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.

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[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 $MgSO_4 \cdot H_2O$(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 $MgSO_4{\cdot}H_2O$ (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 $MgSO_4 \cdot H_2O$ 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 $\mathrm{Fe}_x\mathrm{TiS}_2$ (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 $\mathrm{Fe}_x\mathrm{TiS}_2$ (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_2SO_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 two-domensional 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 $c(2\times 2)$-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 $(3\sqrt{2}\times 3\sqrt{2})R45°$ 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 Au-freier 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 Wasserstofffluss 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 ($\leq$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 $\approx$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 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_2O. 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.

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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.

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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 properities, 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.