A. Stierle[1], I. Costina[1], P. Nolte[1], M. Delheusy[1], H. Dosch[1], E. Lundgren[2] und J. Andersen[2] — [1]Max-Planck Institut für Metallforschung, Heisenbergstraße 1, 70569 Stuttgart — [2]Department of Synchrotron Radiation Research, Institute of Physics, University of Lund, Box 118, SE-221 00 Lund, Sweden

The oxidation behavior of metallic alloy surfaces is of interest for fundamental studies, as well as for numerous applications in a variety of different fields such as heterogeneous catalysis, high temperature resistant coatings, microelectronics and gas sensors. As an example, the stability diagram of gallium oxide on CoGa(100) surface was determined. Surface X-ray Diffraction and High Resolution Core Level Spectroscopy experiments were performed at different temperatures in an oxygen partial pressure range up to 1 bar, following under which conditions the surface oxide starts to transforms into a bulk oxide. It was observed that at $T < 350^oC$, the formation of the bulk oxide is kinetically hindered, the surface gallium oxide layer being stable even at 1 bar oxygen. Oxidation at 650^oC and $2 \cdot 10^{-2}$ mbar oxygen leads to the formation of a smooth and well-ordered epitaxial bulk Ga_2O_3, whereas at temperatures higher than 750^oC the formation of the bulk oxide is accompanied by substrate faceting.

O 26.8 Sa 16:45 TU EB202

Reaction Kinetics on Oxide Supported Metal Nanoparticles: On the Role of Surface Oxygen, Subsurface Oxygen and Surface Oxides — •Tobias Schalow, Mathias Laurin, Swetlana Schauermann, Björn Brandt, Jörg Libuda, and Hans-Joachim Freund — Fritz-Haber-Institut der MPG, Faradayweg 4-6, 14195 Berlin, Germany

The nature and formation of different oxygen species on iron-oxide supported Pd nanoparticles and their influence on catalytic reactions are investigated on well-defined supported model catalysts by combining molecular beam methods and various surface science techniques. IR reflection absorption spectroscopy of adsorbed CO is employed as a sensitive probe in order to identify the different adsorption sites on the metal particles and the support.

Remarkable differences are observed in comparison with previous studies on single crystal surfaces. For example it is found that the interaction with oxygen strongly depends on the particle size, involving e.g. reaction conditions under which the nanoparticle surface becomes only partially covered by surface-oxides. Moreover, the onset of surface-oxide formation is shown to be directly related to morphological transformations of the nanoparticles.

O 27 Phasenübergänge

Zeit: Samstag 15:00–16:45 Raum: TU EB107

O 27.1 Sa 15:00 TU EB107

Surface freezing and surface phase transition studied on the liquid eutectic AuSi surface — •Reinhard Streitel, Alexei Grigoriev, Oleg G. Shpyrko, and Peter S. Pershan — Division of Applied Sciences and Department of Physics, Harvard University, Cambridge, MA 02138

We present x-ray investigations on the liquid surface of the eutectic AuSi alloy. Reflectivity and GID (grazing incidence diffraction) measurements indicate surface freezing well above the bulk melting temperature, $T_m(bulk) = 636K$. A reversible surface phase transition occurs at about $T = 645K$. Measurements performed on other metal or alloy (eutectic) surfaces did not show a similar behaviour to date. In comparison to other metals and alloys, AuSi shows a temperature dependent anomalous behaviour of the specular reflectivity in a range of $q_z = 1.0 - 2.5\AA$. Solid like surface structures on liquids were studied on different alloys before [1]. Surface free energy and entropy play a key role in surface freezing effects [2]. Our measurements were performed at the APS (Advanced Photon Source at Argonne National Lab, Chicago, USA). [1] Two-dimensional freezing in the liquid-vapor interface of dilute Pb:Ga alloy - B. Yang, S.A. Rice et al. [2] Wetting prewetting and surface freezing transitions in fluid Ga-based alloys: a surface light scattering study - W. Freyland et al.

O 27.2 Sa 15:15 TU EB107

Reversible surface phase transitions between quasicrystalline modifications — •K. J. Franke[1,2], W. Theis[1], P. Kury[3], M. Horn-von Hoegen[3], P. Gille[4], and K. H. Rieder[1] — [1]Inst. f. Experimentalphysik, FU Berlin — [2]IPN, EPFL, Lausanne, Switzerland — [3]Inst. f. Experimentalphysik, Uni Essen — [4]Dept. f. Geo- und Umweltwiss., LMU, München

Due to the complexity of quasicrystalline structures and their derivation from periodic lattices in higher dimensional space, mechanisms such as phason flips, which are nonexistent in periodic crystals, play a key role in transitions between quasicrystalline phases. Decagonal $Al_{72.3}Ni_{9.5}Co_{18.2}$ exists in three different modifications between 30 °C and 850 °C. It therefore provides the opportunity to study the effects of phase transitions on the surface. By using low-energy electron microscopy (LEEM), rough and smooth morphologies have been observed on the nanometer scale for all three low-index surfaces at temperatures below and above 650 °C, respectively. The transition between the medium and high temperature modification at 730 °C leads to a structural change at the surfaces. Both surface phase transitions and their relation to the respective bulk transitions will be discussed.

O 27.3 Sa 15:30 TU EB107

Metal-to-semiconductor phase transitions in VO_2 films — •Helena Prima Garcia[1], Tatjana Giessel[1], Emily Hooker[2], Martin Polcik[2], and Wolf Widdra[3] — [1]Max-Born-Institute, Berlin, Germany — [2]Fritz-Haber-Institute der Max-Planck-Gesellschaft, Berlin, Germany — [3]Martin Luther University, Halle, Germany

VO_2 films were grown by subsequent vanadium deposition and oxidation on $TiO_2(110)$ with film thickness' ranging from less than one monolayer to approximately 100 nm and additionally thicker VO_2 films (thickness 200 nm) grown by reactive RF sputtering.

While ultrathin films up to a few monolayers grow nearly epitaxially preserving the structure of the substrate, thicker films grown by subsequent vanadium deposition and oxidation show a polycrystalline structure with a preferential azimuthal orientation of the high symmetry directions in the crystallites parallel to the high symmetry directions of the $TiO_2(110)$ surface. All thermally grown films show only subtle changes in the V 3d region of the valence band as a function of temperature at which VO_2 undergoes a metal-to-semiconductor phase transitions (MSPT at 340 K).

In contrast the thicker VO_2 films grown by reactive RF sputtering show a substantial change in the region of the V 3d level. The spectral analysis of the change at V 3d region reveals the transition temperature around 310K and the width of the hysteresis loop of $\sim 15K$. The relatively broad transition range of $\sim 71K$ could be explained by the different size of the VO_2 particles as observed by AFM.

O 27.4 Sa 15:45 TU EB107

Rastertunnelmikroskopische Untersuchung des Übergangs von amorphem zu kristallinem Eis auf Cu(111) — •Michael Mehlhorn[1], Karina Morgenstern[2] und Karl-Heinz Rieder[1] — [1]Institut für Experimentalphysik, Freie Universität Berlin — [2]Institut für Festkörperphysik, Universität Hannover

Bei 5 K wird mittels hochauflösender Tieftemperatur–Rastertunnelmikroskopie der Übergang von amorphem zu kristallinem Eis auf Cu(111) untersucht. Zunächst werden bis zu 2,5 Doppellagen D_2O bei 85 K aufgedampft. Wegen ähnlicher Wechselwirkungsenergien zwischen den Molekülen untereinander und zwischen Molekül und Substrat erwartet man dreidimensionales Clusterwachstum. Tatsächlich werden bis zu 6 Doppellagen hohe amorphe Cluster beobachtet. Durch Heizen auf definierte Temperaturen unterhalb der Desorptionstemperatur von 160 K kristallisieren die Cluster. Es bilden sich bis zu 2 komplette Doppellagen mit geordneten Strukturen in der dritten, unvollständigen Doppelllage. Bei 150 K entstehen auf den vollständig kristallisierten Eisclustern Bündel von bis zu 4 Doppellagen hohen Eispyramiden. Bei Erreichen der Desorptionstemperatur bilden sich daraus kompakte, über 2 nm bzw. 6 Doppellagen hohe Eistürme.

O 27.5 Sa 16:00 TU EB107

Order-disorder transition of halogens on Pt(110) by I(T)-LEED — •Thomas Loerting, Clemens Deisl, Mariana Minca, Alexander Menzel, and Erminald Bertel — Institute of Physical Chemistry, University of Innsbruck, Austria

We have recorded low-energy electron diffractograms for halogen overlayers on Pt(110) as a function of temperature at constant coverage and electron gun voltage. A sharp decline of the fractional order spots indicates an order-disorder transition from both the (3×1) and c(2×2) phases to a disordered (1×1) phase at approximately 375 K. The peak profiles and the integrated scattered intensities of various spots on these LEED-films have been investigated according to critical scattering theory both in the [110] and [100] direction. The (3×1) as well as the c(2×2) halogen overlayer show a clear anisotropy in their phase transition behaviour, which corroborates our earlier claim of the quasi-one-dimensional nature of these systems. On the other hand, there are also pronounced differences between the phase transitions. Whereas the c(2×2) superstructure shows the expected behaviour for a continuous second-order phase-transition, e.g., the divergence of the correlation length at the critical temperature, the (3×1) superstructure shows a quite different behaviour, which also involves a change in the platinum substrate. Possible mechanisms for the (3×1)→disorder phase transition will be discussed, in particular with respect to a Peierls transition as previously proposed by us.

O 27.6 Sa 16:15 TU EB107

The influence of adsorbates on the Si(111)-In:(4×1) surface — •Karsten Fleischer[1], Sandhya Chandola[1], Norbert Esser[2], and Wolfgang Richter[1] — [1]Technische Universität Berlin, IFP, Sekr. PN 6-1 Hardenbergstr. 36, 10623 Berlin — [2]Institute for Analytical Science, Department Berlin, Albert-Einstein Str. 9, 12489 Berlin

The one dimensional, metallic Si(111)-In:(4×1) surface undergoes a phase transition into a (8×2) symmetry at low temperatures. The nature of this phase transition is explained either as formation of a charge density wave (CDW) or as a merely structural change. With reflectance anisotropy extended into the infrared regime (0.5-6 eV) we are able to monitor the phase transition and also changes to the electronic structure introduced by additional adsorbates such as In or Cs which prevent this phase transition. The current data derived by optical measurements all favour the first model of the surface phase transition – the CDW formation.

O 27.7 Sa 16:30 TU EB107

Submonolayer coverage of long chain alkanes at SiO2/air interfaces: Nucleation, molecular mobility, and structure formation — •Ralf Köhler and Hans Riegler — MPI für Kolloid- und Grenzflächenforschung, Abt. Grenzflächen, 14424 Potsdam

The ordering behavior of submonolayers of long chain alkanes at SiO2/air interfaces is astonishing complex. Two-dimensional nucleation and structure formation occurs below the surface melting point. The observed fractal crystallites (1,2) can be related to a process analogous to diffusion-limited aggregation (3). One observes different growth scenarios depending on the initial thickness of the liquid alkane film, i.e., due to different supply conditions to the growth front. The system also shows a reversible (equilibrium)-coexistence of solid domains and remaining fluid film in between. On-line optical microscopy observations on recent results are presented and analyzed. (1) A.Holzwarth et al., Europhys.Lett.2000,52,653 (2) H.Schollmeyer et al., Langmuir 2003,19,5042 (3) L.Knüfing et al., Langmuir, in press

O 28 Methodisches (Exp. und Theorie)

Zeit: Samstag 15:00–17:00 Raum: TU EB407

O 28.1 Sa 15:00 TU EB407

Coherent x-ray reflectivity using white synchrotron radiation — •Tobias Panzner[1], Ivan Vartanyants[2], Gudrun Gleber[1], and Ullrich Pietsch[1] — [1]Institut für Physik, Universität Potsdam, Am Neuen Palais 10, D-14415 Posdam — [2]HASYLAB at DESY, D- 22603 Hamburg, Germany

In this talk we will present results of x-ray reflectivity measurements with coherent synchrotron radiation. Before application of this method to particular samples one has to analyse precisely the apparatus function of the experimental set-up.

We used a pink beam of 5-20keV and a circular aperture to define the incident wave. Therefore we studied the influence of the diffraction from a circular aperture and the resulting shape of the illumination function approaching the sample. In particular we compare calculated and experimental apparatus function measured at the EDR beamline at BESSY II.

Using this function we show the possibilities and advantages of an energy dispersive set up for static and time resolved coherence experiments and give first results of the investigation of a smooth polymer film covered on silicon.

O 28.2 Sa 15:15 TU EB407

Calculations for a matched photon and photoelectron energy dispersive soft x-ray beamline — •D.R. Batchelor[1], Th. Schmidt[1], R. Follath[2], C. Jung[2], R. Fink[3], and E. Umbach[1] — [1]EP2, Univ. Würzburg — [2]BESSY Gmbh — [3]Phys.Chem. II, Univ. Erlangen

The high brilliance of third generation synchrotron radiation sources and modern developments in monochromator design, combined with 2d-detecting electron energy analysers, allow the simultaneous detection of photoelectron and photon energy: the photon dispersion of the monochromator is imaged onto the specimen, and the 1d-laterally resolving analyser is used to detect this dispersion. Such a combination opens up exploitation of CFS and CIS techniques such as NEXAFS, resonant Auger, and photoelectron spectroscopy. The parallel detection enables the large parameter space to be efficiently sampled such that high energy resolution can be combined with short time scales in the ms range. However, the electron and photon optics of monochromator and electron energy analyser have to be matched and optimised, considering imaging and dispersion characteristics of both. We present calculations for the combination of a collimated, variable cff, PGM monochromator and a Scienta SES 200 analyser with a 2d-detector at the UE52 Undulator at BESSY II, evaluating the limitations and developments necessary to realise the full potential of such an experiment.

Funded by BMBF under contract no. 05KS4WWC/2

O 28.3 Sa 15:30 TU EB407

Resonant inelastic soft x-ray scattering probing semiconductor surface adsorbate dynamics — •Franz Hennies[1], Alexander Föhlisch[1], Annette Pietzsch[1], Mitusuru Nagasono[1], Nadine Wittkowski[2], Stina Matsson[3], Maria-Novella Piancastelli[3], and Wilfried Wurth[1] — [1]Universität Hamburg, Institut für Experimentalphysik, Luruper Chaussee 149, D-22761 Hamburg — [2]Laboratoire d' Optique des Solides, Université Pierre et Marie Curie, Paris, France — [3]Department of Physics, Uppsala University, Sweden

Resonant inelastic x-ray scattering (RIXS) probes the valence electronic structure of a system in an atom specific and symmetry selective manner. Furthermore, the method is sensitive to dynamic properties of the core excited intermediate state. In recent years the method has been utilized to investigate adsorbates on metal surfaces, leading to an improved understanding of the surface chemical bond [1].

We have now investigated adsorbates on a semiconductor surface, i.e. simple hydrocarbons on the Si(001)-(2x1) surface with selectively excited, fully polarization and symmetry resolved RIXS at beamline I511 at MAXLab in Lund, Sweden. The electronic structure information which we obtain supports theoretical adsorption models. In contrast to metals a clear signature of dynamic processes in the core-excited state has been observed. We will present our results and suggest theoretical interpretation schemes. This work is supported by grant Fo343/1-1 of the Deutsche Forschungsgemeinschaft.

[1] A. Nilsson and L.G.M. Pettersson, Surf. Sci. Rep. **55**, 49 (2004)

O 28.4 Sa 15:45 TU EB407

Two-Photon Photoemission Microscopy of Self-organized Ag-Nanostructures on Si(001) — •L. I. Chelaru, O. Heinz, P. Zhou, M. Horn-von Hoegen, D. von der Linde, and and F. Meyer zu Heringdorf — Institut für Laser-und Plasmaphysik, Universität Duisburg-Essen (Campus Essen), 45117 Essen

During epitaxial growth of Silver on Si(001), compact islands and quasi-one-dimensional nanowires are formed. These self-organized nanostructures have been investigated by photoemission electron microscopy (PEEM) where the electrons are generated by femtosecond laser pulses through a two-photon photoemission process (2PPE). Shadow like features are observed around the nanostructures when the Ag islands and wires exceed a certain lateral dimension. The features are different for both directions of the polarization of the incoming light (s- and p-polarization, respectively). In p-polarization the shadows consist of several interference fringes. We interpret the shadows to represent the near field around the islands that is strongly emphasized in photoemission through the nature of the non-linear 2 photon photoemission process. The Ag-nanowire photoemission yield also shows a dependence on the polarization direction of the incoming light with respect to the orientation of the nanowire. Ag-nanowires oriented parallel to the polarization vector of the incoming light are not visible in the microscope images, in contrast to Ag-nanowires that are oriented normal to the vector of polarization. Also, the photoemission yield depends on the size of the islands. We explain these findings with a plasmon state in the silver nanostructures that is the intermediate state for 2 photon photoemission.

O 28.5 Sa 16:00 TU EB407

GW quasiparticle energy calculations for surfaces: the influence of dynamic polarization in a repeated-slab approach — •Philipp Eggert[1], Christoph Freysoldt[1], Patrick Rinke[1], Arno Schindlmayr[1,2], and Matthias Scheffler[1] — [1]Fritz-Haber-Institut der Max-Planck-Gesellschaft, Faradayweg 4-6, 14195 Berlin, Germany — [2]Institut für Festkörperforschung, Forschungszentrum Jülich, 52425 Jülich, Germany

The combination of density functional theory (DFT) and many-body perturbation theory in the GW approximation has become an important tool for *ab-initio* band structure calculations typically in good agreement with experiment. In order to treat surfaces one often employs a repeated slab geometry for computational convenience. However, electric multipole moments may occur in the slabs which then lead to a slowly decaying electrostatic interaction. If present, static dipoles must be corrected for in DFT [1]. In GW however, dynamic dipoles are always created. We present calculations for the hydrogen-saturated silicon (001) slabs and show that slabs smaller than 10 layers are not converged fully with 10-20 Å vacuum thickness. The effect of the dynamic dipoles is slowly decreasing with slab thickness, in accordance with an extension of a simple electrostatic model, that includes these polarization effects [2]. Therefore it is essential to monitor the convergence carefully and if necessary to extrapolate to infinite separation.

[1] J. Neugebauer, M. Scheffler, Phys. Rev. B **46**, 16067 (1992)

[2] C. Delerue, G. Allan and M. Lannoo, Phys. Rev. Lett. **90**, 076803 (2003)

O 28.6 Sa 16:15 TU EB407

The multipole compensation method for slab geometry — •Ferenc Tasnadi — IFW Dresden, ITF Group Numerical Solid State Physics and Simulation

The multipole compensation method developed by M. Weinert[1] to solve the Poisson equation for 3-dimensional periodic crystalline systems is extended for slabs, layer symmetric[2] structures. Unlike in Ref.[1] the presented method assumes localized (compact support), overlapping original charge distributions as introduced in Ref.[3] and non-local (no compact support) Ewald density distributions. The Poisson equation is solved with periodic boundary conditions in the plane and with finite voltage boundary condition in the perpendicular (z) direction. For the $K_{||} \neq 0$ case a Fourier transformation helps to calculate the solution in a three dimensional periodic sense. While for the $K_{||} = 0$ case, the required charge neutrality is the starting point to find the solution. The $K_{||} = 0$ solution connects the z directional potential step with the surface density of the dipole z component. For both cases suitable representations of the spherical harmonics are needed to arrive at expressions that are convenient for numerical implementation.

[1] M.Weinert, J. Math. Phys. **22**,11 (1981).

[2] V. Kopsky and D.B. Litvin, eds., *Subperiodic Groups,* vol. E of *International Tables for Crystallography* (Kluwer Academic Publisher, Dordrecht/Boston/London, 2002).

[3] K. Koepernik and H. Eschrig, Phys. Rev. B. **59**, 1743 (1999).

O 28.7 Sa 16:30 TU EB407

Genetic algorithms in surface cluster expansions — •Ole Wieckhorst und Stefan Müller — Universität Erlangen-Nürnberg, Lehrstuhl für Festkörperphysik, Staudtstr. 7, 91058 Erlangen

The cluster expansion treats the binary alloy problem by mapping DFT-based formation enthalpies of a number of selected input structures onto a finite set of pair and multibody interactions corresponding to characteristic figures like triangulars, tetrahedron, etc. The two critical points of this concept are the selection of an appropriate set of figures and input structures used for the construction, especially when the surface comes into play: The lifting of the symmetry due to the surface causes a lifting of the degeneracy of the figures, thus creating a huge repository of figures and structures to choose from. An effective way of treating such a selection problem are genetic algorithms. It will be demonstrated how the implementation of genetic algorithms in surface cluster expansions allows for a much more efficient and accurate determination of both, energetically relevant figures and input structures compared to conventional fitting procedures. As a first example, we apply this concept to construct a cluster expansion for the (100) surface of the B2-CoAl phase. Here, the segregation profile is controlled by so-called antisite atoms, as we have shown recently [1,2]. (supported by DFG)

[1] V. Blum et al., Phys. Rev. Lett. 89, 266102 (2002)

[2] O. Wieckhorst et al., Phys. Rev. Lett. 92, 195503 (2004)

O 28.8 Sa 16:45 TU EB407

The Nanoworkbench: A Tool to Probe Electronic Properties of Surfaces and Small Structures — •Hubertus Marbach[1,2,3,4], Olivier Guise[1,2,3], Jeremy Levy[2,5], Joachim Ahner[2,6] und John T. Yates, Jr.[1,2,3,5] — [1]Surface Science Center — [2]Center for Oxide Semiconductor Materials for Quantum Computation — [3]Department of Chemistry — [4]Lehrstuhl für Pysikalische Chemie II, Universität Erlangen-Nürnberg, Egerlandstraße 3, D-91058 Erlangen — [5]Department of Physics, University of Pittsburgh, Pittsburgh, PA 15260 — [6]Seagate Technology, Pittsburgh, PA 15222

To investigate the properties of surfaces and small particles in the sub-micrometer range we developed a novel experimental setup: the nanoworkbench (NWB). The core of the NWB consists of an array of four manipulators in UHV which can be positioned individually with nanometer precision. Equipped with sharp metal tips we can use the manipulators to contact the sample electrically. Four terminal measurements like van der Pauw or four-point probe measurements can be performed with the setup. Part of the design is an electron focusing column which enables us to image the sample and the four tips in situ by means of scanning electron microscopy. Running the nanomanipulators in scanning tunnelling microscopy mode provides an additional imaging method. The design of the NWB and first measurements will be presented. Work supported by AFOSR and DARPA

O 29 Hauptvortrag Bauer (Gaede-Preis)

Zeit: Montag 09:45–10:30 Raum: TU EB301

Hauptvortrag O 29.1 Mo 09:45 TU EB301

Femtosecond dynamics of adsorbate-surface interactions studied by means of time-resolved photoelectron spectroscopy — •Michael Bauer — Fachbereich Physik, TU Kaiserslautern, Erwin-Schrödinger-Str. 46, 67663 Kaiserslautern

Time-domain studies of dynamical processes evolving on a sub-picosecond timescale generally require optical pump-probe schemes using pulsed femtosecond light sources. In combination with photoelectron spectroscopy a direct access to ultrafast surface processes is possible. Particularly time-resolved Two-Photon Photoemission (2PPE) has been proven to be very successful in studying the dynamics of the electron relaxation of excited electronic surface states, such as image potential states and adsorbate resonances. For the later case, the alkali adsorption on noble metal surfaces is an ideal model system for investigations regarding the different decay channels of adsorbate excitations. In a time-resolved UPS scheme that allows for probing of the changes in the valence electronic distribution at a surface, we can furthermore study the ultrafast dynamics related to the nuclear motion of the adsorbate and changes in its chemical state during the course of a chemical reaction. This highly promising method has become possible just recently due to the development of laser-driven short-pulse EUV sources. In my talk I will report on experimental results regarding the femtosecond dynamics of adsorbate-surface interactions as probed by means of these two techniques.

O 30 Adsorption an Oberflächen III

Zeit: Montag 10:45–13:00 Raum: TU EB301

O 30.1 Mo 10:45 TU EB301

Fully polarization resolved near edge x-ray absorption fine structure spectroscopy of hydrocarbons adsorbed on Si(001)-(2x1) — •Franz Hennies[1], Alexander Föhlisch[1], Annette Pietzsch[1], Mitusuru Nagasono[1], Nadine Wittkowski[2], Stina Matsson[3], Maria-Novella Piancastelli[3] und Wilfried Wurth[1] — [1]Universität Hamburg, Institut für Experimentalphysik, Luruper Chaussee 149, D-22761Hamburg — [2]Laboratoire d' Optique des Solides, — [3]Department of Physics, Uppsala University, Sweden

The adsorption of simple hydrocarbons on Si(001) has been used as a model system for the Si-C interaction and as such been focus of investigations for more than 20 years. Nevertheless the exact geometrical configuration and the symmetry of the electronic states of several of the investigated adsorbates are still under debate.

We present a fully polarization resolved near edge x-ray absorption fine structure spectroscopy (NEXAFS) study of the adsorption of ethylene, benzene and acetylene on the single domain Si(001)-(2x1) surface which was performed at MAXLab in Lund, Sweden. We give direct experimental proof for ethylene adsorbing in a rotated, so called "dimerized"structure [1]. For benzene, the "butterfly"adsorption model is correct [2]. Acetylene adsorbs at room temperature in more than one configuration [3]. This work has been supported by DFG Fo343/1-1.

[1] F. Hennies, A. Föhlisch et al., Surf. Sci. **529**, 144 (2003)

[2] N. Witkowski, F. Hennies et al., Phys. Rev. B **68**, 115408 (2003)

[3] A. Pietzsch, F. Hennies et al., Surf. Sci. **562**, 65 (2004)

O 30.2 Mo 11:00 TU EB301

Calorimetric Measurements of the Heats of Adsorption of Aromatic Hydrocarbons on Pt(111) — •J.M. Gottfried[1,2], H. Ihm[2], H.M. Ajo[2], P. Bera[2], E.K. Vestergaard[2], and C.T. Campbell[2] — [1]Lehrstuhl fuer Physikalische Chemie II, Universitaet Erlangen-Nuernberg, Egerlandstr. 3, D-91058 Erlangen — [2]Department of Chemistry, Box 351700, University of Washington, Seattle, Washington 98195, USA

The heats of adsorption of benzene and naphthalene on clean Pt(111) at 300 K were measured by microcalorimetry [1]. The initial heats of adsorption were found to be 197 kJ/mol and 314 kJ/mol, respectively. Our data show that the initial and the integral heats are proportional to the number of carbon atoms in these aromatic systems, which lie parallel to the surface. Each bond between a sp^2 hydridized C atom and the surface contributes 30 kJ/mol to the initial heat and 23 kJ/mol to the integral heat at 0.75 ML. Thus, our results disagree with recent DFT calculations [2], in which an integral heat of only 11 kJ/mol per C atom at 0.75 ML was obtained. Sticking probabilities were measured by a modified King and Wells method, giving initial values of 0.97 (benzene) and 0.99 (naphthalene). For both molecules, the sticking probability shows a Kisliuk-type behavior with increasing coverage, which implies that there are precursors to sticking, whose energetics have also been addressed. [1] H.M. Ajo, H. Ihm, D.E. Moilanen, C.T. Campbell, Rev. Sci. Instrum. 75 (2004) 4471. [2] C. Morin, D. Simon, P. Sautet, J. Phys. Chem. B 108 (2004) 12084.

O 30.3 Mo 11:15 TU EB301

Structural transition in Cyclooctatetraene adsorbed on Ru(001) probed by thermal desorption and two-photon photoemission spectroscopy — •P. Tegeder, M. Danckwerts, S. Hagen und M. Wolf — Freie Universtät Berlin

The adsorption behavior of 1,3,5,7-Cyclooctatetraene (COT) on Ru(001) from sub-monolayer coverages up to the multilayer regime has been studied by temperature-programmed desorption (TPD) and work function measurements. The electron dynamics at the COT/Ru(001) interface has been investigated using time- and angle-resolved two-photon photoemission (2PPE) spectroscopy. The TPD data show that COT films grow at 115 K in a metastable phase when the coverage is increased from the chemisorbed monolayer to the bulklike molecular multilayer structure. The metastable states desorb at a temperature which is ~ 9 K lower than the multilayer, followed by an irreversible and thermally activated transformation into a stable multilayer phase. This transition occurs at 165±2 K and is accompanied by the appearance of image potential states and a pronounced increase of the total electron yield in 2PPE by more than one order of magnitude. The image states have binding energies of -0.70 eV and -0.24 eV for the n=1 and n=2 states, respectively, and a lifetime of 20±5 fs for both states. Their appearance is interpreted as an indication of island formation in the stable multilayer regime. 2PPE spectroscopy of the image potential states provides a sensitive probe of structural transitions in the adsorbate layers.

O 30.4 Mo 11:30 TU EB301

Adsorption geometry of hexafluorobenzene on the Cu(111) surface: A polarization dependent NEXAFS study — •Sethuraman Vijayalakshmi[1], Alexander Föhlisch[1], Franz Hennies[1], Annette Pietzsch[1], Mitsuru Nagasono[1], Patrick Kirchmann[2], Martin Wolf[2], and Wilfried Wurth[1] — [1]Institut für Experimentalphysik, Universität Hamburg, Luruper Chaussee 149, 22761 Hamburg, Germany — [2]Department of Physics, FU Berlin, Arnimallee 14, 14195 Berlin

The orientation of hexafluorobenzene (C_6F_6) molecules adsorbed on the Cu(111) surface has been studied by C K-edge near edge x-ray absorption fine structure spectroscopy (NEXAFS) for different adsorbate coverages. Photoelectron spectroscopy and temperature programmed desorption studies indicate distinct multilayer, bilayer, monolayer and half a monolayer phases. NEXAFS on these different coverages shows that the π^* absorption resonance has maximum intensity for the electric field vector perpendicular to the surface whereas it is substantially suppressed for the electric field vector in plane. Thus we propose that C_6F_6 molecules adsorb with the molecular plane parallel to the surface for all the investigated coverages. This observation differs from the adsorption of benzene where the molecules have random orientation in multilayers, interacting only through Van der Waals force. For C_6F_6 our results indicate a significant interaction between the C_6F_6 molecules leading to a preferential orientation in multilayers.

This work was supported by the Deutsche Forschungsgemeinschaft SPP1093.

O 30.5 Mo 11:45 TU EB301

Circular Dichroism in Core Level Photoemission from Tartaric Acid Adsorbed on Cu(110) — •JeongWon Kim, Jan Hugo Dil, Thorsten Kampen, and Karsten Horn — Fritz-Haber-Institut der MPG, Berlin

The adsorption of chiral molecules is an important step in the heterogeneous catalytic conversion of pro-chiral reagents into one of the possible optical isomers. Hence the occurrence of a chiral preference in adsorbed molecules has recently received considerable attention. While the arrangement of chiral molecules into a symmetry-breaking supramolecular structure has been demonstrated in scanning tunnelling microscopy, a direct identification of the presence of chiral centers has so far not been achieved. Here we demonstrate circular dichroism in carbon 1s core level photoemission from the (R,R) and (S,S) enantiomers of tartaric acid $[HOOC-(CHOH)_2-COOH]$ adsorbed on Cu(110). The asymmetry in the core level spectra excited with right- and left circularly-polarized light is readily observed, and changes sign with the handedness of the radiation, or upon changing the nature of the enantiomers. We characterize the circular dichroism in order to differentiate between that induced by the handedness of the experimental geometry (CDAD) and that induced by the chiral center in the adsorbed molecule.

O 30.6 Mo 12:00 TU EB301

Observing enantio selective adsorption: D and L cysteine on Au(17 11 9) — •Richard Schillinger[1], Joachim Wider[1,2], Christoph Quitmann[2], and Thomas Greber[1] — [1]Universität Zürich, Winterthurerstrasse 190, 8057 Zürich, Schweiz — [2]Paul Scherrer Institut, 5232 Villigen PSI, Schweiz

The conformation of chiral D and L cysteine (CYS) on the chiral gold surface Au(17 11 9) is directly determined by angle scanned x-ray photo electron diffraction (XPD).

This is realized by the use of a third generation synchrotron light source (the swiss light source), where the sensitivity of the experiments is pushed forward by two orders of magnitude.

For D and L cysteine we find in the 2π half space above the surface one single scattering maximum, though on different emission angles for L and D CYS, respectively. This demonstrates chiral hetero recognition, i.e. enantio selectivity of the S-kinks on Au(17 11 9).

O 30.7 Mo 12:15 TU EB301

Employing molecules as atomic assemblers under the tip of an STM — •Leo Gross[1], Francesca Moresco[1], Christian Joachim[2], André Gourdon[2], and Karl-Heinz Rieder[1] — [1]Institut für Experimentalphysik, Freie Universität Berlin, Arnimallee 14, D-14195 Berlin, Germany — [2]The Nanoscience Group, CEMES-CNRS, 29 rue J. Marvig, P.O. Box 94347, F-31055 Toulouse Cedex, France

Large organic, custom designed molecules, called HB-HPB (hexa-tert-butyl-hexaphenylbenzene) on Cu(111) are investigated by means of LT-STM. In combination with STM manipulation techniques, the self-ordering properties of the molecules can be exploited to assemble molecules in defined molecular structures. Moreover, the molecules can be utilized to move and aggregate Cu adatoms. This is an example of a single molecular nano-machine, performing the task of an atomic assembler under the operation of the STM tip.

O 30.8 Mo 12:30 TU EB301

XPS study on thiol adsorption on noble metal clusters supported on carbon substrates — •Michael Büttner and Peter Oelhafen — Institute of Physics, University of Basel, Klingelbergstr. 82, 4056 Basel, Switzerland

Submonolayers (0.1A to 1A) of noble metals (Au/Ag) have been deposited onto carbon substrates by means of thermal evaporation. After deposition, thiol vapor was introduced into the vacuum chamber through a leak valve to allow the molecules to adsorb on the metal surfaces. Thiols with long (hexadecanethiol) and short (propanethiol) chains were studied in this work. Additional annealing experiments were performed to investigate thiol desorption as a function of temperature. Between each preparation step the samples were measured with monochromated X-ray Photoelectron Spectroscopy (MXPS) and core-level spectra of the metal and the sulfur were obtained. MXPS valence-band spectra were taken to estimate the metal particle size and to monitor changes in the valence band shape and the Fermi edge upon thiol adsorption.

Shifts towards higher binding energy and changes in the line shape could be observed in the Au 4f core-level spectra after thiol adsorption. We will compare these findings with results for silver particles and comment on the influence of the thiol chain length.

O 30.9 Mo 12:45 TU EB301

Study of the intramolecular deformation of a Lander molecule during its Low Temperature STM manipulation on Cu(211) — •Micol Alemani, Francesca Moresco, Leo Gross, and Karl-Heinz Rieder — Inst. für Exp.physik, FU Berlin, Arnimallee 14, D-14195 Berlin

A detailed Low-Temperature Scanning Tunneling Microscope study of the controlled manipulation of a Lander molecule $C_{90}H_{98}$ adsorbed on Cu(211) is presented. By recording the tunneling current signal I(x) during the manipulation in constant-height-mode and by comparing it with calculations, we demonstrate that I(x) provides information on the mechanical movements of parts of the molecule that are not directly in interaction with the tip apex during the manipulation sequence. This is due to the fact that the intramolecular deformation induced by the manipulation can open other tunneling paths which are not directly located on the point of the molecule in close contact with the tip apex.

O 31 Organische Dünnschichten III

Zeit: Montag 10:45–13:00 Raum: TU EB420

O 31.1 Mo 10:45 TU EB420

Structural investigation of organic monolayers on Ag(111) using NIXSW — •C. Stadler, A. Schöll, S. Hansen, C. Kumpf, and E. Umbach — Exp. Physik II, Uni Würzburg, Germany

The investigation of the interaction of organic molecules with inorganic substrates is a key issue for the understanding of interface effects. We report on new NIXSW measurements on different organic monolayers with flat lying molecules on Ag(111). Information about the bonding distance of different atomic species in the molecule is obtained. In the case of the relaxed monolayer structure of NTCDA a value of 3.02 Å and 3.08 Å for O and C respectively, was measured, demonstrating that the molecule is truely chemisorbed on the surface, not only weakly physisorbed. For the oxygen atoms we also tried to resolve possible differences in the bonding strength for the two different oxygen species in the molecule by identifying core level shifts in the photoemission signal. Measurements on metallo-phthalocyanines have also been performed in order to study the position of the metallic atom with respect to the molecular plane and the substrate. Non-dipolar contributions to the photoemission yield are taken into account as well as electron induced effects on the Auger yield.

O 31.2 Mo 11:00 TU EB420

Epitaktisches Wachstum in organisch-organischen Heterosystemen: line-on-line-Koinzidenz — •T. Fritz, S.C.B. Mannsfeld und K. Leo — Institut für Angewandte Photophysik, TU Dresden, Germany

Die experimentelle Untersuchung des epitaktischen Wachstums zweier unterschiedlicher molekularer Spezies aufeinander führt zu Überstrukturmatrizen, die ein inkommensurables Wachstum nahe legen [1,2]. Dies steht jedoch im Widerspruch zur Tatsache, dass immer wieder die gleichen Anordnungen beobachtet werden. In unserem Beitrag schlagen wir einen neuen Epitaxietyp, die so genannte line-on-line-Koinzidenz (LOL) vor, mit dem sich z.B. das geordnete Wachstum von PTCDA auf HBC auf Graphit erklären lässt. LOL-Koinzidenz entspricht in soweit der bekannten point-on-line-Koinzidenz (POL), als dass die Moleküle der obersten Schicht alle auf parallelen gleichabständigen Gitterlinien der darunter liegenden Molekülschicht liegen. Der wesentliche Unterschied besteht jedoch darin, dass bei LOL im Gegensatz zu POL diese Linien nicht auf primitive Gitterlinien beschränkt sind. Mittels Potentialberechnungen weisen wir nach, dass dieser neue Epitaxietyp tatsächlich durch ein Minimum des Wechselwirkungspotentials zwischen den beiden Molekülschichten charakterisiert ist [2].

[1] T. Schmitz-Hübsch et al., Surf. Sci. **445**, 358 (2000).
[2] S.C.B. Mannsfeld et al., Phys. Rev. Lett., *submitted* (2004).

O 31.3 Mo 11:15 TU EB420

New insight into the physics of organic materials by the absence of surface core level shifts — •M. B. Casu, Y. Zou, S. Kera, D. Batchelor, Th. Schmidt, and E. Umbach — EPII, Universität Würzburg, Am Hubland, 97074 Würzburg

We present highly resolved X-ray photoemission measurements on various different organic materials taken at different photon energies and at different take-off angles in order to investigate Surface Core Levels Shifts (SCLS). Thin films of perylenetetracarboxylic acid dianhydride, coronene, and metal free phthalocyanine were deposited on Ag(111). Photoemission spectra of the C1s core levels evidence the absence of SCLS in organic thin films. We explain these results in terms of very efficient screening. If the molecular interaction is sufficiently strong, the screening of the created charge by rapid delocalisation is quite efficient. This implies that the influence of polarization on the determination of orbitals and gaps and on the electronic and transport properties of organics must be reconsidered taking this delocalization process into account. The idea of the electronic polarisation playing a major role in their electronic properties has to be rediscuss: the usual values considered for the polarisation energy are too high and not supported by the present SCLS nvestigation. This has a strong implication on the characterisation of interfaces in electronic devices, where concepts like band offsets or charge injection should be reconsidered under these new aspect.

O 31.4 Mo 11:30 TU EB420

The in situ observation of organic growth - a spectromicroscopic study of PTCDA and NTCDA on Ag(111) — •Th. Schmidt[1], U. Groh[1], H. Marchetto[2], R. Fink[3], and E. Umbach[1] for the SMART collaboration — [1]Exp. Physik II, Universität Würzburg, 97074 Würzburg — [2]Fritz-Haber-Institut, 14195 Berlin — [3]Phys. Chemie II, Univ. Erlangen, 91058 Erlangen

The growth of two similar molecules - PTCDA and NTCDA - on a Ag(111) surface has been studied *in situ* by the spectroscopic PEEM instrument SMART, using UV-light and polarized monoenergetic synchrotron radiation. Whereas PTCDA grows in a Frank-van der Merwe fashion bellow 300 K, the growth above room temperature is of the Stranski-Krastanov type in both systems: first two closed layers of molecules are formed, followed by three dimensional (3D) growth of islands. Strong differences are observed in the molecular orientations: whereas the PTCDA molecules are always flat-lying on the substrate, the NTCDA behaves differently: the molecules are also flat-lying in the double layer but tilted by about 45° in the islands. We report on surprising observations like reduced sticking coefficient, metastable layers, internal crystal structures, and dynamic changes within the layers. Differences in the growth and the temperature dependence of the two systems are discussed. Funded by BMBF under contract no. 05KS4WWB/4.

O 31.5 Mo 11:45 TU EB420

High resolution STM images of the PTCDA/Ag(111) interface — •A. Kraft, M. Rohlfing, and F. S. Tautz — School of Engineering and Science, International University Bremen, Campus Ring 8, D-28759 Bremen, Germany

We present a combined experimental and theoretical investigation of the detailed atomic structure of the interface between 3,4,9,10-perylene-tetracarboxylic-dianhydride (PTCDA) and Ag(111). The herringbone structure of the PTCDA/Ag(111) interface was imaged in a range of different tunneling conditions with a low-temperature scanning tunneling microscope (T =9K). Experimental images are compared to calculated images based on a density functional study of the complete interface. We use the generalized gradient approximation, localized basis orbitals, and a transfer-matrix formalism to evaluate the local density of states above the surface, which corresponds to the tunneling current (Tersoff-Hamann-theory) We find excellent agreement between experiment and calculations. Implications of our results for the precise structure of the interface are discussed.

O 31.6 Mo 12:00 TU EB420

LEED-IV for the structural investigation of the NTCDA monolayer on Ag(111) — •Christian Kumpf[1], Michael Scheuermann[1], Christoph Stadler[1], Eberhard Umbach[1], and Wolfgang Moritz[2] — [1]Experimentelle Physik II, Physikalisches Institut, Univ. Würzburg — [2]Sektion Kristallographie, Fakultät für Geowissenschaften, LMU München

The Low Energy Electron Diffraction-IV (LEED-IV) technique is a powerful tool for obtaining structural information of surfaces and is often used for the investigation of adsorbate systems or surface reconstructions on an atomic level. In the past this technique was frequently applied to inorganic systems. For organic adsorbates there is a severe demand for detailed structural information, like exact atomic coordinates, which would enable, e.g., detailed quantum chemical calculations. Even though the unit cells of organic adsorbates are often very large and beam damage effects may play an essential role, in some favorable cases LEED-IV can be used to investigate organic adsorbate systems.

We report on a LEED-IV study of a well ordered, coherent monolayer of NTCDA on Ag(111) (the so called relaxed monolayer structure). Important geometric parameters like the position of the molecules (height above the surface), their orientation within the unit cell as well as possible bending and deformation of the molecules were investigated. The effect of radiation damage is also addressed. The data are compared with results from other experimental methods (like, e.g., STM, XSW, NEXAFS and XPS).

O 31.7 Mo 12:15 TU EB420

Molecular resolution in non-contact atomic force microscopy: Experiments and force field calculations — •Tobias Kunstmann[1], Regina Hoffmann[2], Markus Fendrich[1], and Rolf Möller[1] — [1]Universität Duisburg-Essen, D-45141 Essen, Germany — [2]Universität Karlsruhe, D-76128 Karlsruhe, Germany

A scanning force microscope operated in the dynamic force mode has been used to analyze the arrangement of 3,4,9,10-perylenetetracarboxylic-dianhydride (PTCDA) molecules on a KBr surface. The molecules do not form a close-packed layer but crystallites with the shape of truncated pyramids. Even after depositing only 0.3 molecular layers of PTCDA, these crystallites have a height of 20-30 molecular layers. We have been able to resolve individual molecules of the top layer and on some of the crystallite's facets. Additionally, molecular force field calculations simulating a silicon tip on a layer of α-PTCDA(102) have been performed. For the frequency shift, we used the formula given by Garcia et al.[1]. The results agree well with the experimental data.

This work was funded by the SFB616 "Energy dissipation at surfaces"of the Deutsche Forschungsgemeinschaft.

[1] Ricardo García, Rubén Pérez, Surf. Sci. Rep. 47 (2002), 197

O 31.8 Mo 12:30 TU EB420

Effect of substrate structure on organic thin film morphology: Oligo-phenylenes on gold. — •Stefan Müllegger[1], Stefan Mitsche[2], Peter Pölt[2], Kathrin Hänel[3], Alexander Birkner[3], Christof Wöll[3], and Adolf Winkler[1] — [1]Institute of Solid State Physics, Graz University of Technology, Austria. — [2]Research Institute for Electron Microscopy, Graz University of Technology, Austria. — [3]Physikalische Chemie I, Ruhr Universität Bochum, Germany.

Thin films of organic semiconducting materials are attracting a growing interest both from a scientific and an applications point of view. In particular, the structure and morphology of such films are important, as they influence the (opto)electronic thin film properties. Based on our model systems, oligo-phenylene thin films grown on different Au surfaces by physical vapour deposition under UHV conditions, we demonstrate the significance of the geometric substrate structure for the development of highly anisotropic thin films. This is achieved by applying a properly prepared polycrystalline Au substrate, which comprises a large variety of differently oriented single-crystalline grains. We have applied multiple surface-sensitive techniques like secondary electron microscopy (SEM), electron backscattering diffraction (EBSD) and scanning tunnelling microscopy (STM), in order to reveal the effects of geometric anisotropy of the substrate on the structure and morphology of organic crystal growth. In particular, we could relate the orientation and terrace width of stepped (vicinal) Au surfaces to the orientation of the elongated organic crystals and the corresponding growth mode.

O 31.9 Mo 12:45 TU EB420

Die Wechselwirkung von 1,1'-Diisocyanoferrocen mit Gold: Selbstorganisierte Monolagen und supramolekulare Polymerisation — •T. Weidner[1,2], F. Träger[1,2], C. Bruhn[3,2], D. Rother[3,2], U. Siemeling[3,2], D. Fenske[4], A. Rothenberger[4] und A. Priebe[5] — [1]Institut für Physik, Universität Kassel, 34132 Kassel — [2]Center for Interdisciplinary Nanostructure Science and Technology - CINSaT, Universität Kassel, Heinrich-Plett-Str. 40, 34132 Kassel — [3]Institut für Chemie, Universität Kassel, 34132 Kassel — [4]Institut für Anorganische Chemie, Universität Karlsruhe, 76128 Karlsruhe — [5]Kirchhoff Institut für Physik, Universität Heidelberg, 69120 Heidelberg

Isocyanide sind wichtige Liganden in der Koordinations- und in der Oberflächenchemie. Durch unser Interesse an Nanostrukturen redoxaktiver Liganden und sind wir auf das bidentate 1,1'-Diisocyanoferrocene (1) aufmerksam geworden. Wir haben es im Hinblick auf seine Reaktion mit AuCl(SMe$_2$) und die Adsorption auf Goldoberflächen untersucht. Die Reaktion mit AuCl(SMe$_2$) ergibt ein unlösliches Koordinationspolymer $[(1)(\mathrm{AuCl})_2]_\infty$. Die (1)(AuCl)$_2$ Moleküle nehmen hierbei eine 3,4-Diaura-[6]ferrocenophan-Konformation ein. Sie aggregieren reissverschlussartig durch aurophile Wechselwirkungen. Die Adsorption von (1) auf polykristallinem Gold führt zur Bildung selbstorganisierter Monolagen. Messungen mit optischer Frequenzverdopplung ergeben eine Langmuirkinetik erster Ordnung. Mehrlagiges Filmwachstum konnte mit Ellispometrie ausgeschlossen werden. FTIR-Spektren zeigen eine Chemisorption beider Isocyanogruppen. Mit einiger Vorsicht kann die Struktur von $[(1)(\mathrm{AuCl})_2]_\infty$ als Modell der Adsorptionsgeometrie dienen.

O 32 Nanostrukturen III

Zeit: Montag 10:45–13:00 Raum: TU EB202

O 32.1 Mo 10:45 TU EB202

Quantendraht-Verhalten in einem metallischen Einkomponentensystem: monoatomare Cu/Cu(111)-Ketten — •Stefan Fölsch[1], Jérôme Lagoute[1], Per Hyldgaard[2], Fredrik E. Olsson[2], Mats Persson[2] und Klaus H. Ploog[1] — [1]Paul-Drude-Institut für Festkörperelektronik, Hausvogteiplatz 5-7, D-10117 Berlin — [2]Department of Applied Physics, Chalmers University of Technology, S-41296 Göteborg, Schweden

Mittels Tieftemperatur-Rastertunnelmikroskopie und -spektroskopie bei 7 K können monoatomare Cu-Ketten durch laterale Manipulation auf Cu(111) aufgebaut und hinsichtlich ihrer elektronischen Struktur charakterisiert werden. Für einzelne Cu-Adatome finden wir eine sp(z)-artige atomare Resonanz 3.3 eV über dem Fermi-Niveau [1]. In Cu-Ketten führt der Überlapp dieser Resonanzen zur Ausbildung von kettenlokalisierten Quantenzuständen, deren Dispersion vollständig durch ein eindimensionales (1D) Tight-Binding-Energieband einer Bandbreite von 1.8 eV beschrieben wird [2]. Die hier gefundene quasi-1D-Elektronendynamik in einem metallischen Einkomponentensystem stellt einen idealen Modellfall für einen Quantendraht dar, an dem der Effekt geknickter und verzweigter Drähte oder auch deren Wechselwirkung mit organischen Molekülen studiert werden kann. [1] F.E. Olsson et al., Phys. Rev. Lett. 93, 206803 (2004). [2] S. Fölsch et al., Phys. Rev. Lett. 92, 56803 (2004).

O 32.2 Mo 11:00 TU EB202

Kinks and junctions in assembled Cu/Cu(111) quantum wires studied by low-temperature scanning tunneling microscopy and spectroscopy — •Jérôme Lagoute, Xi Liu, and Stefan Fölsch — Paul-Drude-Institut für Festkörperelektronik, Hausvogteiplatz 5-7, D-10117 Berlin

Low-temperature STM-based atomic manipulation at 7 K was used to construct kinks and junctions in monatomic Cu chains on Cu(111). The juncture of these structures is stabilized by a compact Cu trimer while the extremities consist of close-packed monatomic Cu chains along the in-plane $\langle 110 \rangle$ directions (Cu-Cu spacing 255 pm). Starting from the fact that straight Cu/Cu(111) chains exhibit chain-localized quantum states, we have studied the local density of states (LDOS) of these structures of advanced complexity by spatially mapping the dI/dV signal at constant tip height. We find that the LDOS and the eigenstate energies of kinked and branched wires are well described by the LCAO (local combination of atomic orbitals) approach. The wave function confinement in these structures and the electronic implications of the juncture will be discussed in detail.

O 32.3 Mo 11:15 TU EB202

Field controlled growth of nanoscale adsorbate layers — •Carsten Nowak[1], Guido Schmitz[2] und Reiner Kirchheim[1] — [1]Institut für Materialphysik, Friedrich-Hund-Platz 1, D-37077 Göttingen — [2]Institut für Materialphysik, Wilhelm-Klemm-Str. 10, D-48149 Münster

In the presence of strong electrostatic fields at the apex of needle-shaped substrates the formation of amorphous layers with a field-dependent stationary profile can be observed. We attribute this to the attraction of residual gas molecules to the tip due to polarisation.

For a quantitative evaluation we derived a local polarisation potential, describing the polarisation interaction between an uncharged molecule and the tip.

Comparison with the experiment reveals that the shape of the deposited amorphous layers corresponds to equipotential surfaces of the polarisation potential. The formation of a stationary profile, corresponding to a certain tip voltage, can be explained by the transition of the residual gas molecules from the physisorbed to the chemisorbed state and therefore by the necessity to overcome the activation energy of chemisorption.

As this process is restricted to regions of strongest curvature, probably this mechanism can be made responsible also for the growth of nanowires by deposition of molecular gases that has been reported recently [1].

[1] S.-W. Cheng and H.-F. Cheung. Role of electric field on formation of silicon nanowires. J. Appl. Phys., 94(2):1190, 2003.

O 32.4 Mo 11:30 TU EB202

Tip-substrate interaction at the atomic scale — •A.L. Klavsyuk, V.S. Stepanyuk, R.Z. Huang, P. Bruno, and J. Kirschner — Max-Planck-Institut für Mikrostrukturphysik, Weinberg 2, 06120 Halle, Germany

Performing atomic-scale simulations with ab initio based many-body potentials we demonstrate that the concept of size-dependent mesoscopic relaxations introduced for homo-and heteroepitaxy[1] should be used to describe the interaction of the STM tip with adatoms, nanoislands and steps at the atomic scale. We concentrate on Co adatoms, islands on Cu(001), and embedded Co atoms in Cu(100). Strongly inhomogeneous deformations of the substrate and islands are revealed when the tip approaches the surface. The shape of islands, tip and the substrate is found to strongly depend on the island size and the tip-island distance. We show that atomistic processes in the early stages of growth, such as the diffusion of an adatom on a flat surface and on top of islands, are strongly influenced by the tip. The possibility of controlling the dynamics of single adatoms exploiting the tip-substrate interaction is discussed. We reveal an essential role of the mesoscopic stress induced by the tip on a controlled movement of single atoms of Co incorporated in the surface.
[1] O.V. Lysenko, V.S. Stepanyuk, W. Hergert, and J. Kirschner, Phys. Rev.Lett. **89**, 126102 (2002)

O 32.5 Mo 11:45 TU EB202

STM characterisation and tip-induced nanostructuring of surface-frozen interfaces in a Ga-Bi alloy — •Andrey Turchanin[1,2], Alexander Issanin[1], and Werner Freyland[1] — [1]Institut für Physikalische Chemie, Universität Karlsruhe (TH), Kaiserstr. 12, D-76128 Karlsruhe — [2]Fakultät für Physik, Universität Bielefeld, Universitätsstr. 25, D-33615 Bielefeld

We report results of a UHV-STM study of the Bi solid/vapour interface in a solidified Ga-Bi alloy after passing a surface freezing transition. The topology at room temperature is characterized by extended monoatomic Bi terraces with dimensions up to several micrometers. We show for the first time that the application of negative/positive pulses of the bias voltage in the constant current mode results in modification of the Bi interface in the nanometer regime. Particularly unusual is the observation, that deposition and withdraw of Bi is possible by changing the pulse polarity. In this way different nanostructures (cavities, grooves, islands, lines etc.) can be produced. They show unusually high thermal stability at room temperature. For instance, monoatomic cavities with a diameter of 6 nm persist at the surface for at least three weeks. To rationalize the nanostructuring mechanisms different parameters have been studied including the threshold values of the applied pulses and their dynamics. An analysis of these different parameters will be given.

O 32.6 Mo 12:00 TU EB202

STM-Induced Electroluminescence with a Transparent ITO-Tip — •Robert Branscheid[1], Heiko Rochholz[1], Volker Jacobsen[1], Maximilian Scherff[2], Wolfgang Knoll[1], and Maximilian Kreiter[1] — [1]MPI für Polymerforschung, Ackermannweg 10, D-55128 Mainz — [2]Fachbereich Bauelemente der Elektrotechnik, Fernuniversität Hagen, Haldenerstr. 182, D-58084 Hagen

A homebuilt STM combined with an efficient optical detection has been used to investigate photon maps of nano-structured gold substrates and disc-shaped single-particles. Common metal tips like Pt/Ir or W often show photon emission consistent with topographical features but presence of the metallic tip 'felt' by the sample provokes a strong influence on photon emission. Additional distortions caused by multiple-tip phenomena make a correct interpretation almost impossible. Therefore a dielectric tip consisting of indium doped tin oxide (ITO) has been compared with Pt/Ir. This material is assumed to be transparent for optical fields and should thus lead to less tip-induced modifications. As substrate nano-structured triangle patterns have been used showing a plasmon induced field enhancement. Furthermore disk-shaped gold particles have been investigated and isochromat photon maps have provided additionally spectral information.

O 32.7 Mo 12:15 TU EB202

Building Planar Molecular Networks by Polymerization — •Markus Wahl[1], Meike Stöhr[1], Thomas A. Jung[1,2], Hans-Joachim Güntherodt[1], and Lutz H. Gade[3] — [1]Institute of Physics University of Basel, Switzerland — [2]Paul-Scherrer-Institut, Villigen, Switzerland — [3]Institute of Anorganic Chemistry University of Heidelberg, Germany

Self-assembly of molecules on surfaces directed by different supramolecular interactions has been widely explored. Our aim is the formation of covalently linked planar structures by means of polymerization confined in one or two dimensions.

Recent experiments with a perylene derivative (DPDI) using differential thermoanalysis and gravimetry demonstrated that bulk DPDI can polymerize releasing ammonia. Inspired by this observation, we formed covalent networks on metallic surfaces and checked the feasibility of such an approach for the formation of other stable polymer-nanostructures.

For this purpose, thin films of DPDI were prepared on Cu(111) by evaporation in a UHV setup. The molecular arrangements were analyzed with a home-built STM. For a coverage of 1ML DPDI a 1D polymer chain pattern was observed after annealing the sample to 580K. For lower coverage in the range of 0.3 ML only a mobile phase was detected before annealing. However, upon annealing a stable 2D network with a honeycomb-like structure was observed which conveniently matches the angles and distances expected for the chemically feasible polymer structure.

O 32.8 Mo 12:30 TU EB202

Copper-phthalocyanine/Cu(001) as template for cobalt- nanodots — •C.X. Liu, H. L. Meyerheim, J Barthel, and Jürgen Kirschner — Max-Planck-Institut für Mikrostrukturphysik, Weinberg 2, D-06120 Halle

Preparation of metallic nanostructures require a special template for preferential adsorption. While for this purpose vicinal surfaces or dislocation networks are used quite frequently, large organic molecules deposited on flat substrate surface have only recently attracted interest[1]. Here we show that copper-phthalocyanine (CuPc) molecules deposited on Cu(001) at room temperature can be used to prepare a suitable template for preparing a metallic nanostructure. Depending on the CuPc-coverage we find different CuPc-superstructures. A "relaxed"one at a coverage of one monolayer (i.e. a complete layer of molecules), which we assign to a quadratic (5 3 -3 5) unit-cell in matrix notation, and a "compact"one corresponding to a coverage of about 1.5 monolayers. For the latter, STM indicates the formation of a stripe structure, where the stripes are formed by molecules aligned in columns parallel to the $< 110 >$ substrate directions. The stripes are up to 100 nm long, their lateral separation (1.3 and 2.6 nm) gives rise to a (10x1) LEED-diffraction pattern. Subsequently deposited Co ($\approx$ 0.3-0.5 ML; $1ML = 1.53 \times 10^{15} atoms/cm^2$)is found to adsorb in monolayer thick islands (diameter $\approx$ 5nm) aligned parallel to the stripes keeping the short range ordering intact. Magnetic hysteresis loops are observed in longitudinal geometry above about 0.5 ML at 50K.
[1] X. Ma, et al., Appl. Phys. Lett. **84** (2004) 4038

O 32.9 Mo 12:45 TU EB202

One dimensional metal-organic chains on Cu(110): Cu-TMA (trimesic acid) and Fe-TMA — •Thomas Classen[1], Giovanni Costantini[1], Frank Stadler[1], Cheolkyu Kim[1], Klaus Kern[1], Guido Fratesi[2], Stefano Fabris[2], Stefano de Gironcoli[2], and Stefano Baroni[2] — [1]Max-Planck-Institut für Festkörperforschung, Heisenbergstr. 1, 70569 Stuttgart — [2]SISSA and INFM DEMOCRITOS National Simulation Center, Via Beirut 2-4, I-34014 Trieste, Italy

One dimensional (1D) metal-organic coordination networks have been created on Cu(110) using self-organized growth. Trimesic acid (TMA) and Fe have been deposited in ultra-high-vacuum (UHV) by means of organic and conventional molecular beam epitaxy respectively. TMA deposition on Cu(110) results in the formation of metal-organic chains with Cu adatoms supplied from the step edges. The chains are mono-disperse and are oriented along the $\langle 1\bar{1}0\rangle$ substrate direction. By deposition of Fe also Fe-TMA chains were produced with a noticeably different morphology. Both chain types have been investigated using variable temperature scanning tunnelling microscopy in UHV and density functional theory in the generalized gradient approximation (DFT-GGA). The DFT-calculations predict a spin-polarization for the Fe atoms in the Fe-TMA chains. This opens the possibility to study a low dimensional magnetic system thermally stabilized by organic linker molecules.

O 33 Teilchen und Cluster II

Zeit: Montag 10:45–13:00 Raum: TU EB107

O 33.1 Mo 10:45 TU EB107

Optische Eigenschaften von Goldnanopartikelpaaren — •Christian Dahmen, Benjamin Schmidt und Gero von Plessen — I. Physikalisches Institut (IA), RWTH Aachen, D-52056 Aachen

Bei der gegenseitigen Annäherung von Edelmetallnanopartikeln bis auf wenige Nanometer Abstand entstehen aufgrund der elektromagnetischen Kopplung zwischen den Nanopartikeln ausgedehnte Plasmonenmoden. Die dadurch auftretenden hohen Feldstärken in der direkten Umgebung des Nanopartikelpaares werden für die Verstärkung nichtlinearer Effekte z.B. bei der oberflächenverstärkten Raman-Streuung verantwortlich gemacht. In dieser Arbeit werden für Paare sphärischer Goldnanopartikel Extinktionsquerschnitte sowie elektromagnetische Nah- und Fernfelder berechnet. Mittels der Verallgemeinerten Mie-Theorie wird an diesem Modellsystem die elektromagnetische Kopplung zwischen Plasmonenmoden sowie die Entstehung großer elektromagnetischer Feldstärken im Zwischenraum der Partikeloberflächen untersucht.

O 33.2 Mo 11:00 TU EB107

Optische Spektren massenselektierter Goldcluster auf MgO — •Matthias Alschinger[1], Marcel Di Vece[2], Frank Hubenthal[1], Richard E. Palmer[2] und Frank Träger[1] — [1]Institut für Physik und Center for Interdisciplinary Nanostructure Science and Technology - CINSaT, Universität Kassel, Heinrich-Plett-Str. 40, 34132 Kassel — [2]Nanoscale Physics Research Laboratory, School of Physics and Astronomy, The University of Birmingham, Edgbaston, Birmingham B15 2TT, UK

Wir stellen Experimente vor, bei denen die Extinktionsspektren kleiner Golddcluster, die zwischen 300 und 4000 Atomen enthalten, gemessen wurden. Hierzu wurden Goldcluster mit Hilfe einer Magnetron-Sputterquelle hergestellt, anschließend massenselektiert und mit Energien zwischen 0,6 keV und 3,9 keV pro Cluster auf einem Substrat aus Magnesiumoxid deponiert. Aufgrund der Größe der Cluster ist dabei die Energie pro Atom in der Größenordnung von wenigen eV, d.h. im Energiebereich des *soft-landing*. Die optischen Spektren wurden mit p-polarisiertem Licht unter einem Einfallswinkel von 45° gemessen. Goldcluster, die zwischen 300 und 2000 Atome enthalten, zeigen eine sehr schmale Plasmonresonanz bei Photonenenergien um 2,5 eV. Dies steht in Einklang mit Experimenten von Palpant et al. an in Al_2O_3 eingebetteten Goldclustern, die jedoch auf Grund der recht breiten Größenverteilung eine deutlich breitere Plasmonresonanz aufweisen [1]. Für Au_{4000} wurde hingegen eine breite Plasmonresonanz bei 2,2 eV beobachtet.

[1] B. Palpant et al., Phys. Rev. B **57**(3), 1963 (1998)

O 33.3 Mo 11:15 TU EB107

Photoelectron spectroscopy of "free clusters on surfaces" — •T. Irawan[1], D. Boecker[1], F. Ghaleh[1], I. Barke[1], H. Hövel[1], C. Yin[2], and B. von Issendorff[2] — [1]Experimentelle Physik I, Universität Dortmund, D-44221 Dortmund — [2]Fakultät für Physik, Universität Freiburg, D-79104 Freiburg

The interaction with a surface can change the electronic structure of clusters significantly compared to the corresponding free clusters. We plan to study this with the direct comparison of photoelectron spectroscopy for mass selected clusters deposited on surfaces and the same clusters studied in a free cluster beam. Here we present experiments which were performed as a preparatory work for these deposition experiments. Metal clusters (gold and lead) were produced by island growth on rare gas layers on different surfaces (HOPG, Au(111) and Pb(111)) by deposition of metal atoms [1]. The electronic coupling to the surface and charging effects in the photoemission process were studied with UPS. We observed significant energetic shifts if the islands were decoupled from the surface by the rare gas layer and different materials for the substrate and the clusters were used. This can be interpreted as the limit of "free clusters on surfaces".

[1] V.N. Antonov, J.S. Palmer, A.S. Bhatti, J.H. Weaver, Phys. Rev. B **68**, 205418 (2003).

O 33.4 Mo 11:30 TU EB107

Multi-step laser tailoring for the production of monodisperse metal nanoparticles — •D. Blazquez, N. Borg, C. Hendrich, F. Hubenthal und F. Träger — Experimentalphysik I, Institut für Physik und Center for Interdisciplinary Nanostructure Science and Technology - CINSaT, Universität Kassel, Heinrich-Plett-Straße 40, D-34132 Kassel

We have produced metal nanoparticles (NP) by deposition of atoms on dielectric substrates followed by diffusion and nucleation. This usually leads to rotational ellipsoidal NP with broad size and shape distributions. As demonstrated earlier, particles of undesired size can be removed with nanosecond laser pulses. The technique is based on the size and shape dependent surface plasmon resonance (SPR) frequencies of metal NP and allowed us to prepare nanoparticles with a size disribution as narrow as about 10 %. Here, we describe recent experiments to explore the potential of the method to further narrow the size distribution. Using continuously tunable laser light Ag NP on quartz substrates have been tailored in a multi-step process. The nanoparticles were characterized by atomic force microscopy and optical spectroscopy. The potential of the method will be discussed.

O 33.5 Mo 11:45 TU EB107

Preparation and characterization of fully oxidized TiO_2 films on Ru (0001) and of $Au/TiO_2/Ru(0001)$ model catalysts — •zhong zhao, T. Diemant, H. Rauscher, and R.J. Behm — Abt.Oberflächenchemie und Katalyse, Universität Ulm, 89069, Ulm

As part of an effort to study CO oxidation on Au/TiO_2 model catalyst, we investigated the growth, structure and chemical composition of completely oxidized TiO_2 films (thickness ca. 10 monolayers (ML)) on a Ru(0001) substrate, and Au/TiO_2 model catalysts prepared by Au evaporation on these films (catalytic properties of these model systems see [1]). Atomic resolution STM images show that after Ti deposition in O_2 (640 K) and annealing in O_2 , the TiO_x film is closed, relatively flat, and consists of TiO_2 (110). Upon room temperature Au evaporation and at lower Au coverages ($\leq$0.2) ML Au nanoparticles nucleate preferentially at steps, a small fraction of them nucleates at defect sites on the TiO_2 terraces. With higher Au coverages, the Au particles grow increasingly on the whole surface. UHV annealing at 770 K (10 min) causes the Au clusters to grow, but different from Pt/TiO_2 [2] we find no encapsulation by TiO_2. The stability of the Au nanoparticles is discussed, comparing with recent findings for Au/TiO_2 (110) model catalysts [3]. [1] T. Diemant, Z. Zhao, H. Rauscher, and R.J. Behm, DPG Spring Meeting, AKF Surface Physics, Berlin (2005) [2] O. Dulub, W. Hebenstreit, and U. Diebold, Phys. Rev. Lett. 84, 3646 (2000) [3] S. Kielbassa, M. Kinne, and R.J. Behm, J. Phys. Chem. B, in press

O 33.6 Mo 12:00 TU EB107

Einfluß von Substraten auf die elektronischen Eigenschaften ligandenstabilisierter Metallcluster — •Huijing Zhang, Holger Grzeschik und Uwe Hartmann — Fachrichtung Experimentalphysik, Universität des Saarlandes, 66123 Saarbrücken

Anders als Massivmaterialien können die elektronischen Eigenschaften von Clustern sehr von ihrer Umgebung beeinträchtigt werden, insbesondere wenn die Anzahl der Oberflächenatome des Clusters größer als die der inneren Atome ist. Es wurden ligandenstabilisierte Au_{55}-Cluster mittels Rastertunnelmikroskopie und -spektroskopie hinsichtlich des Elektronentransports durch die Cluster und der Energiequantisierung der Cluster jeweils auf 3 verschiedenen Substraten, Au(111), HOPG und $NbSe_2$, untersucht. Die per Spin-Coating deponierten Cluster weisen auf der Au(111) Oberfläche eine lokal geordnete Monolage auf. Diese wurde jedoch bei Verwendung von anderen Substraten nicht beobachtet, was auf eine stärkere Wechselwirkung zwischen Au_{55} und Au(111) als zwischen Au_{55} und HOPG und $NbSe_2$ hindeutet. Tunnelspektren zeigen, daß der Elektronentransport durch Cluster nicht von den elektronischen Eigenschaften der Substrate oder der Ligandenmolekülen sondern vom Einzelelektronen-Tunneleffekt dominiert wird. Die Wechselwirkung zwischen Clustern und Substraten könnte jedoch eine Verschiebung der Energiezustände des Clusterkerns verursachen.

O 33.7 Mo 12:15 TU EB107

Dynamic force microscopy and spectroscopy investigations of Au_{55} on Au(111) — •Georgeta Radu, Dirk Mautes, and Uwe Hartmann — Fachrichtung Experimentalphysik, Universität des Saarlandes, Postfach 151150, D-66041 Saarbrücken, Deutschland

Non-contact atomic force microscopy (NC-AFM) and spectroscopy were used to study thin films of ligand-stabilized Au_{55} clusters deposited on Au(111). The clusters were dissolved in dichlormethane (CH_2Cl_2) and deposited onto a freshly prepared Au(111) substrate by spin coating. The deposit consist of a layer of single cluster height covering the Au(111) substrate. The NC-AFM images show many local areas where the clusters are arranged in a 2D closest packing alternating with areas showing the bare substrate. Frequency shift- and dissipation-versus-distance measurements on individual clusters as well as on the bare substrate were performed. The distance dependence of the interaction force was calculated from the experimental frequency-versus-distance curves for individual clusters as well as for the Au(111) substrate. On the basis of the results, a model of the tip-cluster and tip-substrate interaction force will be presented. Different distance dependencies of the dissipation curves taken on clusters and on the substrate were found. Dissipation mechanisms for the tip-cluster and tip-substrate interaction will be discussed.

O 33.8 Mo 12:30 TU EB107

Herstellung von Gold-Nanoteilchen einheitlicher Form auf dielektrischen Substraten mittels lasergestützten Wachstums — •N. Borg, D. Blazquez, C. Hendrich, H. Ouacha, F. Hubenthal und F. Träger — Institut für Physik und Center for Interdisciplinary Nanostructure Science and Technology - CINSaT, Universität Kassel, Heinrich-Plett-Straße 40, D-34132 Kassel

Auf dielektrischen Oberflächen können metallische Nanoteilchen (NT) durch selbstorganisiertes Wachstum hergestellt werden. Solche Proben weisen in der Regel eine breite Größen- und Formverteilung der NT auf. Dabei besteht ein definierter Zusammenhang zwischen Größe und Form der NT: Kleine NT sind kugelförmig, während große die Form flacher Rotationsellipsoide aufweisen.

Ein in unserer Arbeitsgruppe entwickeltes Verfahren erlaubt es, metallische NT mit vorgegebenem Achsverhältnis und variabler Größe zu präparieren und wurde bereits für Silber-NT auf verschiedenen Substraten demonstriert. Es basiert auf den einzigartigen optischen Eigenschaften und deren Abhängigkeit von Größe und Form metallischer NT. Dabei wird während des Wachstums mittels Einstrahlung von ns-Laserpulsen geeigneter Wellenlänge der Zusammenhang zwischen Größe und Form der NT aufgehoben. Wir haben die Einflüsse von Wellenlänge und Fluenz des Laserlichts auf das Wachstum von Gold-NT auf Saphir- und Quarzsubstraten systematisch mit optischer Spektroskopie und Rasterkraftmikroskopie untersucht. In Abhängigkeit der genannten Parameter lässt sich das mittlere Achsverhältnis der Gold-NT zwischen 0,19 und 0,98 unabhängig von deren Größe stabilisieren.

O 33.9 Mo 12:45 TU EB107

Photoelektronenspektroskopie an PbS- Nanokristalloberflächen — •J. Tobias Lau[1], Arun Lobo[2], Mona Nagel[3], Holger Borchert[3], Stephen Hickey[3], Horst Weller[3] und Thomas Möller[1] — [1]Technische Universität Berlin, IAPF PN 3-1, Hardenbergstraße 36, 10623 Berlin — [2]HASYLAB/DESY, Notkestraße 85, 22603 Hamburg — [3]Universität Hamburg, Institut für Physikalische Chemie, Grindelallee 117, 20146 Hamburg

Viele Eigenschaften von Nanokristallen werden durch die Eigenschaften ihrer Oberfläche bestimmt; daher ist es notwendig, detaillierte Informationen über die Struktur dieser Oberfläche und über die Bindungen zwischen Oberflächenatomen und Liganden zu gewinnen. Dazu wurden unter anderem nasschemisch präparierte PbS-Nanokristalle im Größenbereich von 3–10 nm und mit einer engen Größenverteilung mittels Röntgenphotoelektronenspektroskopie untersucht. Die Pb *4f*- und S *2p*-Niveaus werden sowohl bei oberflächen- als auch volumensensitiven kinetischen Energien analysiert. Dabei ergeben sich die Pb *4f*-Niveaus zwei und die S *2p*-Niveaus vier Komponenten, die jeweils Atomen mit unterschiedlicher lokaler Koordination zugeordnet werden. Es zeigt sich, dass die Bindungsverhältnisse an der Oberfläche des Nanokristalls von der Art der Liganden abhängen.

O 34 Rastersondentechniken II

Zeit: Montag 10:45–13:00 Raum: TU EB407

O 34.1 Mo 10:45 TU EB407

Investigation of the statistics of stick-slip friction on graphite — •Lars Jansen[1,2], André Schirmeisen[1,2], and Harald Fuchs[1,2] — [1]Physikalisches Institut, Westfälische Wilhelms-Universität, Wilhelm-Klemm-Str. 10, 48149 Münster — [2]CeNTech, Center for Nanotechnology, Gievenbecker Weg 11, 48149 Münster

The stick-slip mechanism is believed to be one fundamental process of atomic friction. It is described by the Tomlinson model for zero temperature [1]. In this model a tip jumps between two equilibrium positions of a surface potential. The lateral forces, inducing the jump are called jump heights. For finite temperatures these jump heights follow a statistical distribution due to thermal excitation [2]. We measured stick-slip friction on the atomic scale with an AFM and we will introduce a new analysis method to extract the statistical information i.e. the corresponding jump height histograms from the experimental data, acquired with a Si-tip on a vacuum cleaved HOPG surface under ultra high vacuum conditions. These histograms are in good quantitative agreement with the theoretical model [3]. From the histograms we can extract quantitative values for the effective energy barrier. We find that the energy barrier depends strongly on the exact position of the tip within the surface potential. As a result of this the theoretical model has to be expanded to two dimensions. Furthermore we can confirm that the histogram shape depends sensitively on the measurement parameters like scan speed and normal load, as predicted by the theory. [1] Tomlinson, Phil. Mag. 7 (1929), [2] Gnecco et al., PRL 84 (2000), [3] Sang et al., PRL. 84 (2001)

O 34.2 Mo 11:00 TU EB407

Interface dependent frictional forces: Study of amorphous and crystalline nanoparticles by dynamic scanning force microscopy — •Claudia Ritter[1], Udo D. Schwarz[2], Markus Heyde[1,3], and Klaus Rademann[1] — [1]Humboldt-Universität zu Berlin, Institute of Chemistry, Brook-Taylor-Str. 2, D-12489 Berlin, Germany — [2]Department of Mechanical Engineering, Yale University, P.O. Box 208284, New Haven, CT 06520-8284, USA — [3]Fritz-Haber-Institute of the Max-Planck-Society, Faradayweg 4-6, D-14195 Berlin, Germany

The fundamentals of friction, in particular, the interplay between friction, adhesion, true contact area and crystalline structure at the interface, are still insufficiently understood. In this investigation, antimony nanoparticles grown on HOPG and MoS2 were used as a model system to investigate the contact area dependence of frictional forces. The morphology of the nanoparticles was characterized by Scanning Force Microscopy (SFM) and Electron Microscopy (SEM, TEM). Thus, both the interface structure and the real contact area were accurately determined. The TEM study revealed a size dependent amorphous-polycrystalline phase transition. Controlled translation of the particles was induced by the action of the oscillating tip in dynamic mode SFM. During manipulation, the power dissipated due to tip-sample interactions was recorded. Particles with contact areas below 10000nm2 were much easier to move compared to their larger counterparts. We suggest that structural lubricity might be the reason for the low dissipation in the small amorphous particles, while elastic multistabilities might dominate energy dissipation in the larger polycrystalline particles.

O 34.3 Mo 11:15 TU EB407

Adhesion force measurements for well-defined probe - sample geometries — •Bert Stegemann, Henrik Backhaus, Heinz Kloss, and Erich Santner — Bundesanstalt für Materialforschung, BAM - VIII.1 Tribologie und Verschleißschutz, Unter den Eichen 44-46, D-12205 Berlin

Adhesion is of fundamental importance for the tribological behavior, e.g., in nanomechanical devices. A promising approach to determine interfacial adhesion at sub-micron scale is to measure pull-off forces with an atomic force microscope (AFM). As adhesion depends on numerous factors, such as contact area, environment and dynamics, there is still a lack of reliable quantitative data. Here, we report on a systematic analysis of AFM pull-off forces for well-defined systems under ultrahigh vacuum conditions. Interaction geometry is controlled by means of colloid AFM probes, i.e., microspheres attached at the end of bare AFM cantilevers. Clean sample surfaces of a wide range of single crystal metals and compound materials were prepared by subsequent Ar ion sputtering and annealing as affirmed by surface analytical techniques. The influence of experimental parameters, like applied load, contact time and contact area on the pull-off forces is discussed. The results obtained are compared with predictions from theoretical models and correlated with macroscopic mechanical properties of the materials.

O 34.4 Mo 11:30 TU EB407

Nanoindentation with Atomically Defined Tips — •Andre Schirmeisen[1] und Graham Cross[2] — [1]Center for Nanotechnology (CeNTech), University of Münster, Wilhelm-Klemm-Str.10, 48149 Münster — [2]SFI Trinity Nanoscience Bldg, Trinity College, Dublin 2, Ireland

An atomically defined tungsten asperity of 3 nm radius was fabricated and imaged by field ion microscopy and brought into contact with a Au(111) terrace in ultra-high vacuum conditions. The mechanical evolution of the asperity contact under cyclic indentation testing was monitored by a simultaneous load-displacement and electrical current-displacement measurement. Adhesive forces of 10 nN consistent with short range chemical bonding were measured. Compressive loads of up to 100 nN under displacements of 1.5 nm, equivalent to 5 atomic gold layers, were recorded. Load displacement curves of the pristine surface showed multiple pop-in events during loading, which indicate the creation of nanoscale dislocations in the sample material. More interestingly, during unloading, we found correlated pop-out events, which indicate the occurrence of complete self-healing of the induced dislocation. The energy dissipated during those reversable dislocation creation and healing events can be directly measured in our experiments. These values are in good agreement with recent molecular dynamics simulations of incipient plasticity in asperity contacts.

O 34.5 Mo 11:45 TU EB407

Atomic transfer and single-adatom contacts — •Laurent Limot[1], Jörg Kröger[1], Richard Berndt[1], Aran Garcia-Lekue[2], and Werner A. Hofer[2] — [1]Institut für Experimentelle und Angewandte Physik,Christian-Albrechts-UniversitÄat zu Kiel, D-24098 Kiel, Germany — [2]Surface Science Research Centre, University of Liverpool, Liverpool L69 3BX, United Kingdom

How do mechanical and transport properties change as matter is sized down to the atomic scale? Proximity probes like the Scanning Tunneling Microscope (STM), metal break junctions and related techniques, together with computational methods for simulating tip-sample interactions with atomic detail, have enabled to address this question by investigating atomic-size contacts to the surface. We employed a low temperature STM to investigate the point contact of the tunnel tip when approached towards Ag(111) and Cu(111) surfaces. On these metallic surfaces, a sharp jump-to-contact, random in nature, is observed in the conductance. Images acquired after point contact show that the tip-apex atom is transferred to the surface, suggesting that a one-atom contact is formed during the approach. In sharp contrast, the conductance over single silver and copper adatoms exhibits a smooth and reproducible transition from tunneling to contact regime. Numerical simulations indicate that this is a consequence of the increased stiffness of the adatom-contact.

O 34.6 Mo 12:00 TU EB407

Nanomechanical tuning of an optical near-field interaction resonance — •Thomas Taubner[1], Fritz Keilmann[2], and Rainer Hillenbrand[1] — [1]Nano-Photonics Group, Max-Planck Institut für Biochemie, 82152 Martinsried — [2]Abt. Molekulare Strukturbiologie, Max-Planck Institut für Biochemie, 82152 Martinsried

We use a scattering-type near-field optical microscope (s-SNOM) to experimentally demonstrate the controlled shift of a near-field optical polaritonic resonance. Therefore we study both amplitude and phase of light scattered from a metallic s-SNOM's tip probing a flat SiC sample, at mid-infrared frequencies where surface phonon polaritons resonantly enhance the tip-sample near-field interaction [1]. Especially, we concentrate on effects of varying the gap width between tip and the sample. We find that a decreasing distance causes a red-shift of the resonance, accompanied by strong optical phase changes [2]. Both effects can be explained by theory that treats the system as a point dipole (tip) interacting with its image dipole (sample), in electrostatic approximation. Tuning the polaritonic resonance of a nanosystem by adjusting nanometric distances could be applied to control confinement and transport of light in nanoassemblies [2].

[1] R. Hillenbrand, T. Taubner and F. Keilmann, Nature **418**, 159 (2002)

[2] T.Taubner, F.Keilmann and R. Hillenbrand, Nano Letters **4**, 1669 (2004)

O 34.7 Mo 12:15 TU EB407

Crystallinity Mapping of SiC-surfaces by Infrared Near-field Microscopy — •Andreas Huber, Nenad Ocelić und Rainer Hillenbrand — NanoPhotonics Group, Max-Planck-Istitut f. Biochemie, Martinsried

We exploit phonon-enhanced near-field interaction [1] in an infrared scattering-type scanning near-field optical microscope (s-SNOM) for mapping the structural properties of SiC crystals at nanoscale resolution.

Imaging is done by a s-SNOM in which the probing tip of an AFM is illuminated by infrared light (λ = 9-11 μm). Along with the topography the backscattered light is recorded, thereby measuring the complex-valued optical near-field signal originating from the tip-sample near-field interaction. The scattered light exhibits a phonon-polariton resonance close to the LO-frequency in a polar material. The magnitude and spectral position of this resonance is extremely sensitive to the sample's local dielectric function ϵ. Thus this resonance acts as an optical fingerprint of the materials properties. This is experimentally confirmed by s-SNOM imaging of lattice damage in a 6H-SiC crystal induced by focused ion beam implantation (FIB)[2]. The sensitivty of this method is confirmed by differentiating 4H - and 6H - SiC polytypes at nanoscale resolution.

Altogether, spatial monitoring of the local phonon-resonance in s-SNOM could be a useful tool to characterise SiC.

[1] R.Hillenbrand, T.Taubner, F.Keilmann, Nature 418, 159-162 (2002).

[2] N.Ocelic, R.Hillenbrand, Nature Materials 3, 606-609 (2004)

O 34.8 Mo 12:30 TU EB407

Laterally resolved electrical characterization of ultrathin oxides — •Herbert Wormeester, Marko Sturm, Andrey Zinine, Radko Bankras, Jisk Holleman, Jurriaan Schmitz, and Bene Poelsema — MESA+ Institute for Nanotechnology, Universiteit Twente, Enschede, The Netherlands

A non-contact AFM with a conducting tip was used to image both the topography and electrical properties of a 2.5 nm thick aluminumoxide film on Si(001). These films were grown with Atomic Layer Deposition (ALD). Large protrusions are observed on the surface, whose contrast depends on the applied bias voltage. They are the result of an electrostatic interaction between tip and a fixed charge. A quantitative understanding of these features is only feasible if not only the image charge in the tip is evaluated, but also the image of the tip in the silicon is taken into account. The Contact Potential Difference (CPD) of the surface was evaluated with and without the use of lock-in technique (1f signal). The similarities and differences of these measurements will be discussed. A 60 mV change in CPD over the surface was found to correlate with the topography. The local variation of the capacitance (2f signal) was found to negatively correlate with the topography, i.e. a larger height correlates to a lower capacitance. On a siliconoxide film with similar thickness and roughness, a lower variation of the capacitance was found to be uncorrelated with the roughness. These seemingly conflicting results can be attributed consistently to different growth modes of the oxide films.

O 34.9 Mo 12:45 TU EB407

SNOM-Untersuchungen zur Beeinflussung der Plasmonenausbreitung durch strukturierte dielektrische Deckschichten — •Stefan Griesing, Andreas Englisch und Uwe Hartmann — Fachrichtung Experimentalphysik, Universität des Saarlandes, Im Stadtwald, 66123 Saarbrücken

Oberflächenplasmonen zeichnen sich durch zweidimensionale Ausbreitung an der Grenzschicht Metall/Dielektrikum aus. Im roten Spektralbereich ist die Propagationslänge maximal, und der Betrag der Tangentialkomponente des Wellenvektors (ktan) ist von derselben Größenordnung wie der des Wellenvektors im Dielektrikum. Untersuchungen wurden am System Silber/PMMA durchgeführt. Durch strukturieren mittels Elektronenstrahllithografie wurden im Dielektrikum Gebiete mit unterschiedlichem ktan erzeugt. Über die Änderung der Schichtdicke des PMMA zwischen 30 nm und 250 nm konnte der Wellenvektor im Vergleich zum System Silber/Luft bis zu einem Faktor 1,40 vergrössert werden. Zur Plasmonenanregung diente eine Kretschmann-Raether-Konfiguration. Mit dem SNOM ließ sich die Plasmonenfahne bis zu 100 Mikrometer entfernt vom einkoppelnden Laserspot detektieren. Es wurde das Verhalten der Plasmonen beim Auftreffen auf PMMA-Strukturen studiert. Der einfachste Fall des geradlinigen Übergangs von Gebieten mit PMMA-Deckschicht zu Gebieten ohne PMMA-Deckschicht zeigte eine winkelabhängige Ablenkung des Plasmonenstrahls in der Ebene, was durch ein Brechungsgesetz analog zur klassischen Optik beschrieben werden kann. Weiterhin wurde das Verhalten beim Auftreffen auf aus der klassischen Optik bekannte Elemente wie Linsen, Gitter und Prismen untersucht.

O 35 Hauptvortrag Dose (R.W. Pohl-Preis)

Zeit: Montag 14:00–14:45 Raum: TU EB301

Hauptvortrag O 35.1 Mo 14:00 TU EB301

Die Bayes'sche Variante — •Volker Dose — Max-Planck-Institut für Plasmaphysik, Boltzmannstraße 2, Garching bei München – Träger des Robert-Wichard-Pohl-Preises

Physiker scheuen weder Mühe noch Sorgfalt, um mit Hilfe hoch komplizierter Apparaturen ihre experimentellen Daten zu gewinnen. Vergleichsweise unbedeutend ist dagegen im Allgemeinen der Aufwand, der betrieben wird, um von den gewonnenen Daten zur physikalischen Erkenntnis zu gelangen. Für diesen zweiten Schritt gibt es aber eine systematische Vorgehensweise, nämlich die Bayes'sche Wahrscheinlichkeitstheorie. Die Theorie wird kurz erläutert und ihre Leistungsfähigkeit wird an mehreren Beispielen – u. a. aus der Oberflächenphysik – demonstriert.

O 36 Postersitzung (Elektronische Struktur, Grenzfläche fest-flüssig, Halbleiteroberflächen und -grenzflächen, Nanostrukturen, Oberflächenreaktionen, Teilchen und Cluster, Struktur und Dynamik reiner Oberflächen)

Zeit: Montag 15:00–18:00 Raum: Poster TU F

O 36.1 Mo 15:00 Poster TU F

A Four Point Probe Investigation of the Surface Conductivity of Si(111)-7x7 — •J. Wells[1], T.M. Hansen[2], and Ph. Hofmann[1] — [1]iNano Center, Aarhus University, Aarhus, Denmark — [2]National Institute for Materials Science (NIMS), Nanomaterials Laboratory (NML), Tsukuba, Japan

An in-vacuum 4 point probe has recently been developed which allows more direct measurements of conductivity to be made than is possible with non-contact methods. As a demonstration of the technique, Si(111)-7x7 has been measured under UHV conditions between 70 K and 300 K. Although this surface has already been studied with many techniques, the nature of the surface conductivity still remains unclear and published estimates vary between $10^{-9}\Omega^{-1}$ and $10^{-4}\Omega^{-1}$.

The silicon surface has been modeled as an infinite sheet separated from a semi-infinite bulk by a charge depletion layer. When the probe spacing is sufficiently small, and at low temperatures, the 4 point probe conductivity is saturated by the surface component whereas at higher temperatures (or larger probe spacings), the bulk component dominates the measurement. Between these two extremes, the measurement is limited by the conduction across the charge depletion layer, and this is temperature dependent.

Our measurements show that the temperature dependence of the conductivity is accurately described by this model. Both the high and low temperature saturations are observable, and from this, this surface conductivity is estimated as 6 x $10^{-9}\Omega^{-1}$, consistent with a semiconducting surface state.

O 36.2 Mo 15:00 Poster TU F

H/Pt(110): Atypical chemisorption and its influence on quasi-one-dimensional surface states — •Alexander Menzel[1], Enrico Dona[1], Mariana Minca[1], Zhenrong Zhang[1], Erminald Bertel[1], Rinaldo Zucca[2], and Josef Redinger[2] — [1]Phys. Chemie, Univ. Innsbruck, A-6020 Innsbruck — [2]CCMS, TU Wien, A-1060 Vienna

The quasi-one-dimensional (Q1D) model system Pt(110) is investigated with respect to changes induced by hydrogen adsorption. In striking contrast to the usual expectation of highly coordinated chemisorption sites [2], we show experimental and theoretical evidence that H initially chemisorbs at the *low coordinated* short bridge site on top of the outermost platinum rows. The experimental results on geometry (I/V-LEED), adsorption (TPD) and electronic structure (ARUPS) are supplemented by an ab-initio calculation of the chemisorption geometry [3]. The analysis reveals a strong coupling of the H atom positions to Pt lattice relaxations on the (1x2) missing row surface and an extreme sensibility of the Q1D electronic features upon hydrogen adsorption.

Support by the Austrian Science Fund (FWF) is gratefully acknowledged.

[1] E. Kirsten, G. Parschau,W. Stocker, and K. Rieder, Surf. Sci. **231**, L183 (1990)

[2] G. Burns, Solid State Physics (Academic, New York, 1985); K.Christmann, Surf. Sci. Rep. **9**, 1 (1988).

[3] Z. Zhang et al, Phys. Rev. B **70**, 121401 (2004).

O 36.3 Mo 15:00 Poster TU F

Ternary insulators: adsorption of water on $\mathrm{MgSO_4 \cdot H_2O}$(100) — •C. Tegenkamp[1], V. Maslyuk[1], T. Bredow[2], and H. Pfnür[1] — [1]Institut für Festkörperphysik, Abteilung Oberflächen, Appelstr. 2 — [2]Theoretische Chemie, Im Kleinen Felde 30, 30167 Hannover, Germany

The properties of the clean $\mathrm{MgSO_4 \cdot H_2O}$ (100) surface (geometry, relaxation, electronic structure, stability) were investigated using *ab initio* and semi–empirical methods. Especially the influence of intrinsic water was compared to water molecules adsorbed onto the surface. *Ab–inito* calculations were performed both with density functional theory (DFT), using the Perdew–Wang exchange potential, and with Hartree–Fock (HF). Best agreement with the experimental band gap of 7.4 eV at the Γ–point of the Brillouin zone for the (100) surface was obtained by a linear combination of DFT and HF. The gap was determined with EELS at polycrystalline $\mathrm{MgSO_4 \cdot H_2O}$ samples under UHV conditions.The valence band (VB) is formed mainly by the O2p–levels, whereas the S2p–states contribute mostly to the conduction band. A small electron density is located at the Mg atoms in the valence band region. The energetically preferred adsorption site of water within the unit cell of kieserite is above the Mg–atom. The electrostatic interaction between the Mg and the O–atoms of water is stabilized by two additional hydrogen bonds. The water induced changes of the density of states with respect to the separated systems were mainly limited to small energetic shifts towards lower binding energies (0.3eV). Similar results have been obtained for the chemically bound water, i.e. the DOS for $MgSO_4 \cdot H_2O$ and $MgSO_4$ are almost identical in the energy range around the VB.

O 36.4 Mo 15:00 Poster TU F

Adsorption of benzoic acid and its OH–substituted derivatives on $MgSO_4 \cdot H_2O$(100) — •C. Tegenkamp[1], V. Maslyuk[1], T. Bredow[2], and H. Pfnür[1] — [1]Institut für Festkörperphysik, Abteilung Oberflächen, Appelstr. 2, 30167 Hannover, Germany — [2]Theoretische Chemie, Im Kleinen Felde 30, 30167 Hannover, Germany

The adsorption of organic molecules on the $MgSO_4 \cdot H_2O$(100) surface has been investigated theoretically using *ab inito* and semi–empirical methods. For the *ab initio* method a combination of Hartree–Fock and density functional theory, using the Perdew Wang exchange potential, has been used. As already demonstrated for the clean surface, both methods reveal comparable results and agree well with experimental data. The semi-empirical MSINDO package was "calibrated" by means of the *ab initio* method and can be successfully used to describe large unit cells. Here we present results about the adsorption of the organic molecules, benzoic acid, saliclyic acid (SA), and para-salicylic acid. Both the geometry and the electronic structure have been calculated. For all three acids, the energetically most favorable position is above the Mg-atom with the molecules bound to the surface by the carboxylic O-atom. This leads to dramatic changes in the remaining molecule structure, e.g. the quasi-aromatic system of the SA is distorted. Furthermore, all acids generate new occupied and unoccupied states within the band gap of the insulator and the band gap is reduced to 0.1eV and 1eV depending on the molecule. The origin of these states can be assigned to specific parts of the molecule. The impact of the change in the electronic structure will be discussed in the context of contact charging between insulators.

O 36.5 Mo 15:00 Poster TU F

Surfaces of Aqueous Salt Solutions, Bases and Acids — •B. Winter[1], R. Weber[1], C. Pettenkofer[2], W. Freyer[1], I. V. Hertel[1], M. Faubel[3], S. E. Bradforth[4], L. Vrbka[5], and P. Jungwirth[5] — [1]Max-Born-Institut, Berlin — [2]Hahn-Meitner-Institut, Berlin — [3]MPI für Strömungsforschung, Göttingen — [4]University of Southern California, Los Angeles — [5]Academy of Science, Prague

We report on the measured and calculated lowest electron binding energies (and distributions) of aqueous alkali cations and halide anions. The experimental results, obtained by EUV photoemission (PE) using a liquid microjet, are complemented by ab initio calculations, at the MP2 and CCSD(T) level, of the ionization energies of these prototype ions in the aqueous phase. Adiabatic models perform well only for cationic solvation, in which case there is little change of the water geometry upon photoionization. An explicit charge model gives good results for aqueous anions. For the first time the spectra of protonated and deprotonated water, H3O+ and OH-, have been recorded in the aqueous phase. As opposed to the NaOH solution spectra, the PE spectra of aqueous acids, H2SO4 and HNO3, are rather complex, leaving their interpretation, particularly the spectral fingerprint of the hydrated proton, unclear at this point.

O 36.6 Mo 15:00 Poster TU F

Controlled modification of the surface electronic structure by adsorbates: A high resolution ARPES study — •Johannes Ziroff, Felix Schmitt, Frank Forster, Azzedine Bendounan, and Friedrich Reinert — Experimentelle Physik II, Universität Würzburg, Germany

High energy resolution angular-resolved photoemission (ARPES) is a powerful tool for the direct investigation of electronic states at surfaces. By the example of (111) surfaces of Cu, Ag and Au we study the absorbate derived modification of Shockley surface states as well as the electronic states of the coverage.

We will show that physisorbed rare gases and chemisorbed alkali metals significantly modify the Shockley state binding energies and the band masses. In the case of gold there is an interesting change in the width of the spin-orbit splitting, related to the interaction between adsorbate and surface. Another particular example for an overlayer system are thin films of simple organic molecules on Ag (111). They usually inhibit the formation of Shockley surface states while their own electronic structure is modified by the surface interaction. We discuss the influence of the bonding character on the surface electronic structure.

O 36.7 Mo 15:00 Poster TU F

Surface reconstruction effects on the surface state on noble metals — •Azzedine Bendounan, Frank Foster, Johannes Ziroff, Felix Schmitt, and Friedrich Reinert — Experimentelle Physik II, Universität Würzburg, Am Hubland, 97074 Würzburg, Germany

Noble metal surfaces (Cu, Ag and Au) in (111)-orientation are characterized by the existence of Shockley states which appear in the projected band L gap and form a quasi bi-dimensional system. Our photoemission experiments at low temperature (20 K) with very high energy and angle resolution give precise parameters characterizing the band dispersion of these states (energy of bottom of the surface band, effective mass and hole lifetime) which can be compared to the theory. Here, we present e.g. a study on the photoemission line-shapes of ultra-thin Ag films on Cu(111). Depending on the deposition temperature, the first Ag monolayer surface displays two typical 9 × 9 reconstructions resulting of the large lattice mismatch between Cu and Ag. At low temperature, the Ag monolayer forms an unstrained hexagonal moiré structure defined as a modulation resulting from the superposition of the two commensurate Ag and Cu lattices. Several Ag atoms are in energetically unfavorable on-top positions leading to strongly stressed Cu regions in the substrate. At room temperature, the surface presents a triangular corrugation interpreted as the introduction of a few Cu vacancies. It was shown that the bottom band energy of surface state depends on the type of superstructure present at the surface. In addition, we investigate the lifetime evolution in these highly-ordered reconstructions.

O 36.8 Mo 15:00 Poster TU F

An investigation of Nitrogen interaction at the Iron Pyrite (100) surface — •Dirk Rahn[1], Bridget Murphy[1], Jaroslaw Iwicki[1], Matthias Kalläne[1], Kai Rossnagel[1], Felix Tuczek[2], and Lutz Kipp[1] — [1]Institut für Experimentelle und Angewandte Physik, Universität Kiel, D-24098, Germany — [2]Institut für Anorganische Chemie, Universität Kiel, D-24098, Germany

The intereaction of gasous N_2 on the FeS_2 (100) surface at room temperature was studied using scanning tunneling microscopy (STM) to characterise its structural properties. Furthermore, the electronic structure of the FeS_2 (100) clean substrate and during N_2 deposition has been investigated by angle-resolved photoemission spectroscopy (ARPES) to determine the reactivity of the iron dangling bonds to N_2 exposure at various concentrations up to 1000 Langmuir.

Work supported by the DFG Forschergruppe FOR 353.

O 36.9 Mo 15:00 Poster TU F

Electronic properties of Fe_xTiS_2 (x=0.0, 0.1, 0.33, 0.66) — •Meike Quitzau, Magnus Garbrecht, Kai Rossnagel, and Lutz Kipp — Institut für Experimentelle und Angewandte Physik, Universität Kiel, D-24098, Germany

The electronic properties of the sandwich-layered transition metal dichalcogenide TiS_2 and its intercalation compounds Fe_xTiS_2 (x=0.1, 0.33, 0.66) have been investigated by angle-resolved photoelectron spectroscopy, resistivity measurements, LEED, and STM. While the resistivity measurements confirm magnetic phase transitions at different temperatures as a function of x, no superlatice induced by the iron could be found in the LEED and STM patterns, indicating that there is no long-range order in the distribution of the guest atoms at the surface. The ARPES data show new electronic states just below the Fermi level that appear as two bands with almost no dispersion in $\overline{\Gamma M}$ and $\overline{\Gamma K}$ directions. An opening of a hybridization gap for increasing x between the highest S 3p-band at the $\Gamma(A)$ point and the lowest Ti 3d-band at the $M(L)$ point is observed.

The work is supported by DFG Forschergruppe FOR 353.

O 36.10 Mo 15:00 Poster TU F

Geometric and electronic structure of pentacene on layered materials — •Frank Baehr, Jaroslaw Iwicki, Bridget Murphy, Matthias Kalläne, Kai Rossnagel, and Lutz Kipp — Institut für Experimentelle und Angewandte Physik, Universität Kiel, D-24098, Germany

Organic semiconductors, such as pentacene, are promising candidates for several applications, including electronic devices. In order to develop an understanding for the interaction of pentacene with layered transition metal dichalcogenide surfaces, a combination of experimental techniques was employed. An angle-resolved photoemission (ARPES) investigation of the electronic structure during pentacene deposition on $1T$-TiSe$_2$ and $1T$-TaS$_2$ was carried out using the ASPHERE spectrometer at beamline W3.2 at HASYLAB. The geometric alignment of pentacene molecules on the substrates was studied by scanning tunneling microscopy (STM). ARPES and STM data will be presented and discussed.

Work supported by the DFG Forschergruppe FOR 353.

O 36.11 Mo 15:00 Poster TU F

GW quasiparticle calculations for surfaces: the role of periodicity in the repeated-slab approach — •Christoph Freysoldt[1], Philipp Eggert[1], Patrick Rinke[1], Arno Schindlmayr[1,2], and Matthias Scheffler[1] — [1]Fritz-Haber-Institut der Max-Planck-Gesellschaft, Faradayweg 4-6, 14195 Berlin, Germany — [2]Institut für Festkörperforschung, Forschungszentrum Jülich, 52425 Jülich, Germany

Many-body perturbation theory in the *GW* approximation has become a valuable tool for *ab-initio* band structure calculations that are typically in good agreement with photoelectron experiments. In order to treat surfaces one often employs a repeated slab geometry for computational convenience. If no low-order electric multipole moments are present in the slab, the limit of the isolated slab is quickly reached when increasing the slab separation. Within *GW*, multipoles are induced even if the ground state exhibits no dipole which may lead to slower convergence compared to DFT. We show that certain approximations that are commonly made in GW implementations must be carefully validated in order to capture the physical behaviour of the repeated slabs. Our numerical results give evidence that the periodic arrangement manifests itself noticeably in the bandstructure, which is in agreement with an electrostatic model that incorporates the induced dipole effects. Prospects for realistic GW surface calculations are discussed.

O 36.12 Mo 15:00 Poster TU F

Wave-vector dependent intensity variations of the Kondo peak in $4d \rightarrow 4f$ resonant photoemission from CePd$_3$ — •S. Danzenbächer[1], Yu. Kucherenko[2], M. Heber[1], D.V. Vyalikh[1], S.L. Molodtsov[1], V.D.P. Servedio[3], and C. Laubschat[1] — [1]Institut für Festkörperphysik, TU Dresden, D-01062 Dresden, Germany — [2]Institute of Metal Physics, National Academy of Sciences of Ukraine, UA-03142 Kiev, Ukraine — [3]Sezione INFM and Dip. di Fisica, Università “La Sapienza”, P.le A. Moro 2, 00185 Roma and Centro Studi e Ricerche e Museo della Fisica E. Fermi, Compendio Viminale, Roma, Italy

CePd$_3$(111) films were prepared in UHV by co-adsorption of Pd and Ce on a W(110) surface. The films were characterized by means of LEED, angle-resolved photoemission (ARPES) and resonant ARPES. Strong angle-dependent intensity variations of the Fermi-level Ce-$4f$ feature are observed in $4d \rightarrow 4f$ resonant photoemission spectra of CePd$_3$(111) that reveal the periodicity of the lattice and largest intensity close to the $\overline{\Gamma}$ points of the surface Brillouin zone. In the framework of a simplified periodic Anderson model the phenomena can quantitatively be described by a wave-vector dependence of the electron hopping matrix elements caused by Fermi-level crossings of non-$4f$-derived energy bands.

O 36.13 Mo 15:00 Poster TU F

Subsurface impurities in noble metals - a comparison between STM data and simulations of bulk electron transport — •A. Weismann, M. Wenderoth, N. Quaas, and R. G. Ulbrich — IV. Physikalisches Institut der Universität Göttingen,Friedrich-Hund-Platz 1, 37077 Göttingen

Isolated sub-surface impurities a few monolayers below the (111) surface of noble metals were prepared by codeposition of host metal and impurity compound from two evaporators and investigated with Scanning Tunneling Microscopy at 8 K. The modulations of the surface electronic density in the vicinity of the the defects show signatures of bulk electron properties, i.e. a threefold symmetry and oscillation lengths much shorter than the wavelength λ_F of the surface state. Simulations of bulk electron scattering at point defects based on the host metal band-structure were performed. These calculations are in good agreement with the obtained STM data. The surface patterns are strongly influenced by electron focussing effects due to the non-spherical fermi surface of the host metal.

O 36.14 Mo 15:00 Poster TU F

Rashba Effect at Magnetic Lanthanide Surfaces — •O. Krupin[1], S. Gorovikov[2], J. E. Prieto[1], K. Döbrich[1], G. Bihlmayer[3], S. Blügel[3], G. Kaindl[1], and K. Starke[1] — [1]Institut für Experimentalphysik, Freie Universität Berlin, Germany — [2]MAX-Lab, Lund University, Sweden — [3]Institut für Festkörperforschung, Forschungszentrum Jülich, Germany

A key issue of condensed matter research for future spintronic devices is the control and manipulation of the electron spin without the need to apply an external magnetic field. In a combined experimental and theoretical study, employing valence band photoemission and *ab initio* band structure calculations we demonstrate, at the examples of ferromagnetic rare earth Gd(0001) and Tb(0001) surfaces, that (1) the Rashba spin-orbit effect is a general surface and interface phenomenon which, in case of d-derived surface (interface) states, can lead to substantial Rashba splittings, and that (2) the Rashba splitting of d-derived surface states is strongly enhanced when an epitaxial metal oxide layer is formed on top of a metal surface. The experimental observations are quantitatively described by *ab initio* calculations giving a detailed account of the near-surface charge density gradients. They show that the enhanced Rashba interaction upon oxide layer formation is caused by a spread of the two-dimensional states over a wider interface lattice region, together with a substantial change in orbital character.

O 36.15 Mo 15:00 Poster TU F

Cu-Oberflächenstrukturen in alkalischen Elektrolyten: vom Cu(111)-Einkristall zur Cu-Submonolage auf Au(111) — •Daniel Friebel, Christian Schlaup, Peter Broekmann und Klaus Wandelt — Institut für Physikalische und Theoretische Chemie, Universität Bonn, Wegelerstr.12, D-53115 Bonn

Mit Hilfe der in-situ-Rastertunnelmikroskopie in Kombination mit zyklischer Voltammetrie werden die potentialabhängigen Oberflächenstrukturen von Cu(111)-Elektroden sowie ultradünnen Kupferfilmen auf Au(111)-Elektroden in alkalischen Elektrolyten charakterisiert. Letztere werden sowohl durch Unterpotential- (upd) als auch bulk-Abscheidung aus schwefelsauren CuSO$_4$-Lösungen hergestellt, die anschließend unter Potentialkontrolle zunächst gegen H$_2$SO$_4$ und dann gegen alkalische Lösungen getauscht werden. Eine durch upd gebildete 2/3-Monolage Cu auf Au(111) zeigt in 0.01 M NaOH drastisch veränderte strukturelle Eigenschaften. Neueste Untersuchungen zur Elektrokatalyse der Sauerstoff-Reduktion an Cu-modifizierten Au(111)-Elektroden sowie zur elektrochemischen Erzeugung ultradünner Kupferoxidfilme werden vorgestellt und diskutiert.

O 36.16 Mo 15:00 Poster TU F

Surface design for attachment of biomolecules by adaptive polymer surfaces — •Nikolay Houbenov[1], Alexander Sidorenko[1], Leonid Ionov[1], Sergiy Minko[2], and Manfred Stamm[1] — [1]Leibniz-Institut fuer Polymerforschung e.V., Hohe Str 6, 01069 Dresden, Germany — [2]Clarkson University Potsdam, NY 13699

Surface chemical patterning can be successfully used to control the spatial position of proteins attachment. We applied chemical patterning on stimuli responsive polymer brushes, consisted of a non-polar hydrophobic polymer (polyisoprene (PI)) and a polar one (Poly(2-vynilpyridine) (P2VP)). By patterning the substrate via photo-crosslinking of PI, we were able to generate chemistry driven differences in the adsorption of Bovine Serum Albumin (BSA). The surface micropattern appeared and disappeared interchangeably between pH 4 and 7, caused by swelling/deswelling behavior of P2VP in non-irradiated regions. The adsorption experiments indicated that BSA adsorbs strongly at the non-polar hydrophobic PI parts, where attachment would be expected to occur primarily by hydrophobic interaction. For the hydrophilic P2VP parts (at low pH), protein adsorption appears to occur by polar interactions resulting in a weaker attachment and a different conformation.

O 36.17 Mo 15:00 Poster TU F

In-situ Investigation of Adsorption of Functionalized Base-free Porphyrins at the Solid-liquid Interface using STM technique — •Maxim Smetanin[1], Zakariyya Ishtaiwi[2], Heinrich Lang[2], and Michael Hietschold[1] — [1]Chemnitz University of Technology, Institute of Physics, Solid Surfaces Analysis Group, D-09107 Chemnitz, Germany — [2]Chemnitz University of Technology, Institute of Chemistry, Inorganic Chemistry, D-09111 Chemnitz, Germany

Molecular assemblies on surfaces are one of the key technologies for nanoscale electronic devices. Formation and characterization of ordered adlayers of porphyrin at surfaces is of great importance from the fundamental and technological point of view, since these molecules are closely related to the fields of molecular biology, photosynthesis, electrocatalysis and molecular devices. In this work, we present the adsorption studies of functionalized base-free porphyrins at the solid-liquid interface using Scanning Tunneling Microscopy (STM). We studied functionalized tetraphenyl-21H,23H-porphin (TPP) with (a) SiMe(CH2CH=CH2)2 creating a first generation dendrimer; (b) Si(C6H4SiMeCH2CH=CH2)3 creating a second generation dendrimers. We have observed one and twodomensional self-organization of these molecules from 1-phenyl-octane liquid phase on the basal plane of Highly Oriented Pyrolytic Graphite (HOPG).

O 36.18 Mo 15:00 Poster TU F

Wetting on the well ordered and irregular structured surfaces from core-shell particles — •Alla Synytska[1], Leonid Ionov[1], Sergiy Minko[2], Klaus-Jochen Eichhorn[1], Manfred Stamm[1], and Karina Grundke[1] — [1]Leibniz Institute of Polymer Research Dresden, Germany — [2]Clarkson University, Chemistry Department, Potsdam, USA

Wetting and non-wetting phenomena are ubiquitous in the natural and technological worlds, and their understanding has been the subject of intensive investigations over the past decades. Numerous surface modification techniques are used to control wettability and adhesion of polymer surfaces. A promising strategy to regulate wetting behaviour is the combination of the surface patterning and the chemical surface modification. In the present study we suggest strategy to obtain patterned surfaces with specifically designed surface roughness by using core-shell particles. The surface morphology and roughness is built by self-assembled submicrometer- and micrometer-sized monodisperse core-shell particles forming ordered films on silicon wafer substrates. The shell of the particles is made from polymer brushes covalently grafted onto the particles. The wetting behaviour of both individual liquids and water/methanol mixtures on well ordered structured and irregular fractal surfaces from core shell particles of different size will be discussed.

O 36.19 Mo 15:00 Poster TU F

In-situ Video-STM study of the dynamic behavior of the reconstructed Au(100) surface. — •Christian Haak, Miguel Labayen, and Olaf M. Magnussen — Institut für Experimentelle und Angewandte Physik, Universität Kiel, Leibnizstr. 19, 24098 Kiel

The dynamic of five atomic rows wide, hexagonally arranged strings has been studied by Video-STM on a Au(100) surface in sodium sulphate and hydrochloric acid containing solution. Those "hex"-strings appear during the phase transition from the Au(100)(1x1) to the "hex" reconstruction of the top-most layer when applying negative potential. We have studied the initial stages of the formation of individual strings, the growth of the strings and the formation of larger domains. Isolated "hex"-strings exhibit highly dynamic fluctuations in structure and position. They show a high mobility perpendicular and parallel to the string direction. Surprisingly, the mobility perpendicular to the string direction is independent from string length. This can be explained by simple models where the string moves due to nucleation and propagation of kinks. Furthermore, we discuss potential- and temperature-dependent measurement, which show that the string mobility increases towards more negative potentials and is thermally activated.

O 36.20 Mo 15:00 Poster TU F

STM-Untersuchungen des Redoxverhaltens von 1,1'-disubstituierten 4,4'-Bipyridinen auf chloridbedecktem Cu(100)-Elektrode — •Caroline Safarowsky, Klaus Wandelt und Peter Broekmann — Institut für physikalische und theoretische Chemie, Universität Bonn, Wegelerstr. 12, 53115 Bonn, Germany

Mittels in-situ STM- und cyclovoltammetrischen Untersuchungen wird das Adsorptionsverhalten von dikationischen 1,1'-disubstituierten 4,4'-Bipyridinen auf einer chloridbedeckten Cu(100)-Elektrodenoberfläche untersucht. Die zuvor präparierte $c(2\times2)$-Cl Adsorbatstruktur dient dabei als Templat für die Adsorption der dikationischen Moleküle. STM-Untersuchungen zeigen, dass der Redoxzustand des Bipyridiniumions maßgeblich Einfluss auf die Adsorbat-Substrat-Wechselwirkungen und damit auch auf die Phasenbildung auf der chloridmodifizierten Oberfläche nimmt.

Elektrochemische Messungen auf Graphit und Cu(100) verifizieren eine sukzessive Reduktion in Abhängigkeit des Probenpotentials, welche mit entsprechenden Phasenübergängen einhergeht, die sich letztlich durch veränderte Adsorbat-Adsorbat- bzw. Adsorbat-Substrat-Wechselwirkungen begründen. Mischungsexperimente verdeutlichen die Adsorptionseigenschaften der unterschiedlichen Redoxzustände.

O 36.21 Mo 15:00 Poster TU F

Energy loss of bouncing water drops — •Wolfram Hild, Juergen A. Schaefer, Denis Duft, and Thomas Leisner — TU Ilmenau, Institut für Physik und ZMN, Postfach 100565, 98684 Ilmenau

Water droplets can bounce like an elastic sphere after hitting a super hydrophobic surface. Interestingly, they behave like a spring. The contact time, which corresponds to one period of oscilla-tion of the spring, is independent of impact velocity. However, the velocity of the reflected droplet depends on the impact velocity. Thus, there is a loss of kinetic energy depending on the starting conditions. Energy losses are due to adhesive forces between substrate and droplet and mainly due to excitations of droplet oscillations.

It could be shown that energy losses are due to adhesion at lower velocity. Furthermore, approximately seventy percent of the kinetic energy is transferred to oscillations at higher velocities.

O 36.22 Mo 15:00 Poster TU F

Vibrational Sum-Frequency Spectroscopy of Quartz/Water Interfaces — •Björn Braunschweig and Winfried Daum — Institut für Physik und Physikalische Technologien, TU Clausthal, Leibnizstrasse 4, D-38678 Clausthal-Zellerfeld

We have applied vibrational sum-frequency spectroscopy to examine the ordering of hydrogen-bonded water molecules at quartz/water interfaces and to investigate the structure of the interfacial water layer. Consistent with previous work, our spectra reveal OH stretching bands at $\sim$3200cm^{-1} and $\sim$ 3450cm^{-1} that can be assigned to tetrahedrally and non-tetrahedrally coordinated, hydrogen-bonded water molecules at the interface, respectively. pH-depending variations of the spectra are related to ordering of tetrahedrally coordinated water molecules caused by the electric field of deprotonated silanol groups at the interface. Spectra of thin water films on quartz exhibit a narrow band at 3140cm^{-1} instead of the broad band at $\sim$3200cm^{-1} observed for bulk water on quartz. Analysis of the spectra indicates that the broad resonance at 3200cm^{-1} which in previous work was assigned to the symmetric OH stretching vibration of tetrahedrally bonded water molecules in fact consists of two bands at 3140cm^{-1} and 3240cm^{-1} attributable to the symmetric and antisymmetric stretching vibration of tetrahedrally coordinated H_2O, respectively. Comparison of spectra for water films of different thickness leads us to the following model of the interface: the water molecules right on the quartz surface are tetrahedrally coordinated and oriented. The contribution of non-tetrahedrally H_2O observed in our spectra originates from the interfacial region above the ordered water layer.

O 36.23 Mo 15:00 Poster TU F

Structural changes of a TMPyP layer on a Cu(100)/Cl - Surface within the corrosion region — •Minh Hai Nguyen Thi, Blazenka Gasparovic, Peter Broekmann, and Klaus Wandelt — Institut für Physikalische und Theoretische Chemie, Universität Bonn, Wegelerstr. 12, 53115 Bonn

The self-assembly of 5,10,15,20-Tetrakis-(N-methyl-4-pyridyl)-21H,23H-porphyrin tetrachloride (TMPyP) on an Chloride-Modified Cu(100) electrode within the copper corrosion regime was investigated by using Electrochemical Scanning Tunneling Microscopy (EC-STM). A highly ordered TMPyP adlayer was observed at a potential of E = - 400 mV vs.Ag/AgCl which became disordered when the applied potential was changed more positive into the regime of copper corrosion. This process is reversible, that the highly ordered porphyrin layer is restored when the potential is turned back into the negative direction. The corrosion process was found to be favoured at step-edges and to run along the close-packed chloride rows like in the case of the corrosion of Cu(100) in the pure chloride containing electrolyte. High resolution EC-STM images indicated that the structure of TMPyP on the Cu(100)/Cl surface is $(3\sqrt{2}\times3\sqrt{2})R45^\circ$ with respect to the chloride (2×2) layer or (6×6) with respect to the Cu(100).

O 36.24 Mo 15:00 Poster TU F

In-situ Untersuchungen elektrochemischer Abscheidungsprozesse auf Au-Oberflächen — •Ahmed Ayyad, Klaus Krug, Jochim Stettner und Olaf Magnussen — Institut für Experimentelle und Angewandte Physik, Christian-Albrechts-Universität Kiel, Leibnizstraße 19, 24098 Kiel

Das grundlegende Verständnis elektrochemischer Abscheidungsprozesse ist von hoher grundlegender Bedeutung wie auch relevant für technologische Anwendungen. Insbesondere das komplexe Wechselspiel zwischen der Struktur der Elektrodenoberfläche, dem Wachstumsverhalten und dessen Abhängigkeit von zentralen Wachstumsparametern (Elektrodenpotential, Abscheiderate, Elektrolytzusammensetzung) ist hierbei von Interesse. Wir haben das homoepitaktische Wachstum auf einkristallinen Au(111) und Au(100) Oberflächen in-situ während des Abscheideprozesses mit Hilfe oberflächenempfindlicher Röntgenbeugungsexperimente unter Verwendung von Synchrotronstrahlung untersucht. Die Messungen wurden in Transmissionsgeometrie in einer hierfür entwickelten Probenzelle durchgeführt, die in-situ Strukturuntersuchungen unter reaktiven Bedingungen (d.h. keine Einschränkung des Transports in der Elektrolytlösung) und simultan hochqualitive elektrochemische Messungen erlaubt. Die Experimente zeigen im Vergleich zu Untersuchungen in Aufreier Lösung oder unter UHV-Bedingungen eine starke Beeinflussung der Au-Oberflächenrekonstruktion, insbesondere eine erhöhte laterale Kompression der obersten Au Atomlage.

O 36.25 Mo 15:00 Poster TU F

Growth of ultrathin silver films on Ge(100) — •Olaf Skibbe, Fanzhen Meng, Andreas Priebe, and Annemarie Pucci — Kichhoff-Institut für Physik, Ruprecht-Karls-Universität Heidelberg, Im Neuenheimer Feld 227, 69120 Heidelberg

The growth of ultrathin metal films on semiconductor surfaces is of interest for different reasons. On the one hand for the technical application of conductors at decreasing dimensions, on the other hand for the understanding of the growth mechanism. The system Ag/Ge(100) shows an alloy phase [1] and indications of a superconducting phase at low temperatures [2].

For in situ investigation of the growth of metal films with high thickness resolution infrared spectroscopy provides a particularly suitable method. By measuring the frequency dependent transmission of the film, one can get information about it's metallic properties and morphology. For the growth of a silver film on Ge(100) a coalescence thickness of about 1.3 nm could be determined. The measurement of absorption bands of adsorbed molecules (e.g. CO) gives further knowledge of the physical properties of the film. The preparation of the Germanium sample and the available measurements have been carried out in UHV environment. Ex situ atomic force microscopy was performed afterwards.

[1] L. Chan and E. Altman, Phys. Rev. B 66, 155339 (2002).

[2] K. Hattori, Y. Takahashi, T. Iimori, and F. Komori, Surf. Sci. 357, 361 (1996).

O 36.26 Mo 15:00 Poster TU F

Metallic indium cluster growth on InP(001) — •M. Himmerlich[1], M.C. Zeman[1,2], T. Stolz[1], M. Gubisch[1], M. Eremtchenko[1], S. Krischok[1], R.J. Nemanich[2], and J.A. Schaefer[1] — [1]Institut für Physik und Zentrum für Mikro- und Nanotechnologien, TU Ilmenau, P.O. Box 100565, 98684 Ilmenau, Germany — [2]Department of Physics, North Carolina State University, Raleigh, NC, 27695

We present a microscopic and spectroscopic study of indium cluster formation on the InP(001) surface. AFM investigations reveal the appearance of metallic nanoclusters (10–50 nm in diameter) after Ar^+ sputtering and subsequent annealing steps. The shape and dimension of the clusters were studied using microscopic techniques (AFM, PEEM and SEM). In parallel the chemical composition, the electronic structure of the valence band and the surface plasmon were investigated by spectroscopic methods (laterally resolved UPS, XPS and HREELS). The combination of these techniques provides detailed information about the cluster formation and its evolution during annealing steps. The influence of the metal droplets on the depletion layer of the semiconductor leads to a shift of the surface carrier plasmon frequency.

O 36.27 Mo 15:00 Poster TU F

Surface conductance at metal-semiconductor transitions induced by alkali metal adsorption on Si(001) — •E.P. Rugeramigabo, A.A. Shklyaev, Liu Hong, V. Zielasek, and H. Pfnür — Universität Hannover, Institut für Festkörperphysik, Abteilung Oberflächen, Appelstr. 2, 30167 Hannover

Electrical transport in ultrathin Na and Cs layers on Si(001) has been studied combining macroscopic conductivity measurements with LEED, EELS, and measurements of the work function. EELS has previously identified metal-semiconductor transitions during alkali metal deposition on Si(001) at the occurence of first ordered structures in the submonolayer regime, while at room temperature (RT) only for Cs/Si(001) the transition back to a metallic surface was observed at saturation coverage. In fact we find that the conductance (σ) of the n-type substrate decreases during Na/Si(001) deposition when the first ordered adsorbate structure is observed by LEED, while for Cs/Si(001) a channel for electrical transport in surface states opens up at 0.5 ML coverage, leading to an increase of the surface conductance in the $10^{-5}\Omega^{-1}$ range. Its dependence on temperature indicates that electrical transport is thermally activated. Upon Cs deposition at temperatures below 200 K a structural transition to a stable monolayer configuration is found to be related to the sudden onset of a metal-like conductance in the $10^{-3}\Omega^{-1}$ range. While σ exhibits a similar onset during RT deposition beyond 0.5 ML, it decreases after finishing deposition, indicating the existence of a supersaturation Cs fraction during deposition and a relaxation of the Cs/Si(001) surface to a saturation coverage below 1ML.

O 36.28 Mo 15:00 Poster TU F

Surface vibrations of clean and hydrogen terminated silicon (100) and (110) surfaces — •M. Eremtchenko[1], R. Öttking[1], F. S. Tautz[2], and J. A. Schaefer[1] — [1]TU Ilmenau, Institut für Physik und Zentrum für Mikro- und Nanotechnologien, P.O. Box 100565, 98684 Ilmenau, Germany — [2]School of Engineering and Science, International University Bremen, 28759 Bremen, Germany

We present a comprehensive study of the clean and hydrogen terminated silicon (100) and (110) surfaces by means of high resolution electron energy loss spectroscopy (HREELS). The phonon modes assignment to the calculated atomic displacement patterns and the phonon modification by the surface treatments is emphasized. The measured data of the vibrational modes of clean Si(100) and (110), as well as of the monohydrides of these surfaces are reported. The comparison of the mono- and dihydride phonon spectra of Si(100) reveals the modes related to the dimer bond and the shift of the phonon frequencies due to either hydrogen or deuterium termination is discussed. We discuss the correspondence of the phonon modes of the clean and hydrogen terminated Si(110) surfaces with respect to the assigned calculated data.

O 36.29 Mo 15:00 Poster TU F

Optically excited electronic states of the 2H:Si(001)-(2x1) surface — •Neng-Ping Wang[1], Michael Rohlfing[1], Peter Krüger[2], and Johannes Pollmann[2] — [1]School of Engineering and Science, International University Bremen, P.O. Box. 750561, 28725 Bremen, Germany — [2]Institut für Festkörpertheorie, Universität Münster

We report on ab initio calculations for optically excited electronic states of the 2H:Si(001)-(2x1) surface. The ground-state geometry is addressed by DFT calculations within the local-density (LDA) and generalized gradient (GGA) approximation. Based on this, the optically excited electronic states are described by many-body perturbation theory (MBPT; GW approximation and Bethe-Salpeter equation). Of particular interest are dynamical processes within the excited states that lead to photodesorption of hydrogen atoms [see the experimental results by T. Vondrak and X.-Y. Zhu, Phys. Rev. Lett. 82, 1967 (1999)]. In this work, we try to explain the photodissociation of the adsorbate-surface bond within the framework of MBPT. This requires to calculate the corresponding excited-state forces. One particular issue concerns the local character of the excitation, which we describe by appropriate confinement potentials.

O 36.30 Mo 15:00 Poster TU F

BEEM on Ag/Si(111 — •Christian Bobisch, Amin Bannani, and Rolf Möller — Universität Duisburg-Essen, D-45141 Essen, Germany

BEEM (Ballistic Electron Emission Microscopy) is an STM derived method to obtain information on buried metal/semiconductor interfaces. By applying a tunnelling voltage to the tunnelling tip, electrons are injected into a metal film on a semiconducting substrate. Some of them may reach the interface to the semiconductor without loss of energy and pass the Schottky-barrier if the energy exceeds the barrier height. The ballistic electrons contribute to a current that can be detected between the semiconducting-substrate and the independently contacted metal layer. This current is sensitive to various scattering processes leading to an energy dissipation within the metal film and, or at the interface.

In this work the system Ag on Si(111) has been studied. 3-4nm thick Ag films have been grown on the Si-substrate at 150K and annealed at 300 K to obtain a well defined interface. In addition to the topographic STM-data it was possible to obtain laterally resolved information on the electronic structure of the interface. BEES (Ballistic Electron Emission Spectroscopy) was performed to evaluate the local height of the Schottky-barrier. By fitting the obtained I(V) curves with a power law we find a mean barrier height of about 0.71eV.

This work was funded by the SFB616 of the DFG.

O 36.31 Mo 15:00 Poster TU F

Diamant als Substrat für einen Quantencomputer auf der Basis von Fullerenen — •Kati Hübener[1,2], Wolfgang Harneit[2], Diana Vilchez[2], Rainer Döring[2], Jens Hauschild[2] und Michael Scheloske[2] — [1]Hahn-Meitner- Institut Berlin, Glienicker Str. 100, 14109 Berlin — [2]Freie Universität Berlin, Arnimallee 14, 14195 Berlin

Fullerene mit einem einzelnen eingeschlossenen Stickstoff-bzw. Phosphoratom (endohedrale Fullerene), eignen sich aufgrund ihres langlebigen Spins, als Informationsträger in einem Quantencomputer. Dazu müssen sie in einer festen Orientierung auf einem Substrat aufgereiht werden. Diamant ist als Substrat sehr gut geeignet, da in diesem Material sogenannte NV-Zentren erzeugt werden können. Ihr Spin koppelt mit dem der endohedralen Fullerene und lässt sich durch optische Spektroskopie auslesen. Für das Aufbringen der Fullerene auf das Substrat soll zunächst von einer chemisch inerten, glatten Oberfläche ausgegangen werden. Diese wurde durch eine H-Terminierung des Diamanten, bei 900°C, unter Wasserstoffffluss erzeugt. Zur kovalenten Anbindung der Fullerene an die Diamantoberfläche muss diese chemisch modifiziert werden. Eine O-terminierte und damit chemisch reaktivere Oberfläche erhält man z.B. durch eine Behandlung des Diamanten in einem Gemisch aus Schwefelsäure und Salpetersäure. Entsprechende Versuche zur Passivierungen der Diamantoberfläche wurden an Diamantfilmen, sowie Diamantpulver (¡250nm) durchgeführt. Anschließend wurde die Oberfläche mittels IR-Spektroskopie, XPS und AFM untersucht.

O 36.32 Mo 15:00 Poster TU F

Ultra-trace analysis and speciation of low Z contaminants on silicon wafer surfaces by TXRF-NEXAFS employing monochromatized undulator radiation — •B. Beckhoff, R. Fliegauf, M. Kolbe, M. Müller, J. Weser, and G. Ulm — Physikalisch-Technische Bundesanstalt, Abbestr. 2 - 12, 10587 Berlin, Germany

The Physikalisch-Technische Bundesanstalt (PTB) develops total-reflection x-ray fluorescence (TXRF) analysis in the soft x-ray range, providing a means for the quantitation of low Z contaminants on silicon wafer surfaces at its monochromator beamline for undulator radiation at BESSY II. The absolute lower levels of detection of TXRF analysis for low Z elements such as C, N, Na, Mg and Al range between 100 fg and 1 pg. A dedicated instrumentation fully utilizes these excitation conditions: 300 mm Si wafers, as well as 200 mm wafers, are transported directly from their shipping cassettes via a prealigner into a high vacuum load-lock by an adapted commercial equipment front end module. A vacuum robot located inside the load-lock takes the wafer and places it inside the UHV irradiation chamber on an electrostatic chuck mounted on an 8-axis manipulator. Furthermore, the investigation of near-edge X-ray absorption fine structures (NEXAFS) in conjunction with TXRF is able to contribute to the speciation of minute amounts of low Z and organic compounds. Here, fluorescence count-rates normalized to the incident radiant power were recorded at the K-edges of C, N and O. The PTB instrumentation offers off-line reference measurements to assess surface cleaning procedures and multi-elemental nano-layered systems deposited on wafers.

O 36.33 Mo 15:00 Poster TU F

Construction of a Low Temperature Scanning Tunneling Microscope — •N. Henningsen, C. Roth, I.F. Torrente, and J.I. Pascual — Freie Universität Berlin, Department of Physics, Arnimallee 14, 14195 Berlin, Germany

Scanning Tunnelling Microscopy has become a standard tool for analysing crystal surfaces, or single molecules, even atoms. One of the most surprising capabilities of Scanning Tunnelling Microscopes (STM) is the local measurement of electronic, magnetic and vibrational properties of surfaces and adsorbates. For such spectroscopic measurements it is important to have a very good stability of the tunnel junction, as well as high energy resolution.

Here we present the design of our new low temperature STM, which has been optimised for spectroscopic measurements demanding high stability, as it is the case for Inelastic Tunnelling Electron Spectroscopy (IETS). The system will be used for inducing reactions on individual adsorbed molecular species by means of inelastic scattering of tunnelling electrons as well as by photons. For this purpose, the system will be equipped with a light source, an arc lamp providing power regimes up to 100 mW/mm2 in a continuous spectrum, which will be inserted in the UHV system via an optical fibre.

The STM head is of the Besocke type, and the design and materials are chosen to accomplish maximum stability, required for performing slow spectroscopic measurements. The design allows also the possibility of changing the tip in vacuum. The STM is coupled with a bath cryostat and is properly shielded to reach an equilibrium temperature of 5 K.

O 36.34 Mo 15:00 Poster TU F

Influence of pulsed laser light on metallic nanostructures — •Daniel Schmidt, Juliane König-Birk, Johannes Boneberg, Elke Scheer, and Paul Leiderer — Department of Physics, University of Konstanz, Germany

We introduce a complementary method to the scanning near-field optical microscopy (SNOM) to image optical near-fields below metallic nanostructures. For this method the socalled "optical near-field photography" we use e.g. silicon, glass or polymer films as substrates. The nanostructures on the substrates are illuminated with a femtosecond laserpulse. The intensity is adjusted such that no influence of the illumination is detectable on the bare substrate. When illuminating arrays of metallic nanostructures on substrates we observe ablation of the substrate below and around the nanostructures due to the local intensity enhancement in the optical near-field. The ablation pattern depends on the geometry of the nanostructures (triangular, rectangular, ...) and the polarization of the laser and can thus be used to image the optical near-field of the nanostructures (1).

In a second experiment we test if the optical near-field can also be used to manipulate the current transport through two tips. For example the electrical conductivity through a mechanically controlled break junction can be manipulated. First results are shown.

(1) Paul Leiderer et al., Appl. Phys. Lett. 85, (2004)

O 36.35 Mo 15:00 Poster TU F

Lichtstreuung an einzelnen Nanolöchern in Metallfilmen — •Maximilian Reismann, Christian Dahmen und Gero von Plessen — I. Physikalisches Institut (IA), RWTH Aachen, D-52056 Aachen

Die Lichttransmission durch regelmäßig angeordnete submikrometergroße Löcher in Metallfilmen hat in den letzten Jahren großes Interesse gefunden [1]. In dieser Arbeit wird die Abhängigkeit der optischen Streuspektren einzelner Nanolöcher von Lochgeometrie sowie dem Metall des Films experimentell untersucht. Dazu werden mittels Nanokugel-Lithographie zylindrische Löcher mit 200 nm–300 nm Durchmesser in Metallfilmen mit Dicken von 50 nm–100 nm erzeugt. Streulichtspektren einzelner Nanolöcher werden mit einem Dunkelfeldmikroskop gemessen und der Einfluss von Oberflächenplasmon-Polaritonen auf die Streuung am Nanoloch wird diskutiert.

[1] T.W. Ebbesen *et al.*, Nature **391**, 667 (1998)

O 36.36 Mo 15:00 Poster TU F

Light scattering by thin planar nanostructures on surfaces — •Manuel Gonçalves and Othmar Marti — University of Ulm - Dept. of Experimental Physics, Albert-Einstein-Allee 11, D-89069 Ulm, Germany

The scattering of light by small metallic structures depends strongly on the dielectric constant of the material and on the geometry. Unlike in dielectric structures the scattered radiation is mainly produced by surface plasmons confined in the metallic structures. These plasmons can be excited by an evanescent wave produced by total-internal-reflection. The intensity and location of the scattering centers have been investigated using a confocal microscope. For some materials the scattering patterns depend strongly on the polarization direction. The location of the scattering centers is also dependent on the geometry of the structures and on their relative orientation relative to the direction of incidence. SNOM images of the same metallic particles and structures obtained in illumination mode do not reveal a particular dependency on the geometry or particle orientation.

O 36.37 Mo 15:00 Poster TU F

Stimulated emission of surface plasmons at the interface between a silver film and an optically pumped dye solution — •Jan Seidel, Stefan Grafström, and Lukas Eng — Institut für Angewandte Photophysik, TU Dresden, George-Bähr-Str. 1, 01069 Dresden

Surface plasmons (SPs) are surface-bound electromagnetic waves supported by metals, offering the possibility of strong spatial confinement of electromagnetic fields on the micro- and nanoscale. They suffer, however, from strong damping caused by internal absorption and radiation losses. Here we demonstrate amplification of SPs by stimulated emission, which marks a possible solution to this problem. We use an attenuated-total-reflection setup to detect stimulated emission of SPs at the interface between a silver film and an optically pumped dye solution acting as the amplifying medium. Clear evidence of stimulated emission is provided by an excellent agreement of the experimental observations with a theoretical analysis. Amplification of SPs can be considered analogous to photon amplification in a laser, thereby suggesting novel approaches in the field of nanooptics.

O 36.38 Mo 15:00 Poster TU F

Two-dimensional supramolecular coordination networks at a metal surface — •Sebastian Stepanow[1], Alexandre Dmitriev[1], Magalí Lingenfelder[1], Hannes Spillmann[1], Franck Vidal[1], Nian Lin[1], Johannes V. Barth[2], and Klaus Kern[1,2] — [1]Max-Planck-Institut für Festkörperforschung, Heisenbergstraße 1, D-70569 Stuttgart, Germany. — [2]Institut de Physique des Nanostructures, Ecole Polytechnique Fédérale de Lausanne, CH-1015 Lausanne, Switzerland.

The self-assembly of iron coordinated two-dimensional supramolecular networks at a Cu(100) surface has been investigated by high-resolution scanning tunnelling microscopy under ultra-high vacuum conditions. As organic linkers we applied rod-like symmetric and asymmetric molecules with carboxylate and pyridyl endgroups. Upon annealing the iron-molecule mixture two-dimensional network structures with diiron coordination centers evolve. The iron pairs are bridged by two equatorial carboxylate groups and coordinated by two or four carboxylate oxygen atoms or two pyridyl nitrogen atoms depending on the axial linker. The orientation of the network and alignment of the diiron unit depends on the functional groups of the molecule and their interaction with the substrate and the surface symmetry. The interplay between the adsorbate-substrate and the metal-ligand interaction results in different coordination geometries of the iron dimers and their arrangement in the network. The intradimer spacing for the different ligands amounts to 3.8 Å to 4.7 Å and the interdimer distance varies from 10 Å to 19 Å. These diiron complexes can be considered as model systems mimicking the cofactors of biological enzymes for the design of novel catalysts at the atomic level.

O 36.39 Mo 15:00 Poster TU F

Kombination mizellarer und lithographischer Techniken – ein unkonventioneller Strukturierungsansatz — •Oliver Dubbers[1], A. Ethirajan[1], C. Pfahler[1], H.-G. Boyen[1], A. Plettl[1], P. Ziemann[1], M. Ozawa[2] und P. Walter[2] — [1]Abt. Festkörperphysik, Universität Ulm, D-89069 Ulm — [2]Abt. Elektronenmikroskopie, Universität Ulm, D-89069 Ulm

In Toluol gelöste Diblockcopolymere aus Polystyrol und Poly-2-Vinylpyridin (PS-b-P2VP) formen inverse Mizellen mit einem P2VP Kern und einer PS Korona. Diese können mit Metallsalzen, wie z.B. $HAuCl_4$ beladen werden. Selbstorganisationsprozesse führen bei Deposition auf glatten Oberflächen durch Aufziehen oder Spin Coaten zu einer hexagonalen Anordnung. Nach Entfernung des Polymers in einem H_2- oder O_2-Plasma erhält man so hexagonal geordnete Nanoteilchen, deren Größe und Abstand durch die Salzbeladung und Polymerkettenlängen bestimmt werden. Durch elektrodenloses Wachstum in Chrom- oder Goldsalz-/Reduktionsmittellösungen lassen sich diese Nanoteilchen gezielt vergrößern und als Masken beim anisotropen Plasmaätzen verwenden, um z.B. Nanosäulen oder, in einem komplexeren Prozeß, Nanolöcher in Silizium herzustellen.

Der mizellare Ansatz läßt sich auch mit Elektronenstrahllithographie kombinieren. In definierten Fenstern von Lack- oder Metalltemplaten lassen sich Mizellen einfüllen und anschließend veraschen. Beim Lift-off der Maske werden die darauf liegenden Teilchen mit entfernt, so dass sich nur noch die Teilchen auf der Oberfläche befinden, die direkt auf dem Substrat aufgebracht wurden. Beispiele hierfür werden demonstriert.

O 36.40 Mo 15:00 Poster TU F

STM-Spitzeninduzierte CVD von Fe- und Cu-Nanostrukturen — •Erik Freier[1], Matthias Berse[1], Martin Kneppe[1], Guido Walther[1], Ulrich Köhler[1], Marie-Katrin Schröter[2] und Stephan Hermes[2] — [1]Experimentalphysik IV/Oberflächenphysik, Ruhr-Universität Bochum, 44780 Bochum — [2]Anorganische Chemie II, Ruhr-Universität Bochum, 44780 Bochum

In den hier vorgestellten Experimenten wurde die Erzeugung kleiner Strukturen durch direktes Schreiben mit dem STM untersucht. Die Spitzeninduzierte CVD bedient sich dabei gasförmiger Precursor, um aus diesen gezielt Metalle lokal auf der Substratoberfläche abzuscheiden. Insbesonders lassen sich sowohl Punkt- als auch Linienstrukturen aus Eisen bzw. Kupfer auf Si, $InAs$ und $GaAs$ erzeugen. Als Precursorgase dienten dabei Eisenpentacarbonyl und $Bis(N, N-dimethylaminopropan-2-ol)Cu$. Weiterhin wurde das rein thermisch induzierte Wachstum von Kupfer aus der Gasphase auf Si bzw. SiO_2 und aufgesputterten Zinkoxid-Schichten untersucht. Die so erzeugten Systeme können sowohl im Halbleiter-/Elektronikbereich als auch für katalytische Zwecke eingesetzt werden.

O 36.41 Mo 15:00 Poster TU F

Titanium silicide contacts for nanoengineering — •Svend Vagt, Gernot Gardinowski, Tammo Block, Volkmar Zielasek, and Herbert Pfnür — Institut für Festkörperphysik, Abteilung Oberflächen, Universität Hannover, Appelstr.2, 30167 Hannover, Germany

For the electrical characterization of nanostructures it is vital to connect the mesoscopic to the macroscopic world. The requirements for such contacts are chemical purity, well defined boundaries, and a substrate free of defects for further nanoprocessing.

TiSi$_2$ contacts with a variable separation down to 200nm have been generated by an optimized e-beam lithography process and were studied with SEM, STM, and μ-Auger. Ti was evaporated 50 nm thick on a lithographically structured Si substrate and subsequently annealed to activate the silicide formation at the Si interface. These contacts have been demonstrated to be stable up to 1200K on Si(100) and Si(111). STM measurements reveal atomically clean Si surfaces in the contact gaps and sharp and well-defined contact boundaries.

When the Ti pads are capped by a Si layer prior to thermal silicide formation, step bunching of the substrate due to lattice-mismatch induced strain close to the contact boundaries is reduced, probably because of a reduced consumption of substrate silicon.

Futher analysis focusses on even thinner TiSi$_2$ contacts to improve the connectability between the contacts pads and the nanostructures.

O 36.42 Mo 15:00 Poster TU F

Nanocontacts and Nanowires: Electromigration effects in thin Ag structures — •G. Gardinowski, C. Tegenkamp, and H. Pfnür — Institut für Festkörperphysik, Abteilung Oberflächen, Appelstr. 2, 30167 Hannover, Germany

In order to characterize nanostructures electrically, contacts in the nm - region are of importance. A controlable planar breakjunction technique of high yield is particularly interesting, but requires a nearly total understanding of the fabrication method. We demonstrate that it is possible to produce desireable contacts via electromigration. Experiments with lithographic prestructured Ag-wires on Si (100) with different shapes and thickness were carried out in constant- current and constant - voltage mode monitored by SEM. The procedure can be devided into two phases. The first shows the typical electromigration effects like the void/hillock formation and the influence of defects inside the Ag - structure until the breakdown of the wire. Nanocontacts with reproduceable separation lengths in the range of 10-20 nm can be produced as seen by SEM/AFM. The second phase is typical for the constant - voltage mode and demonstrates a way for the self-assembling of Ag - nanowires. After the formation of a planar breakjunction an interesting growth behavior sets in. Field effects cause a local melting of the silver structure which leads to the formation of a crystalline silver wire with no defects up to length of 200 μm. As seen in AFM - line scans, the width is around 700 nm and the height around 200 nm.

O 36.43 Mo 15:00 Poster TU F

Nanostructured Ag wetting layers on Si via e-beam lithography — •T. Block, V. Zielasek, and H. Pfnür — Institut für Festkörperphysik, Universität Hannover, Appelstrasse 2, 30167 Hannover

o We present a lithography method taking place entirely in UHV for the formation of metal nanostructures of arbitrary shape. A combined SEM-STM instrument is used to perform electron beam lithography and subsequent investigations with STM within the same vacuum system. We employ electron-beam stimulated thermal desorption of oxygen (EBSTD) from ultrathin SiO_2 layers on a Si(111) surface to generate windows of clean Si in a SiO_2 mask, usually in the form of narrow (≤20nm) lines. During subsequent Ag deposition two different morphologies of nanowires are formed, depending on the annealing treatment. Percolated epitaxial crystalline silver islands are observed at low temperatures and a continuous wetting layer emerges at elevated temperatures. The wetting layer forming at 790K shows the well-known $(\sqrt{3}\times\sqrt{3})$ Ag reconstruction, which exhibits a metallic surface state band and a conductivity of about $5-10\times10^{-5}\Omega^{-1}$, as demonstrated elsewhere [1]. Continuous layers are already formed at a coverage of 0.5 ML, indicating accumulation of Ag from the neighboring SiO_2 covered areas, an effect not observed for thicker films deposited at 130K and annealed to ≈700K. The crystalline silver islands as well as the wetting layer appear in our experiment restricted to the size and shape of the prepared Si window areas.

[1] C.-S. Jiang et. al. , Phys. Rev. B **54** 10389 (1996)

O 36.44 Mo 15:00 Poster TU F

Electrical and optical sensors fabricated by thin film fracture — •Mady Elbahri, Shiva Kumar Rudra, Abhijit Biswas, and Rainer Adelung — Lehrstuhl für Materialverbunde, Technische Fakultät der Universität Kiel, Kaiserstrasse 2, 24143 Kiel, Germany

Recently, it was shown how nanowires can be formed by using stress induced cracks in thin films as a template [1]. The fracture of thin films is determined by the strain field. The strain field depends on the design of the film, which can be chosen intentionally to create predetermined breaking points. Such nano structures have the potential to be used as electrical or optical triggered sensors.

The fracture approach is also useful for the generation of thin film cracks in metallic thin films. Those cracks, typically smaller than optical wavelength, show interesting optical properties, making them a promising candidate for optical and sensors applications. Conductivity measurements through nanowire arrays and optical measurement for such nanocracks will be shown and discussed; also using them for the detection of molecules by means of optical measurement.

[1] R. Adelung, M. Elbahri, O.C. Aktas et al., Nature Materials 3, 375, (2004)

O 36.45 Mo 15:00 Poster TU F

Thin layers of donor and acceptor mixture as studied by STM, STS and AFM — •Min Ai[1], Frank Jäckel[1], Peng Wu[1], Wei Zhuang[1], Jishan Wu[2], Klaus Müllen[2], and Jürgen P. Rabe[1] — [1]Humboldt University Berlin, Department of Physics, Newtonstr. 15, 12489 Berlin — [2]Max-Planck-Institut für Polymerforschung, Ackermannweg 10, 55128 Mainz

A new "star" type derivative of hexa-*peri*-hexabenzocoronene (HBC) with rigid arms was investigated as neat system at the interface between its solution in 1,2,4-trichlorobenzene and the basal plane of graphite. STM revealed double layers, where the structure of the first layer was determined by the interaction with the substrate. The second layer exhibits the same lattice parameters as the first layer, but different structure within the unit cell. Structure and electronic properties of layers of the new HBC derivative mixed with an electron acceptor (coronenebis(dicarboximide)) were characterised by STM, STS and AFM.

O 36.46 Mo 15:00 Poster TU F

Evaluation of the Elasticity on Single-Walled Nanotubes on Graphite(0001) with Dynamic Force Spectroscopy — •Timo Behnke, Makoto Ashino, and Roland Wiesendanger — Institute of Applied Physics, University of Hamburg,

Due to their unique mechanical and electronic properties, carbon nanotubes are one of the promising canditates for future functional nanostructures. We study the elasto-mechancial properties of single-walled carbon nanotubes (SWNT) at the nanoscale using dynamic force microscopy and spectroscopy with frequency modulation technique. Site specific frequency shift data were recorded by changing the tip-sample distance at different positions on SWNTs and Graphite, respectivly, and converted into a force versus distance relationship. The results obtained in the attractive and repulsive regime are compared with respect to theoretical estimations. Possible elastic deformation of SWNTs under radial compression will be discussed.

O 36.47 Mo 15:00 Poster TU F

Electronic structure of nano-size iron oxide particles measured by scanning tunneling- and photo electron spectroscopy — •Marcus Preisinger, Michael Krispin, Torsten Rudolf, and Siegfried Horn — Lehrstuhl für Experimentalphysik II, Universität Augsburg, D-86135 Augsburg

We have investigated the electronic structure of nano sized iron oxide by scanning tunnelling microscopy (STM) and spectroscopy (STS) as well as by photoelectron spectroscopy (PES). Nano particles were produced by thermal treatment of Ferritin molecules containing a self-assembled core of iron oxide. Depending on the thermal treatment we were able to prepare different phases of iron oxide nanoparticles resembling γ-Fe_2O_3, α-Fe_2O_3, and a phase which apparently contains both, γ-Fe_2O_3 and α-Fe_2O_3. Changes to the electronic structure of these materials were studied under reducing conditions. We show that the surface band gap of the electronic excitation spectrum can differ from that of bulk material and is dominated by surface effects.

O 36.48 Mo 15:00 Poster TU F

Gold Nanoparticles on Nb/Al_2O_3: An STM Study of Dynamic Charging Effects at Room Temperature — •Christof Dietrich, Berndt Koslowski, Frank Weigl, Hans-Gerd Boyen und Paul Ziemann — Abt. Festkörperphysik, Universität Ulm

In order to obtain a system showing Coulomb Blockade effects at room temperature, in a first step epitaxial Nb(110) films were prepared on Sapphire(0001). These films have an extremely smooth surface (RMS: 0.4 nm for 500x500 nm^2) and atomic resolution can be achieved. Onto this base electrode, 0.9 nm of Al was evaporated and oxidized by flashing the sample several times to 1400K in an oxygen atmosphere. An extremely smooth and epitaxial Al_2O_3 coating was obtained. Small Gold particles (1nm-15nm) were prepared by loading a solution of the diblock-copolymer polystyrene-b-poly(2)vinylpyridin in toluene with $HAuCl_4$. By dip coating, one monolayer of Gold salt loaded inverse micelles could be deposited on the Al_2O_3/Nb (110)/Sapphire(0001) system. In a final step, the polymer was removed in an Oxygen plasma resulting in naked gold particles of controlled size and separation exhibiting a high degree of hexagonal order as revealed by STM. Additional I-V measurements on the particles clearly show Coulomb blockade effects which can be nicely fit to orthodox theory of the Coulomb blockade. We discuss the effect of annealing on the charging behavior.

O 36.49 Mo 15:00 Poster TU F

Study of metal cluster growth on rare gas layers using STM and UPS — •F. Ghaleh[1], D. Boecker[1], T. Irawan[1], H. Hövel[1], C. Yin[2], and B. von Issendorff[2] — [1]Experimentelle Physik I, Universität Dortmund, D-44221 Dortmund — [2]Fakultät für Physik, Universität Freiburg, D-79104 Freiburg

The growth of metal clusters on rare gas films, as described in Ref. 1 was studied using a combination of different techniques on the same sample. UPS was used for monitoring the growth of rare gas layers with a well defined thickness of up to 100 monolayers. Then metal atoms (Au or Pb) were deposited on these surfaces. UPS spectra for different rare gas film thicknesses and different substrate materials (HOPG, Au and Pb) taken in normal and oblique electron emission indicate that several ten monolayers of rare gas are needed for a complete decoupling of the clusters and the substrate. The morphology could be checked also after rare gas desorption using STM. For metal substrates the change of morphology from islands to flat layered structures was observed when the sample had been warmed up to room temperature. In future experiments we will extend these studies to the deposition of mass selected clusters and a comparison to experiments for the same clusters in a free cluster beam.

[1] V.N. Antonov, J.S. Palmer, A.S. Bhatti, J.H. Weaver, Phys. Rev. B **68**, 205418 (2003).

O 36.50 Mo 15:00 Poster TU F

Electronic transport in anisotropic Pb structures grown on Si(557) — •M. Czubanowski, Z. Kallasy, C. Tegenkamp, and H. Pfnür — Institut für Festkörperphysik,Abteilung Oberflächen ,Appelstr. 2, 30167 Hannover, Germany

Transport measurements between 3K and 300K of epitaxially grown Pb–film on Si(557) have been performed. Using the van der Pauw geometry, both the conductivity parallel and perpendicular to the steps of the uniaxial Si(557) surface have been measured and correlated with Pb-structures obtained by LEED and STM.

Different transport mechanisms have been identified: Above the percoloation limit of 0.6ML the electronic transport in annealed Pb films up to 3ML is activated. With respect to the Si(557) step structure the conductance parallel to the steps is higher (50–100%) than in the perpendicular direction. For higher coverages a metallic behavior is seen, i.e. the conductance decreases with increasing temperature. In contrast to this anisotropic 2-D conductivity, a 1-D conduction channel is formed parallel to the steps, after annealing of Pb–multilayers to 640K. The remaining coverage is close to 1ML. As revealed by STM, atomic wires, separated by 14Å, are formed on the Si(557) substrate.

For $T_C \leq$78K, the conductivity shows a (1/T +*const.*) dependency for the parallel direction. This 1D-transport switches back to 2D for temperatures higher than T_C. At this temperature also an insulator-metal transition is seen for the perpendicular direction. This transition at $\mathrm{T_C}$ can be correlated with an order–disorder phase transition in form of a 10–fold periodicity along the atomic wires.

O 36.51 Mo 15:00 Poster TU F

Kontaktieren von Nanoröhrchen mit einer Testelektrode unter dem LEEPS-Projektionsmikroskop — •Dirk Henning Weber, André Beyer, Andreas Eisele, Susanne Schüler, Berthold Völkel und Armin Gölzhäuser — Physik supramolekularer Systeme, Universität Bielefeld

Wir stellen ein Verfahren vor, mit dem das LEEPS-Mikroskop (LEEPS = Low Energy Electron Point Source) zur Charakterisierung der strukturellen, elektrischen und mechanischen Eigenschaften von Nanoobjekten eingesetzt werden kann. Als Testobjekte verwenden wir Kohlenstoff Nanoröhrchen. Das LEEPS-Mikroskop besteht im Wesentlichen aus einer feldemittierenden Spitze als Quelle für kohärente Elektronen, einem Probenhalter und einem Detektorschirm. Die am Objekt gestreuten Elektronen erzeugen auf dem Schirm eine Projektion des Objekts. Ein Vergleich zwischen LEEPS-Aufnahmen und REM-Bildern wird präsentiert. Durch gezielte Annäherung der Punktquelle an ein Objekt kann dieses kontaktiert werden. Da man während der Annäherung die lokale Morphologie der Nanoröhrchen beobachten kann, bildet dieses Verfahren die Grundlage für die Untersuchung des Einflusses der Morphologie auf die Leitfähigkeit. Das Konzept einer zusätzlichen Spitze, die anstelle der Punktquelle als bewegliche Elektrode für diese Messungen dient, wird diskutiert.

O 36.52 Mo 15:00 Poster TU F

Niederenergetische Elektronenholographie mit Nanometerauflösung (LEEPS - Mikroskopie) — •Andreas Eisele, Berthold Völkel und Armin Gölzhäuser — Physik supramolekularer Systeme, Universität Bielefeld

Es wurde die Einsatzfähigkeit der LEEPS - Mikroskopie für die Strukturaufklärung an einzelnen Molekülen und Nanostrukturen untersucht. Bei der Abbildung von DNA-Bündel wurde eine reproduzierbare Auflösung von Objektdetails in der Größe von ∼1nm erreicht. Dabei erhält man durch die Verwendung niederenergetischer Elektronen einen hohen Bildkontrast, sodass LEEPS - Experimente keine zusätzliche kontrastverstärkende Probenpräparationen erfordern. Daher kann die LEEPS - Mikroskopie besonders gut bei der Strukturaufklärung biologischer Moleküle eingesetzt werden.

Messungen an leitfähigen Objekten wie *carbon nanotubes* ergaben eine hohe Sensitivität der Bilder für elektrostatische Felder, die sich an der Oberfläche des Probenmoleküls aufbauen. Dadurch kann indirekt - durch Vergleich mit simulatorischen Rechnungen - auf das Probenpotenzial geschlossen werden. Dies demonstriert die Eignung der LEEPS - Mikroskopie für ortsaufgelöste kontaktlose Leitfähigkeitsmessungen an Netzwerken aus Nanostrukturen.

O 36.53 Mo 15:00 Poster TU F

Investigation of InAs/AlAs(001) quantum dots using X-ray diffraction and FEM calculations — •Andriy Zolotaryov and Robert L. Johnson — Institute of Experimental Physics, University of Hamburg, Luruper Chaussee 149, 22761 Hamburg, Germany

Nanoscale island structures are of great importance for applications exploiting quantum confinement effects. An exact knowledge of the crystalline and chemical properties of such structures plays a crucial role. Here we present a new method for the structural analysis of nanoisland systems using X-ray synchrotron radiation and final element calculation techniques. The InAs/AlAs(001) sample was grown using MBE. InAs final coverage was limited to 2.7 ML at a growth temperature of 500°C. The grazing incidence diffraction experiments were performed at the BW2 wiggler beam line on the DORIS storage ring at HASYLAB, DESY. Two 2D reciprocal space maps in the vicinity of the AlAs (202) and (220) Bragg positions were acquired. In order to analyse the diffraction data the theoretical calculations of the diffraction patterns have been performed based on InAs island growth simulations using finite-element (FEM) computations and the kinematical diffraction approximation. Trial-and-error fitting procedure has revealed the presence of two types of islands with different dimensions, chemical composition and surface density. STM and AFM measurements have confirmed correctness of the proposed model.

O 36.54 Mo 15:00 Poster TU F

Monte-Carlo studies of nanostructures stabilized by surface-state electrons — •N.N. Negulyaev[1], H. Fangohr[2], V.S. Stepanyuk[3], W. Hergert[1], and P. Bruno[3] — [1]Fachbereich Physik, Martin-Luther-Universität, Halle-Wittenberg, Friedemann-Bach-Platz 6, D-06099 Halle, Germany — [2]School of Engineering Sciences, University of Southampton, SO17 1BJ, UK — [3]Max-Planck-Institut für Mikrostrukturphysik, Weinberg 2, 06120 Halle, Germany

Our studies have shown that new magnetic nanostructures can be stabilized by the long-range interactions between adatoms mediated by surface-state electrons[1,2]. Remarkable expereminets of the group of W.-D. Schneider have demonstrated that cerium adatoms, deposited on Ag(111), can self-assemble into large ordered superlattice via the long-range interaction[3]. Here, we present the Monte Carlo(MC) simulations of the coverage and temperature dependent self-organization of the magnetic adatoms on metal surfaces. The ab initio KKR Green's function method is used to find parameters of interactions for the MC simulations. We concentrate on Ce adatoms on Ag(111) and Co adatoms on Cu(111).

[1] V.S. Stepanyuk, A.N. Baranov, D.V. Tsivlin, et. al., Phys. Rev. B **68**, 205410 (2003).

[2] V.S. Stepanyuk, L. Niebergall, R.C. Longo, et. al., Phys. Rev. B **70**, 075414 (2004).

[3] M. Ternes, C. Weber, M. Pivetta, et. al., Phys. Rev. Lett. **93**, 146805 (2004).

O 36.55 Mo 15:00 Poster TU F

Electronic lifetime in quantum corrals — •Matthias Semmelhack and Felix von Oppen — Fachbereich Physik, FU Berlin, Arnimallee 14, D-14195 Berlin

Motivated by experiment [1], we study the electronic lifetime in quantum corrals on noble metal surfaces. We show that the dominant contribution to the lifetime of surface electrons arises from the excitation of surface electron-hole pairs. Using diagrammatic many-body theory combined with Monte Carlo methods, we find that the lifetime as a function of excitation energy exhibits oscillations induced by the quantum corral. We also develop an efficient semiclassical approximation of the free Green function of the corral, which may be helpful in studying further interaction effects in quantum corrals.

[1] K.-F. Braun, K.-H. Rieder, Phys. Rev. Lett. 88, 096801 (2002)

O 36.56 Mo 15:00 Poster TU F

Dynamics of Nanodroplets — •Anja Habenicht[1], Michael Olapinski[2], Frank Burmeister[3], Johannes Boneberg[1], and Paul Leiderer[1] — [1]Universität Konstanz, Fachbereich Physik, LS Leiderer, 78457 Konstanz — [2]LMU München, Sektion Physik, LS Kotthaus / AG Simmel, 80539 München — [3]Fraunhofer Institut Werkstoffmechanik, 79108 Freiburg

Liquid metal nanodroplets are generated by a dewetting induced desorption process: flat metal nanostructures placed on a substrate are illuminated with an intensive short laser pulse. If heated over the melting point, the liquid nanostructures reduce their surface energy by reforming to spheres. For the large aspect ratios used here, this involves a vertical movement of the center of mass and due to inertia the droplets leave the surface. The velocity of the desorbed nanodroplets is measured with a light barrier technique where the scattering signal is converted into a velocity dependent particle density. Results for different structure dimensions and laser energies are shown. Further we show first results of impact experiments, where the liquid or solid droplets are landed on another substrate. The particles cool down during the flight due to thermal radiation. By catching at different distances the landing temperature can be varied and thus different outcomes of droplet impact are achieved.

O 36.57 Mo 15:00 Poster TU F

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 Halle, Germany

Performing the state of art *ab initio* calculations, we study the quantum confinement of surface-state electrons in atomic-scale nanostructures on metal surfaces. Quantum corrals on Cu(111) and fcc Co/Cu(111) are considered. We predict that the spin-polarization of surface state-electrons caused by magnetic adatoms can be projected to a remote location exploiting the quantum confinement of surface-state electrons in corrals. The long-range exchange interaction between magnetic adatoms in quantum corrals is revealed. The possibility of tailoring this interaction at large distances by the confined surface-state electrons is demonstrated. We show that the spin-polarization of surface-state electrons on Co/Cu(111)[1] could be manipulated constructing atomic-scale nanostructures on this substrate.

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

O 36.58 Mo 15:00 Poster TU F

Ab initio approach for atomic relaxations in supported magnetic clusters — •A.L. Klavsyuk[1], V.S. Stepanyuk[1], L. Niebergall[1], W. Hergert[2], and P. Bruno[1] — [1]Max-Planck-Institut für Mikrostrukturphysik, Weinberg 2, 06120 Halle, Germany — [2]Fachbereich Physik, Martin-Luther-Universität, Halle-Wittenberg,Friedemann-Bach-Platz 6, D-06099 Halle, Germany

We present a newly developed scheme for atomic relaxations of magnetic supported clusters. Our approach is based on the full potential Korringa-Kohn-Rostoker Green's function method and the second moment tight-binding approximation for many-body potentials. We demonstrate that only a few iterations in ab initio calculations are necessary to find an equilibrium structure of supported clusters. As an example, we present our results for small Co clusters on Cu(001). Changes in electronic and magnetic states of clusters due to atomic relaxations are revealed.

O 36.59 Mo 15:00 Poster TU F

Transport through a benzene-dithiolate molecule — •Volodymyr Maslyuk[1], Thomas Bredow[2], and Ingrid Mertig[1] — [1]Fachbereich Physik, Marthin-Luther-Universität Halle-Wittenberg, Von-Seckendorff-Platz 1, 06099 Halle — [2]Theoretische Chemie Institut, Universität Hannover, Am Kleinen Felde 30, 30167 Hannover

We present the results of a theoretical investigation of the transport properties of a benzene-dithiolate molecule between Cu contacts. The electronic properties were calculated within the framework of density functional theory using a linear combination of atomic orbitals. The structure relaxation of the molecule at the surface and between the leads was performed by means of a semi-empirical method MSINDO [1]. The parameters were fitted to various experimental data and results of first principles calculations of structure and energy. The non-equilibrium Green's function formalism was applied to investigate the transport properties. The conductance is discussed as a function of the deformation of the molecule.

[1] B. Ahlswede, K. Jug, J. Comput. Chem. 20 (1998) 563; B. Ahlswede, K. Jug, J. Comput. Chem. 20 (1998) 572.

O 36.60 Mo 15:00 Poster TU F

Direct and indirect manipulation of small water clusters on Ag(111) — •H. Gawronski[1], K. Morgenstern[2], M. Mehlhorn[1], and K.-H. Rieder[1] — [1]Freie Universität Berlin, Institut für Experimentalphysik, Arnimallee 14, 14195 Berlin — [2]Universität Hannover, Institut für Festkörperphysik, Appelstr. 2, 30167 Hannover

Scanning tunneling microscopy (STM), ineleastic tunneling spectroscopy (IETS), and electron induced manipulation at low temperature are used to investigate the dynamics of small D_2O clusters of 6 to 12 molecules formed by deposition of water at 25 K. To get information about the formational changes of the clusters, their excitation energy, and their vibrational modes we use electron induced manipulation at a temperature of 5 K. Formational changes of the D_2O clusters are induced by injecting electrons directly into the cluster with an energy of 180 meV. The energies needed for indirect excitation of a cluster at manipulation distances of a few Ångstrom from the cluster are about a factor 1.5 to 2 higher than those for direct excitation. IETS allows us to identify vibrational modes, namely the frustrated translations and rotation, of D_2O clusters on the Ag(111) surface. Furthermore the gap of the water molecule is visible in the spectra. The results are related to previous IETS and EELS measurements for H_2O bilayers and clusters on the (111) faces of Au, Ag, and Cu.

O 36.61 Mo 15:00 Poster TU F

Corrosion of chemical and mechanical stressed aluminium components studied with MIES, UPS, XPS and AES — •Florian Voigts[1], Martin Frerichs[1], Volker Kempter[1], Sven Hollunder[2], Alfons Esderts[2], and Wolfgang Maus-Friedrichs[1] — [1]Institut für Physik und Physikalische Technologien, TU Clausthal, Leibnizstrasse 4, 38678 Clausthal — [2]Institut für Maschinelle Anlagentechnik und Betriebsfestigkeit, TU Clausthal, Leibnizstrasse 32, 38678 Clausthal

The corrosion of aluminium by exposure to different gases, liquids and especially commercially available disinfectants was studied by means of Auger Electron Spectroscopy (AES), X-Ray Photoelectron Spectroscopy (XPS), Ultraviolet Photoelectron Spectroscopy (UPS), Metastable Impact Electron Spectroscopy (MIES) and fatigue tests. Aluminium components from industrial application as well as aluminium films produced in ultrahigh vacuum (UHV) were used as specimen.

Fatigue tests show a massively reduced lifetime of aluminium components when exposed to disinfectants regularly. Commonly applied protective coatings decrease the lifetime even further.

Our measurements are able to provide information on the state of oxidation, the progress of the corrosion and the influence of various elements present at the surface. Experiments under controlled conditions yield a picture of the reaction mechanisms with selected elements like water, oxygen and salt. We attempt to provide a model for the mechanism of the corrosion and its effect on the durability of the components.

O 36.62 Mo 15:00 Poster TU F

Langreichweitige Granulatstruktur von Gläsern in Beziehung zu deren Oberflächeneigenschaften — •Chun Wang, Andreas Spörl und Georg Krausch — Physikalische Chemie II, Universität Bayreuth, 95440 Bayreuth

Kalknatronsilikat-Floatglas, Borosilikat-Rohrglas und Bleikristallglas zeigen eine gemeinsame charakteristische Granulatstruktur (20-100 nm). Diese Struktur wurde mit Feld-Emissions-Rasterelektronenmikroskopie und Rasterkraftmikroskopie auf den Glasoberflächen untersucht. Die Bereiche zwischen den Granuliten wurden mit dem schwachen Ätzmittel Wasser erodiert. Die Experimente legen nahe, dass die Granulatstruktur aufgrund thermischer Dichtfluktuationen gebildert wird. Das anomale Diffusionverhalten vom Sn aus Floatglas, Pb aus Bleikristall und die Clusterung der Korrosionsprodukte kann mit der Granulatstruktur erklärt werden.

O 36.63 Mo 15:00 Poster TU F

Transport of matter with a chemical wave-the influence of alkali metals on catalytic surface reactions — •Hubertus Marbach[1,2], S. Günther[3,2], T. Neubrand[2], R. Hoyer[2], B. Luerssen[2], G. Lilienkamp[4], Y. Suchorski[4,2], L. Gregoratti[3], M. Kiskinova[3], and R. Imbihl[2] — [1]Lehrstuhl für Pysikalische Chemie II, Universität Erlangen-Nürnberg, Egerlandstraße 3, D-91058 Erlangen — [2]Institut für Physikalische Chemie und Elektrochemie, Universität Hannover, Callinstraße 3 - 3A, D-30167 Hannover — [3]Sincrotrone Trieste, Italy — [4]Institut für Physik und Physikalische Technologien, TU Clausthal

Heterogeneous catalysed reactions as O2+H2 and NO+H2 on Rh(110) are known for their ability to form spatiotemporal concentration patterns on the surface. In this work the influence of coadsorbed alkali metals (AM), namely K and Cs on these reactions were studied experimentally. It turned out that under certain reaction conditions a mass transport of AM occurs. Starting with an initial homogenous distribution of the AM this effect can lead to a condensation of stationary K-O concentration patterns during the O2+H2 reaction. Other selforganized patterns were found in the NO+H2 reaction. All experiments were carried out in UHV-chambers driven as continuous flow reactors. To clarify the underlying processes the following experimental methods were applied: LEEM, XPS, SPEM and PEEM. The driving force of the occurring selforganizing processes will be discussed by presenting experimental results showing chemical, electronic and structural aspects of the substrate and the involved reacting species.

O 36.64 Mo 15:00 Poster TU F

Catalytic Oxidation of Ammonia on RuO$_2$(110) Surfaces: Mechanism and Selectivity — •Yuemin Wang[1,2], Karl Jacobi[2], Wolf-Dieter Schöne[2], and Gerhard Ertl[2] — [1]Lehrstuhl für Physikalische Chemie I, Ruhr-Universität Bochum — [2]Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin

The selective oxidation of ammonia on RuO$_2$(110) surfaces was studied by a combination of vibrational spectroscopy (HREELS), thermal desorption spectroscopy (TDS), and steady-state rate measurements. The stoichiometric RuO$_2$(110) surface exposes coordinatively unsaturated (cus) Ru atoms onto which either adsorption of NH$_3$ (NH$_3$-cus) or dissociative adsorption of oxygen (O-cus) may occur [1]. In the absence of O-cus ammonia desorbs completely thermally without any reaction. However, interaction between NH$_3$-cus and O-cus starts already at 90 K by hydrogen abstraction and hydrogenation to OH-cus, leading eventually to N-cus and H$_2$O. The N-cus species either recombine with each other to N$_2$ or with neighboring O-cus leading to strongly held NO-cus which desorbs around 500 K [2]. Under steady-state flow condition the product selectivity was found to depend on temperature and relative partial pressures of the reactants: Excess oxygen favors the production of NO and at 530 K almost 100 percent selectivity for NO formation is reached. [1] C.Y.Fan, J. Wang, K. Jacobi, G. Ertl, J. Chem. Phys. 114 (2001) 10058. [2] Y. Wang, K. Jacobi, G. Ertl, J. Phys. Chem. B, 107 (2003) 13918.

O 36.65 Mo 15:00 Poster TU F

Pressure Gap in Ammonia Oxidation on Platinum — •Sebastian Günther[1], Axel Scheibe[2], Axel Knop-Gericke[3], Yingfeng Zeng[2], and Ronald Imbihl[2] — [1]Department Chemie, Ludwig-Maximilians-Universität München — [2]Institut für Physikalische Chemie und Elektrochemie, Universität Hannover — [3]Fritz-Haber-Institut der MPG

In an attempt to bridge the pressure gap in ammonia oxidation on platinum, in situ X-ray photoelectron spectroscopy (XPS) was used to follow the adsorbate coverage on Pt(533) in the 10^{-4} mbar range and at about 1 mbar. The N 1s regimes show that at 100 - 300 °C NH_x species are presented; at high temperature atomic nitrogen is dominant, adsorbed NO decompose already below T = 80 °C. The results are compared with the simulations of a realistic mathematical model. For bridging the material gap kinetic studies of N_2 and NO formation on Pt(533) are compared with measurements on a polycrystalline Pt foil. The overall kinetics are very similar, but pronounced differences exist with respect to the hysteretic behavior.

O 36.66 Mo 15:00 Poster TU F

Silizium Cluster auf Oberflächen — •Tim Fischer, Rainer Dietsche, Nils Bertram, Felix von Gynz-Rekowski, Dong Chan Lim, Ignacio Lopez, Young Dok Kim und Gerd Ganteför — Universität Konstanz, 78457 Konstanz

Für Oberflächenprozesse in Chemie, Optik und Elektronik werden immer neuere Werkstoffe gesucht. Stabile "supermagische" Cluster, wie C_{60} oder Sb_4[1], eignen sich für eine Entwicklung solcher neuer Materialien mit ungewöhnlichen elektronischen und chemischen Eigenschaften.

Mögliche Kandidaten sind die magischen Silizium Cluster Si_4[2] und Si_7. Diese werden mit einer Magnetronquelle erzeugt, massenselektiert und auf unterschiedlichen Substraten weich gelandet ($E_{kin} \leq 0{,}3$ eV/Atom). Die auf Graphit (amorph oder kristallin) oder einen Silbereinkristall deponierten Cluster werden mit PES, STM, AES, LEED und HREELS untersucht.

Die Spektren weisen auf eine inerte Cluster-Spezies auf der Oberfläche hin. Eine Carbidisierung auf amorphen Graphit und Oxidierung bei Sauerstoffzugabe wird nicht beobachtet. Im Gegensatz dazu ist bei deponierten Si-Atomen eine Reaktion zu erkennen[3].

[1] B. Stegemann, B. Kaiser and K. Rademann New Journal of Physics 4, 89 (2002)

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

[3] M. Mathes, M. Grass, Y.D. Kim and G. Ganteför Surf. Sci. 552, L58, (2004)

O 36.67 Mo 15:00 Poster TU F

Synchrotron x-ray studies of metal and semiconductor clusters — •C. Hendrich[1], D. N. Ievlev[1], F. Meneau[2], W. Bras[2], P. Lievens[1], and K. Temst[1] — [1]Laboratory of Solid State Physics and Magnetism, K.U. Leuven, Celestijnenlaan 200 D, 3001 Leuven, Belgium — [2]DUBBLE@ESRF, 6 Rue Jules Horowitz, 38043 Grenoble, France

Ensembles of nanometer sized clusters were investigated with synchrotron x-ray radiation (small angle x-ray scattering (SAXS) and wide angle x-ray scattering (WAXS)) at the DUBBLE beam line at the European Synchrotron Radiation Facility (ESRF).

The investigated samples consisted of metal and semiconductor clusters embedded in a MgO matrix. The Co, Pb and Si clusters were produced by a laser vaporization source and their size-distribution was determined by time-of-flight mass spectrometry. Embedded cluster films were grown on mica substrates by co-depositing the clusters with MgO evaporated from a Knudsen cell.

Analysis of the data from the SAXS measurements allows to estimate the cluster radii by using Guinier plots. The results are compared with the sizes obtained from time-of-flight mass spectrometry.

The WAXS data reveal information about the chemical composition of the samples, i.e. about oxidation of the clusters. The diffraction peaks from the different lattice orientations can be identified and their shifts compared to the bulk values yield information on changes in the lattice constants of the cluster material.

O 36.68 Mo 15:00 Poster TU F

Superconducting properties of cluster-assembled Pb-films — •M.J. Van Bael, D.N. Ievlev, A.N. Dobrynin, C. Hendrich, K. Temst, V.V. Moshchalkov, and P. Lievens — Laboratorium voor Vaste-Stoffysica en Magnetisme, Katholieke Universiteit Leuven, Celestijnenlaan 200D, B-3001 Leuven, Belgium

We have prepared Pb cluster assembled films and studied their superconducting properties. The clusters were produced in a laser vaporization cluster source and deposited at low kinetic energy (<1 eV/atom) at UHV conditions [1, 2]. The mass abundance distribution was monitored by time-of-flight mass spectrometry. By changing the source parameters the mass distribution peak was shifted in the range from 100 to 1500 atoms per cluster. The superconducting properties of the Pb-cluster films were measured in a SQUID magnetometer and by ac-susceptibility. Pb is a superconducting material with a bulk critical temperature of 7.2K. A reduced critical temperature is observed in the cluster-assembled Pb films. We have measured the superconducting phase boundary and magnetic hysteresis curves with the applied magnetic field parallel and perpendicular to the film plane. The dependence of the superconducting properties on the size of the constituent clusters will be discussed.

[1] N. Vandamme, E. Janssens, F. Vanhoutte, P. Lievens, C. Van Haesendonck, J. Phys.: Cond. Matter 15, S2983 (2003).

[2] W. Bouwen, P. Thoen, F. Vanhoutte, S. Bouckaert, F. Despa, H. Weidele, R.E. Silverans, and P. Lievens, Rev. Sci. Instrum. 71, 54 (2000).

O 36.69 Mo 15:00 Poster TU F

Highly correlated STM and 2PPE-imaging of defined cluster-substrate System. — •M. Rohmer, C. Wiemann, M. Munzinger, L. Guo, M. Aeschlimann, and M. Bauer — FB Physik,Technische Universität Kaiserslautern, Erwin-Schrödinger-Straße, D-67663 Kaiserslautern

Conventional PE-experiments probe electronic properties of deposited clusters integral over a macroscopic sample area and give, in general, rise to inhomogeneous broadening due to e.g. local substrate inhomogenities or a spread in the cluster properties. To overcome this problem we combined a STM and a PEEM to enable in situ characterization of a surface with respect to topography and lateral distribution of the photoemission yield. The STM allows to set local markers which can be identified in the PEEM images. In this way local highly correlated STM/Photoemission experiments of deposited clusters are possible. We used threshold PE- and 2PPE-PEEM to record the lateral distribution of the photoemission yield from selected areas of Ag clusters on HOPG which had been characterized by STM before. Furthermore, data are presented that correlate local spectroscopic data (in terms of PES and a scan of the laser wavelength) of the Ag/HOPG surface using our PEEM with STM images obtained from identical areas. These results show that the combination of PEEM and STM is an efficient tool for the investigation of nanoscopic systems additional to conventional PES.This work was supported by the DFG, SPP1153.

O 36.70 Mo 15:00 Poster TU F

Two-photon-photoemission spectroscopy of supported silver clusters — •Mihai E. Vaida[1], Tobias Gleitsmann[1], Bert Stegemann[2], Thorsten M. Bernhardt[1], and Ludger Wöste[1] — [1]Freie Universität Berlin, FB Physik, Arnimallee 14, D-14195 Berlin, Germany — [2]Bundesanstalt für Materialforschung und -prüfung, BAM VIII.1 Tribologie und Verschleißschutz, Unter den Eichen 44-46, D-12205 Berlin, Germany

In order to get an insight into the electronic properties of atomic silver clusters, we set up the technique of time-resolved two-photon-photoemission spectroscopy (2PPS) to a well-defined cluster-support system consisting of silver clusters on an atomically flat insulating thin film of magnesia. The goal is to determine the electronic level structure of the supported silver clusters as a function of cluster size as well as the corresponding excited state lifetimes to identify possible radiative and non-radiative transitions. For this purpose we set up a new experimental arrangement combining a high intensity continuous sputter clusters source (CORDIS) with an UHV-chamber for surface analysis. The cluster ions are mass-selected via quadrupole mass-filter, thermalized, deflected out of the beam production line and subsequently guided by electrostatic lenses and an octopole ion guide onto a MgO/Mo(100) surface. The 2PPS experiments will be carried out by utilizing a home-built field free time-of-flight electron spectrometer. The light source consists of an amplified kHz femtosecond laser system and an optical setup for pump-probe measurements with a typical pulse length of about 40 fs.

O 36.71 Mo 15:00 Poster TU F

Growth and properties of Ag nanoparticles on HOPG — •Ignacio Lopez-Salido, Dong Chan Lim, Tim Fischer, Rainer Dietsche, Felix v. Gynz-Rekowski, and Young Dok Kim — Department of Physics, University of Konstanz, D.78457, Konstanz, Germany

Growth of Ag nanoparticles on Highly Oriented Pyrolytic Graphite (HOPG) surfaces were studied using Scanning Tunneling Microscopy (STM). The Ag particles show quite narrow size distributions on the HOPG surface, and the particle sizes can be controlled using variation of Ag coverage. Detailed analysis of the STM images reveals that Ag nanoparticles grow three-dimensionally from the initial stage of the particle growth, and no significant changes in the ratio of the particle height and width can be observed as a function of particle size. This result is quite in contrast to those of Ag on other van der Waals surfaces such as Wse2, on which Ag prefers two-dimensional growth above a certain particle size, indicating that small changes in metal-support interactions can alter the particle shape significantly. Due to the extremely weak metal support interactions of this system, information of intrinsic size effects of Ag nanoparticles on electronic and chemical properties can be obtained. High-Resolution Electron Energy Loss Spectroscopy and core level shift data show significant alteration of the electronic and chemical properties of Ag nanoparticles as a function of particle size.

O 36.72 Mo 15:00 Poster TU F

Photoelectron spectra of quantized states on cluster facets — •I. Barke, T. Irawan, and H. Hövel — Experimentelle Physik I, Universität Dortmund, D-44221 Dortmund

Gold clusters grown on prestructured Highly Oriented Pyrolytic Graphite (HOPG) have been investigated by Scanning Tunneling Spectroscopy (STS) and Ultraviolet Photoelectron Spectroscopy (UPS). In earlier STS studies the pronounced patterns of standing waves in the dI/dV maps measured on the top facets of large Au clusters have been identified with a Shockley surface state confined to the facet area [1]. Here we present new results of combined UPS and STM studies using the same sample which are discussed in the context of the respective characteristics of the experimental methods. Spatial (UPS) and momentum (STS) averaging is taken into account explicitly, as well as the dynamic final state effect in the photoemission process [2]. Quantized states could now be clearly observed not only in the STS curves, but also in angle resolved UPS (ARUPS) measurements of the same cluster sample. Utilizing a sophisticated deconvolution technique based on the Maximum Entropy Method (MEM) we achieve a unified description of the different spectra.

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

[2] H. Hövel, I. Barke, H.-G. Boyen, P. Ziemann, M.G. Garnier, P. Oelhafen, Phys. Rev. B **70**, 045424 (2004).

O 36.73 Mo 15:00 Poster TU F

Surface enhanced infrared absorption (SEIRA) of spherical gold nanoparticles on SiO_2 — •Dominik Enders[1], Andreas Priebe[1], Swen Rupp[1], Alexander Küller[2], Gerhard Fahsold[1], and Annemarie Pucci[1] — [1]Kirchhoff-Institut für Physik, Ruprecht-Karls-Universität Heidelberg, Im Neuenheimer Feld 227, 69120 Heidelberg — [2]Angewandte Physikalische Chemie, Ruprecht-Karls-Universität Heidelberg, Im Neuenheimer Feld 253, 69120 Heidelberg

The properties of spherical gold nanoparticles with regard to SEIRA were studied in IR transmission-, IRRAS- and ATR geometry. The gold nanoparticles were prepared by citrate reduction of $HAuCl_4$ and deposited on the SiO_2 surface by immersion of the samples (respectively the ATR crystal) into the nanoparticle solution. Time resolved ATR measurements of the SiO_2-water interface during deposition of the nanoparticles on the SiO_2 surface show, that the absorption peaks of the water molecules increasingly get enhanced, as the nanoparticles assemble on the surface. Furthermore, an estimation of the enhancement factor is made by comparing IR transmission spectra of antibodies on nanoparticles/SiO_2 to IRRAS spectra of antibodies on 40 nm thick reflective gold films.

O 36.74 Mo 15:00 Poster TU F

Präparation und optische Charakterisierung von Core-Shell- und Legierungs-Nanopartikeln aus Gold und Silber — •Frank Hubenthal, Torsten Ziegler, Nils Borg, Matthias Alschinger und Frank Träger — Uni Kassel

Aufgrund ihrer besonderen optischen Eigenschaften werden nasschemisch hergestellte metallische Core-Shell-Nanopartikeln seit einigen Jahren intensiv untersucht. In unserem Beitrag stellen wir unsere neuesten Untersuchungen an Core-Shell- und Legierungspartikeln aus Au und Ag vor, die wir mittels Volmer-Weber-Wachstum im UHV hergestellt haben. So wurden u.a. $20{,}85 \cdot 10^{15}$ Ag-Atome/cm^2 auf einem Quarzsubstrat deponiert und das optische Spektrum gemessen. Anschließend wurden schrittweise bis zu $14{,}9 \cdot 10^{15}$ Au-Atome/cm^2 aufgedampft, was zur Bildung von Core-Shell-Partikeln führt. Abhängig von der Au-Dicke kann die Oberflächen-Plasmonen-Resonanz (SPR) präzise zwischen 2,8 eV und 2,1 eV eingestellt werden, ohne dass sich die Extinktion signifikant ändert. Deponiert man hingegen Ag auf Au, so zeigt sich, dass die SPR trotz wachsender Ag-Dicke konstant bei 2,2 eV verbleibt, die Extinktion hingegen deutlich zunimmt. Anschließendes Ausheilen der Core-Shell-Partikel führt zu einer kontinuierlichen Verschiebung der SPR zu 2,6 eV und zur Bildung von Legierungspartikeln. Wir sind somit in der Lage die SPR in einem weiten spektralem Bereich einzustellen und für mögliche Anwendungen (z.B. SERS) zu optimieren.

O 36.75 Mo 15:00 Poster TU F

Molecular dynamics simulations of Si(001) surfaces excited by fs laser pulses — •Jan van Heys and Eckhard Pehlke — Institut für Theoretische Physik und Astrophysik, Universität Kiel

The ultrafast dynamics of Si(100) surface atoms in response to strong electron-hole pair excitation by fs laser pulses has been simulated *ab initio*. The time-dependent Kohn-Sham equations are integrated numerically, while the atomic positions follow Ehrenfest dynamics. The adiabatic approximation is applied to the time-dependent exchange-correlation functional.

The excitation frequency has been chosen in such a way as to maximize the absorption by electronic transitions involving surface dangling-bond states. It turned out that the wave-vector dependence of the optical absorption plays a crucial role for the magnitude of electron-hole pair excitation. The effect of different laser-pulse shapes, widths, and intensities on the dynamics of the Si(001) dimer-buckling angle has been studied in detail. Notably, the magnitude of the electronic excitation as well as the buckling-angle amplitude vary non-monotonically with, e.g., laser intensity.

O 36.76 Mo 15:00 Poster TU F

Van der Waals interaction: Semi-*ab initio* description of graphite and its surface — •Frank Ortmann, Wolf G. Schmidt, and Friedhelm Bechstedt — Institut für Festkörpertheorie und -optik, Friedrich-Schiller-Universität, Max-Wien-Platz 1,07743 Jena, Germany

Graphite is one of the most interesting and demanding model systems for *ab initio* calculations because of the strong sp^2 -hybridized intralayer bonds and the weak van der Waals bonded layers. Density-functional calculations within the generalized-gradient approximation (DFT-GGA)

fail to yield a converged lattice constant perpendicular to the graphene sheets[1].
Therefore we investigate the influence of an additional long-range attractive term based on the London description of van der Waals forces[2]. It is found that one obtains the correct c lattice constant of graphite while the changes of the bulk properties of diamond due to the inclusion of the van der Waals term are negligible. Results for the relaxation of the graphite surface will be presented.
[1] K. R. Kganyago and P. E. Ngoepe, Molecular Simulation **29**, 39 (1999)
[2] F. London, Z. Phys. Chem. **Abt. B11**, 222 (1930)

O 36.77 Mo 15:00 Poster TU F

DFT studies of charged gold surfaces — •Martina Nothacker[1], Ferdinand Evers[1], Klaus-Peter Bohnen[2], Rolf Heid[2], Florian Weigend[1], Christian Elsässer[3], and Jörg Weissmüller[1] — [1]Institut für Nanotechnologie, Forschungszentrum Karlsruhe, 76021 Karlsruhe, Germany — [2]Institut für Festkörperphysik, Forschungszentrum Karlsruhe, 76021 Karlsruhe, Germany — [3]Frauenhofer Institut für Angewandte Festkörperphysik, 79108 Freiburg, Germany

The study of surface and interface properties, electronic and structural, has a long history. Surprisingly, very little is known about the change of these propertities, for instance in bandstructure, surface atom configuration etc. when the surface is being charged. In view of recent experiments, we use density functional methods in order to analyze how the reconstruction of a planar gold surface is modified with increasing surface excess charge. Our results for the planar surface will be compared to data for charged gold clusters, where we find a behavior in qualitative agreement with the experimental findings.

O 36.78 Mo 15:00 Poster TU F

The aqueous-solution gas interface of sodium halogenides — •Michael Paulus[1], Christian Gutt[1], Michael Sprung[2], Christoph Krywka[1], and Metin Tolan[1] — [1]Experimentelle Physik I, Universität Dormund, Maria-Goeppert-Mayer Str. 2, 44227 Dortmund, Deutschland — [2]c/o 8ID/IMMY-XOR-CAT, APS/ANL, Argonne, IL, 60439, USA

We present an in-situ grazing incidence diffraction (GID) experiment to study the aqueous-solution gas interface of the sodium halogenides, NaCl, NaBr and NaI. The aim of our experiment was to investigate the microscopic structure of the aqueous-solution gas interface and its changes for different types of salt in comparison with a water surface. Besides the appearance of the ion structure factor we observe a reduction of the surface energy at short length scales as it was calculated by Mecke et al PRE 59 (6) 6766 (1999).

O 36.79 Mo 15:00 Poster TU F

Dynamics of ice surface morphologies close to the melting point — •Sebastian Schöder, Harald Reichert, Simon Engemann, and Helmut Dosch — Max-Planck-Institut für Metallforschung, Heisenbergstrasse 3, D-70569 Stuttgart

Ice surfaces play an important role in many natural and technical systems. In order to get access to the dynamics of ice surface structures, we have investigated a vincinal ice surface. The dynamics of the facets was examined with dynamic light scattering in a specially designed experimental chamber. This setup allows us to accurately control the sublimation rate of the observed surface. The results were compared for different temperatures. For low temperatures (-12.5 degrees) no dynamics was found. For temperatures close to the melting point we found dynamic correlations with a correlation time in the order of ten minutes. We attribute this temperature dependent behaviour to the surface melting of ice.

O 37 Hauptvortrag Soukiassian

Zeit: Dienstag 09:45–10:30 Raum: TU EB301

Hauptvortrag

O 37.1 Di 09:45 TU EB301

Silicon Carbide Surfaces: Metallization versus Passivation — •Patrick Soukiassian — Commissariat à l'Energie Atomique, Laboratoire SIMA associé à l'Université de Paris-Sud/Orsay, DSM-DRECAM-SPCSI, Saclay, Bâtiment 462, 91191 Gif sur Yvette Cedex, France

Silicon carbide (SiC) is an advanced semiconductor especially promising in high power, high temperature, high voltage and high frequency micro-electronics devices and sensors. Cubic and hexagonal SiC surfaces exhibit many reconstructions (over 10). SiC nanochemistry with oxygen and hydrogen is studied by atom-resolved scanning tunneling microscopy and spectroscopy, synchrotron radiation based- core level and valence band photoemission spectroscopies, and infrared absorption spectroscopy. The following results will be presented and discussed: i) Atomic scale understanding of O2 interaction and initial oxide interface formation. ii) The first example of H-induced semiconductor surface metallization. This unprecedented behavior results from H-creating a specific defect coming from competition between hydrogen termination of surface dangling bonds and hydrogen-generated steric hindrance below the surface. In addition, such a H-induced metallization is not removed by oxygen exposures and most interestingly, also takes place on a pre-oxidized SiC surface. This H-induced metallization directly impacts the ability to eliminate electronic defects at semiconductor interfaces critical for microelectronics, provides means to develop electrical contacts on high band-gap chemically passive materials, particularly exciting for interfacing with biological systems where oxygen is unavoidable, and gives control of surfaces for lubrication, e.g. in nanomechanical devices.

O 38 Halbleiteroberflächen und -grenzflächen

Zeit: Dienstag 10:45–13:00 Raum: TU EB301

O 38.1 Di 10:45 TU EB301

Atomic structure of the GaAs(001)-$c(4\times 4)$ surface: first-principles evidence for diversity of heterodimer motifs — •E. Penev[1,2], P. Kratzer[1], and M. Scheffler[1] — [1]Fritz-Haber-Institut der Max-Planck-Gesellschaft, Faradayweg 4–6, D-14195 Berlin — [2]Institut für Physik, Universität Basel, CH-4056 Basel, Schweiz

The atomic structure of the $c(4\times 4)$ reconstruction, formed on the GaAs(001) surface under high arsenic overpressure, has recently been attracting renewed interest. This has lead to a revision of the commonly accepted $c(4\times 4)$ structural model but a definitive understanding of the driving force for the newly proposed structure[1] was lacking. Targeting the later problem, the talk will present a state-of-the-art theoretical study of the GaAs(001)-$c(4\times 4)$ surface employing *ab initio* atomistic thermodynamics based on density-functional theory calculations. We shall demonstrate[2] that in a range of stoichiometries, between those of the conventional three As-dimer and the new three Ga-As dimer model[1], there exists a diversity of atomic structures featuring Ga-As heterodimers, *driven by surface configurational entropy.* These results fully explain the experimental scanning tunneling microscopy images and are likely to be relevant also to the $c(4\times 4)$-reconstructed (001) surfaces of other III-V semiconductors.
[1] A. Ohtake *et al.*, Phys. Rev. Lett. **89**, 206102 (2002).
[2] E. Penev *et al.*, Phys. Rev. Lett. **93**, 146102 (2004).

O 38.2 Di 11:00 TU EB301

InP growth on $c(4 \times 4)$ and (1×3) reconstructed GaAsSb(100) surfaces — •Z. Kollonitsch[1], U. Seidel[1], S. Neumann[2], F.-J. Tegude[2], F. Willig[1], and T. Hannappel[1] — [1]Hahn-Meitner-Institut, SE 4, Glienicker Strasse 100, D-14109 Berlin — [2]Universität Duisburg/Essen, Halbleitertechnik/Halbleitertechnologie, Lotharstr. 55, ZHO, Gebäude LT, D-47048 Duisburg

Lattice matched $GaAs_{0.5}Sb_{0.5}$/InP(100)-layers were grown by MOVPE at 770K. Contamination free sample transfer into ultrahigh vacuum (UHV) allowed for the correlation of in-situ reflectance anisotropy/difference (RA/RD) spectra with LEED and photoelectron spectra (XPS/UPS). The in-situ signals indicated that the $GaAs_{0.5}Sb_{0.5}$ surface was Sb-rich during growth and turned preferably into an As-rich surface after growth. The group-V rich surface reconstructions formed $c(4 \times 4)$ and (1×3) symmetries, which are well known from the related binaries GaAs and GaSb. Energy dependent UP spectra of the $c(4 \times 4)$ reconstruction showed a prominent peak near the valence band maximum which was attributed to a surface state. There were similarities between the $c(4 \times 4)$ reconstructed surfaces of $GaAs_{0.5}Sb_{0.5}$ and GaAs. XPS measurements of InP/GaAsSb interfaces taken in UHV and I-V curves of InP/GaAsSb resonant tunneling diodes indicated that Sb segregation into a subsequent InP layer was significantly lower when the InP film was grown on the $c(4 \times 4)$ reconstructed $GaAs_{0.5}Sb_{0.5}$ surface compared to the (1×3) reconstructed surface.

O 38.3 Di 11:15 TU EB301

A study on the surface structure of CuInSe2 (001) — •thalia Deniozou[1], Norbert Esser[1], Thomas Schulmeyer[2], and Ralf Hunger[2] — [1]Institute for Analytical Sciences, Albert-Einstein-Str. 9, 12489 Berlin-Adlershof, Germany — [2]Surface Science Division, Institute of Materials Science, Darmstadt University of Technology, Petersenstr. 23, 64287 Darmstadt, Germany

In contrast to most other semiconductor surfaces the atomic structure of chalcopyrite (001) surfaces is practically unresolved. Reconstructions have not been reported yet. The (001) surface structure of the chalcopyrite semiconductor CuInSe2 was studied by means of Low Energy Electron Diffraction, Auger Electron Spectroscopy and Synchrotron X-ray Photoelectron Spectroscopy. For the study heteroepitaxial CuInSe2/GaAs (001) films were employed which were grown by molecular beam epitaxy and capped with a protective Se layer. The CuInSe2 surfaces were initially decapped and then treated by simultaneous Ar+-ion bombardment and annealing. Two different reconstructions in dependence of the preparation time were observed for the first time, namely a (2x4) and a mixed (2x4)/(4x2) reconstruction. The chemical state and composition of the CuInSe2(001) surfaces were monitored by the photoelectron spectra of the Cu2p, Se3d, and In4d core levels. The observed surface core level shifts are discussed in relation to possible surface geometries.

O 38.4 Di 11:30 TU EB301

Electronic structure of Ge(001) surface studied by room temperature scanning tunneling spectroscopy — •Oguzhan Gurlu[1,2], Harold J.W. Zandvliet[1], and Bene Poelsema[1] — [1]Solid State Physics Group, MESA+ Research Institute, University of Twente, PO. Box. 217, 7500AE Enschede, The Netherlands — [2]Max-Planck Institut fur Festkorperforschung, Heisenbergstrasse 1, D-70569 Stuttgart, Germany

The surface electronic structure of Ge(001) has been studied by scanning tunneling spectroscopy. The measured surface densities of states unequivocally reveals the presence of a metallic state on the (2x1) domains, which is absent on the c(4x2) domains. This metallic state, so far only observed in integral measurements, is attributed to the flip-flopping dimers, which constitute the (2x1) domains. Our data also reveals a set of previously unresolved surface states, in perfect agreement with published theoretical predictions.

O 38.5 Di 11:45 TU EB301

Photoelektronenbeugungsuntersuchungen an der SiO_2/4H-SiC(0001)-Grenzfläche — •Mark Schürmann, Stefan Dreiner, Ulf Berges, Daniel Weier, Abner de Siervo und Carsten Westphal — Universität Dortmund, Experimentelle Physik 1, Otto-Hahn-Straße 4, 44221 Dortmund

Thermisch oxidierte Siliziumkarbidoberflächen wurden mittels Photoelektronenbeugung untersucht. Dazu stand intensives Synchrotronlicht mit hoher Energieauflösung zur Verfügung, so daß es möglich war, die lokale atomare Struktur der verschiedenen chemisch verschobenen Komponenten im Si2p-Photoemissionsspektrum getrennt zu untersuchen. Insbesondere war so das Signal der Siliziumatome an der Siliziumoxid/Siliziumkarbid-Grenzfläche der Analyse zugänglich.

Die Ergebnisse der Messungen zeigen, daß auch thermisch oxidierte Proben, die keine langreichweitige Ordnung zeigen, an der Grenzfläche lokal durchaus geordnet sein können. Ein Vergleich mit Messdaten von einer Probe mit geordneter Silikatschicht zeigt, daß die lokale atomare Struktur in der Umgebung der Grenzflächenatome in beiden Proben gleich ist.

O 38.6 Di 12:00 TU EB301

Diffusion Pathways of Hydrogen across the Steps of a vicinal Si(001)-Surface — •P. Kratzer[1], M. Lawrenz[2], C. Schwalb[2], M. Dürr[2], and U. Höfer[2] — [1]Fritz-Haber-Institut der Max-Planck-Gesellschaft, Faradayweg 4–6, D-14195 Berlin — [2]Fachbereich Physik und Zentrum für Materialwissenschaften, Philipps-Universität, D-35032 Marburg

Surface diffusion of hydrogen on vicinal Si(001) surfaces is an interesting system to test theoretical results against experimental data, because selective hydrogen adsorption *at the step sites only* opens the experimental possibility to prepare a well-defined initial state. Diffusion of H away from the D_B step sites has been observed by real-space STM studies at elevated temperatures. We have investigated the diffusion pathways by performing density-functional theory calculations using the gradient-corrected PW91 functional and the plane-wave+pseudopotential approach. While H atoms bind more strongly to the lower terrace sites than to the upper terrace sites, the calculated energy barriers show that H diffusion onto the upper terrace is strongly preferred, in agreement with the experimental findings. We learn from the calculations that a metastable intermediate where hydrogen binds weakly to an already fourfold coordinated Si atom at the step is responsible for the lowering of the "upward" diffusion barrier.

O 38.7 Di 12:15 TU EB301

Untersuchung der Struktur der SiO_2/Si-Grenzschicht in Abhängigkeit von der Oberflächenorientierung — •Stefan Dreiner, Mark Schürmann, Ulf Berges, Martin Krause, Christian Flüchter und Carsten Westphal — Universität Dortmund, Experimentelle Physik I, 44221 Dortmund

Die Methode der Photoelektronenbeugung benötigt im Gegensatz zu vielen anderen Beugungsmethoden keine perfekte Periodizität, um Informationen über die lokale atomare Struktur zu gewinnen. Daher ist sie ideal zur Untersuchung des Übergangs zwischen kristallinem Silizium und seinem amorphen Oxid.
Die untersuchten Grenzschichten wurden auf Si-Proben mit (100)-,(111)- und (110)-Orientierung durch thermische Oxidation hergestellt (wenige Å SiO_2-Schichtdicke). Am U41-PGM Meßplatz bei BESSY II wurden hochaufgelöste Si2p-Photoemissionsspektren über nahezu den gesamten Halbraum bei einer Photonenenergie von $h\nu = 180$ eV aufgenommen. Diese Spektren ermöglichen die Trennung der verschieden Oxidationsstufen des Siliziums (Si^{1+}, Si^{2+}, Si^{3+}, Si^{4+}) vom Volumensignal (Si^{B}). Aus den Intensitäten der Si^{x+}-Signale in Abhängigkeit vom Polarwinkel ergibt sich die Tiefenverteilung der Oxidationsstufen in der Grenzschicht. Die Si^{x+}-Beugungsmuster liefern weitere Informationen über die atomare Umgebungsstruktur der Si-Oxidationsstufen. Die Daten der verschiedenen Oberflächenorientierungen werden miteinander verglichen.

O 38.8 Di 12:30 TU EB301

Investigation of the geometrical properties of NiMnSb-Half-Heusler thin films. — •Andreas Stahl[1], Christian Kumpf[1], Eberhard Umbach[1], Peter Bach[2], Georg Schmidt[2], and Laurens Molenkamp[2] — [1]Experimentelle Physik II, Univ. Würzburg — [2]Experimentelle Physik III, Univ. Würzburg

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

We present a series of x-ray measurements on MBE-grown NiMnSb thin films from 15 to 120nm thickness. Reciprocal space mapping was performed using the six-circle-diffractometer at BW2, HASYLAB, Hamburg. Structural properties like the critical thickness for pseudomorphic growth, relaxation, and the poisson ratio of the Half-Heusler layers are discussed.

[1] A. Koveshnikov et al.: submitted to J. Appl. Phys. (2004).

O 38.9 Di 12:45 TU EB301

Characterization of the growth peculiarities of Physical Vapor Deposited CdS on Cu(In,Ga)Se_2 Thin Film Solar Cells Using Kelvin Probe Force Microscopy in Ultrahigh Vacuum — •Ferdinand Streicher, Marin Rusu, Christian A. Kaufmann, Axel Neisser, Susanne Siebentritt, Martha Ch. Lux-Steiner, and Thilo Glatzel — Hahn-Meitner-Institut Berlin, Glienicker Strasse 100, 14109 Berlin, GERMANY

High-efficiency thin-film solar cells based on Cu(In,Ga)Se_2 absorber material have been developed using CdS buffer layers deposited by chemical bath deposition (CBD). However, for industrial production, an inline vacuum deposition such as, e.g. physical vapour deposition (PVD) is preferred. This contribution reports on the preparation and characterization of highly-efficient ZnO/CdS/Cu(In,Ga)Se_2 solar cells with PVD-deposited CdS buffer layers. The PVD-CdS preparation conditions were optimized for the deposition of the CdS layers suitable for highly-efficient (14%, AM1.5, total area) thin film solar cells. Compared to the CBD deposition the ZnO/PVD-CdS/Cu(In,Ga)Se_2 solar cell devices show an increased short circuit current while open circuit voltage is decreased. The surface analysis of the CdS growth process with Kelvin probe force microscopy (KPFM) reveals, that the CdS deposition is retarded at the grainboundaries of the absorber which could be a reason for the observed device behavior.

O 39 Nanostrukturen IV

Zeit: Dienstag 10:45–13:00 Raum: TU EB420

O 39.1 Di 10:45 TU EB420

Formation and decay of Si/Ge nanostructures at the atomic level — •Bert Voigtländer, Neelima Paul, Vasily Cherepanov, and Josef Myslivec̆ek — Institut für Schichten und Grenzflächen (ISG 3) and cni - Center of Nanoelectronic Systems for Information Technology, Forschungszentrum Jülich, 52425 Jülich, Germany

The step-flow growth mode is used to fabricate two-dimensional Si and Ge nanowires with a width of ≈3.5 nm and a thickness of one atomic layer (0.3 nm) by self-assembly on a Si(111) surface. Alternating deposition of Ge and Si results in the formation of a nanowire superlattice covering the whole surface. Also different kinds of two-dimensional Si/Ge nanostructures like alternating Si and Ge nanodots and nanorings having a width of 5-10 nm were grown. One atomic layer of Bi terminating the surface is used to prevent intermixing between Si and Ge and to distinguish between these elements. A difference in apparent height is measured in scanning tunneling microscopy (STM) images for Si and Ge, respectively. The method to distinguish between Si and Ge allows to study intermixing on the nanoscale and to identify the fundamental diffusion processes giving rise to the intermixing.

O 39.2 Di 11:00 TU EB420

STM contrast between Ge and Si atoms incorporated in the Si(111)-$\sqrt{(3)} \times \sqrt{(3)}$-Bi surface — •Josef Myslivec̆ek, Neelima Paul, and Bert Voigtländer — Institut für Schichten und Grenzflächen (ISG 3) and cni - Center of Nanoelectronic Systems for Information Technology, Forschungszentrum Jülich, 52425 Jülich, Germany

The termination of the Si(111) surface by 1 ML Bi prevents intermixing between subsequently deposited Ge and Si atoms that incorporate below the Bi layer. At the same time, apparent height difference between the incorporated Ge and Si monolayers is observed in the scanning tunneling microscope, allowing the control of the formation of lateral Ge-Si nanostructures on the Si(111)-$\sqrt{(3)} \times \sqrt{(3)}$-Bi surface. Using scanning tunneling spectroscopy techniques we study the origin of this apparent height difference. While the densities of electronic states measured over the incorporated Ge and Si layers do not differ significantly, a significant lowering of the inverse decay length is observed for the unoccupied electron states over the incorporated Ge layer. This indicates, that the presence of the incorporated Ge layer on the Si(111)-$\sqrt{(3)} \times \sqrt{(3)}$-Bi surface decreases the electron affinity on this surface.

O 39.3 Di 11:15 TU EB420

Strukturelle Untersuchungen von Dysprosiumsilizid-Nanodrähten auf vizinalen Si(001)-Oberflächen mittels Rastertunnelmikroskopie und LEED — •N. Tschirner, S. K. Becker, H. Eisele und M. Dähne — Technische Universität Berlin, Institut für Festkörperphysik, PN4-1, Hardenbergstr. 36, 10623 Berlin

Seltenerdsilizid-Nanodrähte zeichnen sich durch eine geringe Schottkybarriere auf der Si(111)- und der Bildung von Nanodrähten auf der Si(001)-Oberfläche aus. Wie aus früheren Untersuchungen bekannt[1], lassen sich durch Anpassen der Präparationsbedingungen verschiedene Arten von Drähten bilden. Bei niedrigen Temperaturen bilden sich dünne Drähte mit einer 2×7-Uberstruktur, bei höheren Temperaturen formen sich breitere und längere Drahttypen aus.

Auf vizinalen Oberflächen kann man ein paralleles Wachstum der Drähte aufgrund von Doppelstufen beobachten. Diese Drähte wurden mit LEED als auch mit STM untersucht und ihre atomare Struktur für unterschiedliche Wachstumstemperaturen und Dysprosium-Bedeckungen analysiert.

[1] C. Preinesberger, S. Vandré, T. Kalka, and M. Dähne. J. Phys. D: Appl. Phys **31**, L43 (1998)

O 39.4 Di 11:30 TU EB420

Local electronic properties of the one-dimensional Si(557)-Au surface — •M. Sauter[1], M. Schöck[2], R. Hoffmann[1], C. Sürgers[1], and H. v. Löhneysen[1,3] — [1]Physikalisches Institut and DFG Center for Functional Nanostructures (CFN), Universität Karlsruhe, D-76128 Karlsruhe, Germany — [2]Institut for Fysik og Astronomi, Aarhus Universitet, DK-8000 Århus, Denmark — [3]Forschungszentrum Karlsruhe, Institut für Festkörperphysik, D-76021 Karlsruhe, Germany

The local electronic properties of the Si(557)-Au surface, obtained by deposition of 0.2 monolayers Au on vicinal Si(111) and subsequent annealing, are investigated by scanning tunneling microscopy (STM) and spectroscopy at different temperatures. Images taken at room temperature show the characteristic surface structure of chains adjacent to diffuse stripes. At $T = 77$ K the images show a voltage dependent contrast which disagrees with the previously reported interpretation in terms of a Peierls-like transition occurring below 260 K [1]. The voltage-dependent contrast is is confirmed by atomically-resolved tunneling spectra which indicate metallic or semiconductor-like behavior depending on the type of protrusion. The results are discussed by comparison with a recent calculation of the electronic surface-band structure of Si(557)-Au [2].

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

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

O 39.5 Di 11:45 TU EB420

Lead on hydrogen terminated Si(111)1x1: STM and surface x-ray diffraction — •C. Rettig[1], V. Chamard[2], T.-L. Lee[3], J. Zegenhagen[3], and H. Hövel[1] — [1]Universität Dortmund, Experimentelle Physik I, D-44221 Dortmund — [2]CNRS, laboratoire de thermodynamique et physico-chimie metallurgique, B.P. 75, F-38402 St Martin d'hères — [3]European Synchrotron Radiation Facility (ESRF), B.P. 220, F-38043 Grenoble

We studied the growth of Pb on Si(111):H 1x1. The hydrogen termination leads to a chemically inert surface and results in a well defined modification of the Pb/Si interface if we compare our data to experiments for Pb on Si(111)7x7 deposited at T<270K in UHV. Recently for this system a uniform-height island growth was observed due to quantum well states, which lead to energy minima every second ML in height [1]. We characterised the growth mode of Pb on Si(111):H 1x1 at room temperature, changing the deposition amount from 2ML to 20ML, by using STM and SXRD (Surface X-Ray Diffraction) without breaking insitu UHV conditions. The SXRD data show the growth of exclusively Pb(111) planes parallel to the Si(111) plane and exhibit a beating pattern similar to the results of Pb on Si(111)7x7 [2], which may indicate a quasibilayer growth of the Pb clusters already at room temperature. In addition we characterised the morphology for different deposition temperatures (10K, 50K, 150K, 300K) with STM at 77K. In all cases we observed a 3D island structure of the Pb deposit.

[1] M. Hupalo et al., Phys. Rev. B **64**, 155307 (2001).
[2] P. Czoschke et al., Phys. Rev. Lett. **93**, 036103 (2004).

O 39.6 Di 12:00 TU EB420

Annealing induced 2D nano-patterning of Ga/Si(111) studied by STM — •Subhashis Gangopadhyay, Thomas Schmidt, and Jens Falta — Institute of Solid State Physics, University of Bremen, P. O. Box 330440, Bremen 28334, Germany

Annealing induced two dimensional nano-patterning was observed on Si(111) after submonolayer deposition of Ga at room temperature (RT) followed by annealing cycles. The evolution of the surface structure was studied using variable temperature scanning tunneling microscope (VT-STM). After RT Ga deposition, self-organized Ga induced magic clusters are found. Excess Ga leads to the formation of small 2D islands. The magic clusters are thermally stable up to 400°C (transition temperature). Depending on Ga deposit, two types of 2D pattern formation are observed located at the surface steps and the domain boundaries of the former Si(111)-7×7 reconstruction. For Ga coverages below 1/3 ML, Si(111)-7×7 domains are surrounded by $\sqrt{3}\times\sqrt{3}$-Ga structure which decorates the former domain boundary and step edges. If the Ga coverage exceed 1/3 ML, domains of $\sqrt{3}\times\sqrt{3}$-Ga structure are found surrounded by a 6.3×6.3-Ga structure.

O 39.7 Di 12:15 TU EB420

Stöchiometriebestimmung von III-V Halbleiternanostrukturen mittels Querschnittsrastertunnelmikroskopie — •Holger Eisele[1], Rainer Timm[1], Andrea Lenz[1], Oliver Flebbe[1], Ernst Lenz[2], Ferdinand Streicher[1] und Mario Dähne[1] — [1]Inst. F. Festkörperphysik, Technische Universität Berlin, Hardenbergstr. 36, D-10623 Berlin — [2]Inst. f. Technische Informatik u. Mikroelektronik, Technische Universität Berlin, Einsteinufer 17, D-10587 Berlin

Verspannte III-V Halbleiternanostrukturen bauen nach dem Spalten einer Querschnittsfläche ihre Verspannungsenergie über eine Relaxation dieser Spaltfläche ab. Diese Relaxation kann sowohl lateral in der Oberfläche als auch vertikal zu ihr mit dem Rastertunnelmikroskop gemessen werden.

Über die laterale Ralaxation erhält man Informationen, die mit der durchmischungkonzentrattion der Nanostrukturen in der Querschnittsfläche korreliert sind. Aus der vertikalen Verspannungrelaxation erhält man weiterhin Aussagen über die Konzentration und Form der weiter unterhalb der Spaltfläche liegenden berteiche der Nanostrukturen. Mit hilfe numerische Verfahren kann sowohl die laterale als auch vertikale Verspannungsrelaxation zur Konzentrationsbestimmung von durchmischten III-V Halbleiternanostrukturen genutzt werde.

O 39.8 Di 12:30 TU EB420

Querschnitts-Rastertunnelmikroskopie an stickstoffhaltigen InAs/GaAs-Heterostrukturen — •M. Müller[1], A. Lenz[1], L. Ivanova[1], R. Timm[1], H. Eisele[1], M. Dähne[1], O. Schumann[2], L. Geelhaar[2] und H. Riechert[2] — [1]Technische Universität Berlin, Institut für Festkörperphysik, PN4-1, Hardenbergstr. 36, 10623 Berlin — [2]Infineon Technologies, Corporate Research Photonics, 81730 München

Die Rastertunnelmikroskopie an Querschnittsflächen ist eine geeignete Methode zur Untersuchung vergrabener Heterostrukturen, ihrer Struktur und chemischen Komposition[1]. Untersucht wurden mittels Molekularstrahlepitaxie gewachsene, vergrabene InAs/GaAs Quantenpunkt-Dopplestapel, die unter verschiedenen Wachstumsparametern, insbesondere Stickstoffbeimengungen in der Quantenpunktschicht und der Zwischenschicht hergestellt wurden.

Beobachtet wurde eine zunehmende Veränderung der Quantenpunktform und eine teilweise Auflösung der Benetzungsschicht. Ferner wurden Oberflächendefekte beobachtet, die beim Spalten des Kristalls aufgrund von Verspannungen durch den Stickstoffeinbau entstehen[2]; ebenso konnte der Einbau von Stickstoff in das GaAs-Substrat auf atomarer Ebene untersucht werden.

[1] A. Lenz, R. Timm, H. Eisele, M. Dähne et al.,
Appl. Phys. Lett. **81**, 5150 (2002)
[2] H. A. McKay, R. M. Feenstra, J.Vac.Sci.Technol. B **19**, 1644 (2001)

O 39.9 Di 12:45 TU EB420

Raman spectroscopy on double-walled carbon nanotubes — •Wencai Ren[1,2], Feng Li[1], Huihong Qian[3], Hui Qian[3], Thorsten Staedler[2], Achim Hartschuh[3], Xin Jiang[2], and Hui-Ming Cheng[1] — [1]Institute of Metal Research,Chinese Academy of Sciences, Shenyang 110016, China — [2]Chair of Surface and Materials Technology, University of Siegen, Siegen 57068, Germany — [3]Department of Chemistry, University of Siegen, Siegen 57068, Germany.

Double-walled carbon nanotube (DWNT) provides a new platform for fundamental studies and nanodevice applications, due to their special double wall structure and one-dimensional (1D) character. In this work, we developed a sulfur-assisted floating catalytic decomposition method to directly synthesize DWNT bundles with high purity, narrow diameter distribution and good alignment. In a first step Raman spectra of DWNT bundles were studied. The results indicate that (1) the radial breathing mode (RBM) and G-band profiles can all be decomposed into two intrinsic independent single-walled carbon nanotube (SWNT) components constituting the DWNT, and (2) D-band and G'-band were composed of four well-resolved peaks, which are considered to originate from the curvature effect related to the tube diameter and relative atom stacking effect of the two constituent tubes.

In a second step, Raman measurements at a single nanotube level were carried out. The correlation between the Raman spectra of the individual nanotubes and their bundles will be discussed. All results indicate that DWNTs possess unique and characteristic Raman spectra different from other sp2 carbon materials.

O 40 Adsorption an Oberflächen IV

Zeit: Dienstag 10:45–13:00 Raum: TU EB202

O 40.1 Di 10:45 TU EB202

CO adsorption on Ag and Co nanoparticles monitored by SFG and TDS — •Frank Höbel, Günther Rupprechter, and Hans-Joachim Freund — Fritz-Haber-Institut, Faradayweg 4-6, 14195 Berlin

CO adsorption on Al_2O_3 supported Ag nanoparticles and Nb_2O_5 supported Co nanoparticles was studied by sum frequency generation (SFG) vibrational spectroscopy from ultrahigh vacuum (UHV) to 100 mbar, at temperatures from 90 K to 450 K. Under UHV conditions CO binding energies and coverages were examined by thermal desorption spectroscopy (TDS).

Under UHV CO adsorbs on silver only at temperatures below 60 K. Adsorption studies at higher temperature therefore require higher gas pressure, e.g. terminal CO was detected at 50 mbar and 150 K. Results of CO adsorption on a Co-Nb_2O_5 Fischer-Tropsch model catalyst under reaction conditions will be presented.

O 40.2 Di 11:00 TU EB202

Alloy surface segregation in reactive environments via density-functional theory and atomistic thermodynamics — •John Kitchin, Karsten Reuter, and Matthias Scheffler — Fritz-Haber-Institut, Faradayweg 4-6, D-14195 Berlin

The chemical and materials properties of an alloy surface depend sensitively on its detailed surface composition and structure, which in turn can differ substantially from the one of the bulk alloy due to segregation of one species to the surface. Concerning the alloy function e.g. in catalytic or corrosive environments, this surface segregation can furthermore depend on the partial pressures and temperatures in the surrounding, if one alloy component interacts more strongly with a gas-phase species than the other. Instead of solely predicting the chemical and materials properties on the basis of the formal bulk composition, this requires a theory that explicitly considers the effect of the reactive environment.
As a first step in this endeavor, we are extending the concepts of *ab initio atomistic thermodynamics* to address segregation in binary transi-

tion metal alloys in the presence of a reactive gas phase. We apply the approach to the (111) surface of Ag_3Pd in an O_2 atmosphere, and find that contrary to the situation in ultra-high vacuum, Pd segregates to the surface at high oxygen pressures. We discuss the difficulties and possible inaccuracies of the *ab initio atomistic thermodynamic approach* with respect to the limited exploration of configuration space and the steps necessary to proceed beyond it.

O 40.3 Di 11:15 TU EB202

Hydrogen-induced relaxations in epitaxial Ni-films on Cu(001) — •W. Meyer[1], M. Krause[1], A. Klein[1], S. Müller[1], L. Hammer[1], K. Heinz[1], D. Sander[2], and J. Kirschner[2] — [1]Lehrstuhl für Festkörperphysik, Universität Erlangen-Nürnberg, Staudtstr. 7, D-91058 Erlangen — [2]Max-Planck-Institut für Mikrostrukturphysik, Weinberg 2, D-06120 Halle/Saale

We have investigated the atomic structure and morphology of epitaxial Ni-films on Cu(001) in the coverage regime 2-12 monolayers (ML) as well as their changes upon hydrogen adsorption. Quantitative Low-Energy Electron Diffraction (LEED) and Scanning Tunnelling Microscopy (STM) were applied in-situ. The STM studies show layer-by-layer growth in the coverage range up to 5 ML while thicker films exhibit an increased roughness. The LEED structure determinations reveal a tetragonal distortion (-3.1% on average) of the hydrogen-free Ni-films very close to the predictions of elastic theory (-3.2%). For all coverage values the first layer spacing is reduced even further (by -4.5%). Yet, by adsorption of 1 ML of hydrogen it increases to a value larger than that of deeper spacings whereas the latter are rather unaffected, i.e. the films subsurface tetragonal distortion remains.

The LEED fit allows to detect also the hydrogen atoms. They reside in the 4-fold hollow sites at 0.3 Å above the top Ni layer. It has been proposed that these H-induced changes are also decisive for the accompanied spin reorientation-transition from in- to out-of-plane [1].

[1] D. Sander, W. Pan, S. Quazi, J. Kirschner, W. Meyer, M. Krause, S. Müller, L. Hammer, K. Heinz, Phys. Rev. Lett., in press

O 40.4 Di 11:30 TU EB202

Formation of Fe Clusters on Superstructured Al_2O_3 Films on $Ni_3Al(111)$ — •Anne Lehnert, Regis Decker, Katharina Franke, Stefano Rusponi, and Harald Brune — IPN, EPF Lausanne, Switzerland

Common industrial catalysts consist of small metal particles dispersed on oxide surfaces. In order to prepare a model system to study systematically the catalytic properties as a function of size, shape, and composition, we grow a well-ordered Al_2O_3 film on $Ni_3Al(111)$. The alumina film is known to exhibit a long-range ordered superstructure, partly of electronic origin.

On top of the oxide layer we deposit iron. By using STM, we investigate the formation of iron clusters in dependence of several parameters, such as coverage, deposition and annealing temperature.

O 40.5 Di 11:45 TU EB202

Nanostrukturiertes Eisenwachstum auf einem Aluminiumoxidfilm auf $Ni_3Al(111)$ — •Aleksander Krupski, Stefan Degen, Marko Kralj, Conrad Becker und Klaus Wandelt — Institut für Physikalische und Theoretische Chemie, Wegelerstr. 12, 53115 Bonn

Ein bei einer Temperatur von 1000 K in einer Sauerstoffatmosphäre auf einer $Ni_3Al(111)$-Oberfläche gewachsener doppellagiger Aluminiumoxidfilm weist eine hexagonale Überstructur der Gitterkonstante 2,40 nm auf [1] und erweist sich dadurch als Templat für nanostrukturiertes Eisenwachstum. Die mittels eines Metallverdampfers im UHV bei Raumtemperatur aufgewachsenen Eisenschichten wurden mit Rastertunnelmikroskopie bei Raumtemperatur sowie bei 23 Kelvin untersucht. Es findet ausschließlich Clusterwachstum statt, und die Nukleation der Cluster wird von der Oxidüberstruktur bestimmt. Die aufgewachsenen Cluster besetzen genau die Gitterpunkte dieser hexagonalen Überstructur. In früheren Experimenten wurde bereits Mangan und Vanadium auf den gleichen Oxidilm aufgewachsen [2]. Die Ordnung der Eisencluster ist nicht ganz so gut wie diejenige der Vanadiumcluster, aber deutlich besser als die der Mangancluster. Bei sehr niedrigen Eisenbedeckungen konnte der Templateffekt, den der Oxidfilm auf die Eisennukleation ausübt, deutlich gezeigt werden. Weiterhin wurden tunnelspektroskopische Messungen an einzelnen Eisenclustern durchgeführt, deren Interpretation sich aufgrund der Komplexität des Systems als schwierig erwiesen hat.

[1] A. Rosenhahn et al., J. Vac. Sci. Technol. A 18 (2000) 1923.

[2] C. Becker et al., New J. Phys. 4 (2002) 75.

O 40.6 Di 12:00 TU EB202

Adsorption of superheavy elements on metal surfaces using relativistic density functional theory — •Cristina Sarpe-Tudoran[1], Josef Anton[1], Valeria Pershina[2], and Burkhard Fricke[1] — [1]Institut für Physik, Universität Kassel, D-34109 Kassel, Germany — [2]Gesellschaft für Schwerionenforschung, D-64291 Darmstadt, Germany

The production of isotopes with half-lives of up to 30 min. for element 112 justifies chemical experiments. Using the gas-phase-chromatography technique the adsorption energy of element 112 on an Au surface is aimed to be measured. The theoretical prediction is very complicated. We present here an ab initio embedded-cluster relativistic density functional calculation of this quantity for the element 112 and for its homologue Hg on an Au(100) surface.

Different clusters were designed, corresponding to a top-, hollow-, and bridge-position of the adsorbate relative to the metal lattice in order to check at which position the ad-atom is adsorbed. We present the potential energy curves and the corresponding values of the binding energies and bond lengths. The geometry of the cluster was kept unchanged during the self-consistent calculations.

Our analysis shows that the adsorption energy of element 112 on a gold surface is about 0.12 eV smaller than the corresponding value for the adsorption of Hg on the same surface. This result offers a benchmark to the experimentalist for this value, which is helpful in designing the chemical experiment with element 112.

O 40.7 Di 12:15 TU EB202

Observation of two states of Ce adparticles on Ag(100) — •Markus Ternes, Marina Pivetta, François Patthey, and Wolf-Dieter Schneider — Institut de Physique des Nanostructures, École Polytechnique Fédérale de Lausanne, CH-1015 Lausanne, Switzerland

We report on intriguing experimental results obtained with a scanning-tunneling microscope after evaporation of a small amount of Ce on a Ag(100) surface at low temperature (5K). Some adparticles (about 5%) can be switched from their initial state, where they appear large and with featureless dI/dV spectra around E_F, to a state where they appear smaller and with a narrow dip at the Fermi level in the dI/dV spectra. The latter is tentatively interpreted as a Kondo resonance with a Kondo temperature of about 30K. This observation may be related to a change in the 4f electron-valence band hybridization when passing from one state to the other.

O 40.8 Di 12:30 TU EB202

Coverage-dependent adsorption phases of Cs on Cu(111) — •Thomas von Hofe, Jörg Kröger, and Richard Berndt — Institut für Experimentelle und Angewandte Physik, Universität Kiel, D-24098 Kiel

While the adsorption structure of several alkali metals on noble metal surfaces is well examined, little is known about Cs on Cu(111). We report about atomically resolved STM images of Cs on Cu(111) with coverages $0 < \Theta \leq 0.25$ ML at 9 K. Depending on coverage, we observe four incommensurate rotated and a commensurate phase similar to Cs on Ag(111). We explain the observed rotation angles of the incommensurate phases with a model by McTague and Novaco [1] which was originally developed to explain adsorption structures of argon on graphite.

[1] J.P. McTague, A.D. Novaco, Phys. Rev. B **19**, 5299 (1979)

O 40.9 Di 12:45 TU EB202

Alkali Intercalation in Transition metal dichalcogenides via Steps — •Claudia Ramirez[1], Rainer Adelung[2], Lutz Kipp[3], and Wolfgang Schattke[1] — [1]Institut für Theoretische Physik und Astrophysik, Christian-Albrechts-Universität zu Kiel, Leibnizstrasse 15, 24098 Kiel, Germany — [2]Technische Fakultät, Christian-Albrechts-Universität zu Kiel, Kaiserstrasse 2, 24143 Kiel, Germany — [3]Institut für Experimentelle und Angewandte Physik, Christian-Albrechts-Universität zu Kiel,Leibnizstrasse 19, 24098 Kiel, Germany

The aim of this work was to understand how alkali metal atoms intercalate into transition metal dichalcogenides (TMDCs). To this end, a detailed investigation into the geometrical and electronic effects on TMDCs caused by adsorption and intercalation of alkali atoms was carried out by means of ab initio density-functional theory. The question of whether the alkali atoms can reach the van der Waals gap from the plain surface through the atomic planes was addressed. Because of the huge energy barrier involved in this process (3.81 eV), this type of intercalation can be excluded. The high value of the barrier suggests that the most probable path of intercalation must be through the edges or defects of the crystal such as steps or dislocations. The diffusion of Li adatom across and along two different steps, $(10\bar{1}0)$ and $(\bar{1}2\bar{1}1)$, was studied. STM experiments favor mainly the two step here considered. A model of alkali intercalation into TMDCs was obtained, namely via a $(10\bar{1}0)$ step.

This work was supported by the Deutsche Forschungsgemeinschaft (DFG), Forschergruppe FOR 353.

O 41 Elektronische Struktur III

Zeit: Dienstag 10:45–13:00 Raum: TU EB107

O 41.1 Di 10:45 TU EB107

Systematic ARPES study of the influence of different adsorbates on surface states — •Frank Forster, Azzedine Bendounan, Johannes Ziroff, Felix Schmitt, and Friedrich Reinert — Experimentelle Physik II, Universität Würzburg, Germany

On the example of the (111) surfaces of Cu, Ag and Au we demonstrate that high and angle resolved photoemission spectroscopy (ARPES)($\Delta E = 3$ meV, $\Delta\Theta = 0.3°$) is a powerful tool for the study of the influence of differnt absorption processes on the electronic structure of these systems.

We discuss that only one monolayer of weak-interacting rare gases is reponsible for a characteristic shift of the Shockley-states towards and even above the Fermi level whereas bulk states of the substrates remain – except for band back-folding – almost unimpressed. Furthermore, the Au(111) surface state experiences an increase in the spin-orbit splitting up to 30%.

In contrast to the physisorption process of rare gases, a coverage of alkali metals on the nobel metal surfaces leads to a opposite effect on the Shockley-states, i.e., a decrease of the still detectable spin-orbit splitting and an increase in binding energy, until they reach the bottom of the L-gap and vanish in the bulk states.

These experimental results are supported by theoretical considerations which allow a deeper understanding of the electronic processes on adsorbate-substrate interfaces.

O 41.2 Di 11:00 TU EB107

Electronic structure of misfit layer chalcogenides — •Matthias Kalläne[1], Hans Starnberg[2], Kai Rossnagel[1], Sven Stoltz[2], and Lutz Kipp[1] — [1]Institut für Experimentelle und Angewandte Physik, Universität Kiel, D-24098, Germany — [2]Department of Physics, Göteborg University and Chalmers University of Technology, SE-412 96 Göteborg, Sweden

Misfit layer chalcogenides $(\mathrm{MX})_{1+x}(\mathrm{TX}_2)_m$ (M=Sn, Pb, Sb, Bi; T=Ti, V, Cr, Nb, Ta; X=S, Se; $0.08 < x < 0.28$; m=1,2,3) result from an alternate stacking of MX and TX_2 slabs where the cubic MX layers are incommensurate with the hexagonal TX_2 layers in one of the two crystallographic directions parallel to the layers. To reach a better understanding of the electronic structure of these compounds we have performed angle-resolved photoelectron spectroscopy and photoelectron spectromicroscopy experiments. Our results reveal details about charge transfer from the MX to the TX_2 layers, interlayer bonding, possible effects of the incommensurability, and the domain structure of the cleavage planes. The photoemission experiments were carried out at HASYLAB (Germany), MAXLAB (Sweden), and the ALS (USA). Work at the University of Kiel is supported by DFG Forschergruppe FOR 353.

O 41.3 Di 11:15 TU EB107

Unoccupied electronic states on oxidized SiC(0001)-surfaces determined by inverse photoemission — •Kathrin Wulff, Ralf Ostendorf, Carsten Benesch, and Helmut Zacharias — Physikalisches Institut, Universität Münster, Wilhelm-Klemm Strasse 10, 48149 Münster

Starting from the silicon rich (3×3) reconstruction of SiC(0001) we prepared oxidized surfaces by hydrogen etching as well as molecular oxygen exposure ranging from 5000 L to 30000 L. LEED pictures show a (1×1)-reconstructed surface with a faint $(\sqrt{3}\times\sqrt{3})$R30° structure after oxidation, indicating a mainly disordered surface with only few patches of long range order. A distinct change in the shape of the $\mathrm{Si}_{\mathrm{LVV}}$ AES peak which is similar to spectra taken on pure SiO_2 refers to the existence of Si-O bonds on the surface.

By applying inverse photoemission spectroscopy we find four electronic resonances above the Fermi level. Decreasing intensities with time caused by residual gas phase contaminants identify these structures as possible surface states. Finally, wave-vector resolved measurements show a flat dispersion for each resonance throughout the whole surface Brillouin zone.

O 41.4 Di 11:30 TU EB107

Rechnungen zur energie- und winkelaufgelösten Photoemission an GaN(0001) Oberflächen — •Thomas Strasser und Wolfgang Schattke — Institut für Theoretische Physik und Astrophysik, Leibnizstr. 15, 24098 Kiel

Galliumnitrid hat in der Optoelektronik erheblich an Bedeutung gewonnen. Jedoch sind Fragen zur elektronischen und geometrischen Struktur seiner Oberfläche offen. Die Photoelektronenspektroskopie ist aufgrund ihrer Oberflächenempfindlichkeit ein geeignetes Mittel zu ihrer Klärung.

Ausgangspunkt der Untersuchung sind theoretische Oberflächenmodelle der 1x1 aus Gesamtenergierechnungen von Wang et. al. [1]. Für diese werden gerechnete Spektrenserien in nichtnormaler Emission entlang verschiedener hochsymmetrischer Richtungen gezeigt und mit Hilfe von Matrixelementen, Zustandsdichten und komplexen Endzustandsbändern analysiert.

Zum Vergleich stehen experimentelle Ergebnisse von Dhesi und Chao zur Verfügung [2,3]. Beide Experimente wurden an 1x1 GaN Oberflächen durchgeführt, zeigen aber dennoch charakteristische Unterschiede. Ziel ist es, diese mit Hilfe des Einstufenmodells auf mikroskopischer Ebene zu verstehen.

[1] Fu-He Wang et al.; Phys. Rev. B 64, 035305 (2001).

[2] S.S. Dhesi et al.; Phys. Rev. B 56, 10271 (1997).

[3] Y.-C. Chao et al.; Phys. Rev. B 59, R15586 (1999).

O 41.5 Di 11:45 TU EB107

Polarization-Dependent Domain Contrast on cesiated Si(100) in Photoemission Electron Microscopy — •D. Thien, M. Horn-von Hoegen, and F.-J. Meyer zu Heringdorf — Institut für Laser und Plasmaphysik, Universität Duisburg-Essen (Campus Essen), 45117 Essen

On the Si(100) surface, two types of terraces are present with either (2x1) or (1x2) reconstruction. In Low Energy Electron Microscopy (LEEM) dark-field contrast can be observed if a diffraction spot of only one of the two superstructures is used for imaging of the related domain. In Photoelectron Emission Microscopy (PEEM), however, such contrast has not yet been observed. Using a polarized light source such as a 532nm-laser (2.4eV) for illumination of a Cs covered Si(100) surface, however, we observe a polarization dependent photoemission signal of the two different terraces. Ultraviolet Photoemission Spectroscopy (UPS) and Medium Energy Ion Spectroscopy (MEIS) studies of Cs on Si(100) indicate the transfer of the Cs 6s electron to the previously unoccupied upper dangling bond state of the Si(100) surface [1], which acts as initial state for the photoemission process. This lowers the work function while leaving the geometry of the silicon substrate unchanged. The polarization dependence of this contrast is strong enough to be observed even with a green laser pointer.

[1] J.Günster et al., Surf.Sci.359(1996)155-162

O 41.6 Di 12:00 TU EB107

The electron-phonon coupling on Mg(0001) — •T. Kim[1], T.S. Sørensen[1], E. Wolfring[1], H. Li[2], E.V. Chulkov[3], and Ph. Hofmann[1] — [1]Institute for Storage Ring Facilities, University of Aarhus,8000 Aarhus C, Denmark — [2]Department of Physics, Zhejiang University,Hangzhou 310027, China — [3]Donostia International Physics Center (DIPC), 20018 San Sebastián/Donostia, Basque Country, Spain

The influence of many-body effects on surface state lifetimes, and in particular the role of the electron-phonon coupling, has recently attracted considerable attention. Work has mostly concentrated on surface states located in wide gaps of the projected band structure, such as the L-gap surface states of the (111) noble metal surfaces or the surface state on Be(0001). Here we report results from the deeply penetrating surface state which is located in a narrow gap at the Brillouin zone centre of

Mg(0001). The temperature-dependent photoemission linewidth of this state is used to determine the electron-phonon mass enhancement parameter λ. λ, as well as the electron-electron contribution to the surface state linewidth at zero temperature, are compared to first-principles calculations and good agreement is found.

O 41.7 Di 12:15 TU EB107

Influence of electron-phonon-coupling on the spectral function of nitrogen induced adsorbate states on Cu(100) — •Christian Bumiller, Thordis Michalke, Christian Kant, and René Matzdorf — Institut für Physik, Universität Kassel

We investigated the self organized surface of the adsorbate system nitrogen on copper (Cu(100)c(2×2)N) by means of angle resolved photoelectron spectroscopy (ARPES). Temperature dependent photoelectron spectra reveal a very strong electron-phonon-coupling of the nitrogen induced states on Cu(100). The strong coupling is very interesting for electronic states close to the Fermi level. One adsorbate state shows exceptional behaviour when approaching the Fermi energy. The spectral function changes drastically with the energy position. Here the real part of the self energy for the electron-phonon-coupling is visible. We show the influence of the self energy at different temperatures and binding energies. The characteristic features of the spectra are explained with the Eliashberg theory using the Einstein and Debye models for the phonon density of states.

O 41.8 Di 12:30 TU EB107

PES and LEED-IV measurements of Cu(100)c(2×2)N in comparison with theoretical studies — •Ch. Kant[1], Th. Michalke[1], Ch. Bumiller[1], J. Braun[2], A. Postnikov[3], and R. Matzdorf[1] — [1]Institut für Physik, Universität Kassel — [2]Universität Münster — [3]Universität Osnabrück

The atomic structure of the self organized nanopatterned adsorbate system Cu(100)c(2×2)N is still under discussion and the electronic bandstructure was not measured so far. Although it is known since 30 years, that nitrogen adsorbs at the fourfold hollow site, the positions of the outermost copper-atoms, which may undergo a strong reconstruction due to the incommensurate adsorption of nitrogen, is not clarified completely. We present the first angle resolved photoemission spectra of this system. The measurements are compared with detailed theoretical calculations based on the one-step model of photoemission. These calculated spectra are very sensitive to the positions of N- and Cu-atoms. The results from the calculations may help to understand the atomic structure of the adsorbate system. In addition we use LEED-IV analysis to evaluate the models of the surface structure.

O 41.9 Di 12:45 TU EB107

Energy and angle resolved measurement of the $(1\pi)^{-1}$ photoemission cross section of CO adsorbed on Pt(111) — •Grigorios Tsilimis, Sebastian Wegner, Jörg Kutzner, and Helmut Zacharias — Physikalisches Institut, Westfälische Wilhelms-Universität, Wilhelm-Klemm-Straße 10, D-48149 Münster

The c(4×2)-2CO-covered Pt(111) surface is investigated by energy and angle resolved photoelectron spectroscopy (ARUPS) using high-order harmonic radiation. Femtosecond pulses of a table–top, high–repetition rate (1 kHz) Ti:sapphire laser system are focussed into rare gases to generate high-harmonic radiation in the range of $h\nu = 20$ to 120 eV (60 − 11 nm). Both the coarse tunability in steps of 3.1 eV as well as a fine tuning within a single harmonic are utilized in the measurements.

The photoemission cross section of the CO-induced structures, in particular the pronounced $CO(1\pi)^{-1}$-emission at photon energies around $h\nu = 32$ eV is analyzed by means of partial wave decomposition. The influence of the surface on the electronic structure of the adsorbed CO leads to a different $(1\pi)^{-1}$-emission compared to oriented gas phase CO molecules.

O 42 Oberflächenreaktionen II

Zeit: Dienstag 10:45–13:00 Raum: TU EB407

O 42.1 Di 10:45 TU EB407

Chemically induced electronic excitations during scattering and Eley Rideal reaction of hydrogen on gold surfaces — •Beate Mildner[1], Yanka Yeliazova[1], Eckart Hasselbrink[1], and Detlef Diesing[2] — [1]Institute of Physical and Theoretical Chemistry, University of Duisburg-Essen, Campus Essen — [2]Institut für Schichten und Grenzflächen 3, Forschungszentrum Jülich

It is well known that highly exothermic reactions on metal surfaces can cause electron emission, if an electron is ejected with an energy exceeding the metal workfunction. Electrons with low excitation energy can be detected using thin film Schottky or tunnel diodes with barrier energies $E_B < \Phi_{metal}$. At first, we studied the scattering of H-atoms at room temperature. On the gold surface of a $Ta/Ta_2O_5/Au$ tunnel junction we observed a H-atom induced tunnel current at 0 V bias voltage. Exposure to H_2 does not cause any detectable currents. When the sample temperature is lowered to 170 K (≈ desorption temperature of atomic hydrogen) the hydrogen induced tunnel current increases by a factor of 6. Moreover, the shape of the transient current caused by the adsoption of hydrogen from a pulsed atom beam changes from a simple square form to a shape with an initial overshoot followed by a slow decay. We assign the overshoot and the increase of the tunnel current to an Eley Rideal reaction ($H_{gas} + H_{ad} \rightarrow H_2$). Applying a bias voltage to the tunnel junction, we compared the energetic structure of the electronic excitation during ER reaction with the one from a scattering process. The bias dependence reveals that electrons with increased energy are produced during the ER-reaction .

O 42.2 Di 11:00 TU EB407

Reversible isomerization of an individual photochrome molecule by tunneling electrons — •Jörg Henzl[1], Karina Morgenstern[2], Heiko Gawronski[1], Michael Mehlhorn[1], and Karl-Heinz Rieder[1] — [1]Freie Universität Berlin, Institut für Experimentalphysik, Arnimallee 14, 14195 Berlin — [2]Universität Hannover, Institut für Festkörperphysik, Appelstr. 2, 30167 Hannover

Azobenzene molecules are well known for the light-stimulated cis-trans isomerization. We have investigated Disperse Orange 3 on the Au(111) surface at 5K under UHV conditions with a scanning tunneling microscope. Disperse Orange 3 ($C_{12}H_{10}N_4O_2$) is an azobenzene derivate ($C_6H_4N{=}NC_6H_4$) with a NO_2 and a NH_2 endgroup. At a deposition temperature of about 230K the molecules form dimers, which can be separated into monomers. We induce isomerization of individual molecules between the cis- and trans-state for several times both within dimers and monomers by tunneling electrons. Detailed insights in the switching process will be presented in this talk.

O 42.3 Di 11:15 TU EB407

The adsorption of gold on gold surfaces – where does the binding energy go ? — •Michael Kayser[1], Eckart Hasselbrink[1], and Detlef Diesing[2] — [1]Institute of Physical and Theoretical Chemistry, University of Duisburg-Essen, Campus Essen — [2]Institut für Schichten und Grenzflächen 3, Forschungszentrum Jülich

The chemistry and physics of the deposition of a metal atoms on a metal surface is not only interesting for the understanding of fundamental processes like charge transfer, chemical bonding and energy dissipation but also for altering or even tailoring properties and behaviour of surfaces [1] for their industrial application. The deposition of a metal atom on a metal surface leads to the release of the heat of sublimation which is completely transferred to the substrate. The question to be answered is to which extend the binding energy is transferred to the electronic system and to the phononic system of the gold. Electronic excitations within their short lifetime of several tens of fs [2] can be detected using a tunnel junction realized by a metal-insulator-metal system. We present measurements which prove that the binding energy is at least partly transferred to the electronic system of the gold substrate. The adsorption induced electronic excitation is measured as a tunnel current at 0 V bias voltage across the tunnelling barrier. The observed tunnel current is directly proportional to the gold atom flux. Additional processes as photo induced tunnelling play a minor role in the experiment.

[1] M. Ø. Pedersen, S. Helveg, A. Ruban - Surf. Sci. 426 (1999) 395 - 409

[2] S. Meyer et al., Phys. Rev. Lett. 93, 137601 (2004)

O 42.4 Di 11:30 TU EB407

Kinetic electron excitation in atomic collision cascades — •Stefan Meyer[1], Detlef Diesing[2], and Andreas Wucher[1] — [1]Institut für experimentelle Physik, Universität Duisburg- Essen, 45117 Essen — [2]Institut für Schichten und Grenzflächen 3, Forschungszentrum Jülich, 52425 Jülich

In atomic collision cascades, initiated by the impact of a fast particle onto a solid surface, a part of the deposited energy is transferred into the electronic system and leads to the creation of hot electrons. Recently we have shown [1] that Metal- Insulator- Metal (MIM) tunnel junctions are an appropriate tool to investigate low energy electron excitation. Electrons which are excited by particle bombardment in the top electrode of the junction travel elastically within their mean free path to the insulator interface and tunnel to the base electrode where they are detected as a tunnel current. By applying a dc- voltage across the junction, it is possible to compare the energy distribution of excited electrons caused by collision reactions with different kinetic energies. Comparative collision experiments with neutral atoms will distinguish which part of the energy transferred into the substrate is due to potential energy effects.

[1] S. Meyer, D. Diesing, A. Wucher, Physical Review Letters 93 (2004) 137601

O 42.5 Di 11:45 TU EB407

Detection of low energy electronic excitations($E < E_{\mathrm{vacuum}}$) during the interaction of metastable rare gas atoms with metal surfaces. — •Domokos Kovacs[1], Johannes Berndt[1], Jörg Winter[1], and Detlef Diesing[2] — [1]Experimentalphysik 2, Ruhr-Universität Bochum — [2]Institut für Schichten und Grenzflächen 3, Forschungszentrum Jülich

The interaction of metastable rare-gas atoms with a metal surface gives rise to deexcitation accompanied by electron emission. While the electron emission into the vacuum is well investigated, the low energy electronic excitations cannot be detected by classical spectroscopic methods. For their detection, a thin film tunnel junction was used. It consists of a silver film (15 nm) exposed to the metastable atom beam and of an aluminum film (30 nm), separated by a very thin (2-3 nm) aluminum-oxide layer. In such a multilayer system, low energy electronic excitations can be detected as a pulsed tunnel current in the base aluminum electrode by chopping the metastable atom beam. A bias induced reversible polarity change in the metastable induced tunnel current was observed. It depends strongly on the intrinsic properties of the metastable atoms (excitation energy), but does not depend on the intensity of the metastable atom beam. In order to explain the experimental data a theoretical model considering tunnel processes between a ground state electron gas and an excited free electron gas is proposed.

O 42.6 Di 12:00 TU EB407

Energy partitioning in the femtosecond-laser induced $D_{\mathrm{ads}} + D_{\mathrm{ads}} \rightarrow D_2$ desorption reaction from Ru(001) — •S. Wagner[1], M. Rutkowski[2], H. Zacharias[2], C. Frischkorn[1], and M. Wolf[1] — [1]Freie Universtät, Berlin — [2]Westfälische Wilhems-Universität, Münster

The energy transfer to different degrees of freedom during the recombinative desorption of D_2 from a deuterium covered Ru(001) surface induced by femtosecond-laser excitation has been investigated with (1+1') resonance enhanced multi-photon photoionization (REMPI) and time-of-flight (TOF) measurements. Rovibrational population distributions of the reaction product are detected via various $B\ ^1\Sigma_u^+ \leftarrow X\ ^1\Sigma_g^+$ Lyman bands using tunable vacuum ultraviolet (VUV) laser radiation in the excitation step. Rotational quantum states in the vibrational ground state and the first excited state are measured yielding rotational temperatures of $E_{\mathrm{rot}}/k_{\mathrm{B}} = 800\,\mathrm{K}$ and $1500\,\mathrm{K}$, respectively, at an absorbed laser fluence F of 85 J/m^2. Also, a vibrational temperature of the desorbing molecules is extracted which amounts to $E_{\mathrm{vib}}/k_{\mathrm{B}} = 1200\,\mathrm{K}$. In addition, comprehensive TOF results ($E_{\mathrm{trans}}/k_{\mathrm{B}} = 2500\,\mathrm{K}$ at $F = 85$ J/m^2) enable complete energy balancing and underline the non-thermal and anisotropic energy partitioning during reaction. The effects of multi-dimensional friction between substrate and adsorbate layer and peculiarities of the potential energy landscape governing the D_2 recombination are discussed.

O 42.7 Di 12:15 TU EB407

Ellipsometric Confirmation of the Phase Transition in Methanol Oxidation over Copper Surface — •Ling Zhou[1], Sebastian Günther[2], and Ronald Imbihl[1] — [1]Institut für Physikalische Chemie und Elektrochemie, Universität Hannover — [2]Department Chemie, Ludwig-Maximilians-Universität München

The kinetics of methanol oxidation over metallic and oxidized copper surface has been studied in the 10^{-2} mbar range. It was found that the different phases over the copper sample lead to different reactivity. Comparing with the metallic copper surface, the partially oxidized copper surface has higher reactivity to produce formaldehyde whereas the deep oxidized surface shows more total oxidation to CO_2. The phase transition during the reactions can be well defined by the optics and ellipsometer which is in favour of determining the active phase in methanol selective oxidation to formaldehyde.

O 42.8 Di 12:30 TU EB407

A RAIRS investigation of methanol dehydrogenation on a Rh(111)/V islands surface — •Robert Schennach, Hans Peter Koch, and Georg Krenn — Institute of Solid State Physics, Graz University of Technology, Petersgasse 16/2, 8010 Graz, Austria

Fundamental insights in the dehydrogenation reaction of methanol is of interest due to the importance of this reaction in methanol powered fuel cells. In this work the methanol dehydrogenation on a Rh(111) surface with V islands has been investigated using reflection absorption infra red spectroscopy (RAIRS). The surface consists of two to four layer high V islands with an average island diameter of about 9 nm, which cover about 25% of the Rh(111) surface. The reactivity of this surface for methanol dehydrogenation is about 6 times as high as the reactivity of the V free Rh(111) surface. But the reactivity of the Rh(111)/V islands surface decreases over time due to CO dissociation on the V islands. However, the deactivated islands are still significantly more reactive towards methanol dehydrogenation than Rh(111). The RAIRS measurements show that the reaction mechanism changes markedly going from Rh(111) to the Rh(111)/V islands surface. This is mainly due to an increased stability of methanol on the V islands. In addition a new reaction pathway via methanol C-O bond opening yielding CH_3 on the surface has been found on the Rh(111)/V islands surface. The reactivity of the deactivated islands seems to be due to a slight stabilization of methanol on this surface.

O 42.9 Di 12:45 TU EB407

Elektronen induzierte Isomerisierung: Direkte Visualisierung einer chemischer Reaktion innerhalb eines einzelnen Moleküls — •V. Simic-Milosevic[1], K. Morgenstern[2], M. Mehlhorn[1] und K.-H. Rieder[1] — [1]Freie Universität Berlin, Institut für Experimentalphysik, Arnimallee 14, 14195 Berlin — [2]Universität Hannover, Institut für Festkörperphysik, Appelstr. 2, 30167 Hannover

Der Tunnelstrom eines Tieftemperatur-Rastertunnelmikroskops wurde genutzt, um Dipolmoment und 2D- Chiralität von einzelnen Chlornitrobenzol ($C_6H_4ClNO_2$)-Molekülen auf Cu(111) bei 5 K zu verändern. Die hohe submolekulare Auflösung des RTM erlaubt die Identifizierung des Phenylrings und der verschiedenen Substituenten. Durch direkte Injektion von Tunnelelektronen in die Bindung zwischen Kohlenstoff und Chlor ist es möglich, die Position des Chlors innerhalb des Moleküls zu ändern. Als Folge ändern sich 2D-Chiralität und Dipolmoment des Chlornitrobenzols. Die Abhängigkeit der Reaktionswahrscheinlichkeit von der Anregungsenergie und dem Strom wurde untersucht. Dies erlaubt die Identifizierung des zugrunde liegenden Mechanismus. Detailierte Ergebnisse werden im Ramen des Vortrags präsentiert.

O 43 Hauptvortrag Witte

Zeit: Dienstag 14:00–14:45 Raum: TU EB301

Hauptvortrag O 43.1 Di 14:00 TU EB301

Structure and growth of thin films of aromatic molecules on solid surfaces — •Gregor Witte — Physikalische Chemie I, Ruhr-Universität Bochum, 44801 Bochum

The increasing interest in molecular electronics has expressed a necessity of understanding the microstructure and growth properties of ordered organic films. Of particular interest for the fabrication of organic thin film transistors (OFETs) are polycyclic aromatic hydrocarbons (PAHs) which reveal a large variety of structures upon growth on inorganic substrates [1]. In this talk I will mainly focus on the structural properties of thin films of various poly-acenes (Pentacene, Perylene and Rubrene) grown by organic molecular beam deposition on different metal and insulator substrates. By combining various surface sensitive techniques we have been able to derive the molecular microstructure developing with increasing film thickness. In case of planar molecules a characteristic molecular reorientation from substrate controlled thin film phases towards bulk-like phases was identified and on particular surfaces even epitaxial film growth has been obtained [2]. Moreover, with increasing thickness and/or rising substrate temperature a characteristic dewetting of the organic films takes place leading to a formation of distinct nanoscale crystallites which can be further studied.

[1] G. Witte and Ch. Wöll, J. Mat. Res. 19, 1889 (2004).

[2] S. Söhnchen, S. Lukas and G. Witte, J. Chem. Phys. 121, 525 (2004).

O 44 Hauptvortrag Ristein

Zeit: Dienstag 14:45–15:30 Raum: TU EB301

Hauptvortrag O 44.1 Di 14:45 TU EB301

Diamond surfaces: familiar and amazing — •Jürgen Ristein — Institute of Technical Physics, University of Erlangen, Erwin-Rommel-Str. 1, D-91058 Erlangen, Germany

Diamond is the only wide band gap representative of the elemental semiconductors, with a crystal structure identical to its more common relatives silicon and germanium. On first glance one might expect also similar surface properties in terms of reconstructions, surface states and surface band diagrams. In part this expectation is indeed fullfilled, but diamond also exhibits a number of unusual and potentially very useful surface properties. Particularly when the surface dangling bonds are saturated by by monovalent hydrogen atoms, (donor-like) surface states are removed from the gap, the electron affinity changes sign and becomes negative, and the material becomes susceptible to an unusual type of transfer doping where holes are injected by acceptors located at the surface instead of inside the host lattice. These surface acceptors can in the simplest case be adsorbed molecules conveniently chosen by their electron affinity, but they can also be solvated ions within atmospheric water layers or electrolytes in contact with the hydrogenated diamond surface. The understanding of those phenomena requires in fact concepts of surface science, semiconductor physics and electrochemistry, which makes the diamond surface a true 'interdisciplinary' research topic.

O 45 Organische Dünnschichten IV

Zeit: Dienstag 15:45–18:30 Raum: TU EB301

O 45.1 Di 15:45 TU EB301

Molecular distortions and chemical bonding of a large π-conjugated molecule on a metal surface — •F. S. Tautz[1], A. Hauschild[2], K. Karki[1], B.C.C. Cowie[3], M. Rohlfing[1], and M. Sokolowski[2] — [1]International University Bremen, School of Engineering and Science, PO Box 750761, D-28725 Bremen — [2]Institut für Physikalische und Theoretische Chemie, Universität Bonn, Wegelerstr. 12, D-53115 Bonn — [3]European Synchrotron Radiation Facility, Bote Postale 220, 38043 Grenoble Cedex, France

We report an experimental and theoretical investigation of the chemical bonding of 3,4,9,10-perylene-tetracarboxylic-dianhydride (PTCDA) on Ag(111). Normal incidence x-ray standing wave experiments and density functional theory reveal that PTCDA chemisorbs on Ag(111) in a non-planar, vertically distorted configuration. The carboxylic O atoms are 0.018 nm closer to the surface than the perylene core. The distortion is related to weak local bonds between carboxylic O atoms and the Ag surface which are coupled - through charge transfer into the former lowest unoccupied molecular orbital - to the primary, extended chemisorption bond via the perylene skeleton.

O 45.2 Di 16:00 TU EB301

Diffusion and Chemical Reaction at the Interfaces between Metals and the PTCDA — •Gianina Gavrila[1], Mihaela Gorgoi[1], Reinhard Scholz[1], Walter Braun[2], and Dietrich R.T. Zahn[1] — [1]Institut für Physik, Technische Universität Chemnitz, D-09107, Chemnitz, Germany — [2]BESSY GmbH, Albert-Einstein-Straße 15, D-12489 Berlin, Germany

The electronic and chemical and properties of interfaces in organic devices are decisive for charge carrier injection and transport. Metal/organic interfaces can undergo complex and spatially extended chemical interactions. In and Mg metals were deposited onto 3,4,9,10-perylene tetracarboxylic-dianhydride (PTCDA). The interface formation is analyzed via High Resolution Soft X-ray Photoemission Spectroscopy. The experimentally observed C1s, O1s, In4d and Mg2p core level emission intensities together with the valence band evolution upon metal deposition are compared to data from previous study [1]. Additionally, the differences between the two metals are emphasized and a new model for the formation of the In/PTCDA interface is proposed. The photoemission results are correlated with the near edge X-ray absorption spectroscopy spectra taken at the C K-edge and O K-edge. [1] Y. Hirose, A. Kahn, V. Aristov, P. Soukiassian, Appl. Phys. Lett. 68 (2), 1996.

O 45.3 Di 16:15 TU EB301

Ordered (dppy)BF films grown on Ag(110): From submonolayer to multilayer — •Dingyong Zhong[1], Feng Lin[1], Lifeng Chi[1], Yue Wang[2], and Harald Fuchs[1] — [1]Institute of Physic and Center for Nanotechnology (CeNTech), Universität Münster, Wilhelm-Klemmstrabe 10, 48149 Münster, Germany — [2]Key Laboratory for Supramolecular Structure and Materials of Ministry of Education, College of Chemistry, Jilin University, 130012 Changchun, P. R. China

Ordered molecular films of a blue light-emitting material, 1,6-bis(2-hydroxyphenyl) pyridine boron complex [(dppy)BF], grown on the Ag(110) surface by means of organic molecular beam epitaxy, were investigated by scanning tunneling microscopy (STM) and low energy electron diffraction (LEED) under an ultrahigh vacuum. Two commensurate structures exist in the monolayer film grown at 300 K, as found by STM. In the monolayer film, two types of hydrogen bonds are formed between the molecules, which, in addition to the molecule-substrate interaction, essentially determine the monolayer structures. The structural evolution of the (dppy)BF films from submonolayer to 3 monolayers was monitored by LEED in situ and in real time. The results indicate that the growth of the first two monolayers is affected by the periodic potential on the substrate surface, while such a template effect is weakened beyond the second monolayer.

O 45.4 Di 16:30 TU EB301

Structural and spectroscopic investigations of the laterally structured heterorganic system alkanethiol/PTCDA/Ag(111) — •Florian Pollinger, Stefan Schmitt, Christian Kumpf, and Eberhard Umbach — Exp. Phys. II, Univ. Würzburg, 97074 Würzburg

The planar organic molecule 3,4,9,10-perylenetetracarboxylic acid dianhydride (PTCDA) is well known to form commensurate thin films on Ag(111) surfaces. Furthermore, it has been demonstrated that PTCDA induces faceting on vicinal Ag(111) surfaces by step bunching. For an appropriate choice of coverage, self-organization leads to a grating-like morphology with a periodicity down to several nanometres. This enables the use of these surfaces as pre-patterned templates [1].

Other model systems important for designing organic nanostructures are alkanethiols like 1-Decanethiol and 1-Octadecanethiol. They grow as self-assembled monolayers (SAMs) on clean Au and Ag(111) surfaces. In the study presented here, however, we also deposited them on pre-patterned sub-monolayer PTCDA/Ag(111) substrates. These *laterally structured* heterorganic systems were investigated using standard surface characterization techniques, like TPD, XPS and LEED.

[1] X.Ma et al., Appl. Phys. Lett. 84 (2004) 4038

O 45.5 Di 16:45 TU EB301

A standing wave study of the PTCDA-precursor state on the Ag(111) surface — •A. Hauschild[1], R. Temirov[2], M. Sokolowski[1], and F. S. Tautz[2] — [1]Institut für Physikalische und Theoretische Chemie der Universität Bonn, Wegelerstr. 12, 53115 Bonn, Germany — [2]International University Bremen, School of Engineering and Science, PO Box 750 561, 28725 Bremen, Germany

PTCDA deposited on Ag(111) can lead to two different adsorption states: At room temperature (RT) the commonly-known stable chemisorbed state is formed, deposition at temperatures below 160 K, however, yields a meta-stabile "precursor state". This state is also chemisorbed, but no long-range order exists. Photoemission spectroscopy also shows significant differences of the electronic structures of both states [1]. From an earlier normal incidence x-ray standing wave (NIXSW) study, we know that the "RT state" involves a significant distortion of the planar PTCDA molecule. The aim of the present experiment was to investigate the different bonding geometry of the precursor state in comparison to that of the RT state. A first data evaluation actually confirms the existence of differences. However, in contrast to the RT-state, the precursor also undergoes a reversible transition to a second state under exposure to the intensive x-rays, which complicated the experiments. Supported by the DFG. [1] L. Kilian, Doctoral thesis, Universität Würzburg 2002.

O 45.6 Di 17:00 TU EB301

High resolution ARPES study of thin organic films on metallic substrates — •Azzedine Bendounan, Johannes Ziroff, Frank Foster, Felix Schmitt, Eberhard Umbach, Achim Schöll, and Friedrich Reinert — Experimentelle Physik II, Universität Würzburg, Am Hubland, 97074 Würzburg, Germany

We study by high energy and angular resolution photoemission (ARPES) the electronic properties of ultrathin organic films deposited on metal surfaces. Our interest is focused on large π-conjugated planar molecules like 3,4,9,10-perylene-tetracarboxylic dianhydride (PTCDA) and 1,4,5,8-naphthalene-tetracarboxylic dianhydride (NTCDA). On noble metal surfaces, characterized by flat density of states close to the Fermi energy, these molecules form a highly ordered superstructure and grow in layer-by-layer mode. Ag(111), for example, is an ideal substrate since the molecule can diffuse over large distances and form ordered islands. After deposition of one monolayer of PTCDA, the Ag-Shockley surface state disappears and new spectrae features appear. One of these features is associated with the formation of a chemical bond suggesting an hybridization between the metal and the molecule which fills the lowest unoccupied molecular orbital (LUMO). The second feature is described as the highest occupied molecular orbital (HOMO) peak modified also by the bonding. Moreover, we observe an important modification in the photoelectron intensity as function of the emission angle. The observed structures are significantly narrower than in previously published investigations on similar systems.

O 45.7 Di 17:15 TU EB301

Tetracene and pentacene growth on Ag(111) — •Moritz Sokolowski[1], Andreas Langner[1], Annegret Hauschild[1], Russlan Temirov[2], Stefan Tautz[2], Maxim Eremtchenko [3], D. Bauer[3], and Jürgen-A. Schaefer[3] — [1]Institut für Physikalische und Theoretische Chemie der Universität Bonn — [2]School of Engineering and Science, International University Bremen — [3]Institut für Physik und Zentrum für Mikro- und Nanotechnologien, Technische Universität Ilmenau

The growth of the two polyacenes tetracene (Tc) and pentacene (Pc) on Ag(111) was investigated by SPA-LEED, STM, HREELS, XPS, and TPD. Although the two molecules are chemically similar, their growth behaviour on Ag(111) turns out to be significantly different. Tc forms two long-range ordered monolayer structures at temperatures below 230 K, which contain one (planar) and two (slighly tilted) Tc molecules per unit cell, respectively [1]. From the second layer onward, a pronounced cluster-growth occurs. Quite differently, the monolayer of Pc appears to be disordered, possibly due to kinetic limitations. Interestingly, the second layer exhibits a long range ordered structure, whereby the growth directions are templated by surface steps. Supported by the DFG. [1] A. Langner et al., Surf. Science (2004), in press.

O 45.8 Di 17:30 TU EB301

Growth and electronic structure of pentacene films deposited on polycrystalline gold surfaces — •V. Yanev, Ch. Weis, M. Himmerlich, S. Krischok, M. Eremtchenko, and J.A. Schaefer — Institut für Physik und Zentrum für Mikro- und Nanotechnologien, TU Ilmenau, P.O. Box 100565, 98684 Ilmenau, Germany

Pentacene is a promising material for organic thin film transistors due to its high carrier mobilities. Therefore, for organic electronics, it is of great interest to gain a basic understanding of the pentacene growth on evaporated or sputtered metal films, similar to the contacts in electronic devices. We examined the structure and electronic properties of pentacene films on evaporated gold surfaces. The molecular layer structure was investigated using atomic force microscopy (AFM). An upright molecular orientation was observed. The structure of the films is compared to that of pentacene grown on Ag(111). The dependence of the grain size on the deposition conditions is discussed. The electronic structure of the molecular-metal interface was investigated using X-ray and ultraviolet photoelectron spectroscopy (XPS and UPS).

O 45.9 Di 17:45 TU EB301

Orientation of substituted phthalocyanines on polycrystalline gold: distinguishing between the first layers and thin films — •Indro Biswas[1], Heiko Peisert[1], Lei Zhang[1], Martin Knupfer[2], Michael Hanack[3], Danilo Dini[3], Thomas Schmidt[4], David Batchelor[4], and Thomas Chassé[1] — [1]Universität Tübingen, IPC, Auf der Morgenstelle 8, 72076 Tübingen — [2]Leibniz Institute for Solid State and Materials Research Dresden, P.O. Box 270116, , D-01171 Dresden — [3]Universität Tübingen, Inst. Organ. Chem., Auf der Morgenstelle 18, D-72076 Tübingen — [4]Universität Würzburg, Am Hubland, D-97074 Würzburg

We have studied the molecular orientation of substituted phthalocyanines (Pc's) grown as ultra-thin films on a polycrystalline gold substrate. For about 10-20 nm thick films of Pc's with small substituents, a high degree of molecular orientation has been observed. Similar to unsubstituted PcCu, the orientation of the molecules is perpendicular to the sample surface. Importantly, however, the molecular orientation is different for low coverages, the molecules lie on the substrate surface. Thus, the orientation of organic molecules directly at the interface cannot be deduced from the orientation in typical thin film systems. The growth mode is discussed in terms of different molecule-molecule and molecule-substrate interactions. We are grateful for helpful discussions and the synthesis of organic materials to M. Cook and I. Chambrier. Financial support by BESSY is acknowledged.

O 45.10 Di 18:00 TU EB301

Structural and Topographic Study of clean Porphyrin films — •Karmen Comanici, Florian Maier, Hubertus Marbach , and Hans-Peter Steinrück — Lehrstuhl für Pysikalische Chemie II, Universität Erlangen-Nürnberg, Egerlandstraße 3, D-91058 Erlangen

Organic molecules play a prominent role for the development of new materials and molecular devices. An important group of such molecules are porphyrins. Their versatility and distinct chemical and electronic properties makes them promising candidates for tailored catalytic processes and as building blocks for nanoscaled electronic devices.The properties of porphyrins can be modified e.g. by introducing or changing a central metal atom and different ligands. We studied different porphyrins on silver surfaces by means of scanning tunneling microscopy (STM) and low energy electron diffraction (LEED) in ultra high vacuum (UHV). The preparation of the porphyrin layers were done in UHV via sublimation techniques. Ordered porphyrin layers as well as tip induced structural changes in the STM image of the adsorbed fims were observed. One topic to be presented and discussed will be the first time observation of ordered porphyrin layers on an Ag(111) surface.

This work has been funded by Sonderforschunsbereich 583

O 45.11 Di 18:15 TU EB301

Conjugated organic molecules on Au(111): Effect of molecular geometry and conformational changes — •Carsten Busse[1], Sigrid Terkelsen[1], Lars Petersen[1], Morten Nielsen[2], Kurt V. Gothelf[2], Trolle R. Linderoth[1] und Flemming Besenbacher[1] — [1]Department of Physics and Astronomy and iNANO, University of Aarhus, 8000 Aarhus C, Denmark — [2]Department of Chemistry and iNANO, University of Aarhus, 8000 Aarhus C, Denmark

We have performed a UHV-STM study of structures formed by a family of geometrically different, but chemically similar, molecules adsorbed on Au(111). The molecules consist of a central benzene ring with three or two ethynylene spokes, each terminating in a tert-butyl substituted salicylaldehyde moiety. After adsorption at 300 K a variety of close-packed phases is observed which can be rationalized by a common motif of molecules adsorbed with their backbone parallel to the surface and optimized side-to-side interactions. These results constitute a platform for ongoing experiments where conformational changes of the adsorbed molecules are studied and the molecular parameters governing this flipping process are determined, and where covalent cross-linking is induced through co-adsorption with reactive amines.

O 46 Adsorption an Oberflächen V

Zeit: Dienstag 15:45–18:30 Raum: TU EB420

O 46.1 Di 15:45 TU EB420

Investigation of water adsorption on different low index ZnO surfaces — •Tilo Plake, Stefan Andres, and Christian Pettenkofer — Hahn-Meitner-Institut, Glienicker Straße 100, 14109 Berlin

The influence of Zn(OH)$_x$ is reported to play a considerable role regarding the electronical properties of ZnO semiconductor structures. We present x-ray and ultraviolet photoelectron spectroscopy data of ZnO (0001), $(000\bar{1})$, $(10\bar{1}0)$, and $(11\bar{2}0)$ surfaces that have been cleaned under ultrahigh vacuum conditions by Ar$^+$ sputtering and subsequent annealing. Adsorption of H_2O is performed on the samples which have been cooled down to 77 K. Temperature is gradually raised until all water desorbes completely. The changes in the spectral emissions are discussed with respect to the formation of a hydroxide capping. Alternatively, samples are exposed to water at temperatures ranging from 300 K to 600 K. Adsorbate spectra are compared to data obtained from hydroxide exposed samples. Decomposition of Zn(OH)$_x$ to ZnO and H_2O during annealing is monitored and compared to data obtained from polycrystalline samples.

O 46.2 Di 16:00 TU EB420

Partial Dissociation of Water on the ZnO$(10\bar{1}0)$ Surface — •B. Meyer[1], D. Marx[1], O. Dulub[2], U. Diebold[2], M. Kunat[3], D. Langenberg[3], and Ch. Wöll[3] — [1]LS für Theoretische Chemie, Ruhr-Universität Bochum — [2]Dept. of Physics, Tulane University, New Orleans, USA — [3]LS für Physikalische Chemie I, Ruhr-Universität Bochum

The delicate interplay between chemical bonding, van der Waals forces, and hydrogen bonding gives rise to complex phenomena such as complete dissociation, partial dissociation at defects, molecular adsorption, and multilayer formation when H_2O interacts with solid surfaces. Recently, an intriguing, yet controversial, intermediate scenario was advanced, where the interaction between water molecules results in a partial dissociation of H_2O on perfect surfaces, leading to superlattices with long-range order. In a combined theoretical and experimental study, applying DFT calculations, Car-Parrinello molecular dynamics simulations, and STM computations, together with diffraction (He-atom scattering, LEED), STM, and thermodynamic measurements we give conclusive evidence that such a phenomenon is encountered for H_2O on the perfect ZnO$(10\bar{1}0)$ surface. At monolayer coverage, every second water molecule is found to auto-dissociate, subject to a low activation barrier, upon a favorable hydrogen-bonding interaction with a neighboring water molecule, i.e. without the need to invoke defects or impurities. This process leads to a (2×1) superlattice with long-range order which is stable from below 200 K up to temperatures close to the boiling point of liquid water. [1] B. Meyer, D. Marx, O. Dulub, U. Diebold, M. Kunat, D. Langenberg, Ch. Wöll, Angew. Chem., in print.

O 46.3 Di 16:15 TU EB420

Alternative Gate Oxide Pr_2O_3: Growth characterization on Si(111) and Si(113) — •N.M. Jeutter[1], M. Hennemeyer[1], L. Libralesso[2], T.-L. Lee[2], J. Zegenhagen[2], A. Stierle[3], and W. Moritz[1] — [1]Dept. of Earth- and Enviromental Sciences, LMU Munich, Germany — [2]ESRF, Grenoble, France — [3]MPI MF, Stuttgart, Germany

GIXRD measurements of a 0.6 nm thick Pr_2O_3 -layer on Si(111) show that the interface is formed by an Pr-O-Si bond with oxygen on top of Si. Evidence is found from XRD and LEED measurements that Pr_2O_3 grows at 500 ° C in double layers, corresponding to one unit cell of the hexagonal Pr_2O_3 bulk phase. Annealing up to 760 ° C of the thicker layers leads to island growth and formation of $PrSi_2$. The p(2x1) and the coexisting p($\sqrt{3}x\sqrt{3}$) structures, occurring in the LEED pattern after annealing, are probably due to submonolayer coverage of Pr on Si (111)[1].

The growth of Pr_2O_3 on Si(113) has been investigated by LEED and X-ray diffraction. Pr_2O_3 was evaporated at a substrate temperature of 600 ° C. After deposition of 0.2 nm of Pr_2O_3, the reconstruction of the clean surface is removed and the LEED pattern exhibits a streaky (4x1) superstructure. AFM images show flat islands of triangular to trapezoid form. First GIXRD measurements did not show any superstructure reflections indicating that the (4x1)pattern seen in LEED arises from the oxygen ordering.

[1] L. Grill, M.G. Ramsey, J.A.D. Matthew, F.P. Netzer, Surface Science 380 (1997) 324-334

O 46.4 Di 16:30 TU EB420

Towards ultimate resolution in surface stress measurements — •Peter Kury and Michael Horn-von Hoegen — Institut für Laser- und Plasmaphysik, Universität Duisburg-Essen, 45141 Essen

Surface stress is one of the most important physical quantities for the evolution of structure and morphology on the surfaces of solids due to its large contribution to the total energy. Unfortunately, the 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 in the order of 1N/m, corresponding for example to a biaxially by 4.2% compressed germanium film of one monolayer thickness, can be easily achieved if proper mechanical isolation of the system and vibration damping are implemented. To reach an instrumental resolution in the order of 0.01N/m, however, it is necessary also to consider effects which are far from obvious in this context. Here we present modifications of SSIOD that allow the determination of surface stress with a resolution of 0.005N/m [2] corresponding to a sensitivity of less than 1% of a monolayer in typical adsorbate systems. Experimental results are shown for Sb/Si(001), Cs/Si(001) and Si/Si(111).

[1]: A. Schell-Sorokin et al., Phys. Rev. Lett. **64**(9), 1039 (1990)

[2]: P. Kury et al., Rev. Sci. Instrum., in press (2004)

O 46.5 Di 16:45 TU EB420

Nanostructuring with silver on Au-Si(111) — •C. Seifert, C. Wiethoff, F.-J. Meyer zu Heringdorf und M. Horn-von Hoegen — Universität Duisburg-Essen, Standort Essen

Self-assembly of 1D nanostructures on surfaces usually requires anisotropic qualities of the substrate e.g. vicinial cut of the surface. Gold adsorption over 350°C on the non-anisotropical Si(111) surface produces anisotropically formed (5x2) domains, with domain shapes rounding up at higher temperatures. Adsorption or annealing in temperature regions of around 750 °C, well below the transition of the (5x2) to (1x1) reconstructed areas, leads to creation of a surface with the 2-fold direction mainly aligned along the step direction of the remaining steps. In order to use these surfaces as template for silver wire growth - atoms diffuse faster along the 2-fold direction of the (5x2) reconstruction - the alloying of silver with gold on this surface has to be understood better. Measurements on the formation of Ag/Au alloys have been done with RT-STM and high resolution LEED. A phasediagram for Silver on Au(5x2)-Si(111) is provided.

O 46.6 Di 17:00 TU EB420

Photodesorption of molecules adsorbed on ultrathin Au — •Claudia Wesenberg and Eckart Hasselbrink — FB Chemie, Universitaet Duisburg-Essen, Universitaetstr. 5, 45117 Essen, Germany

Ultrathin Au films (20-100ML) deposited on Si(100) are suited to study the electron dynamics in such films and the influence of the film thickness on charge transfer to the adsorbate and subsequent photodesorption. In our experiments, NO is chosen as the probe molecule. Its adsorbtion is performed at 100K on the Au-covered Si(100) surface. Photodesorption is induced using a Nd:YAG laser and the desorbed molecules are detected by QMS. The film thickness is varied in order to obtain information about the charge transfer dynamics between the ultrathin Au film and the NO adsorbate. The photodesorption crosssection of NO is expected to decrease with increasing film thickness.

O 46.7 Di 17:15 TU EB420

CO-Adsorption auf der Pt(111)-Oberfläche: Vergleich eines gradientenkorrigierten Funktionals und eines Hybridfunktionals — •Klaus Doll — Institut für Mathematische Physik, TU Braunschweig, Mendelssohnstraße 3, D-38106 Braunschweig

Die CO-Adsorption auf der Pt(111)-Oberfläche in einem $(\sqrt{3} \times \sqrt{3})$-Muster wurde mit dem gradientenkorrigierten Funktional von Perdew und Wang (PW91) und dem Hybridfunktional B3LYP studiert. Dazu wurde das System mit einem Modell mit Periodizität in zwei Raumrichtungen beschrieben. Das PW91 Funktional gibt den falschen Adsorptionsplatz (fcc), in Übereinstimmung mit einer Reihe früherer Rechnungen [1]. Das B3LYP-Funktional gibt den top site als den bevorzugten Platz an. Dies bestätigt Resultate von Cluster-Rechnungen, wo vorgeschlagen wurde, dass die unterschiedliche (je nach Funktional) Energielücke zwischen höchstem besetzten und tiefsten unbesetzten Orbital verantwortlich sein könnte für diese Veränderung [2]. Die Resultate werden unterstützt durch projezierte Zustandsdichten und Populationsanalysten.

[1] P. J. Feibelman, B. Hammer, J. K. Nørskov, F. Wagner, M. Scheffler, R. Stumpf, R. Watwe and J. Dumesic, J. Phys. Chem. **105**, 4018 (2001).
[2] A. Gil, A. Clotet, J. M. Ricart, G. Kresse, M. García-Hernández, N. Rösch, and Ph. Sautet, Surf. Sci. **530**, 71 (2003).

O 46.8 Di 17:30 TU EB420

A comparative study of prenal on Pt(111), $Pt_2Sn(111)$ and $Pt_3Sn(111)$ surface alloys — •Jan Haubrich, Alexander Krupski, Conrad Becker und Klaus Wandelt — Inst. f. Phys. u. Theo. Ch., Wegeler. 12, D-53115 Bonn

It is known that the selectivity of the hydrogenation processes of α,β-unsat. aldehydes like acrolein or prenal depends not only on the molecule itself, but also on the catalyst employed. To understand the different selectivities, the adsorption of prenal on Pt(111) and two Pt-Sn surface alloys is investigated with HREELS, TPD and LEED.

After adsorption of prenal at 100K the desorption of fragments up to 100 amu is studied with TPD. While on Pt(111) the desorption of prenal is detected at 160K (Multilayer), 177K and 199K, also a fragmentation reaction is observed giving rise to desorption of H_2 and CO in several peaks. On Pt_2Sn and Pt_3Sn surface alloys this fragmentation process is suppressed. HREELS experiments carried out between 100K and 500K on the three surfaces show highly complex spectra of adsorbed prenal. On Pt(111) also the fragmentation process starting at 300K can be examined with HREELS. Also on the Pt_xSn surfaces complex HREEL spectra of prenal are recorded.

O 46.9 Di 17:45 TU EB420

CO adsorption on stepped Pt(355) and Pt(644) - the dissimilar twins — Barbara Tränkenschuh, Thomas Fuhrmann, Christian Papp, Junfa Zhu, •Reinhard Denecke, and Hans-Peter Steinrück — Lehrstuhl für Physikalische Chemie II, Universität Erlangen-Nürnberg, Egerlandstr. 3, 91058 Erlangen

The adsorption and thermal desorption of CO on stepped Pt surfaces was studied by the combination of a supersonic molecular beam and in-situ high resolution XPS. Using synchrotron radiation as excitation source, we are able to clearly distinguish between adsorption sites at steps and at terraces in C 1s spectra, even at fast measuring times (about 4 s per spectrum). Both surfaces studied contain five atom wide (111) terraces separated by monatomic steps. While on Pt(355) these steps have (111) orientation, they are in (100) orientation on Pt(644). Interestingly, these very similar surfaces exhibit differences in CO adsorption behaviour not only at step sites, as expected, but also on the nominally equal terraces. Here, the distribution between bridge and on-top bound species on Pt(644) is quite similar to the situation found for Pt(111)[1], whereas for the (355) surface the adsorbate-adsorbate interactions modify the occupation ratio significantly. Thus, an influence on surface reactions such as the CO oxidation, can be expected. Supported by the DFG (STE 620/4-2). [1] M. Kinne et al., J. Chem. Phys. 117, 10852 (2002).

O 46.10 Di 18:00 TU EB420

Accurate prediction of the CO adsorption site on Cu(111) from first-principles calculations — •Qing-Miao Hu, Karsten Reuter, and Matthias Scheffler — Fritz-Haber-Institut, Faradayweg 4-6, D-14195 Berlin

It is well known that density-functional theory (DFT) with present-day jellium-based local or gradient-corrected exchange-correlation (xc) functionals fails to predict the correct adsorption site of CO on most close-packed metal surfaces, including Pt(111) and Cu(111). Motivated by earlier findings, e.g. [1], that showed that the error of these functionals is “nearsighted”, we present here a systematic study of the correction of the xc energy for CO adsorption. The clue is to use appropriate *energy differences* and appropriately chosen clusters around the adsorption site. Again [1] we find that *the xc correction* (not the total energy) converges rapidly with cluster size. Calculations using DFT-LDA, PBE, and B3LYP as well as HF+MP2 are presented.

For the example of low-coverage adsorption of CO at Cu(111) we therewith indeed obtain the correct on-top adsorption site. We also explain our results, as well as the failure of standard DFT calculations in a simple physical picture.
[1] C. Filippi, S.B. Healy, P. Kratzer, E. Pehlke, and M. Scheffler, Phys. Rev. Lett. **89**, 166102 (2002)

O 46.11 Di 18:15 TU EB420

MIES (=Metastable Induced Electron Spectroscopy) als Methode zur mechanistischen Untersuchung der heterogenen Katalyse — •YanChun Liu, Andrea Berlich und Harald Morgner — Wilhelm-Ostwald-Institut für Physikalische und Theoretische Chemie der Universität Leipzig, Linnestr.2, 04103 Leipzig

Der Mechanismus von Reaktionen an Metall-Träger-Katalysatoren ist bis heute nicht eindeutig verstanden. Insbesondere ist zu klären, welchen Einfluß die Belegung von Metallclustern mit Molekülen und Oxidpartikeln hat. Die perfekt oberflächenempfindliche Methode MIES (=Metastable Induced Electron Spectroscopy) kann einen Beitrag zur Aufklärung zu leisten. Wir haben begonnen mit Arbeiten an dem System Nickel/Nickeloxid. MIES erlaubt die Aussage, dass dabei das NiO teilweise zu Metall reduziert wird. Dies ist im Einklang mit früheren Befunden, dass der Übergang zwischen Oads/Ni(100) und NiO reversibel ist und von der Sauerstoffkonzentration abhängt[1]. Unter welchen Umständen sich auf der Oxidschicht Ni-Cluster bilden können, wird untersucht. Das Angebot von CO zur Adsorption zeigt kaum einen merkbaren Einfluss zwischen Raumtemperatur und ca. 200°C. Experimente zur Adsorption von NH3 sind in Vorbereitung. Die quantitative Analyse der Oberflächenbeschaffenheit in allen Stadien der Präparation mit Hilfe von MIES wird präsentiert[2]. [1]R.Kubiak, H.Morgner and O.Rakhovskaia, Surf. Science 321 (1994) 229-36 [2]H. Morgner, Adv. At. Mol. Opt. Physics 42B (2000) 387-488

O 47 Rastersondentechniken III

Zeit: Dienstag 15:45–18:30 Raum: TU EB202

O 47.1 Di 15:45 TU EB202

Optical interaction between tip and substrate in apertureless SNOM — •Ruben Esteban, Ralf Vogelgesang und Klaus Kern — Max Planck Institute für Festkörperforschungg

Scanning near field optical microscopes (SNOM) have proved able to overcome the resolution limit and study light-matter interaction in nanometer sized structures. Resolution of $\sim 10nm$ is achievable at optical and infrared frequencies using the apertureless configuration (a-SNOM), which detects the fields scattered when a sharp tip is approached to a substrate under focused illumination. We use numerical simulation to better understand the phenomena involved. In our modelling we go significantly beyond the "spherical tip" model towards realistic, extended, conical tips. We can approach the experimental, "infinite-tip" case very well, including the presence of a large background field from the tip bulk. We also simulate the behavior of an efficient demodulation scheme that helps to discriminate the field generated in the strongly localized tip-substrate interaction. Good qualitative agreement with experimental measurements is found.

O 47.2 Di 16:00 TU EB202

Scattering scanning near-field optical microscopy on anisotropic dielectrics — •Susanne Schneider, Stefan Grafström, and Lukas Eng — Institute of Applied Photophysics, University of Technology Dresden, D-01062 Dresden

Scattering scanning near-field optical microscopy (s-SNOM) is based on the interaction between an optically scattering nano-cluster (AFM tip) and a dielectric sample. The size of the cluster defines the resolution of the microscope, which is in the order of nanometers. On this scale the optically anisotropic properties of the sample have to be taken into account, even if the sample is isotropic on the macroscopic scale.

We discuss the interaction between a cluster and an anisotropic sample using an analytical dipole-dipole model by taking the following contrast mechanisms into account:

1. The reflection on the surface of the anisotropic sample, which causes a change in the external electric field at the position of the probe.
2. The modification of the polarizability of the tip by interaction with the anisotropic sample. Here we use the image charge method for anisotropic samples, which was developed in 1997 by I. Lindell.
3. The formation of a resulting dipole which is the superposition of the tip dipole and the image dipole induced in the sample.

In these calculations not only the influence of the sample anisotropy is included but also the anisotropy that the probe may exhibit for geometrical or material-specific reasons.

O 47.3 Di 16:15 TU EB202

Resonant light scattering by near-field induced localized phonon polaritons — •Jan Renger[1], Stefan Grafström[1], Lukas M. Eng[1], and Rainer Hillenbrand[2] — [1]Institute of Applied Photophysics, University of Technology Dresden, D-01062 Dresden — [2]Nano-Photonics Group, Max-Planck-Institut für Biochemie, Am Klopferspitz 18, D-82152 Martinsried

In the vicinity of a SiC surface the scattering of light at a metallic nanoparticle shows a strong peak around the surface phonon polariton resonance of the SiC substrate [1] in the mid-infrared spectral region. Close to the surface the polarized particle couples to localized phonon polaritons. This near-field interaction shifts the peak to lower frequencies and causes a splitting into two modes for distances below 5 nm. We analyze this phenomenon by applying an accurate numerical 3D model based on the multiple-multipole method. The results are compared with the predictions of the analytical dipole model as frequently used to explain the contrast in aperture-less scattering- type scanning near-field optical microscopy. We find a qualitative agreement but the dipole model turns out to underestimate the spectral shift quantitatively, which is significant for small separations between the sphere and the SiC interface.

[1] R. Hillenbrand, T. Taubner, and F. Keilmann, Nature **418**, 159 (2002).

O 47.4 Di 16:30 TU EB202

Quantitative investigation of tip-sample interaction on single-walled carbon nanotubes in the attractive force regimes — •Makoto Ashino, Timo Behnke, and Roland Wiesendanger — Institute of Applied Physics and Microstructure Research Center, University of Hamburg, Jungiusstrasse 11, D-20355 Hamburg

The three-dimensional force field spectroscopy measurement combined with atomic-resolution dynamic force microscopy imaging has allowed us to evaluate interaction forces acting between a foremost atom of the silicon-cantilever tip and specific atomic sites of a single-walled carbon nanotubes (SWNT) [1]. Quantitative analysis using a simple Lennard-Jones (L-J) potential leads to the finding that the short-range interatomic van der Waals forces are responsible for the atomic-scale contrast. The analysis also shows that the interaction forces deviate from the L-J fits at closer tip-sample distances than that showing the maximum attractive forces. The degree of deviation is site dependent as well. Using some model calculations, we try to analyze tip-sample interactions at closer distances. By taking softness and tip-induced relaxations of SWNTs into account, we discuss the dynamic response of the SWNT to variation of the tip-sample distance.

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

O 47.5 Di 16:45 TU EB202

First-priciples simulations of NC-AFM image contrast on InAs(110) surface — •Vasile Caciuc[1], Hendrik Hölscher[1], Stefan Blügel[2], and Harald Fuchs[1] — [1]Physikalisches Institut der Universität Münster, Wilhelm-Klemm-Str. 10, 48149 Münster — [2]Institut für Festkörperforschung, Forschungszentrum Jülich, 52425 Jülich

In the present contribution we report *ab initio* pseudopotential calculations based on density functional theory to investigate the non-contact atomic force microscopy (NC-AFM) image contrast on InAs(110) surface. The foremost tip structure is modeled by a SiH_3 tip. The influence of long-range van der Waals forces on the simulated AFM images due to the macroscopic part of the tip was taken into account by an empirical model. The effect of the tip-induced surface relaxations on the calculated forces was investigated for the tip above As and In atoms. The displacement curves corresponding to these vertical scans exhibit an hysteretic behaviour. At the tip-surface separations where the instability induced by this hysteresis is not present, the force curves obtained for relaxed (due to tip-sample interaction) and unrelaxed InAs(110) surface exhibit the same qualitative behaviour. From the calculated forces on a large number of grid points in real space (≈ 1300) we obtained maps of constant frequency shifts. The overall structure and the corrugation of the simulated NC-AFM images are in good agreement with the experimental results and allow us to explain the experimentally observed features of the image contrast mechanism on the basis of the calculated short-range chemical tip-sample interaction forces.

O 47.6 Di 17:00 TU EB202

Tip Models and Surface Atoms in DFT Simulations of AFM Scans — •Vladan Buš and Josef Redinger — Center for Computational Materials Science, Institut f. Allgemeine Physik, Vienna University of Technology, Getreidemarkt 9/134, 1060 Vienna, Austria

Non-contact Atomic Force Microscope operated under ultra-high vacuum conditions is able to display atomic features of insulating or semiconductor surfaces. Oscillations of the cantilever are influenced by forces acting between the surface atoms and the probe tip. In the close-to-contact operation region and for small amplitudes, forces describing the on-set of chemical bonding stand behind the contrast formation in this experiment.

We employ the DFT VASP code, using PAW and PW91 GGA, to simulate probing of surface atoms of GaAs(110) and Si(100) surfaces with a Si tip. Changes in structure during the approaching and withdrawing move lead to abrupt changes in normal and lateral forces and cause a hysteresis in the interaction energy.

O 47.7 Di 17:15 TU EB202

Q-Control in der dynamischen Kraftmikroskopie — •D. Ebeling[1], H. Hölscher[1], U.D. Schwarz[2], B. Anczykowski[3] und H. Fuchs[1] — [1]Center for Nanotechnology (CeNTech) und Physikalisches Institut, Universität Münster — [2]Department of Mechanical Engineering, Yale University, New Haven, USA — [3]nanoAnalytics GmbH, Münster

Der Cantilever kann in der dynamischen Kraftmikroskopie sowohl als extern angeregter als auch als selbsterregter Oszillator betrieben werden. Das so genannte Q-control kombiniert beide Ansätze und erlaubt eine aktive Modifikation der Dämpfung des Federbalkens und damit der Güte des Systems [1]. Diese Eigenschaft kann auf verschiedene Arten genutzt werden, um die Möglichkeiten der dynamischen Kraftmikroskopie zu verbessern.

Wir präsentieren eine Analyse des Q-controls in der dynamischen Kraftmikroskopie. Basierend auf der analytischen Lösung der Bewegungsgleichung geben wir explizite Formeln an, mit denen man die relevanten Parameter wie Verstärkungsfaktor, Phase und Amplitude berechnen kann. Anhand der eingehenden Analyse dieser Formeln lassen sich die bekannten Vorteile des Q-controls (wie z.B. Kontrolle des Q-Faktors, erhöhte Scangeschwindigkeit, Reduktion der Spitze-Proben Kräfte) erklären. Zum Schluss vergleichen wir die theoretischen Ergebnisse mit den experimentellen Resultaten.

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

O 47.8 Di 17:30 TU EB202

Calculation of STM images of defect and adsorbate structures on the ZnO(10$\bar{1}$0) surface — •Roman Kovacik, Bernd Meyer, and Dominik Marx — Lehrstuhl für Theoretische Chemie, Ruhr-Universität Bochum, D-44780 Bochum, Germany

The interpretation of scanning tunneling microscopy (STM) experiments is often difficult since STM images are not a direct probe of the atomic structure of a surface but of its electronic properties. To determine STM images from electronic structure calculations we have implemented the two most common methods, the Tersoff–Haman approach and the evaluation of Bardeens tunneling formula, into the density–functional based Car–Parrinello Molecular Dynamics (CPMD) code. As first applications we have calculated STM images together with selected I(V)–profiles (scanning tunneling spectroscopy – STS) for (i) the clean ZnO(10$\bar{1}$0) surface, (ii) the surface with oxygen, zinc and ZnO vacancies and (iii) the adsorbate–covered surface considering different coverages of water molecules. Characteristic differences between the Tersoff–Haman and the Bardeen approach will be discussed, and the calculations will be compared to recent experimental results.

O 47.9 Di 17:45 TU EB202

STM induced light emission spectroscopy of individual C_{60} molecules — •Elizabeta Ćavar, Marie-Christine Blüm, Marina Pivetta, François Patthey, and Wolf-Dieter Schneider — Institut de Physique des Nanostructures, Ecole Polytechnique Fédérale de Lausanne (EPFL), CH-1015 Lausanne, Switzerland

The tunneling electrons from a Pt/Ir STM tip were used as an excitation source to locally investigate optical transitions of individual C_{60} molecules. Experiments were performed with a home built STM operating in ultra-high vacuum and at a temperature of 50 K. The C_{60} molecules were sublimated on ultrathin NaCl(001) film on Au(111). Topography images revealed C_{60} nanocrystals in the hexagonal and truncated triangular form with an average side length between 30 and 80 nm and a maximal height of 4 layers. The molecules form hexagonal layers with an intermolecular distance of 1nm. Light emission spectra from individual C_{60} molecules show several peaks in the wavelength range between 670 and 900 nm which are assigned to the characteristic C_{60} luminescence.

O 47.10 Di 18:00 TU EB202

Untersuchung der Bandstruktur und der Injektionscharakteristik von Elektronen am Beispiel Niob mittels Rastertunnelspektroskopie — •Berndt Koslowski, Christof Dietrich und Paul Ziemann — Abtl. Festkörperphysik, Universität Ulm

Die Volumen-Bandstruktur von Nb wurde mittels Rastertunnelspektroskopie auf Nb(110) und Nb(100) untersucht. Zur Anwendung kamen sowohl die herkömmliche I-V-Spektroskopie als auch die selten benutzte Z-V-Spektroskopie. Letztere erweitert den adressierbaren Energiebereich auf ±5 eV. In diesem Energiebereich können viele Signaturen in der experimentell bestimmten lokalen Zustandsdichte gefunden werden, die sich kritischen Punkten der Volumenbandstruktur von Nb zuordnen lassen. Unter anderem kann eine bislang unverstandene Signatur bei +1eV auf der Nb(110) auf einen Oberflächenzustand zurückgeführt werden. Hier vergleichen wir die auf der (110)-Oberfläche gewonnenen Erkenntnisse mit der Spektroskopie auf der (100)-Oberfläche und versuchen Informationen über die Injektions-Charakteristik der Elektronen in die Elektroden abzuleiten.

O 47.11 Di 18:15 TU EB202

Visualisierung und Manipulation ferroelektrischer Domänen in Lithiumniobat mit dem Rasterkraftmikroskop* — •Tobias Jungk, Elisabeth Soergel und Karsten Buse — Physikalisches Institut, Universität Bonn, Wegelerstr. 8, 53115 Bonn

Lithiumniobat ist ein Ferroelekrikum, das aufgrund seiner piezoelektrischen, pyroelektrischen, elektrooptischen und nichtlinear-optischen Eigenschaften von großem Interesse für viele technische Anwendungen ist. Da die Domänenstruktur einen direkten Einfluss auf die Eigenschaften des Materials hat, ist es von besonderem Interesse diese bis hin zur kleinstmöglichen Skala zu untersuchen. Hier bietet das Rasterkraftmikroskop (RKM) die Möglichkeit der zerstörungsfreien Domänenvisualisierung auf der Nanometerskala. Wir untersuchen die Mechanismen zur Abbildung ferroelektrischer Domänen mit dem RKM in Lithiumniobat-Kristallen. Dazu wird im Kontaktmodus eine Wechselspannung an die RKM-Spitze angelegt und mittels Lock-In-Technik die lokale Antwort des Kristalls ortsaufgelöst analysiert. Die erreichte Ortsauflösung beträgt ca. 100 nm. Neben der Charakterisierung und Optimierung des Abbildungsverfahrens wird das RKM auch zur Strukturierung ferroelektrischer Domänen im Submikrometerbereich eingesetzt. Mit dem an der RKM-Spitze inhomogenen, stark überhöhten elektrischen Feld ist es möglich, gezielt Domänen zu schalten und somit künftig Strukturen für die integrierte Optik zu realisieren. *Gefördert von der DFG und von der Deutschen Telekom AG.

O 48 Oxide und Isolatoren II

Zeit: Dienstag 15:45–18:30 Raum: TU EB107

O 48.1 Di 15:45 TU EB107

Ordered alumina film on NiAl(110): Structure and nucleation centers — •E. Napetschnig[1], G. Kresse[2], L. Köhler[2], M. Schmid[1], and P. Varga[1] — [1]Institut f. Allgemeine Physik, Vienna University of Technology, Austria — [2]Institut fuer Materialphysik, University of Vienna, Austria

Transition metal clusters on alumina support are one of the most frequently used model systems for investigations of heterogenous catalysis. Oxidation of the (110) surface of NiAl at elevated temperatures leads to the formation of an alumina film of uniform thickness and structure [1]. In spite of many attempts of structural analysis, the atomic structure of the unit cell was unknown until now. Unexpectedly our atomically resolved STM images of the topmost oxygen layer show squares with oxygen atoms at the edges in addition to areas with hexagonal structure. The unit cell has a p2g symmetry. This is an atomic arrangement not found in the known bulk structures of alumina. Based on these STM images the complete determination of the oxide film structure was possible by ab-initio calculations [2]. This was the starting point to determine the nucleation centers of platinum clusters on the alumina film.

[1] M. Bäumer et al., Prog. Surf. Sci. 61 (1999) 127

[2] G. Kresse et al, to be published

O 48.2 Di 16:00 TU EB107

Growth of vanadium oxides on $Cu_3Au(111)$ — •Michael Hafemeister, Jürgen Middeke, Ralf-Peter Blum, and Horst Niehus — Humboldt-Universität zu Berlin, Institut für Physik/ASP, Newtonstraße 15, D-12489 Berlin

Systematic studies of the deposition of transition metals on different oxidic substrates illustrate the trend of increased wetting and enhanced growth depending on the oxygen affinity of the deposit. According to the concept of an oxygen-containing substrate we found that different transition metal oxide films (VO_x, NbO_x, MoO_x) of high quality can be obtained on $Cu_3Au(100)$. In order to analyze the influence of structural factors of the substrate, the growth of VO_x on $Cu_3Au(111)$ has been investigated. STM studies show the 2D growth of a single-phase VO_x film with a honeycomb structure (2.7nm), that can be recognized as a Moiré pattern created by a hexagonal superlattice with a lattice parameter of 0.3nm. This structure could be confirmed by LEED images. The evaluation of AES data suggests a VO stoichiometry. From low energy ion scattering we conclude that the top layer is composed of oxygen. Finally the formation of a VO(111) layer is proposed, exposing a lattice of 0.3nm which is just slightly lager than 0.28nm known from the bulk vanadium monoxide.

O 48.3 Di 16:15 TU EB107

Oxidation and reduction of thin molybdenum oxide layers on $Cu_3Au(100)$ — •Jürgen Middeke, Ralf-Peter Blum, and Horst Niehus — Humboldt-Universität zu Berlin, Institut für Physik, ASP, Newtonstr. 15, 12489 Berlin

Recently it has been shown that well defined two dimensional vanadium oxide layers can be created on a $Cu_3Au(100)$ surface [1]. The most important step of the preparation technique seems to be oxygen implantation and subsequent annealing of the alloy substrate prior to the transition metal evaporation. Meanwhile the technique was also successfully applied to niobium oxide and molybdenum oxide formation. In this presentation we will focus on oxidation and reduction processes observable at different phases of MoO_x that exhibit either rectangular or hexagonal symmetry. The oxidation and reduction has been followed in situ on an atomic scale by scanning tunneling microscopy.

[1] H. Niehus R.-P. Blum and D. Ahlbehrendt, phys. stat. sol. (a) **187** (2001) 151

O 48.4 Di 16:30 TU EB107

Structural Studies of thin VO_x films grown on TiO_2 using NIXSW — •Emily Kröger[1], Francesco Allegretti[2], Martin Polcik[1], Matthew Knight[2], Vin Dhanak[3], and Phil Woodruff[1,2] — [1]Fritz-Haber-Institut, Faradayweg 4-6, 14195, Berlin — [2]Department of Physics, University of Warwick, Coventry CV4 7AL, UK — [3]Daresbury Laboratory, UK

The aim of this project is to use quantitative structural techniques to obtain information on transition metal oxide surfaces. The Normal Incidence X-Ray Standing Waves (NIXSW) technique is used to investigate the growth of sub-nanometre vanadia films on the rutile titanium dioxide (110) surface. The bulk NIXSW structural parameters for TiO_2 have been successfully fitted. Three different Bragg reflections were used to triangulate the V atom positions and epitaxial film growth for vanadia films grown by post-oxidation has been confirmed. The measurements allowed the decrease in film quality with film thickness to be monitored. In addition, a series of experiments on as-deposited sub-monolayer films were completed. Two components in the X-ray photoelectron spectrum of the V 2p suggest two different V species on the surface and this NIXSW study shows that they take different surface positions.

O 48.5 Di 16:45 TU EB107

Tieftemperatur-STM-Untersuchungen der Morphologie und Defektstruktur von dünnen MgO-Filmen — •Martin Sterrer, Markus Heyde, Niklas Nilius, Hans-Peter Rust und Hans-Joachim Freund — Fritz-Haber-Institut der Max-Planck-Gesellschaft, Abteilung Chemische Physik, Faradayweg 4-6, 14195 Berlin

Die genaue Kenntnis der Struktur und elektronischen Eigenschaften von Defekten ist unumgänglich für die Aufklärung des Zusammenhangs zwischen Struktur und Reaktivität von Oberflächenzentren. Mittels Raster-Tunnel-Mikroskopie bei 4K wurde die Morphologie eines 4 Monolagen dünnen MgO-Films auf Ag(100) untersucht. Mindestens 4 atomare Lagen des Films sind exponiert, wobei die Terrassen nahezu perfekt georndet sind, Stufen jedoch eine hohe Anzahl von Defekten wie Kinken und Ecken aufweisen. Es wird gezeigt, dass mittels Landungsinjektion von der STM-Spitze elektronische Defekte auf der Oberfläche erzeugt werden können, deren Energieniveaus innerhalb der Bandlücke von MgO liegen. Durch geeignete Wahl der Polarität der Probenspannung ist es möglich, den Ladungszustand der Defekte gezielt zu verändern. Der Vergleich mit theoretischen Berechnungen legt den Schluss nahe, dass es sich bei den Defekten um Farbzentren handelt.

O 48.6 Di 17:00 TU EB107

ESR-spektroskopische Untersuchung zur Bildung und Reaktivität von Oberflächen-Farbzentren auf dünnen MgO-Filmen — •Esther Fischbach, Martin Sterrer, Thomas Risse und Hans-Joachim Freund — Fritz-Haber-Institut der Max-Planck-Gesellschaft, Abteilung Chemische Physik, Faradayweg 4-6, 14195 Berlin

Die chemischen und physikalischen Eigenschaften von Oxid-Oberflächen werden entscheidend von der Anwesenheit von Defekten beeinflusst. Die Aufklärung der Reaktivität der Oberfläche erfordert daher eine genaue Untersuchung der Natur und elektronischen Eigenschaften von Defektstrukturen. Farbzentren, i.e. neutrale oder einfach positiv geladene Anionenfehlstellen auf MgO, sind in diesem Zusammenhang von herausragender Bedeutung, da sie einerseits durch die Möglichkeit eines Elektronentransfers auf molekulare Adsorbate zur chemischen Reaktivität der Oberfläche beitragen, andererseits die elektronischen Eigenschaften von adsorbierten Metallclustern verändern.

In der vorliegenden Arbeit wurden dünne MgO-Filme (20ML) auf einkristallinen Substraten hergestellt und mittels Elektronen-Spin-Resonanz-Spektroskopie untersucht. Während auf den frisch gewachsenen MgO-Filmen keine Farbzentren detektiert werden konnten, bewirkt Elektronenbeschuss eine deutliche Veränderung der Oberflächen-Morphologie und führt zu einem den Farbzentren zuzuordnenden ESR-Signal. Die Reaktivität der Oberflächen-Farbzentren gegenüber einfachen molekularen Adsorbaten wie O_2, CO, N_2O und NO wurde untersucht.

O 48.7 Di 17:15 TU EB107

On the electronic structure of LiCoO2 and related compounds used as battery cathodes — •Thissen Andreas[1], David Ensling[1], Qi-Hui Wu[2], Francisco Javier Fernandez Madrigal[1], Stefan Laubach[1], Peter C. Schmidt[1], and Wolfram Jaegermann[1] — [1]FB Material- und Geowissenschaften, Fachgebiet Oberflächenforschung, TU Darmstadt, Petersenstr. 23, D-64287 Darmstadt — [2]Lehrstuhl für Physikalische Chemie I, Ruhr-Universität Bochum, Universitätsstr. 150, D-44780 Bochum

Electronic structure of transition metal oxides is often discussed in terms of ionic bonding in a rigid band model. In this approach the introduction of electrons by alkaliation leads to filling of metal 3d states. In most cases those two approximations are too simple, because of polar-covalent bonding, electron correlation, localization, polaron formation and structural influences, like Madelung-potentials, ligand-field effects and Jahn-Teller-distortion. Stoichiometric, polycrystalline LiCoO2 thin films in the high temperature modification have been prepared by RF magnetron sputtering. From XPS data it has been shown, that the Co-ions are in the formal 3+ low-spin oxidation state. The interpretation of the ResPES data is complicated, because of ligand-hole screening effects. At the Co3p-3d threshold an anti-resonance occurs, from that the O2p and Co3d PVBDOS have been derived, showing good agreement with DFT calculations. Via the preparation of an all solid state micro-battery a route to in-situ measurements of the electronic structure as a function of the lithium content in parallel to electrochemical measurements is presented. This work is funded by DFG (SFB595) and BMBF.

O 48.8 Di 17:30 TU EB107

Surface x-ray analysis of Co grown on NiO(100) — •Christian Tusche[1], Holger Meyerheim[1], Jürgen Kirschner[1], Ulrich Hillebrecht[2], and Carlos Quiros[3] — [1]Max-Planck-Institut für Mikrostrukturphysik, Weinberg 2, D-06120 Halle — [2]Institut für Festkörperforschung, Forschungszentrum Jülich, D-52425 Jülich — [3]ESRF, 6 rue Jules Horowitz, F-38043 Grenoble

Ultra-thin ferromagnetic films grown on antiferromagnetic oxides are of interest for fundamental studies of exchange biased systems. Still the role of the microscopic structure of the metal/oxide interface is subject to discussion. Of particular interest is the well known antiferromagnet NiO with thin overlayers of the ferromagnetic elements Fe, Co, Ni.

We have carried out a surface x-ray structure analysis of the Co/NiO(100) interface. About one monolayer of Co was deposited at room temperature on the nonpolar NiO(100) surface. The formation of two layer high CoO islands covering about 25% of the surface area is observed. The interfacial region consists of about one monolayer of a substoichiometric mixed oxide $[NiCo]O_x$ with $x \approx 0.5$. Comparing with bulk NiO the interlayer spacing is expanded by 9%.

The oxygen deficiency in the interface region gives strong evidence for the presence of metal-like Ni and Co in the interface. By formation of uncompensated interfacial spins, this is generally considered to play a major role in exchange bias effects.

O 48.9 Di 17:45 TU EB107

Field emission resonances investigated by scanning tunneling spectroscopy on Ag(001) surfaces and CoO islands on Ag(001) at low temperatures — •Stephan Grosser, Christian Hagendorf, and Wolf Widdra — Martin-Luther-Universität Halle-Wittenberg, FB Physik, Hoher Weg 8, D-06120 Halle(Saale)

Scanning tunneling microscopy (STM) and scanning tunneling spectroscopy (STS) have been applied to study the clean Ag(001) surface and CoO islands on Ag(001). CoO has been grown by reactive deposition of Co in an O_2 atmosphere. dI/dV and z(V) spectra in the range from 0 to 19 eV are used to investigate field emission resonances. In constant current mode the STS spectra on Ag(001) show up to 44 resonances.
The influence of the surface band structure, the tip radius and the tip structure on the field emission resonances have been examined. Qualitativ different spectra for the metallic Ag(001) surface and different structural phases of CoO islands have been obtained and will be discussed with respect to the different electronic band structures and work functions.

O 48.10 Di 18:00 TU EB107

A Tensor LEED Structure Determination of a CoO Ultrathin Film on Ag(100) — •Karl-Michael Schindler, Jian Wang, Wolf Widdra, and Henning Neddermeyer — Martin-Luther-Universität Halle-Wittenberg, FB Physik, D-06099 Halle, Germany

A four monolayer thick CoO film has successfully be grown in nearly layer by layer mode on a Ag(100) substrate by evaporating Co in 10^{-6} mbar oxygen with the substrate heated to 470 K. Previous LEED and STM investigations have shown that such films grow pseudomorphic i.e. the CoO accepts the lattice of the substrate, Furthermore, they exhibit maximal long range order and minimal variation in thickness. This makes them the most suitable systems for a structure determination by the analysis of LEED I(V) curves. The one of this study is based on the measurement of 5 inequivalent beams in the range from 30 to 400 eV, with a total energy range of 1025 eV. The calculation of the I(V) curves was performed using the Barbierie-van Hove Symmetrized Automated Tensor LEED(SATLEED) package. As an initial structure bulk values were assumed for the Ag substrate and the CoO film. Regarding the lattice relations at the interface, all three possibilities of high symmetry were tried as initial model structures. In addition films with a thickness of 2, 3, 4, and 5 layers were tried. In the optimization the z positions of the atoms in the two topmost layers, the distance between the CoO film and the Ag substrate, the inner potential and the Debey temperatures were optimized. The structural results of the best-fit model (r-factor: 0.20) will be discussed in comparison to related systems.

O 48.11 Di 18:15 TU EB107

Submonolayer growth of KCl on pristine and oxygen covered Cu(110) — •Michael Vogelgesang, Lars Diekhöner, Vitali Lucia, M. Alexander Schneider, and Klaus Kern — Max-Planck-Institut für Festkörperforschung, Heisenbergstraße 1, 70569 Stuttgart

By forming insulating ultrathin films on metal surfaces one can decrease the interaction of adsorbates with the metal electron system. In the monolayer regime these films are transparent enough to allow electron tunneling. As an example of such a system potassium chloride on Cu(110) has been investigated by low temperature scanning tunneling microscopy. For submonolayer growth at room temperature we find that KCl (100) forms large islands on Cu terraces and grows with its [010] direction along the $[2\bar{2}1]$ direction of the Cu(110) substrate. On a Cu(110) O(2x1) substrate the nucleation can be steered as KCl nucleates preferentially on the oxygen covered regions. First results of spectroscopic measurements will also be presented.

O 49 Epitaxie und Wachstum II

Zeit: Dienstag 15:45–18:30 Raum: TU EB407

O 49.1 Di 15:45 TU EB407

In-situ STM Measurements during MOVPE — •M. Breusing, B. Rähmer, M. Pristovsek, R. Kremzow, and W. Richter — TU-Berlin, Institut für Festkörperphysik, Hardenbergstr. 36, 10623 Berlin

Although numerous ex-situ and in-situ studies on nanostructures have been done the effects taking place on the surface during epitaxy are not completely understood. Most severe is the lack of in-situ tools for the Metal-Organic Vapour Phase Epitaxy (MOVPE) providing more information about the sample's topography then mean roughness.

Scanning Tunneling Microscopy (STM) is a technique which would directly give quantitative information about the topography and could work under a typical MOVPE reactor pressure of 100 mbar. However, an in-situ STM in a MOVPE growth environment has not been realized so far, because of many unsolved problems.

Indeed, the development of a STM for in-situ MOVPE measurements requires a completely new set-up. The limited space in the MOVPE reactor and the high temperatures during growth near the susceptor, caused by the thermal conductivity of the carrier gas, require a special design of the STM. On the other hand the influence of the STM on the growth (flow pattern in the reactor) must be minimized.

For these conditions we developed an in-situ STM which can resist sample-temperatures up to 550°C continuously. We were able to make the first STM measurements during InAs MOVPE growth on a GaAs stebpunching surface, showing resolution better than 4 nm vertically and 20 nm laterally.

O 49.2 Di 16:00 TU EB407

Modelling of ultrathin Si_xGe_{1-x} film growth on Si(111) by chemical vapour deposition — •Selvi Gopalakrishnan, H. Rauscher, and R.J. Behm — Abt. Oberflächenchemie und Katalyse, Universität Ulm, 89069

Experimental studies on step width, temperature and gas ratios established [1] that these properties are important factors for epitaxial growth by chemical vapour deposition (CVD). We investigated the effect of these factors on the sticking coefficients of the Si and Ge containing species and on the growth morphology of ultrathin Si_xGe_{1-x} films grown on the Si(111) substrate by CVD with Si_2H_6 and GeH_4 as precursor gases. The CVD films were grown from a 7:3 GeH_4:Si_2H_6 gas mixture at temperatures of 750K and 850K, a deposition pressure of 2.5 × 10^{-5} mbar and with wafers of differing terrace width of 1500A and 6000A, were investigated by STM and XPS. The data on the sticking coefficients of the Si and the Ge containing species and the total (STM) and the Ge (XPS) coverages were used to model the kinetics of the ultrathin Si_xGe_{1-x} film growth at low CVD deposition pressures. Ref:[1] H.Rauscher, J.Braun and R.J. Behm, Si_xGe_{1-x} ultrahigh-vacuum chemical vapour deposition on Si(111)-7×7 from GeH_4/Si_2H_6 mixtures. Appl. Phys. A. 76, 711-719(2003)

O 49.3 Di 16:15 TU EB407

Thin $CuInS_2$ films prepared by MOMBE: Interface and surface properties — •Carsten Lehmann[1], Christian Pettenkofer[1], and Wolfram Calvet[2] — [1]Hahn-Meitner-Institut, Glienicker Straße 100, 14109 Berlin — [2]SPECS GmbH, Voltastrasse 5, 13355 Berlin

$CuInS_2$ (CIS) films were prepared by MOMBE on Si (111) with TBDS as an organic sulfur source. Film properties were investigated in situ by LEED, XPS and UPS with respect to morphology, chemical composition and electronic structure. Film growth starts with a In-S bufferlayer on H-terminated Si(111) substrates. No carbon contaminations from the sulfur precursor are incorporated in the samples. Depending on the deposition conditions metallic In precipitations or Cu_2In phases were detected for the In rich film. A Cu_2S surface phase is found for Cu rich films. Cu to In rato and growth temperature were varied and optimised to obtain near stoichiometric CIS films. A bandalignment for the interface with respect to the bufferlayer and Si will be discussed.

O 49.4 Di 16:30 TU EB407

Facet and layer formation of II-VI semiconductors on GaSe van der Waals terminated Si(111) — •Bengt Jaeckel, Rainer Fritsche, Andreas Klein, and Wolfram Jaegermann — Darmstadt University of Technology, Surface Science Division, Department of Materials Science, Petersenstr. 23, 64287 Darmstadt

The growth of II-VI-semiconductors on GaSe terminated Si(111) is investigated with Scanning Tunneling Microscopy (STM) and Low Energy Electron Diffraction (LEED). CdS, CdSe, ZnS and ZnSe are evaporated from effusion cells filled with compound material. The growth temperature is varied from room temperature up to 300°C. Annealing steps are

also performed to investigate reorganization phenomena.
Nucleation occurs preferred at step-edges or defect sites. On the bare terraces nearly no nucleation takes place. For higher temperatures larger clusters are observed which are better orientated to the substrate. Annealing of films deposited at room temperature leads to a reorganization and to an increased crystallinity with orientation to the GaSe passivated Si(111)-substrate surface.
Interestingly, during the annealing procedures of high temperature films the surface morphology passes through highly facetted surfaces with different kinds of facet-planes. In the case of CdS a closed (111)-orientated film is formed at higher annealing temperatures (300°C) and is also well oriented towards the GaSe:Si(111)-substrate.

O 49.5 Di 16:45 TU EB407

Real-time study of orientational transitions during organic thin film growth — •Stefan Kowarik[1], Alexander Gerlach[1], Stefan Sellner[2], Frank Schreiber[1], Leide Cavalcanti[3], and Oleg Konovalov[3] — [1]Physical and Theoretical Chemistry, Oxford University, United Kingdom — [2]Max-Planck-Institut für Metallforschung, Stuttgart, Germany — [3]European Synchrotron Radiation Facility, Grenoble, France

We study thin films of the semiconductor diindenoperylene on silica during organic molecular beam deposition (OMBD) using synchrotron surface X-ray scattering. The molecular orientation within the thin film and the related anisotropy in electrical conductivity is of practical relevance for electronic devices. Further, the molecular tilt angle is an additional and qualitatively new degree of freedom in growth compared to inorganic / atomic systems. To understand and therefore control growth in OMBD important alterations from inorganic growth have to be included in established growth models. For example, molecular tilt may change scaling laws, which relate surface roughness to lateral and vertical (film thickness) length scales (1). We report on our in-situ and real-time experiment during OMBD growth. It provides evidence for changes of the out-of-plane and in-plane lattice parameters with time, and, importantly, with changes of the molecular tilt angle. We discuss our findings on the orientational transition, combining structural knowledge from the real time measurements with post-growth information on film roughness and morphology.

1. A. C. Dürr et al., Phys. Rev. Lett. 90 (2003) 016104

O 49.6 Di 17:00 TU EB407

Mechanisms of grain growth, coarsening and texture formation in Ag-films on an amorphous Substrate — •Celia Polop[1], Christian Rosiepen[1], Enrique Rodriguez-Cañas[2], and Thomas Michely[1] — [1]I.Physikalisches Institut RWTH-Aachen — [2]Instituto de Ciencia de Materiales de Madrid, CSIC, Spain

In order to study grain growth and texture evolution of a polycrystalline thin metal film, a well defined substrate was carefully constructed. The Si(001) 2x1 surface was prepared under UHV conditions and subsequently amorphised by a dose of 1,4*E15 ions/cm2 of 5 keV Ne+. Then Ag was deposited at 300K. The thin film morphological evolution was investigated for films up to 32nm thickness. Analysing the film with scanning tunneling microscopy (STM) an x-ray diffraction (XRD), three distinct stages of grain growth, grain coalescence and film formation are quantitatively characterized by roughness and length scale determination. Key elements of film evolution are also identified directly in the STM topographs.

O 49.7 Di 17:15 TU EB407

Fe on GaN: Growth investigations — •Ralph Meijers[1], Raffaella Calarco[1], Hans Lüth[1], Matthias Buchmeier[2], and Daniel Bürgler[2] — [1]Institute of Thin Films and Interfaces (ISG1) and CNI - Centre of Nanoelectronic Systems for Information Technology, Research Center Jülich, 52425 Jülich, Germany — [2]Institute of Solid State Research (IFF) and CNI - Center of Nanoelectronic Systems for Information Technology, Research Centre Jülich, 52425 Jülich, Germany

Spintronics is a rapidly evolving research field, which aims to combine ferromagnets with semiconductors to develop devices with new functionality. One of the main goals is achieving an efficient spin-polarized carrier injection into semiconductors at room temperature. One method is to inject carriers from ferromagnetic metals into a semiconductor. The Fe/GaN hybrid system is an interesting layer system, since recent theoretical calculations predict a large spin lifetime in pure GaN. However the lattice mismatch between Fe and GaN is large. The crystalline quality of the heterostructure and the nature of the metal/semiconductor interface are very important.

The epitaxial relation of Fe to GaN was investigated using LEED and XRD together with simulations. The α-Fe(110) plane was found to be parallel to the GaN(0001) plane and formation of three equivalent domains, rotated 120^0 against each other, was observed. Using AFM and STM, the surface morphology was investigated and flat domains with sizes up to 500nm were found. SQUID measurements showed ferromagnetic behavior and good homogeneity of the magnetic properties was concluded from ferromagnetic resonance data.

O 49.8 Di 17:30 TU EB407

Growth of NiO on Ag(100) Studied by In-Situ X-Ray Scattering — •E. Schierle, E. Weschke, A. Gottberg, and S.R. Krishnakumar — Institut für Experimentalphysik, Freie Universität Berlin, Arnimallee 14, D-14195 Berlin, Germany

The growth of NiO on Ag was studied by specular x-ray diffraction *in situ* at ID 10 A of the European Synchrotron Radiation Facility, using a small UHV chamber mounted on the diffractometer. Films where prepared by Ni evaporation in oxygen atmosphere, with the substrate held at 500 K. In agreement with earlier results, we find that on Ag(111), layer-by-layer growth occurs only up to ≈ 6 monolayers, while extended growth is observed for Ag(100). On this surface, films were grown with thicknesses of up to 180 monolayers. Pronounced Laue oscillations of the (100) Bragg peak and rocking widths from 0.6 to 1.2 degrees indicate good crystalline quality of the films, particularly at film thicknesses below ≈ 30 monolayers. We observe a gradual change of the lattice parameter from a strained value to the bulk value of NiO.

This work was supported by DFG, Sfb 290 (TPA06).

O 49.9 Di 17:45 TU EB407

Growth and atomic structure of NiO and MnO films on Pt(111): In-situ STM experiments at elevated temperatures — •Christian Hagendorf, Henning Neddermeyer, and Wolf Widdra — Martin-Luther-Universität Halle-Wittenberg, FB Physik, Hoher Weg 8, D-06120 Halle (Saale)

Growth, atomic structure and phase transitions of NiO and MnO thin films on Pt(111) have been studied using scanning tunneling microscopy and spectroscopy (STM/STS), low-energy electron diffraction (LEED), and Auger electron spectroscopy (AES). Mn and Ni have been deposited in an O_2 atmosphere ($10^{-8} - 10^{-6}$ mbar) at substrate temperatures between $300 - 600$ K. In-situ STM experiments were performed at elevated temperatures during film growth.

Depending on the substrate temperature, one-dimensional network-like Ni/O adsorbate structures or islands with (7x1) and (4x2) reconstruction are formed during the initial stages of growth. These structures transform *reversibly* to a (2x2) reconstruction by varying the O_2 pressure between $1.5 - 2 * 10^{-6}$ mbar which has been followed by in-situ STM. After further reduction of the O_2 pressure to $< 10^{-10}$ mbar metallic Ni islands are obtained. At higher coverages (111) oriented NiO islands are stabilized in a 3-dimensional growth mode.

MnO grows on Pt(111) at 450 K in a layer-by-layer mode. Characteristic reconstructions are observed at different coverages which are stable after deposition. Structural changes can be induced by annealing to 600 K. The results will be compared to previous investigations of NiO and MnO on Ag(001).

O 49.10 Di 18:00 TU EB407

Bestimmung des Koinzidenzgitters eines Aluminiumoxidfilms auf Ni_3Al(111) — •Stefan Degen, Aleksander Krupski, Marko Kralj, Andreas Langner, Conrad Becker, Moritz Sokolowski und Klaus Wandelt — Institut für Physikalische und Theoretische Chemie, Wegelerstr. 12, 53115 Bonn

Ein bei einer Temperatur von 1000 K in einer Sauerstoffatmosphäre auf einer Ni_3Al(111)-Oberfläche gewachsener doppellagiger Aluminiumoxidfilm [1] wurde mittels hochaufgelöster Elektronenbeugung (SPA-LEED) und Tieftemperaturrastertunnelmikroskopie (LT-STM) untersucht. Mit beiden Methoden findet man Überstrukturen mit Gitterkonstanten von 2,40 (Netzwerkstruktur) bzw. 4,16 nm (Punktstruktur). Die Punktstruktur ist eine $(\sqrt{3} \times \sqrt{3})R30^0$-Überstruktur der Netzwerkstruktur. Das gemessene Beugungsbild kann unter Berücksichtigung des Substrats und der gefundenen Einheitszellen der Oxidüberstrukturen sehr gut simuliert werden. Die Punktstruktur erweist sich als kommensurabel zum Substrat und die Überstrukturmatrix wurde bestimmt. Durch Variation der Tunnelparameter ist es möglich, mit dem Rastertunnelmikroskop sowohl durch den Film hindurch das Substrat mit atomarer Auflösung sowie an der gleichen Stelle die Oxidüberstrukturen aufzulösen. Aufgrund der hohen Driftstabilität des LT-STM (0,24 nm/Stunde) konnte so die laterale Position der Überstruktur relativ zum Substrat eindeutig bestimmt werden. Die bereits durch SPA-LEED bestimmten Überstrukturrelationen wurden bestätigt.

[1] A. Rosenhahn et al., J. Vac. Sci. Technol. A 18 (2000) 1923

O 49.11 Di 18:15 TU EB407

Formation, propagation and stability of stacking fault defects in Iridium thin films — •Sebastian Bleikamp[1], Celia Polop[1], Arne Thoma[1], Gerhard Pirug[2], and Thomas Michely[1] — [1]I. Physikalisches Institut, RWTH Aachen, 52056 Aachen — [2]Institut für Oberflächen und Grenzflächen, Forschungszentrum Jülich, 52425 Jülich

During homoepitaxial growth stacking fault islands are readily found on Ir(111). Upon coalescence defect structures are formed, which induce stacking fault propagation in subsequent layers.

To follow the fate of the twinned domains, a low energy electron diffraction (LEED) method is applied, which decomposes LEED I/V spectra into linear combinations of the non-equivalent first order diffraction peaks of the clean surface. The method was successfully calibrated versus STM measurements.

At 350K a film thickness of 50 monolayers is sufficient to create a nearly random mixture of twinned and untwinnned crystallites. Such films possess an impressive stability against thermal healing. Only at temperatures above 0.5 of the melting temperature, the fraction of twin crystallites gradually decreases. The stability of the faulted domains is discussed in relation to the structure of the twin boundaries formed.

O 50 Postdeadline-Session

Zeit: Dienstag 20:00–21:00 Raum: TU A151

O 50.1 Di 20:00 TU A151

New twists of a never-ending story: Water on Ru(001) — •Dietrich Menzel[1], Nadir Faradzhev[2], Krassimir L. Kostov[1], Peter Feulner[1], and Theorore E. Madey[2] — [1]Physik E20, TU München, Germany — [2]Physics Dept, Rutgers Univ., Piscataway, NJ, USA

Conflicting reports and views exist on the stability of molecular layers of H_2O and D_2O on Ru(001), a model system. The original bilayer model of Madey et al. is not compatible with the LEED geometry; Feibelman concluded from DFT calculations that partial dissociation has to occur for wetting. Further calculations and experiments agreed in some aspects but not in others. Two very recent PRLs (93,196101/2) drew opposite conclusions from nominally identical techniques. We therefore conducted carefully controlled experiments with TPD and XPS in two laboratories, comparing the situation before and after defined irradiation with slow electrons and photons. We find wetting molecular layers on the clean surface for both H_2O and D_2O. D_2O is thermally stable to desorption; H_2O partially dissociates thermally to variable extent, but also re-associates upon desorption. Thus the free energies of the various layers are very close and separated by low, mass-dependent barriers. Both layers are extremely sensitive to electron irradiation; even energies of a few eV are effective. This and the influence of small amounts of impurities explain the conflicting experimental results.

O 50.2 Di 20:15 TU A151

New magnetism of Fe, Co and Ni monolayers grown with oxygen surfactant — •H. Wende, C. Sorg, N. Ponpandian, A. Scherz, R. Nünthel, and K. Baberschke — Institut für Experimentalphysik, Freie Universität Berlin, Arnimallee 14, D-14195 Berlin-Dahlem, Germany

Surfactant assisted growth of nanoscale structures on surfaces is a well established technique. Moreover, it is known that for a few atomic layers of Fe, Co, and Ni ultrathin films the magnetic properties are highly sensitive to minimal structural changes: If the nearest neighbor distance varies by 0.03-0.05 Å only, the magnetic anisotropy energy may change by $10^2 - 10^3$. So the question arises: Can the growth of the 3d ferromagnets on metallic substrates be improved using oxygen as a surfactant or will an antiferromagnetic metal oxide be formed? The answer is threefold: i) We could indeed show by MEED and XAS that the growth is improved up to >20 ML and that finally the O atoms "float"on top of the ferromagnetic film (see recent perspectives in Surface Science [1] and references therein). ii) Recent measurements demonstrate that the magnetic anisotropy energy is significantly enhanced using this surfactant. Theory reveals that this is mainly due to the decrease in the magnitude of the surface anisotropy. iii) Preliminary experiments of last month at the new BESSY undulator beamline show that the chemisorbed oxygen atoms on the surface of the ferromagnetic film carry an induced magnetic moment. Supported by BMBF (05 KS4 KEB 5) and DFG (Sfb290).

[1] M. Farle, Surf. Sci. Perspectives *in press* (http://dx.doi.org/10.1016/j.susc.2004.10.055)

O 50.3 Di 20:30 TU A151

Switching between one and two dimensions: conductivity of Pb–induced chain structures on Si(557) — •C. Tegenkamp, Z. Kallassy, L.H. Gúnter, V. Zielasek, and H. Pfnär — Institut für Festkörperphysik, Abteilung Oberflächen, Appelstr. 2, 30167 Hannover, Germany

The conductivity of epitaxially grown Pb–structures on Si(557) has been measured using a modified 4-point van der Pauw method. For this sytsem different characteristic transport mechanisms have been found: For coverages above the percolation limit(0.6ML) up to 3ML the electronic transport in the annealed Pb–films is activated. Furthermore, the uniaxial symmetry of the Si(557) surface is reflected directly in a higher conductance in the parallel direction compared to the direction perpendicular to the steps. For coverages higher than 3ML a metallic behavior is found for both directions, i.e. the conductance decreases with increasing temperature.

In contrast, already one ML, but annealed to 640K, leads to the formation of atomic wires, as seen by STM, with an extremely high and quasi one–dimensional surface state conductance along the wire direction. At a critical temperature of $T_c = 78K$, the system switches from a low to a high conductance anisotropy, with a metal–insulator transition in the direction perpendicular to the chain structure, while in the direction along the chains conductance with a (1/T + const.) temperature dependence was found.

STM has shown further, that the 1D/2D transition is associated with an order–disorder phase transition of a 10- fold superperiodicity along the Pb chains as revealed by mesurements done at 40K and 100K, respectively.

O 50.4 Di 20:45 TU A151

Generation and Detection of Coherent Surface Currents — •J. Güdde, M. Rohleder, and U. Höfer — Fachbereich Physik und Zentrum für Materialwissenschaften, Philipps-Universität, D-35032 Marburg

We demonstrate the generation and detection of lateral electron currents at a metal surface with a contact-free experimental setup. The currents are induced by two phase-locked ultrashort laser pulses with frequencies ω and 2ω that generate a population of excited states states which is asymmetric with respect to the direction $+k_\parallel$ and $-k_\parallel$. The relative phase between the two excitation pulses controls the direction of the coherent dc current. The current is detected by time-delayed probe-pulses in terms of an anisotropy of the angle-resolved photoemission yield. This procedure allows to investigate electron transport at surfaces with extremely high sensitivity and gives direct access to the relevant carrier scattering processes. In a first experiment we have excited electrons into the image-potential states of Cu(100) that move with parallel velocities of ~ 1 Å/fs and carry a current of up to 10^7 A/cm^2.

O 51 Hauptvortrag Kampen

Zeit: Mittwoch 09:45–10:30 Raum: TU EB301

Hauptvortrag

O 51.1 Mi 09:45 TU EB301

Electronic structure of organic interfaces — •Thorsten Ulrich Kampen — Fritz-Haber-Institut der Max-Planck-Gesellschaft, Faradayweg 4-6, D-14195 Berlin, Germany

The energy level alignment at organic interfaces determines the efficiency of charge injection into organic films. Quite often the vacuum level alignment rule has been used to determine the energy level alignment at organic interfaces. Here, barrier heights can simply be calculated using the ionisation potentials or electron affinities of semiconductors materials and work functions of metals. For organic interfaces a conclusion has been reached that in general the vacuum levels do not align. This difference in vacuum levels is attributed to interface dipoles. Another important issue is the occurrence of a band-bending like electrostatic energy shift in organic layers, which has been observed in many metal/organic systems. In most cases this shift is confined to a regime of only a few nanometers, which cannot be accounted for using the conventional band bending theory of inorganic semiconductors. Shifts occurring in such small thickness ranges can be due to a change in the intermolecular interaction, namely, due to a change in the molecular orientation as a function of the film thickness. At intimate, abrupt, and defect free interfaces of organic semiconductors which show a band like dispersion in the highest occupied energy levels interface induced gap states govern the energy level alignment.

O 52 Elektronische Struktur IV

Zeit: Mittwoch 10:45–13:00 Raum: TU EB301

O 52.1 Mi 10:45 TU EB301

A photoelectron spectro-microscopy investigation of singleMoS$_2$ nanotubes — •A. Gloskovskii[1], M. Chincetti[1], S. A. Nepijko[1], G. Schönhense[1], H. A. Therese[2], G. H. Fecher[2], H. C. Kandpal[2], C. Felser[2], W. Tremel[2], and M. Klimiankou[3] — [1]Institut für Physik, Johannes Gutenberg -Universität, 55099 Mainz — [2]Institut für Anorganische und Analytische Chemie,Johannes Gutenberg - Universität, 55099 Mainz — [3]Institut für Materialforschung I, Forschungszentrum Karlsruhe GmbH, 76021 Karlsruhe

Nanostructured MoS$_2$ was prepared by thermal decomposition of $(NH_4)_2Mo_3S_{13}$ x H$_2$O in sealed tubes and nanotubes of MoS$_2$ were prepared by coating technique using SiO$_2$ rods as template. The samples were characterized by XRD, HRTEM, EELS, and XANES techniques. The electronic structure of MoS$_2$ was investigated by means of two photon photoemission spectroscopy (2-PPE) performed with a time-of-flight photoemission electron microscope (TOF-PEEM). The spatially resolved 2-PPE spectra show distinguished features arising in emission from the nanotubes. These features are explained by emission from the valence band via resonant excitation of an intermediate state in the conduction band. The size of the gap in semiconducting nanotubes will be discussed on hand of the 2-PPE spectra in comparison to electronic structure calculations. The electronic structure was calculated self-consistently by means of LMTO and FLAPW techniques. Comparing experimental and theoretical findings, we conclude that full potential methods are necessary to calculate electronic properties in particular for sulfide and oxide based nanotubes. (Funded by DFG in SFB 625 TP9.)

O 52.2 Mi 11:00 TU EB301

Quasi-one-dimensional surface states on Pt(110) — •Mariana Minca, Enrico Dona, Zhenrong Zhang, Alexander Menzel, and Erminald Bertel — Phys. Chemie, Univ. Innsbruck, A-6020 Innsbruck

Experimental investigation of the electron correlation responsible for the rich and technologically highly interesting phase diagram [1] of low-dimensional or even quasi-one-dimensional (Q1D) materials is difficult on account of the complex structure, surface reconstructions, and sensitivity to radiation damage of most model systems. Here we show that the clean missing-row reconstructed (1x2) Pt(110) surface can be used as a Q1D model system. The electron dispersion as measured by ARUPS at different photon energies reveals a Tamm-type Q1D surface resonance [2], which is derived from the very high bulk-DOS between the L and W point in the volume band structure [3]. Upon increasing the temperature, the corresponding quasiparticle peak at the Fermi Energy decays rapidly, as is seen in other weakly coupled Q1D systems. We discuss the unusual temperature dependence in terms of a coherent-incoherent transition.

Support by the Austrian Science Fund (FWF) is gratefully acknowledged.

[1] M. Imada, A. Fujimori, and Y. Tokura, Rev. Mod. Phys. **70**, 1039 (1998).

[2] S.D. Kevan (Ed.), *Angle-Resolved Photoemission* (Elsevier, Amsterdam 1992), p.99

[3] O.K. Andersen, Phys. Rev. B **2**, 883 (1970).

O 52.3 Mi 11:15 TU EB301

Fermi contours of a quasi-periodic 1-D film structure — •P. Moras[1], L. Ferrari[1], S. Gardonio[1], C. Carbone[1], J. Fuji[2], W. Theis[3], and K. Horn[4] — [1]Istituto di Struttura della Materia, Consiglio Nazionale delle Ricerche, Trieste, Italy — [2]Laboratorio TASC, I.N.F.M, Trieste, Italy — [3]Freie Universitaet, Berlin, Germany — [4]Fritz-Haber-Institut, MPG, Berlin, Germany

Ag(111) films grown on GaAs(110) present in high-resolution STM images a quasi-periodic distribution of stripes running along the GaAs[1-10]-direction with two characteristic separations of 17 Å and 12 Å. The resulting one-dimensional superstructure can be described by a golden-mean Fibonacci sequence with a coherence length of about 125 Å. Angle-resolved photoemission has been used to examine the spectral functions of the sp-derived Ag electronic states as a function of the photoelectron momentum. While the dispersion of the Ag sp-quantum well states along the stripe direction is close to a free-electron-like parabola, it displays flatter bands and a complex branching structure perpendicularly to them. A close correspondence is found between the incommensurate wave vectors derived from the LEED pattern and those characterizing the Fermi contours of the Ag films in the two-dimensional reciprocal space.

O 52.4 Mi 11:30 TU EB301

Electron dynamics in vacancy islands — •J. Kröger[1], H. Jensen[1], R. Berndt[1], and S. Crampin[2] — [1]Institut für Experimentelle und Angewandte Physik, Universität Kiel, D-24098 Kiel, Germany — [2]Department of Physics, University of Bath, Bath BA2 7AY, United Kingdom

The dynamics of Ag(111) surface state electrons confined to nanoscale hexagonal and triangular vacancy islands are investigated using scanning tunneling spectroscopy. The lifetimes of quantised states with significant amplitude near the centers of the vacancies are weakly affected by the geometry of the confining cavity. A model that includes the dependence of the lifetime on electron energy, vacancy size, step reflectivity and the phase coherence length describes the results well. For vacancy islands with areas in the range ≈ 40–$220\,\mathrm{nm}^2$ lossy scattering is the dominant lifetime-limiting process. This result and a corrected analysis of published experimental data improve the consistency of experimental and calculated surface state lifetimes.

O 52.5 Mi 11:45 TU EB301

Disorder induced local density of states oscillations on narrow Ag(111) terraces — •Karina Morgenstern[1], Karl-Heinz Rieder[1], and Gregory A. Fiete[2] — [1]Institut fuer Experimentalphysik, FB Physik, Freie Universitaet Berlin, Arnimallee 14, D-14195 Berlin, Germany — [2]Kavli Institute for Theoretical Physics and Department of Physics, University of California, Santa Barbara,CA 93106, USA

The local density of states of Ag(111) has been probed on disordered terraces of varying width by dI/dV-mapping with a scanning tunneling microscope at low temperatures. Shifts of the bottom of the surface state band edge lead to varying differential conductance for terraces of different widths. In contrast to perfect terraces, standing wave patterns are observed parallel to the step edges, i.e. in the non-confined direction. Scattering calculations for disordered terraces reproduce these spatial oscillations and all the qualitative features of the standing wave patterns and, thus, reveal the underlying reason for these obwervations.

O 52.6 Mi 12:00 TU EB301

Electrons in the competing potentials of a Moiré-type — •Christian R. Ast[1], Daniela Pacilé[1], Marco Papagno[1], Gero Wittich[2], Klaus Kern[1,2], and Marco Grioni[1] — [1]Ecole Polytechnique Fédérale de Lausanne, Lausanne — [2]Max-Planck-Institut für Festkörperforschung, Stuttgart, Germany

The effects of weak changes in the periodic potential on the electronic structure can be nicely studied in overlayer structures showing a Moiré-type superlattice. Angular resolved photoemission spectroscopy is used to study the valence bands of Pb on Ag(111), which produces a hexagonal Moiré superlattice at monolayer coverage having a lattice constant incommensurate with the surface. The measured electronic structure of the Pb monolayer is hardly influenced by the substrate due to the mismatch in lattice constants. However, within the monolayer the electrons feel the presence of two competing periodicities: The hexagonal primitive cell in the plane of the monolayer as well as the characteristic modulation of the Moiré structure normal to the monolayer plane with a much larger unit cell. A scenario will be proposed in which the superimposed modulation is not strong enough to change the Brillouin zone but does influence the overlap of orbitals normal to the monolayer plane.

O 52.7 Mi 12:15 TU EB301

Quantum Well States in thin films of In on Si(100) — •Jan Hugo Dil, Jeong-Won Kim, Thorsten Ulrich Kampen, and Karsten Horn — Fritz-Haber-Institut der Max-Planck-Gesellschaft, Abteilung Molekülphysik, Faradayweg 4-6, 14195 Berlin

Experiments with ultrathin metal layers on metal or semiconductor substrates have recently resulted in a wide variety of discoveries; anomalous behaviour of the hall effect, self organisation into magic or preferred layers, and strong electron correlation effects are just a few of them. Moreover the quantum well states (QWS) formed in these structures allow for detailed studies of electron-phonon coupling. Here, we present a study of atomically flat layers of indium grown on a Si(100) substrate. QWS are readily observed for a wide range of coverages. These can be discriminated into QWS lying above and below a bandgap. This bandgap corresponds to the one observed in the valenceband of bulk indium. In the direction parallel to the interface the QWS show a free electron like behaviour as expected from DFT calculations. In the energy region where the QWS cross the Fermi energy with free electron like behaviour electron-phonon coupling may be observed.

O 52.8 Mi 12:30 TU EB301

Characterization of nearly free electron bands in thin Al-Mg alloy films on Si(111) — •Massimo Tallarida[1], Lucia Aballe[2], Ashwani Kumar[1], Sudipto Roy Barman[3], and Karsten Horn[1] — [1]Fritz-Haber-Institut der MPG, Berlin — [2]ELETTRA SpA, Trieste, Italy — [3]UGC-DAE Consortium, Indore, Indien

Thin films of Al-Mg alloys have been grown on Si(111) by MBE over a wide range of compositions, and were characterized by angle-resolved photoemission. For Al-rich alloys, electron confinement leads to the occurrence of quantum well states, and a surface state similar to that in the Al/Si(111) film is found. For Mg-rich compositions, only a broad surface state is observed. The occurrence of quantum well states and the surface state, and their binding energy dependence on alloy composition is explained in terms of the virtual crystal approximation, with an average electron density in the alloy system. The dispersion of the quantum well states in a direction parallel to the film shows a nearly free electron behaviour similar to that found in Al/Si(111). The variation of electron density in these alloy films open the way for a study of more complex metallic systems, e.g. an investigation of the influence of electron density of the electromagnetic response.

O 52.9 Mi 12:45 TU EB301

Molecular orbital shift of PTCDA on Au(111) and Au(788) — •Henning Jensen[1], Jörg Kröger[1], Riccardo Rurali[2], Nicolás Lorente[2], and Richard Berndt[1] — [1]Institut für Experimentelle und Angewandte Physik, Christian-Albrechts-Universität Kiel, D-24098 Kiel, Germany — [2]Laboratoire Collisions - Agrégats - Réactivité, Université de Toulouse, F-31062 Toulouse, France

Scanning tunnelling microscopy of 3,4,9,10-perylenetetracarboxylic-dianhydride adsorbed on Au(111) and Au(788) reveals two coexisting superstructures with different coordination numbers. Using single-molecule tunnelling spectroscopy we find that the energy of the second-to-lowest unoccupied molecular orbital varies significantly with coordination geometry. Theoretical modelling attributes this variation to a dipole moment induced by deformation of the molecular plane.

O 53 Organische Dünnschichten V

Zeit: Mittwoch 10:45–13:00 Raum: TU EB420

O 53.1 Mi 10:45 TU EB420

Dynamics of colloidal thin films at the nanometer scale using surface XPCS — •Simone Streit[1], Henning Sternemann[1], Virginie Chamard[2], Michael Sprung[1], Christian Gutt[1], Anders Madsen[3], and Metin Tolan[1] — [1]Exp. Physik I, Universität Dortmund, 44221 Dortmund — [2]LTPCM, St Martin d'Hères, France — [3]ESRF, Grenoble, France

The surface dynamics at the nanometer scale of thin polymer films decorated with gold clusters was investigated using x-ray photon correlation spectroscopy (XPCS) in grazing incidence geometry. The scattering signal from polystyrene films (80-100 nm thick) with different molecular weights (34.4 and 220 kg/mol) and rather large nominal gold thicknesses (1-2 nm) was measured by a CCD as a function of time for temperatures in the range of 290 to 450 K. Capillary waves motion at the polymer surface as well as surface diffusion of the nanoparticles have already been observed for length scales of about 10 nm, leading to viscosity values much higher than the ones already known for the bulk. In this experiment we confirmed the large surface viscosity and investigated the q-parallel dependence of the relaxation time for different temperatures. q-parallel values from 0.1 to 1 nm^{-1} were measured simultaneously, thus leading to the direct observation of surface dynamics on nanometer length scales.

O 53.2 Mi 11:00 TU EB420

PE and NEXAFS study of self-assembled bacterial surface-layer proteins — •Denis Vyalikh[1], Alexander Kirchner[2], Steffen Danzenbächer[1], Michael Mertig[2], Wolfgang Pompe[2], Yuriy Dedkov[1], and Serguei Molodtsov[1] — [1]Inst. f. Festkörperphysik, TU Dresden — [2]Inst. f. Werkstoffwissenschaft, TU Dresden

Electronic structure of regular bacterial cell wall proteins (S layer) of *Bacillus sphaericus* was studied by photoemission (PE) and near-edge x-ray absorption fine structure (NEXAFS) spectroscopies [1]. Both the occupied and unoccupied valence electronic states were characterized and found to represent a series of PE and NEXAFS peaks, respectively, related to the molecular orbitals of individual amino acids. It was shown that the NEXAFS data could be interpreted applying a phenomenological "building block"model, whereas understanding of the valence-band PE structures can be achieved on the basis of electronic density-of-states calculations performed for rather small proteins. It was found that the π clouds of aromatic rings contribute both to the lowest unoccupied and the highest occupied molecular orbitals (LUMO and HOMO). The studied S layer reveals semiconductor-like behavior with a gap value of ~ 3 eV. The Fermi level is pinned close to the bottom of the LUMO.

We expect that the position of the Fermi level can be shifted across the gap by insertion of dopants into the pores in the S layers. First experiments on intercalation of alkali and transition metals into S layer are under way in our cooperation. The obtained results will be reported.

[1] D.V. Vyalikh *et al.*, Phys. Rev. Lett. (2004) in print

O 53.3 Mi 11:15 TU EB420

Radiotracer diffusion measurements of noble metal atoms in semiconducting crystalline organic films — •Michael Scharnberg[1], Jörn Kanzow[1], Klaus Rätzke[1], Stefan Meyer[2], Jens Pflaum[2], Rainer Adelung[1], and Franz Faupel[1] — [1]Lehrstuhl für Materialverbunde, CAU Kiel, Kaiserstr. 2, D-24143 Kiel — [2]3. Physikalisches Institut, Universität Stuttgart, Paffenwaldring 57, D-70569 Stuttgart

The application of organic field effect transistors (OFETs) for large scale low-cost electronic devices has lead to intense research. Diindenoperylene (DIP) thin films on SiO2 are a prominent system due to their high structural out-of-plane order. Preparation of top contacts might cause diffusion of metal atoms (typically Au or Ag) deep into the organic film changing the injection properties at the interface, which are of great importance for the device performance. Only by understanding the diffusion behaviour of metal in the organic layer, formation of well defined interfaces and control of their properties will become possible. Therefore, diffusion profiles for Ag [1] and Au diffusion in DIP films with different crystalline properties, e.g., Rocking widths, were obtained using a radiotracer technique. The results indicate similarities in the diffusion behaviour of noble metals in polymers and organic crystalline films. They will be discussed with respect to the crystalline structure of the DIP films.

[1] M. Scharnberg et al, APL 2004, in press

O 53.4 Mi 11:30 TU EB420

Crystal Face Resolved Oxidation of Pentacene with Ozone — •S. Rentenberger[1], H. Weiss[2], A. Vollmer[3], J. Niemax[4], J. Pflaum[4], I. Salzmann[5], J. P. Rabe[5], and N. Koch[5] — [1]TU-Graz, Institut f. Festkörperphysik, A-8010 Graz, Austria — [2]Universität Magdeburg, Lehrstuhl f. Physikalische Chemie, D-39106 Magdeburg — [3]BESSY GmbH., D-12489 Berlin — [4]Universität Stuttgart, 3. Physikalisches Institut, D-70550 Stuttgart — [5]Humboldt-Universität zu Berlin, Institut f. Physik, D-12489 Berlin

While the oxidation of pentacene by molecular oxygen proceeds very slowly, ozone (produced by illumination with ultraviolet light) leads to a rapid oxidation of this prototypical conjugated organic molecule, successfully used in flexible thin film transistors. We have studied the ozone-induced oxidation kinetics of pentacene thin films by infrared absorption spectroscopy in transmittance and reflection, and the accompanied evolution of the film morphology by atomic force microscopy. In order to selectively probe individual pentacene crystal faces, thin films were grown on silicon oxide [exposing the (ab) plane] and on highly oriented pyrolytic graphite [exposing the (bc) plane]. We find in both cases substantial loss of pentacene mass-thickness, indicating that ozone produces highly volatile reaction products, however, on a faster time scale for films grown on graphite.

O 53.5 Mi 11:45 TU EB420

A new approach to the determination of the transport gap in organic semiconductors using a combination of IPES and UPS — •Stefan Krause, Benedetta Casu, and Eberhard Umbach — Experimentelle Physik II, Universität Würzburg, Am Hubland, 97074 Würzburg

Organic semiconductors are in general believed to be strongly correlated systems. The value for the transport gap is somewhere between the measured value of optical absorption and the one, which one gets from the energetic distance of the HOMO in UPS and the LUMO in IPES. If one uses the peak positions of the HOMO and LUMO the gap is about 1 eV larger than the one of optical absorption. This is then explained with the strong correlation and polarization [1].

We compared the measurements of organic semiconductors with those of inorganic to find a hint on which side of these two boundaries one has to search. Surprisingly the data for the inorganic semiconductors showed the same trend and the UPS-IPES gap was much larger than the optical gap. This can no longer be explained with correlation because these materials are solids with strong covalent bonds and small (Mott-Wannier-) exciton binding energies. However, the distance of the peak onsets perfectly fits the optical data.

[1] E.V. Tsiper et al. Chem. Phys. Lett. 360 (2002), 47-52

O 53.6 Mi 12:00 TU EB420

The self-assembly of alkyl-trichlorosilanes on model surfaces of biphenylthiols — •Svetlana Stoycheva[1], Jörg Fick[1], Steffen Franzka[2], Nils Hartmann[2], Alexander Kornviakov[3], Avi Ulman[3], Michael Himmelhaus*[1], and Michael Grunze[1] — [1]Angewandte Physikalische Chemie, Universität Heidelberg — [2]Institut für Physikalische und Theoretische Chemie, Universität Essen — [3]Dept. of Chemical Engineering, Polytechnic University, Brooklyn, New York

Despite of its technological relevance, the self-assembly of monolayers of alkyl-trichlorosilanes onto oxidized metal or semiconductor surfaces is still not fully understood. Phenomena, such as island formation and polymerization, hamper the formation of densely packed and well-oriented self- assembled monolayers (SAM) in many cases. In particular, it has been found that the amount of surface-adsorbed water plays a crucial role for the process of film formation. In our study we have used rigid 4-mercaptobiphenyls (MBP) to prepare stable, molecularly engineered SAM surfaces, and used them as substrates for the study of the assembly mechanism of alkyltrichlorosilanes. SAM of 4-Methyl-4'-MBP, 4-Hydroxy-4'-MBP and MBP (as a reference system) as well as the bilayer assemblies were characterized by contact angle measurements, spectral ellipsometry, infrared reflection absorption spectroscopy, X-ray photoelectron spectroscopy, sum frequency generation, and atomic force microscopy. In combination with a frequency analysis based on ab initio calculations, insight into the structure of the MBP as well as a detailed picture of the film formation of the silane overlayer could be achieved.

O 53.7 Mi 12:15 TU EB420

Functionalized para-phenylene nanofibers — •Frank Balzer[1], Katharina Al-Shamery[2], Arne Luetzen[2], Manuela Schiek[2], Ralf Frese[3], and Horst-Günter Rubahn[3] — [1]Humboldt-Universität zu Berlin, Institut für Physik / ASP — [2]University of Oldenburg, Institute of Pure and Applied Chemistry, Oldenburg — [3]SDU Odense, Fysisk Institut, Denmark

Growth of mutually aligned, several tens to hundreds of μm long organic nanofibers from functionalized molecules has been demonstrated for the first time. The fibers from 4,4'''-Dimethoxy-1,1':4',1'':4'',1'''-quaterphenyl (MOP4) are grown on mica by vacuum sublimation and they resemble more the well organized growth of long para-hexaphenyl (p-6P) nanofibers as compared to the rather unorganized growth of short para-quaterphenyl (p-4P) aggregates. Atomic force microscopy reveals typical heights of the MOP4 nanofibers of a few ten nanometers and typical widths of a few hundred nanometers. The MOP4 fibers show intense, polarized blue light emission with well resolved higher order vibronic peaks and a morphology that is slightly different from that of p-6P nanofibers.

O 53.8 Mi 12:30 TU EB420

Electron-vibron coupling in the NEXAFS spectra of naphthalene in the condensed and gas phase — •Dominique Hübner[1], F. Holch[1], A. Schöll[1], R. Fink[2], K.C. Prince[3], S. Stranges[4], and E. Umbach[1] — [1]Univ. Würzburg, Exp. Phys. II — [2]Univ. Erlangen, Phys. Chem. II — [3]Sincrotrone Trieste — [4]CNR-Istituto di Metodologie Inorganiche e dei Plasmi

High-resolution NEXAFS spectroscopy is ideally suited to investigate the electronic structure of large organic molecules in both, the condensed and the gas phase. In ideal cases one observes distinct fine structures which are attributed to the coupling of electronic transitions to vibronic excitations [1]. We present NEXAFS data on naphthalene and deuterated naphthalene both in the gas and condensed phase. In order to identify vibronic modes, especially the C-H modes, in the electronic transitions deuterated naphthalene has been utitlized. In contrast to previous studies [1], a manifold of vibronic states efficiently couple to the core excitation which makes the analysis difficult.Comparison with benzene data sufficiently explain most of the structures. The differences between gas and condensed phase spectra are explained by Van-der-Waals like bonding in the condensed phase. The project is financed by BMBF (contracts 05 KS1 WWA5 and 05 KS4 WWC/2).

[1] A. Schöll et al. PRL 93, 146406 (2004)

O 53.9 Mi 12:45 TU EB420

Interaction of Self-Assembled Monolayers of Oligo(ethylene glycol)-Terminated Alkanethiols with Water studied by Vibrational Sum Frequency Generation (VSFG) — •Jörg Fick[1], Rongyao Wang[2], Sascha Herrwerth[1], Wolfgang Eck[3], Michael Himmelhaus*[1] und Michael Grunze[1,3] — [1]Angewandte Physikalische Chemie, Universität Heidelberg — [2]Department of Physics, National University of Singapore — [3]Institute for Molecular Biophysics, University of Maine

In einer kürzlichen Studie konnte nachgewiesen werden, daß die Proteinresistenz selbstaggregierender Monolagen (SAM) aus Oligoether-terminierten Alkanthiolen von verschiedenen Faktoren, wie der Hydrophilie der Molekül-Endgruppen und der Hydrophilie des Molekülinneren, abhängt. Außerdem wurde gezeigt, daß die laterale Packungsdichte der Moleküle einen Einfluß auf die Repulsion von Proteinen hat.

In diesem Beitrag analysieren wir mit Hilfe der Breitband-IR-Vis-Summenfrequenzerzeugung (BB-SFG) den Einfluß von Packungsdichte und Hydrophilie auf die Proteinresistenz der Filme, indem wir Konformations-änderungen der SAMs vor, während und nach Wasserkontakt in-situ verfolgen. Dabei zeigt sich, daß die Proteinresistenz nicht substratabhängig, sondern in der Tat ein reiner Dichteeffekt ist. Die BB-SFG-Resultate werden durch Ellipsometrie- und IR-Messungen ergänzt, mit deren Hilfe das Adsorptionsverhalten von Modelproteinen in den unterschiedlichen Präparationsstadien der Filme untersucht wurde. Darüber hinaus wurde ein Degradationsmechanismus für OEG-SAMs in wäßrigen Lösungen erforscht und aufgeklärt.

O 54 Adsorption an Oberflächen VI

Zeit: Mittwoch 10:45–13:00 Raum: TU EB202

O 54.1 Mi 10:45 TU EB202

Dissociation of Oxygen at Al(111): The Role of Spin Selection Rules — •Jörg Behler[1], Bernard Delley[2], Sönke Lorenz[1], Karsten Reuter[1], and Matthias Scheffler[1] — [1]Fritz-Haber-Institut, Faradayweg 4-6, D-14195 Berlin — [2]Paul-Scherrer-Institut, CH-5232 Villigen PSI

The description of the dissociative adsorption of molecular oxygen at the Al(111) surface remains a most basic and puzzling enigma in surface science. The very low sticking probability of thermal oxygen molecules found experimentally is in strong conflict with the results of state-of-the-art first-principles calculations. We show that this is caused by hitherto unaccounted spin selection rules, which give rise to a highly non-adiabatic behavior in the oxygen-aluminium interaction. As a consequence, the molecular trajectory does not follow the barrier-free adiabatic potential energy surface (PES), but maintains the diabatic triplet state up to close distances to the surface. Detailed density-functional calculations within an appropriate spin-constrained formulation clearly show that the latter PES exhibits sizeable energy barriers, yielding a sticking curve in agreement with experiment. Problems caused by the insufficient accuracy of present-day exchange-correlation functionals and the effects of electronic transitions are also discussed.

O 54.2 Mi 11:00 TU EB202

The relevance of sub-nanometer thin oxide films in the CO oxidation on Pd(100) — •Jutta Rogal, Karsten Reuter, and Matthias Scheffler — Fritz-Haber-Institut, Faradayweg 4-6, D-14195 Berlin

There is an increasing awareness that oxides may form at the surface of transition metal (TM) catalysts under the oxygen-rich environmental conditions of oxidation catalysis. What is, however, still an open question is, if the metal is fully oxidized or if only nanometer thin surface oxide films are formed and which of these different phases are crucial for the catalytic activity of the material.

On Pd(100) the oxidation of the surface proceeds through several different stages, including a $(\sqrt{5} \times \sqrt{5})R27^{O}$ surface oxide structure. The stability of this surface oxide and other oxidation states of Pd(100) in an O_2 gas phase up to ambient pressures was recently analyzed in a combined experimental and theoretical study [1]. We now use density-functional theory and atomistic thermodynamics to also account for the other reactant in CO oxidation catalysis by considering the surface structure and composition in a *constrained* equilibrium with an O_2 and CO gas phase. Under gas phase conditions typical of technological CO oxidation the surface oxide results then as the most stable structure. However, this may be significantly affected by the on-going reactions, which continuously drive the system away from equilibrium. Such kinetic effects under steady-state conditions are discussed on the basis of preliminary kinetic Monte Carlo simulations.

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

O 54.3 Mi 11:15 TU EB202

NO laserdesorption of excited C_{60} — •Tim Hoger[1], Carsten Marzok[2], and Helmut Zacharias[1] — [1]Uni Münster Wilhelm-Klemm Str. 10 48149 Münster — [2]Uni Tübingen

Motivated by long living excited states (exiton states) of a fullerene surface we investigated the desorption of NO rotationally and vibrationally resolved. In a pump / probe experiment we excited the NO covered C_{60} surface with 355 nm ns pulses and detected desorbed NO by (1+1)REMPI. The spectra yield two desorption channels with different characteristics: a 'fast' desorption channel produces a typical non thermal laser desorption spectrum with highly excited rotational and vibrational states ($T_{rot} \sim 430$ K, $T_{vib} \sim 610$ K, E_{kin}(J)~ 1500 m/s) and a second 'slow' desorption channel with low rotational temperatures ($T_{rot} \sim 110$ K) as well as an extremily delayed arrival time.

O 54.4 Mi 11:30 TU EB202

Adsorption-Induced Distortion of F_{16}CuPc on Cu(111) and Ag(111): An X-ray standing wave study — •A. Gerlach[1], F. Schreiber[1], S. Sellner[2,3], H. Dosch[2,3], I. A. Vartanyants[4], B. C. C. Cowie[5], T.-L. Lee[5], and J. Zegenhagen[5] — [1]Physical and Theoretical Chemistry Laboratory, Oxford University, South Parks Road, OX1 3QZ, United Kingdom — [2]Max-Planck-Institut für Metallforschung, Heisenbergstr. 3, 70569 Stuttgart, Germany — [3]ITAP, Universität Stuttgart, Pfaffenwaldring 57, 70550 Stuttgart, Germany — [4]HASYLAB, DESY, Notkestr. 85, 22607 Hamburg, Germany — [5]ESRF, 6 Rue Jules Horowitz, B.P. 220, 38043 Grenoble Cedex 9, France

The adsorption geometry of perfluorinated copper-phthalocyanine molecules (F_{16}CuPc) on Cu(111) and Ag(111) is studied using X-ray standing waves. A detailed, element-specific analysis taking into account non-dipolar corrections to the photoelectron yield shows that the molecules adsorb in a lying down configuration, but with a significant distortion of the molecule on both surfaces. While on copper (silver) the central carbon rings reside 2.61 Å (3.25 Å) above the substrate, the outer fluorine atoms are located 0.27 Å (0.20 Å) further away from the surface. We propose that the outer carbon atoms in F_{16}CuPc undergo a rehybridization ($sp^2 \rightarrow sp^3$) which results in a non-planar adsorption.

O 54.5 Mi 11:45 TU EB202

Influence of the alkyl-chain length on the electronic structure and interface properties of 1,4-octasubstituted Zinc Phthalocyanine thin films on gold — •Indro Biswas[1], Heiko Peisert[1], Sonja Dick[1], Danilo Dini[2], Michael Hanack[2], and Thomas Chassé[1] — [1]Institut für Physikalische und Theoretische Chemie, Universität Tübingen, Auf der Morgenstelle 8, 72076 Tübingen — [2]Institut für Organische Chemie, Universität Tübingen, Auf der Morgenstelle 18, 72076 Tübingen

We compare the interface properties of various 1,4,8,11,15,18,22,25-octa-alkyl-substituted zinc phthalocyanines [$(\mathrm{But})_8$PcZn, $(\mathrm{Hep})_8$PcZn, $(\mathrm{Dec})_8$PcZn] with those of unsubstituted zinc phthalocyanine (PcZn) on gold using X-ray photoemission spectroscopy (XPS) and valence band ultraviolet photoemission spectroscopy (UPS). Although the separation between the aromatic cores in the evaporated thin films clearly depends on the alkyl chain length, it is found that the nature of the substituents causes only minor changes of electronic properties, such as optical gap and ionization potential. It is shown that the observed small energetic shifts for film thicknesses larger than the molecule size cannot be understood in terms of a band bending-like mechanism. Influences of a different orientation of the molecules at the interface and in thin films are discussed. We are grateful for helpful discussions and the synthesis of organic materials to M. Cook and I. Chambrier.

O 54.6 Mi 12:00 TU EB202

Self-assembled two-dimensional supramolecular structures: Rubrene on Au(111) — •Marie-Christine Blüm, Elizabeta Ćavar, Marina Pivetta, François Patthey, and Wolf-Dieter Schneider — Institut de Physique des Nanostructures, École Polytechnique Fédérale de Lausanne (EPFL), CH-1015 Lausanne, Switzerland

We report on the study of the polycyclic aromatic hydrocarbon rubrene (5,6,11,12-Tetraphenylnaphthacene) deposited on a reconstructed Au(111) surface by means of low-temperature STM and STS under UHV conditions. The topographic images measured at 5K reveal a surprising variety of 2D self-assembled structures with different geometries and sizes ranging from dimers up to large ordered islands. A striking feature of this formation is the coexistence of 5- and 6-fold symmetries, i.e. the bonding of the molecules into pentagons, hexagons, honeycomb patterns and hexagonal close packed islands. Furthermore, the molecular pentagons act as new building blocks and line up into chains with lengths of up to 100 nm. The differential conductance spectra acquired on top of a molecule exhibit characteristic peaks which reflect the occupied and unoccupied molecular orbitals and show the presence of an energy bandgap between the HOMO and the LUMO of rubrene adsorbed on Au(111).

O 54.7 Mi 12:15 TU EB202

STM and STS studies of planar and non-planar Naphthalocyanines (Nc) on Graphite (0001) — •T. G. Gopakumar and M. Hietschold — Chemnitz University of Technology, Institute of Physics, Solid Surfaces Analysis Group, D-09107 Chemnitz, Germany.

Adsorption of base free naphthalocyanine (Nc), planar molecule and tin-naphthalocyanine (SnNc), non-planar molecule were studied using a STM on freshly cleaved highly oriented pyrolytic graphite (HOPG) surface at low temperature (50 K) in UHV conditions. Planar Nc molecules form large areas of defect free ordered superstructure [1] with larger molecular packing density (0.3 molecule/nm2) while the non-planar molecules show different phases of adsorption with comparatively less molecular packing density (0.18 molecule/nm2). Tip-sample distance dependent current voltage spectroscopy has been conducted and its normalized differential conductivities have been characterized. The general current voltage curves show an asymmetrical diode like nature. A distant dependent HOMO-LUMO gap shrinking have been observed in the case of Nc, in which it is shown that the HOMOs of the molecules are pinned and the LOMOs are moving towards the Fermi energy. But there is no subsequent HOMO-LUMO gap shrinking in the case of SnNc but an increased current of almost one order of magnitude has been observed in the current voltage characteristics.

[1]. M. Lackinger, T. Müller, T. G. Gopakumar, F. Müller, M. Hietschold, G. W. Flynn, J. Phys. Chem. B. 2004, 108, 2279-2284.

O 54.8 Mi 12:30 TU EB202

Rasterkraftmikrokopie und Mikroquarzwaage: Vergleichende Untersuchungen zur Adsorptionskinetik von Proteinen — •Martin Görlich[1], Peter Schön[2], Lorenz Walder[3] und Marika Schleberger[1] — [1]Universität Duisburg-Essen, Fachbereich Physik, 45117 Essen — [2]Radboud University Nijmegen, Institute for Molecules and Materials, 6525 ed Nijmegen — [3]Universität Osnabrück, Fachbereich Chemie, 49069 Osnabrück

Das Adsorptionsverhalten des Proteins von F_1-ATPase auf Gold ist *in situ* mit einem Rasterkraftmikroskop (*Atomic Force Microscope, AFM*) und einer Mikroquarzwaage (*Quarz Crystal Microbalance, QCM*) untersucht worden. Die Ergebnisse wurden quantitativ ausgewertet und gegenübergestellt. Dabei zeigten die beiden Techniken unterschiedliche Adsorptionskinetiken. Die Gründe dafür sind in den verschiedenen Messmethoden zu suchen: Im AFM-Experiment sorgen spitzeninduzierte Deformationen für einen scheinbar langsameren Adsorptionsverlauf, während im QCM-Experiment der scheinbar schnellere Verlauf auf Wassereinlagerungen in der Proteinschicht zurückzuführen ist.

O 54.9 Mi 12:45 TU EB202

Adsorption isotherms and capillary waves of molecularly thin liquid films - an x-ray reflectivity study — •Michael Paulus[1], Christian Gutt[2], Michael Sprung[3], Christoph Krywka[1], and Metin Tolan[1] — [1]Experimentelle Physik I, Universität Dortmund, Maria-Goeppert-Mayer Str. 2, 44227 Dortmund — [2]Department of Physics 0350, University of California, San Diego, 9500 Gilman Drive, La Jolla, CA 92093-0350, USA — [3]c/o 8ID/IMMY-XOR-CAT, APS/ANL, Argonne, IL, 60439, USA

We present an x-ray reflectivity study of molecularly thin films of liquid iso-butane adsorbed on bulk liquid glycerol. The glycerol-isobutan interface serves as a model system to study the influence of the substrate-adsorbate interactions on both adsorption isotherms and capillary wave fluctuations. The low condensation pressure of isobutane (approximately 1.6bar at 288K) allows to adsorb thin liquid isobutane layers on the glycerol surface. The layer thickness is adjustable between monolayer coverages and 2-3 nm by varying the gas pressure at constant temperature. A special sample cell has been designed which guarantees the high degree of pressure and temperature stability needed for these experiments. From the x-ray reflectivity data film thickness and the capillary wave induced surface roughness as a function of pressure have been determined. A strong coupling between the first monolayers of isobutan and the glycerol surface leads nearly to a complete suppression of capillary waves in the monolayer.

O 55 Epitaxie und Oberflächenreaktionen

Zeit: Mittwoch 10:45–13:00 Raum: TU EB107

O 55.1 Mi 10:45 TU EB107

Surface diffusion and nucleation on Si(111) and Ge(111) 7x7 reconstructed surfaces — •Vasily Cherepanov, Sergey Filimonov, and Bert Voigtländer — Institut für Schichten und Grenzflächen ISG 3, Forschungszentrum Jülich, 52425 Jülich, Germany

Submonolayer deposition on the 7x7 reconstructed Si and Ge surfaces results in formation of two types of objects: the usual 2D islands and small metastable clusters occupying the half unit cells of the surface reconstruction. Using a coarse grain approach we propose a theoretical model with a unified treatment of the coupled system of small clusters and 2D islands. It follows from the model that the densities of 2D islands and small clusters are determined by competition for adatoms. The main energetic parameters determining the measured densities are the diffusion barrier for a single adatom, the energy barrier to reorder the stacking fault unit of the surface reconstruction, and the binding energy of adatoms to the stable small clusters. Simultaneous measurements of the density of 2D islands and the density of small clusters with scanning tunneling microscopy are used to estimate the relevant energetic barriers and to reveal on a quantitative level the influence of the compressive strain, film/substrate material, and surface reconstruction on the island formation and growth.

O 55.2 Mi 11:00 TU EB107

A kmc study of the steering effect in Cu(001) homoepitaxy — •Frits Rabbering, Herbert Wormeester , and Bene Poelsema — MESA+ Institute for Nanotechnology, University of Twente, Enschede, The Netherlands

One of the key assumptions in the description of growth is the homogeneous distribution of the incoming particle flux. The analysis of high resolution LEED measurements after the deposition of 40 ML of Cu on Cu(001) at various polar deposition angles led to the conclusion that attractive forces between the surface and the incoming particle have a dramatic effect on the trajectory of the incoming particle, called steering [1]. The result of the steering effect is that incoming particles are attracted towards protruding structures. This leads to an increased roughening with pronounced changes in morphology for glancing incidence deposition. The steering effect introduces two additional parameters in the growth process: the polar angle of incidence and the velocity of the incident particles. We developed a Kinetic Monte Carlo program that describes well the growth at normal incidence (only small influence of steering). The first results on the influence of both polar incidence angle and the velocity of the incoming particles on the growth morphology in the temperature range of 180 to 250K will be presented. [1] S. van Dijken, L.C. Jorritsma and B. Poelsema, Phys. Rev. Lett. 82 4038 (1999)

O 55.3 Mi 11:15 TU EB107

A Theoretical study of Nanoporous Carbon for Styrene Catalysis — •Johan M. Carlsson[1], Suljo Linic[2], and Matthias Scheffler[1] — [1]Fritz-Haber-Institut der Max-Planck-Gesellschaft, Faradayweg 4-6, 14195 Berlin — [2]Department of Chemistry, University of Michigan, Ann Arbor, MI 48109-2136, USA

Dehydrogenation of Ethylbenzene(EB) to produce Styrene is one of the most important processes in chemical industry. Iron-oxide is widely used as catalyst, but it has recently been proposed that Nanoporous carbon (NPC) deposited on the surface is the actual active material for this reaction. We have therefore studied how motives present in NPC, can change an inert graphene sheet into a chemically active NPC. Our Density Functional Theory (DFT) calculations shows that undercoordinated C-atoms surrounding a vacancy tend to rebind next-nearest neighbours (NNN) forming a larger pore like, structure in the graphene sheet. The strain in the lattice prevent the NNN to form proper sp^2-bonds, such that the defects lead to local curvature and lattice contraction. The cohesive energy of such a defective graphene sheet is comparable to perfect nanotubes in spite of the large E_{form} for the individual defects. This suggests that NPC may concist of graphitic sheets with a significant amount of defects frozen in during growth. The presence of these defects may leave dangling bonds and perturbs the π-band such that a defect state appears close to E_F. Subsequent calculations for oxidation of NPC has confirmed that the vacancies has an increased activity towards adsorption of O_2. These oxidized vacancies furthermore appears promissing as an active sites for oxidative dehydrogenation of EB.

O 55.4 Mi 11:30 TU EB107

Static and Dynamic Self-Organization of Dendron Monolayers on Graphite Monitored with Scanning Tunneling Microscopy — •B. A. Hermann[1], L. Merz[2], L. J. Scherer[3], C. E. Housecroft[3], and E. C. Constable[3] — [1]Dept. of Physics / CeNS, LMU Munich and WMI,Walther-Meissner-Str. 8, 85748 Garching, Germany — [2]on leave from: Inst. of Physics, Uni. Basel, Klingelbergstrasse 82, 4056 Basel, Switzerland — [3]Dept. of Chemistry, Uni. Basel, Spitalstrasse 51, 4056 Basel, Switzerland

The direct imaging of chemical species at molecular and submolecular levels allows to probe self-organized structures using scanning tunneling microscopy (STM). The evaporation of solutions of bipyridine-dendrons and dendron wedges on graphite give highly ordered monolayers.

The near atomic resolution of the 1st and 2nd generation bipyridine dendron permits us to assign conformers, which spontaneously and rapidly form molecular domains under ambient conditions. Within a molecular domain, only one conformer is present and domains of different conformers are observed side by side. No preference for one conformer was observed.

The long-chain alkyl-decorated Fréchet-type dendron wedges initially form a pattern based on trimeric units, organized into hexagonal host structures with a pseudo-unit cell of seven molecules, one of which remains highly mobile. Over time, it changes into a dimeric pattern. The chirality arising from the adsorption of the dendrons onto the surface is discussed.

O 55.5 Mi 11:45 TU EB107

Water Formation from H_2 ad O_2 on Pt(111) — •Timo Jacob[1,2] and William A. Goddard III.[1] — [1]MSC, Caltech, Pasadena, USA — [2]Fritz-Haber-Institut der MPG, Berlin, Germany

Using density functional theory (DFT) with the B3LYP gradient-corrected exchange-correlation functional, the reaction of $H_2+{}^1\!/_2O_2 \longrightarrow H_2O$ was studied on Pt(111), which was represented by a 35 atom cluster. In order to study possible reaction pathways, first binding structures and energetics of each possible intermediate were calculated separately (O, H, O_2, H_2, OH, OOH, H_2O) and afterwards combined with the corresponding dissociation barriers.

Between the two dominant reaction pathways the rate-determining step of the O_2-Dissociation is $O_{ad}+H_{ad} \longrightarrow OH_{ad}$ with a barrier of 31.66 kcal/mol. Along the OOH-Formation pathway $OOH_{ad} \longrightarrow OH_{ad}+O_{ad}$ dissociation has the highest barrier with 17.13 kcal/mol. Although the OOH-Formation is preferred, the oxygen atom, which remains after this reaction without further use, would lead to surface termination. Thus, it also has to use the other reaction channel, or recombine to O_2, which then can be used within the OOH-Formation process.

O 55.6 Mi 12:00 TU EB107

Das Wachstum von Titandioxid auf einer Re(10-10) und einer Ru(0001) Oberfläche — •Dirk Rosenthal[1], Wilhelmine Kudernatsch[1], Klaus Christmann[1], Harry Hoster[2], Hubert Rauscher[2] und R. J. Behm[2] — [1]FU Berlin, Institut für Chemie, Bereich Physikalische und Theoretische Chemie, 14195 Berlin — [2]Abt. Oberflächenchemie und Katalyse, Universität Ulm, 89069, Ulm

Im Rahmen einer Studie zur CO-Oxidation auf goldgeträgertem Titandioxid wurden Titandioxidfilme durch Koadsorption von Titan und Sauerstoff auf einer „glatten“ Ru(0001) und einer grabenförmigen Re(10-10) Oberfläche dargestellt. Morphologie und Wachstum dieser Filme wurden mit LEED, XPS, STM und LEIS untersucht. Auf beiden Substraten wächst Titandioxid in einem Stranski-Krastanov-Modus auf, wobei die benetzende Schicht eine andere Struktur besitzt als die Inseln. Während sich auf dem Ru-Substrat die thermodynamisch günstigste Oberfläche (Rutil(110)) ausbildet, führt die Grabenstruktur des Rheniums zu einer Titandioxidstruktur mit einer Gleitspiegelebene. Sowohl die Rutil(011) als auch die Brookit(001) Oberfläche besitzen diese Symmetrieeigenschaft. Die Einheitsmasche der (2x1) rekonstruierten Rutil(011) Oberfläche ist praktisch gleich groß wie die von Brookit(001). Die Nichtunterscheidbarkeit mit „normalen“ Methoden der Surface Science als auch die Wahrscheinlichkeit des Brookit-Wachstums werden genauso wie der Substrateinfluss diskutiert.

O 55.7 Mi 12:15 TU EB107

Etch figure analysis by scanning force microscopy — •Christian Motzer and Michael Reichling — Fachbereich Physik, Universität Osnabrück, Barbarastr. 7, 49069 Osnabrück

The method of etching crystals was established to determine crystalographic information like orientation of unknown crystals and later to detect structural defects. Etching analysis strongly assisted the semiconductor industry to produce crystals being free from dislocations and other defects. Analysing etching figures is usually done with optical microscopy hence strongly limited in resolution. For high resolution analysis of etch figures we applied the scanning force microscope. We investigated ex-situ CaF_2(111) cleavage plates which were etched in several acids like sulfuric acid, phosphoric acid, hydrochloric acid and nitric acid. SFM reveals new and profound details of the etched plates which are specific to the surface reaction chemistry which is sensitive to surface and bulk defects. AFM measurements allowed to detect ditrigonal etch pit formation and delayed precipitation formation after etching.

O 55.8 Mi 12:30 TU EB107

Dynamics of Surface Defects observed on CeO_2 (111) by Dynamic Force Microscopy — •S. Gritschneder[1], Y. Namai[2], Y. Iwasawa[2], and M. Reichling[1] — [1]Fachbereich Physik, Universität Osnabrück, Barbarastraße 7, 49076 Osnabrück, Germany — [2]Department of Chemistry, The University of Tokyo, 7-3-1 Hongo, Bunkyo-ku, Tokyo 113-0033, Japan

The (111) surface of CeO_2 in various oxidation states is important for catalytic activity and some of its details relating to surface oxygen atoms have already been studied with dynamic scanning force microscopy. The remarkable catalytic properties of ceriumdioxide are strongly connected to the creation, diffusion and healing of oxygen vacancies and, hence, CeO_2 is used as an oxygen storage device in various technical applications like for instance the three-way-catalyst and the solid oxide fuel cell. We demonstrate that dynamic force microscopy is perfectly suitable to investigate nanoscale and atomic size defects on this insulating oxide surface. Our experiments reveal a rich variety of surface defects in form vacancies and protrusions localized at single, well defined lattice sites as well as extended defect formations involving several surface or sub-surface ions. Many of the defects are very stable, but we can show in series of consecutively recorded images that defects can also appear, disappear and change their morphology. Aiming for a chemical identification of the defects, we exposed slightly reduced CeO_{2-x}(111) surfaces to molecular oxygen and observed the changes in the apparent surface structure. Already at very low dosages of less than 10 Langmuir, we observe effects that we interpret as healing of oxygen vacancies.

O 55.9 Mi 12:45 TU EB107

STM studies on the electronic properties of single Au atoms and Au dimers on a thin Al_2O_3 film on NiAl(110) — •Maria Kulawik, Niklas Nilius, Hans-Peter Rust, and Hans-Joachim Freund — Fritz-Haber-Institut der MPG, Abteilung Chemische Physik, Faradayweg 4-6, 14195 Berlin

The adsorption and diffusion of metal atoms on oxide surfaces play key roles in heterogeneous catalysis, notably for the regeneration of the catalytically active species. Despite the importance of these processes, only little is known on the atomic level, which is mainly due to the high complexity of real catalysts. Therefore, the study of model systems is essential to gain a fundamental understanding of these processes.

Here, we have investigated the electronic structure of single Au atoms on a thin Al_2O_3 film on NiAl(110) by Scanning Tunneling Microscopy and Spectroscopy (STM/STS) at 5 K. STS spectra of Au monomers exhibit single resonances between 2 and 3 eV whereby the energy position depends on the adsorption site. For Au dimers, a split of this peak is observed. Conductance images reveal the spacial distribution of the LDOS.