O 18: Poster Session I - MA 141/144 (Atomic Wires; Size-Selected Clusters; Nanostructures; Metal Substrates: Clean Surfaces+Adsorption of Organic / Bio Molecules+Solid-Liquid Interfaces+Adsorption of O and/or H; Surface or Interface Magnetism; Oxides and Insulators: Clean Surfaces)

Time: Monday 18:30–19:30 Location: Poster F

O 18.1 Mon 18:30 Poster F

Infrared studies of gold nanochains on the Si(557) stepped surface — •Chung Vu Hoang, Markus Klevenz, Robert Lovrincic, Olaf Skibbe, Frank Neubrech, and Annemarie Pucci — Kirchhoff-Institut für Physik der Universität Heidelberg

Gold nanochains on Si(557) will be fabricated under ultra high vacuum conditions. The terraces of the stepped surface serve as one-dimensional diffusion channels, which leads to the formation of parallel monoatomic chains. Due to the appearance of metallic chains an anisotropic change of the conductivity of the substrate surface can be expected. The chain growth process and conductivity dependence versus gold composition will be investigated in-situ by using transmittance infrared spectroscopy (IRS) with light polarized parallel and perpendicular to the chains, respectively. IRS is a well-established method to observe conductivity changes on surfaces. The temperature dependent behaviour of gold chains will be studied as well.

O 18.2 Mon 18:30 Poster F

Self-assembled Pt nanowires on Ge(001) — •Cosima Schuster and Udo Schwingenschlögl — Institut für Physik, Universität Augsburg, D-86135 Augsburg

Semiconductor surfaces attract great attention due to various effects of self-organization. For example, adsorption of Pt on the Ge(001) surface results in stable Pt nanowires. Because self-organization of adsorpted atoms relys on strong interaction with surface states, accounting for the full structural relaxation is a prerequisite for describing the electronic properties of a covered surface in an adequate manner.

In a first step, we have thus investigated the surface electronic structure of the $c(4\times 2)$ reconstructed Ge(001) surface by means of DFT band structure calculations In particular, it is possible to attribute each state to either the Ge dimer bonds or the dangling surface bonds. The Ge–Pt surface is investigated in a second step. The formation of Pt chains on Ge(001) is accompanied by the partial breakup of the Ge surface dimers. We show that the surface electronic structure is significantly perturbed due to Ge–Pt interaction. Especially, we find remarkable shifts of Ge states towards the Fermi energy. As a consequence, the topmost Ge layers are subject to a metal-insulator transition.

O 18.3 Mon 18:30 Poster F

CVD synthesis of isolated carbon nanotube peapods on substrates — •Christian Spudat, Carola Meyer, and Claus Schneider — Research Centre Jülich, Institute for Solid State Research, Electronic Properties, 52425 Jülich

Carbon nanotubes filled with C_{60} Fullerenes, so-called "peapods", form a model system for studying one-dimensional molecular chains coupled to a ballistic conductor. C_{60} interacts only weakly with the surrounding SWCNT. Thus, small interactions such as phonon or spin coupling should be observable in transport measurements. In general, these peapods are synthesized by filling *bulk* material, and they are successively dispersed on a substrate from solution. The disadvantage of this method is that the nanotubes are rather short due to prior sonication and bundle together in ropes. Thus, characterisation of individual peapods including transport measurements is rather difficult. Clean and isolated SWCNTs for transport measurements can be grown using chemical vapour deposition. Here, we present a method to fill such SWCNTs with Fullerenes directly on substrates using vacuum filling in an evaporation chamber. We characterize the SWCNTs and peapods after each processing step using AFM, Raman and HRTEM. The main focus is the investigation of defects caused by thermal oxidation and the purification of the synthesized peapods.

O 18.4 Mon 18:30 Poster F

Atomic Nanowires of Self-Organized Pt on Ge(001) – Structural Elements and Electronic Properties — •Marc Wisniewski[1], Jörg Schäfer[1], Sebastian Meyer[1], Andrei Stekolnikov[2], Ralph Claessen[1], and Friedhelm Bechstedt[2] — [1]Physikal. Institut, Universität Würzburg, D-97074 Würzburg — [2]Inst. f. Festkörpertheorie u. -optik, Universität Jena, D-07743 Jena

A special class of nanowires is formed by Pt on the Ge(001) surface. Its low-energy electron states have been explored by scanning tunneling microscopy (STM). A dimerization along the chains is observed at high bias, which might suggest a charge density wave. However, dimer elements also exist with sideways orientation, thus being inconsistent with such picture and instead indicating dimerized back-bonding. Most significantly, for states near the Fermi level, such dimerization along the nanowires is no longer observed. Here a spatially rather uniform charge density is detected. The nanowires can be imaged down to the millivolt regime, indicating metallic character, and tunneling spectroscopy shows finite zero-bias conductivity at room temperature. Ab-initio simulation of the structure has been performed, and a model for the reconstruction at 0.25 ML coverage has been derived. It well reproduces the STM data for various biases. We find that Pt-Ge bonds are favored over Pt-Pt bonds. The prominent dimers along the chain are explained by Ge dimers, while a row of alternating Pt and Ge atoms is identified next to them. This novel tetramer-dimer-chain model consistently explains the wire geometry and its subtle asymmetry. It also accounts for the differential conductivity near the Fermi level.

O 18.5 Mon 18:30 Poster F

Adsorbate induced refacetting: Pb chains on Si(557) — •Annemarie Schuster, Marcin Czubanowski, Shima Akbari, Herbert Pfnür, and Chistoph Tegenkamp — Leibniz Universität Hannover, Institut für Festkörperphysik, Appelstr. 2, 30167 Hannover

The adsorption of monolayers (ML) of Pb on Si(557) followed by annealing to 640K results in the formation of an atomic wire structure. Recently performed transport measurements have shown, that below 78K only along the wires transport occurs, whereas in the perpendicular direction an insulating behavior is found [1]. This finding depends sensitively on the Pb chain structure. Therefore, we have investigated the structure on the atomic and mesoscopic scale by high-resolution low energy electron diffraction (SPA-LEED). Depending on Pb coverage in the range between 1.2 and 1.6ML, formation of various facets [(112), (335), (223)] is induced by the Pb layers, in agreement to recent STM results [2]. The facet orientation in general does not coincide with the macroscopic orientation of the (557) surface. After an initial annealing step to 600 K, starting with 1.2ML of Pb, this new vicinality can be tuned gradually and reversibly even at temperatures below 180K by further adsorption, but also by desorption of Pb. Superstructures of the Pb layers on the terraces were identified on the most stable (223) facets, showing a correlation of adjacent terraces. Here parts of the devil's staircase and the striped-incommensurate (SIC) phases known from Si(111) surfaces develop [3]. [1]C. Tegenkamp et.al. PRL 95 (2005) 176804 [2] H. Murikawa et.al. PRB 76 (2007) 165406 [3]Yakes et.al. PRB 69 (2004) 224103

O 18.6 Mon 18:30 Poster F

Two-dimensional electronic structure of dysprosium silicide nanowires on Si(557) — •Martina Wanke[1], Karolin Löser[1], Gerd Pruskil[1], Petar Stojanov[2], Eric Huwald[2], John Riley[2], and Mario Dähne[1] — [1]Institute of Solid State Physics, Technical University Berlin, D-10623 Berlin, Germany — [2]School of Physics, La Trobe University, Bundoora, VIC 3086, Australia

Rare earth silicide nanostructures are of high interest because of their extremely low Schottky barriers on n-Si(111) [1] and the formation of nanowires with one-dimensional metallicity on Si(001) [2]. In this work, the self-organized growth of monolayer-thick dysprosium silicide nanowires on Si(557) has been studied by scanning tunnelling microscopy and angle-resolved photoelectron spectroscopy. The bare Si(557) surface is characterized by (111) and (112) facets [3]. Accordingly, we observed the nanowires forming on the (111) facets. For coverages of 2 Å dysprosium, nanowire lengths exceeding 1 μm and widths around 5 nm were found. Their electronic structure shows a strong dispersion both parallel and perpendicular to the nanowires, which is assigned to the band structure of $DySi_2$ monolayers on Si(111). At higher coverages similar nanowires are observed at the (111) facets, which show characteristic structural properties of the multilayer growth and also the Dy_3Si_5 multilayer band structure.

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

[1] S. Vandré et al., Phys. Rev. Lett. **82**, 1927 (1999).

[2] C. Preinesberger et al., J. Appl. Phys. **91**, 1695 (2002).

[3] A. Kirakosian et al., Appl. Phys. Lett. **79**, 1608 (2001).

O 18.7 Mon 18:30 Poster F

Structural influence towards transport: Pb wires on Si(557) — •Marcin Czubanowski, Annemarie Schuster, Christoph Tegenkamp, and Herbert Pfnür — Institut für Festkörperphysik, Leibniz Universität Hannover, Deutschland

The adsorption of 1.3 ML of Pb on Si(557) substrates followed by annealing at 640K leads to the formation of an anisotropic metallic structures as revealed by conductivity, STM and ARPES measurements. Those structures below 78K show metallic conductance along the Pb-chains, whereas in the direction perpendicular to the chain-structure an insulating behavior has been found. Additionally, ARPES measurements have shown that below T_c, those structures undergo complete Fermi nesting in the direction normal to the structure. In our recent LEED experiments, the chain structure has been systematically investigated as a function of temperature by means of SPA-LEED analysis. The adsorption of Pb transforms (locally) the surface into a regularly stepped (223) facet below T_c. This structure undergoes reversibly a commensurable-incommensurable phase transition at T_c = 78K as judged from changes in position of step diffraction spots in the $[\bar{1}\bar{1}\ 2]$ direction and also the periodicity of domain wall reflexes in the $[1\bar{1}\ 0]$ direction. Furthermore, the transition depends crucially on the Pb coverage. If the steps are decorated by excess Pb, e.g. 1.5ML, the transition is strongly suppressed.

O 18.8 Mon 18:30 Poster F

Metastable Impact Electron Spectroscopy (MIES) of intermediate nanocatalytic states — •Christopher Harding, Vahideh Habibpour, Sebastian Kunz, and Ulrich Heiz — Lehrstuhl für Physikalische Chemie, Technische Universität München,

Metastable ion electron spectroscopy (MIES) is a well established spectroscopic technique that can be applied in a new and novel way to nanocatalysts. It has several interesting benefits which include a dramatically enhanced sensitivity to electron orbitals with low ℓ-values (compared with UPS) and very low collision velocities leaving the surface virtually untouched.

Thin oxide films and mass-selected metal clusters form the basis of nanocatalysts and are thus of primary importance. In the MIES spectra high sensitivity to sub-1%ML coverages of clusters and also a strong enhancement of various spectral regions which give information on intermediate states in oxidation reactions can be seen.

According to theoretical predictions cluster-oxides intermediates are formed and play an important role in the catalysis of the CO oxidation reaction. These important and interesting predictions are made, based on size selected Pd clusters on MgO films. Using a laser vaporisation cluster source size selected clusters of Pd_9 and Pd_{30} were deposited onto MgO films and this mechanism investigated. The experimental MIES studies confirm the intermediate oxide formation and illustrates other intriguing aspects of the Pd-oxide intermediate state.

O 18.9 Mon 18:30 Poster F

Size-selected clusters on surfaces studied by local probe: An experimental setup and first results — •Markus Bieletzki[1], Marina Pivetta[1], Clemens Barth[2], and Ulrich Heiz[1] — [1]Lehrstuhl für Physikalische Chemie, Technische Universität München, Lichtenbergstr. 4, D-85748 Garching, Germany — [2]CRMCN-CNRS, Campus de Luminy, Case 913, 13288 Marseille Cedex 09, France

During the last decade it has been shown by several groups that clusters with sizes of up to about 30-40 atoms reveal distinct chemical properties which change as function of the precise number of atoms[1,2]. In these experiments the model catalysts were prepared by the deposition of size-selected clusters from the gas phase at low temperatures. Whereas there is strong indication that the clusters remain intact upon deposition, little is known about the dynamics (stability, diffusion, agglomeration) of the clusters at elevated temperatures and under reaction conditions. In order to study the stability of size-selected clusters on oxide surfaces and thin oxide films we built a cluster deposition experiment with size-selection which is coupled to an OMICRON variable temperature scanning probe microscope. In this contribution we present the technical details and specifications of the new experimental setup and show first AFM- and STM-images of cluster assembled materials.

[1] K. Judai, S. Abbet, A. S. Wörz, U. Heiz, C. R. Henry, Journal of the American Chemical Society 2004, 126, 2732.

[2] S. S. Lee, C. Y. Fan, T. P. Wu, S. L. Anderson, Journal of the American Chemical Society 2004, 126, 5682.

O 18.10 Mon 18:30 Poster F

Calculations of two-particle correlation functions at surfaces — •Yaroslav Pavlyukh and Jamal Berakdar — Institut für Physik, Martin-Luther-Universität Halle-Wittenberg, Heinrich-Damerow-Str. 4, 06120 Halle

The spectra of the electron-induced electron pair from surfaces [1] carry information on the short-range charge and spin correlations.

We show in this contribution how the measured angular and energy correlation within the electron pair relates to the spin-resolved spectral density of the sample and the screened Coulomb interaction. Both quantities we inspect theoretically by means of a combination of many-body theory and quantum chemistry methods based on the configuration interaction.

[1] Schumann *et al.*, Physical Review Letters **95**, 117601 (2005)

O 18.11 Mon 18:30 Poster F

Spatially resolved bonding and antibonding states on a silver dimer on Ag(111) — •Alexander Sperl[1], Jörg Kröger[1], Nicolas Neél[1], Henning Jensen[1], Richard Berndt[1], Andreas Franke[2], and Eckhard Pehlke[2] — [1]Institut für Experimentelle und Angewandte Physik, Christian-Albrechts-Universität zu Kiel, D-24098 Kiel, Germany — [2]Institut für Theoretische Physik und Astrophysik, Christian-Albrechts-Universität zu Kiel, 24098 Kiel, Germany

Individual silver dimers were fabricated by single-atom manipulation using the tip of a low-temperature scanning tunneling microscope. Combining spatially resolved scanning tunneling spectroscopy of the dimer with density functional theory calculations bonding and antibonding electron states are identified. While bonding states contribute to the local density of states mainly in the center of the dimer, antibonding states are localized at the atom sites. The evolution of monomer to dimer unoccupied resonances was monitored as a function of decreasing mutual silver atom distance and found to shift toward the Fermi level.

O 18.12 Mon 18:30 Poster F

Reaction Properties of Size-selected Silver Clusters Supported on LTA Zeolite — •Amgalanbaatar Baldansuren and Emil Roduner — Institute of Physical Chemistry, University of Stuttgart, Stuttgart, Germany

Size-selected clusters are important to fundamental investigations. Silver containing catalysts were prepared by aqueous ion exchange of Ag^+ against Na^+ cations in an LTA zeolite. A recent project deals with continuous wave and pulse EPR investigations into adsorption interactions of ethylene, oxygen, and nitrogen monoxide with supported silver clusters. EPR is quite straightforward to analyze structures and electronic properties of paramagnetic clusters. The present work is restricted to monitoring the activity of the Ag_6^+ cluster; however, depending on the metal loading, Ag^0, Ag_3^0 and Ag_4^+ clusters have been formed in the LTA pores as well. The aim of the project is to discern size-dependent effects by directly looking at the centre of potentially catalytic activity.

A well-defined cluster composed of 6 equivalent silver nuclei was obtained after oxidation and hydrogen reduction. As the unpaired spin density distribution is strongly affected by reactions with gas molecules, the symmetric structure of Ag_6^+ turns into less-compact or smaller clusters. After ethylene adsorption a weak proton hyperfine coupling was resolved by ENDOR. HYSCORE experiments determined that the unpaired spin density is mostly on the adsorbed ethylene and no longer on the cluster. Products of the catalytic conversion, e.g. the NO_2 formed on the cluster surface after NO adsorption, exhibits molecular motion at temperatures between 30 K and 125 K.

O 18.13 Mon 18:30 Poster F

Oxidation/Reduction of Au_n (n=2-13) clusters on SiO_2/Si and HOPG — •Rainer Dietsche[1], Dong Chan Lim[1], Moritz Bubek[1], Thorsten Ketterer[1], Young Dok Kim[2], and Gerd Ganteför[1] — [1]Dep. of Physics, University of Konstanz, Konstanz, Germany — [2]Dep. of Chemistry, Sungkyunkwan University, Suwon, Korea

Gas phase Au clusters with less than 20 atoms show a pronounced even-odd alternation in their oxidation behaviour. This behaviour is due to the unpaired electron in case of even-numbered anions. For clusters deposited on metal oxides this pattern vanishes. In our experiment Au cluster anions are soft-landed on silica and graphite. Oxidation and reduction are studied by X-Ray Photoelectron Spectroscopy (XPS).

For Au$_n$ (n=2-13) clusters on Si wafers covered with native oxide layers the even-odd pattern in oxidation behaviour still is observed. This indicates that the cluster-substrate interaction is weak enough to preserve some of the gas phase properties of the clusters [1].

In a second step, the samples are removed from the UHV system and immersed into water or NaOH solution. The samples exposed to water still exhibit similar chemical properties, whereas treatment with NaOH solution results in an inversion of the even-odd alternation.

In case of Au$_n$ (n=2-9) clusters on sputtered HOPG an even-odd pattern is not observed. However, Au$_8$ more readily reacts with atomic oxygen compared to the other clusters. STM measurements of Au$_7$ clusters show that this cluster exhibits two layer, 3D structures [2].

[1] D.C. Lim et al., *ChemPhysChem* **7**, 1909 (2006)
[2] D.C. Lim et al., *Chem. Phys. Lett.* **439**, 364 (2007)

O 18.14 Mon 18:30 Poster F

Softlanding and STM imaging of Ag$_{309}$ clusters on 1 and 2 monolayers C$_{60}$/HOPG — •L. Patryarcha[1], S. Duffe[1], T. Richter[1], B. Sieben[1], H. Hövel[1], C. Yin[2], B. von Issendorff[2], and M. Moseler[3,4] — [1]Technische Universität Dortmund, Experimentelle Physik I — [2]Universität Freiburg, Fakultät für Physik — [3]Fraunhofer-Institut für Werkstoffmechanik IWM, Freiburg — [4]Freiburg Materials Research Center

At 165 K Ag$_{309}$ clusters were deposited on HOPG functionalized with C$_{60}$ and imaged with STM at 77 K. With HOPG at room temperature (RT) during C$_{60}$ evaporation areas of some 100 nm stayed uncovered, and 2 ML islands were formed on 1 ML C$_{60}$ planes. On areas with 1 and 2 ML C$_{60}$ we observed very narrow cluster height distributions with h=(2.4 ± 0.2) nm. By annealing Ag$_{309}$/C$_{60}$/HOPG we observed that the cluster height stayed stable for more than 12 h at RT on 1 and 2 ML C$_{60}$. The clusters on free HOPG areas became mobile during annealing at 265 K and moved to the edges of the C$_{60}$ areas. The RT stability of Ag$_{309}$/C$_{60}$/HOPG is in contrast to the observations for Ag$_{561}$ and Ag$_{309}$ on 1 and 2 ML C$_{60}$/Au(111) which were deposited at 165 K and annealed up to RT. For the samples with an Au(111) substrate we observed that the cluster height on 1 ML C$_{60}$ decreased and finally all clusters disappeared [1]. Molecular dynamics calculations show that there is a low barrier height for the transport of Ag atoms through the C$_{60}$ film on 1 ML C$_{60}$/Au(111) which should be much higher for clusters on 1 ML C$_{60}$/HOPG.

[1] S. Duffe et al., Eur. Phys. J. D (2007), published online

O 18.15 Mon 18:30 Poster F

Size-dependent Photoabsorption and Photoemission of Supported Silver Clusters and Silver Cluster-Biomolecule Hybrid Systems — •Roland Mitric, Christian Bürgel, Jens Petersen, Alexander Kulesza, and Vlasta Bonacic-Koutecky — Humboldt-Universität zu Berlin, Institut für Chemie, Brook-Taylor-Str. 2, D-12489 Berlin, Germany

Silver clusters interacting with different environments such as surfaces or biomolecules exhibit fascinating absorption and emissive properties which can be exploited for biosensing and optoelectronic applications. We address theoretically size dependent structural and optical properties of silver clusters Ag$_n$ (n=2,4,6,8) suppported on MgO surface as well as optical properties of silver-cluster tryptophan hybrid systems Trp-Ag$_n^+$ (n=1-9). Our results on supported silver clusters provide insight into the mechanism responsible for absorption and emission patterns arising from interaction between the excitation within the cluster and the environment. We demonstrate that small clusters such as Ag$_4$ are good candidates for fluorescence centers in the visible regime. Furthermore, in the Trp-Ag$_n^+$ hybrid system we identified different types of charge transfer between the silver and biomolecule subunits. Remarkably, we observe a strong reduction of the photofragmentation yield in Trp-Ag$_9^+$ in comparison with free Ag$_9^+$ which may be attributed to energy dissipation by fluorescence. Thus, the unique optical properties of supported silver nanoclsuters combined with the specific bio-recognition of biomolecules will provide fundamentals for the future development of fluorescent nanocluster-based biochips.

O 18.16 Mon 18:30 Poster F

Comparing Resonant 2p X-ray Absorption of Size-selected Cobalt Clusters on Cu(100) and in a Linear Paul Trap — •Vicente Zamudio-Bayer[1], Leif Glaser[2], Konstantin Hirsch[1], Philipp Klar[1], Andreas Langenberg[1], Fabian Lofink[1], Robert Richter[1], Jochen Rittman[1], Marlene Vogel[1], Wilfried Wurth[2], Thomas Möller[1], Bernd von Issendorff[3], and J. Tobias Lau[1] — [1]Technische Universität Berlin, Institut für Optik und Atomare Physik, EW 3-1, Hardenbergstraße 36, D-10623 Berlin — [2]Universität Hamburg, Institut für Experimentalphysik, Luruper Chaussee 149, D-22761 Hamburg — [3]Albert-Ludwigs-Universität Freiburg, Fakultät für Physik/FMF, Stefan-Meier-Straße 21, D-79104 Freiburg

Its element specificity makes resonant X-ray absorption spectroscopy an ideal tool to study deposited clusters at low coverage. At the $2p$ absorption edges of small, size-selected cobalt clusters on Cu(100), two separate sets of lines are observed which can be interpreted in terms of atomic-like multiplet splitting. For very small clusters ($n = 1, 2, 3$), these absorption lines show a strong size dependence. The size evolution of $2p$ X-ray absorption will be discussed in comparison to size-selected free cobalt clusters, recorded recently on mass selected cluster ions in a linear Paul trap at BESSY. Direct comparison of free and deposited clusters under well defined conditions allows to distinguish size-specific properties from cluster–substrate interaction effects. A shift to higher photon energies in deposited clusters indicates screening by substrate valence electrons.

O 18.17 Mon 18:30 Poster F

EUV/XUV-Radiation: a New and Versatile Tool for Structural and Chemical Surface Analysis — •Armin Bayer, Frank Barkusky, Stefan Döring, Christian Peth, Michael Reese, and Klaus Mann — Laser-Laboratorium Göttingen e.V., Hans-Adolf-Krebs-Weg 1, 37077 Göttingen

One of the most distinct features of EUV/XUV radiation in the regime of 2...20 nm is the strong interaction cross section to almost every material giving rise to penetration depths of about a few hundred nanometers for normal incidence light. Since the order of magnitude of the applied wavelength is comparable to typical dimensions of nanostructures, EUV/XUV light serves as an ideal tool for surface near probing of nanostructured samples.

The Laser-Laboratorium Göttingen e.V. has developed a laser-driven plasma source for generation of soft x-rays in the above mentioned spectral range. A Nd:YAG laser (1064 nm, 800 mJ, 6 ns) is focused into a gas-target leading to plasma formation which in turn emits characteristic soft x-ray radiation. Depending on the employed target gas, narrow-band as well as broad-band spectra can be obtained.

Based on this light source, a Θ-2Θ-reflectometry setup as laboratory metrology tool for in-band characterization of surfaces is currently being developed, enabling the future determination of both the chemical composition (reflectometry and NEXAFS experiments) and surface morphology (scatterometry and diffractometry experiments).

In this contribution we present the experimental concept, possible measurement techniques, numerical simulations as well as first results.

O 18.18 Mon 18:30 Poster F

Probing correlated electron-pair emission from a W(001) surface — •Milton Muñoz-Navia, Carsten Winkler, Michael Birke, Ram Shanker Patel, Frank Oliver Schumann, and Jürgen Kirschner — Max-Planck-Institut für Mikrostrukturphysik, Weinberg 2, 06120 Halle, Germany

An electronic system which is excited by a photon can respond by the simultaneous emission of an electron-pair also called Double Photoemission (DPE). It has been established theoretically that a non-zero DPE intensity requires electron-electron interaction. Besides the simultaneous ejection of two electrons upon photon absorption, another possible pathway of pair emission is that the photon is absorbed by a single electron which scatters from another electron. To study their relative contributions we have analysed the pair emission from a W(001) surface excited by 25 eV and 29.5 eV photons in comparison with 20 eV and 25 eV electrons. The experiments were performed with a coincidence time-of-flight setup with two channelplate detectors in back-reflection geometry. In the (γ,2e) experiments BESSY II synchrotron facility operated in single-bunch mode was used as pulsed light source, while for the (e,2e) experiments, a pulsed electron gun was employed. We find that the 2D-energy distributions for photon absorption or electron excitation are markedly different. Qualitatively this difference can be understood by the selection rule for DPE. Hence, the (γ,2e) intensity has a significant contribution due to the DPE process.

O 18.19 Mon 18:30 Poster F

Aluminum oxide etching with hydrogen — •Markus Reinl, Andreas Assmuth, Rudolf Nüssl, Tanja Stimpel-Lindner, Torsten Sulima, Hermann Baumgärtner, and Ignaz Eisele — Universität der Bundeswehr, Institut für Physik, Werner-Heisenberg-Weg 39, 85577 Neubiberg, Germany

In modern semiconductor production Al is still used as material for the probing and bonding pads. It is widely spread that the difficulties during probing are caused by the native Al_2O_3 on top of the Al pads. In order to improve the probing performance different hydrogen processes to remove the native oxide were investigated on sputtered Al.

The first experiments were implemented in an UHV chamber. The Al was exposed to H* radicals to investigate the etching behavior. Therefore pure hydrogen was piped through a 1900 K hot tantalum tube into the process chamber. With this configuration a dissociation rate of 90 % can be achieved. The in-situ analysis was done by an x-ray photoelectron spectroscopy (XPS).

The hydrogen plasma experiments were performed in a modular UHV cluster tool with Ar as plasma gas and H_2 as etching component. In the purpose of analysis with secondary ion mass spectrometry (SIMS) the cleaned surface needs to be covered with a protective layer in order to avoid a recontamination respectively re-oxidation. Therefore a cap of pure Al was deposited.

As expected the results show that the pure chemical reaction does not lead to a sufficient etching rate. In fact ion bombardment is necessary to achieve a significant etching effect.

O 18.20 Mon 18:30 Poster F

About the existence of the Au(110) surface state at the $\bar{Y}$ point — •Andreas Nuber[1], Frank Forster[1], Friedrich Reinert[1], and Kenya Shimada[2] — [1]Universität Würzburg, Experimentelle Physik II, Am Hubland, 97074 Würzburg, Germany — [2]Hiroshima Synchrotron Radiation Center, Hiroshima University, Japan

Presently there are some discussions and inconsistent results about the existence of the Shockley-type surface state at the $\bar{Y}$ point of the surface Brillouin zone on the (1×2) reconstructed Au(110) surface. We investigated this surface by high-resolution angle-resolved photoelectron spectroscopy (ARUPS). In our investigation we could not find any evidence of a surface state on the clean Au(110) surface, neither at the $\bar{\Gamma}$ point nor at the $\bar{Y}$ point. Furthermore we deposited thin films of Xe and Ag in order to investigate the changes of the surface electronic structure. With about 2 ML of Ag adsorbed, a surface state at $\bar{Y}$ shows up with $E_0 = 450$ meV which is surprisingly a lot higher than the reported binding energy of the surface state on a clean Ag(110) surface. Adsorbing noble gases on the clean (1×2) reconstructed Au(110) surface induced a coverage dependent backfolding effect.

O 18.21 Mon 18:30 Poster F

Inelastic Electron Tunnelling Spectroscopy in studies of complex metal-organic interfaces: The case of PTCDA/Ag(111) — •Adam Lassise[1], Ruslan Temirov[2], and Stefan Tautz[2] — [1]Jacobs University, Bremen, Germany — [2]Forschungszentrum Jülich, Jülich, Germany

Recently it has been proposed that the STM-based Inelastic Electron Tunnelling Spectroscopy (STM-IETS) can solve the long standing problem of the STM chemical insensitivity. However, due to the problems with the interpretation of the IETS data, the potentials of this method in application to the large organic adsorbates are not yet well understood. Here we apply STM-IETS to the well studied model case of complex organic adsorption - PTCDA/Ag(111). We analyse the IETS data obtained on PTCDA molecules in different adsorption states and show that the variations of the local electronic structure of the molecule mostly affect the intensity of IET spectral features but not their energetic positions. Finally, we use the IET imaging in order to identify the strongest vibrational modes observed in IET spectra.

O 18.22 Mon 18:30 Poster F

Ferrocene-1,1-dithiol (FDT) between perfect and defective Ag electrodes — Thomas Bredow[1], Jörg Meyer[2], Volodymyr Maslyuk[3], •Gernot Gardinowski[4], Christoph Tegenkamp[4], Herbert Pfnür[4], and Ingrid Mertig[3] — [1]Institut f. Physikalische und Thoeretische Chemie, Universität Bonn, Germany — [2]Fritz-Haber-Institut - Abtl. Theorie, Berlin, Germany — [3]Fachbereich Physik, Martin-Luther-Universität Halle-Wittenberg, Germany — [4]Institut f. Festkörperphysik, Leibniz Universität Hannover, Germany

The role of surface defects on the energetic and electronic structure of a molecule between two electrodes is of high intrest. We present a theoretical study of the interaction of ferrocene-1,1-dithiol (FDT) with two perfect or defective (vacancies, steps, etc.) parallel Ag(111) surfaces using DFT. We demonstrate, that the adsorption geometry has a strong effect on the electronic levels and conductivity. Furthermore, we show that the presence of point defects strongly enhances the molecule-surface interaction but has a suprisingly small effect on the density of states. Ferrocene dithiolate preferably binds to low-coordinated Ag atoms, which leads to significant shifts of the molecular orbitals and to a decrease of the electronic conductivity compared to the adsorption at perfect surfaces due to increased splitting of molecular levels. The latter leads to a decrease of the overlap with the metal levels near Fermi energy, and therefore to a reduction of the conductivity. Finally, we conclude that highly conducting molecules need collective stabilization by a significant amount of FDT molecules saturating the energetically favorable, but less conducting sites on an Ag electrode.

O 18.23 Mon 18:30 Poster F

C_{68} deposits on Cu(111): Topography and Electronic Properties — •Albert F. Takacs[1,2], Timofey Balashov[1], Wulf Wulfhekel[1,2], Daniel Löffler[3], Artur Böttcher[3], and Manfred M. Kappes[2,3] — [1]Physikalisches Institut, Universität Karlsruhe, D-76131, Germany — [2]CFN-DFG Centrum für Funktionelle Nanostrukturen — [3]Institut für Physikalische Chemie, Universität Karlsruhe, D-76131, Germany

Non-IPR fullerenes (Isolated Pentagon Rule) have very recently attracted attention as stable building blocks for carbon-based nanotechnology. In contrast to classic fullerenes, the smaller C_n cages, n<70 and n>60, are functionalised by terminating reactive sites. We focus here on the C_{68} species which is the largest fullerene to have only non-IPR cage isomers. Ultraviolet photoionization spectroscopy reveals the HOMO-LUMO gap of the C_{68} layers of 1.7 eV and thermal desorption spectroscopy evidences a high intercage binding energy of ≈2 eV. We also used scanning tunnelling microscopy(STM) to determine the geometry and electronic properties of C_{68} deposits on Cu(111). The STM images confirm that C_{68} deposits comprise cages linked in polymeric chains as determined by the geometry of the reaction centers terminating individual cage. By proper positioning and approaching of the STM tip over an individual molecule we have investigated the conductance across the cage-substrate interface. The resulting current-voltage (I-V) and differential conductance (dI/dV) characteristics reveal two distinct trends which indicate the unique role of the non-IPR sites as responsible for the strong interactions with the substrate.

O 18.24 Mon 18:30 Poster F

Characterization of FDT molecules and its binding properties on metallic surfaces — •Jedrzej Schmeidel, Gernot Gardinowski, Christoph Tegenkamp, and Herbert Pfnür — Institut für Festkörperphysik, Universität Hannover, Abteilung Oberflächen, Appelstrasse 2, 30167 Hannover, Germany

Recently performed VASP calculations concerning the adsorption of ferrocene-1,1'-dithiol (FDT) molecules on perfect and defective Ag(111) surfaces show that details of the chemical bond have a large influence on the DOS near Fermi energy, i.e the transport behavior. Furthermore, at defect sites the thiolate bonded FDT is energetically favored. We have experimentally investigated FDT on metallic surfaces, to gain insight into this subject. FDT molecule was chosen due to its large conductance and a high structural flexibility with respect to rotation of the two cyclopentadienyl (Cp) rings. As substrate Au(111) and epitaxially grown Ag/Si(111) were used. On both surfaces the adsorption process and the stoichiometry of the FDT was controlled and checked by XPS/UPS. On Au surfaces, self assembled monolayer (SAM) structures have been investigated by means of STM, where assembled structures have been partly seen in form of parallel oriented lines with average spacings of 1.7nm. Submonolayer coverages, generated by thermal evaporation, have been investigated on Ag $\sqrt{3} \times \sqrt{3}$/Si(111). First results about the preferred adsorption at characteristic defect sites (grain boundaries, steps) will be presented and their electronic structure, obtained by STS, correlated with theoretical results.

O 18.25 Mon 18:30 Poster F

Single molecule manipulations: PTCDA on Ag(111) — •Olga Neucheva[1], Ruslan Temirov[1], Adam Lassise[2], Sergey Soubatch[1], and Stefan Tautz[1] — [1]Forschungszentrum Jülich, Jülich, Germany — [2]Jacobs University, Bremen, Germany

Manipulations of atoms and molecules with the low temperature scanning tunneling microscope open new opportunities for creating nanodevices. The size of molecules and type of their interaction with the substrate play an important role in manipulation process. For PTCDA molecules chemisorbed on Ag(111) surface, we developed a protocol of controllable and reproducible manipulation which includes a creation of stable contact between a molecule and STM-tip, tearing it from the substrate and transporting to a chosen position, and finally locating it on the surface. The reproducibility of these stages is controlled by measuring the I(t) spectra. Using this protocol, we formed different types of molecular corrals and chains in order to modify the Ag(111) surface state. Performed experiments allow us to study substrate-molecule interaction in more details.

O 18.26 Mon 18:30 Poster F

X-ray absorption spectroscopy of spin-crossover complexes on metallic surfaces. — •D. Ball[1], M. Bernien[1], M. Piantek[1], J. Miguel[1], J. Kurde[1], W. Kuch[1], H. Wende[2], M. Haryono[3], S. Hain[3], and A. Grohmann[3] — [1]Freie Universität Berlin, Inst. f. Experimentalphysik, Arnimallee 14, D-14195 Berlin — [2]Universität Duisburg-Essen, Fachbereich Physik, Experimentalphysik - AG Wende, Lotharstr. 1, D-47048 Duisburg — [3]Technische Universität Berlin, Inst. f. Chemie, Straße des 17. Juni 135, D-10623 Berlin

Many six-coordinate iron(II) complexes with an Fe–N$_6$ core show a spin-crossover (SCO) behaviour. The transition between an antiparallel alignment of the electron spins (low spin) and a parallel alignment (high spin) is triggered by temperature, pressure, or optical excitation. We present Near Edge X-ray Absorption Fine Structure (NEXAFS) measurements of mono-molecular layers of Fe(II) 2,6-bis(pyrazol-1-yl)pyridine and 2-phenyl-4,6-di(pyridin-2-yl)-1,3,5-triazine SCO complexes deposited from solution onto Au(111) surfaces. The binding of these complexes to the surfaces is established via different linker groups such as SH, SAc, and SCN. The resulting degree of order and the adsorption geometry are determined by angle-dependent NEXAFS measurements at the C- and N-K edges. The nature of the S–Au bond is studied by X-ray Photoelectron Spectroscopy. The electronic properties of the Fe center are probed by NEXAFS at the Fe L$_{2,3}$ edges. Their spin state is deduced by comparing these spectra to measurements of bulk samples. We find that the interaction with the surface significantly influences the switching behaviour.

O 18.27 Mon 18:30 Poster F

Investigation of the interface between aromatic thiolate SAMs and the Au(111) surface — •Daniel Weier[1], Axel Beimborn[1], Christian Flüchter[1,2], Frank Schönbohm[1], Ulf Berges[1,2], Sven Döring[1,2], Tobias Lühr[1] und Carsten Westphal[1,2] — [1]Fakultät Physik - Universität Dortmund, Otto-Hahn-Str.4, D 44221 Dortmund, Germany — [2]DELTA - Fakultät Physik - Universität Dortmund, Maria-Goeppert-Mayer-Str. 2, D 44227 Dortmund, Germany

SAMs (Self-assembled-monolayers) of aromatic thiolates have been intensively studied in the last three decades. The amphiphilic molecules with a chainlike structure consist of a hydrophobic head group and a hydrophilic carbon chain part. The structure of the molecules allows molecular chemisorption in close packed arrays onto well prepared surfaces due to the high affinity of the sulphur head group to the Au surface. An important trait of the molecules is their strong interaction with x-ray radiation and electrons. The problem of radiation damage within the focus of an undulator beamline is well known. In this project the photon flux density was reduced by moving the sample behind the focus. The out-of-focus measurements showed a significant reduction in the radiation damage at the adsorbed molecules and long data acquisition times became possible. We present first full angle photoelectron diffraction data of the sulphur 2p peak of SAM thiolates on Au(111). The diffracted S 2p signal clearly displays intensity variations. We compare the experimental data with the results of a first simulation of a structure model of the thiolate/Au(111) interface.

O 18.28 Mon 18:30 Poster F

Growth and electronic characterization of TMTTF-TCNQ on metal surfaces — •Dagmar Kreikemeyer Lorenzo, Isabel Fernández Torrente, Katharina Jennifer Franke, and Jose Ignacio Pascual — Institut für Experimentalphysik, Freie Universität Berlin, Berlin, Germany

Here we investigate the adsorption properties and growth of the Bechgaard salt TMTTF-TCNQ on a Au(111) surface by means of Low Temperature Scanning Tunneling Microscopy. TMTTF (tetramethyltetrathiafulvalene) is a charge donor and TCNQ (7,7,8,8- tetracyanoquinodimethane) is an acceptor. The bulk structure is formed by parallel chains of TMTTF and TCNQ, giving rise to one-dimensional conduction bands along the molecular rows. The electronic structure of TMTTF is essentially the same as the well known donor TTF, but the addition of the four methyl groups gives it more three-dimensional shape and increases the decoupling between the chains. The submonolayer growth of pure TMTTF on Au(111) shows a repulsive interaction between molecules as a consequence of its charged state [1]. On the contrary, pure TCNQ self-assembles in close-packed islands. When co-deposited on a metal surface, TMTTF and TCNQ show a strong tendency to mix in ordered domains with alternating rows of each molecule, similar to bulk. By Scanning Tunneling Spectroscopy we identify the molecular resonances of TMTTF and TCNQ and a depopulation of the surface state. Our data indicates that donor-acceptor interactions are still present on a metallic surface. [1] Torrente et al, Phys. Rev. Lett. 99, 176103 (2007)

O 18.29 Mon 18:30 Poster F

Scanning tunnelling microscopy study of nitrobiphenylthiol self-assembled monolayers on Au(111) — •Heiko Muzik, Andrey Turchanin, and Armin Gölzhäuser — Department of Physics, Physics of Supramolecular Systems, University of Bielefeld, D-33615 Bielefeld

Electron beam/extreme UV patterning of 4*-nitro-1,1*-biphenyl-4-thiol self-assembled monolayers (NBPT SAM) on gold surfaces results in the transformation of the terminal nitro groups into amino groups and in the crosslinking of the underlying aromatic cores [1,2]. Such chemical nanolithography has a great potential for nanobiotechnological applications (e.g. fabrication of protein chips[3]), where the post-processing of amino-terminated and pristine areas results in the formation of complex supramolecular assemblies with lateral dimensions of periodic structures down to 30 nm. The understanding of the formation of NBPT SAM at the molecular level is important for a further implementation of chemical nanolithography in different areas. In this contribution we show the first results of a UHV scanning tunneling microscopy (STM) study of NBPT SAMs on Au(111). We present a detailed data evaluation procedure for a non-orthogonal Multiscan-type scanner (Omicron Nanotechnology). The structural polymorphism of NBPT SAMs will be discussed subjecting to the preparation conditions of the samples and their subsequent temperature treatment in UHV. [1] W. Eck et al., Adv. Mater. 2000, 12, 805 [2] A. Turchanin et al., Small 2007. [3] A. Turchanin et al., Adv. Mater. 2007.

O 18.30 Mon 18:30 Poster F

Methanethiolate diffusion on Au(100) and Au(111) — •Andreas Franke and Eckhard Pehlke — Institut für Theoretische Physik und Astrophysik, Christian-Albrechts-Universität zu Kiel

Alkanethioles on unreconstructed Au(111) and Au(100) surfaces are studied as model systems for the bonding and diffusion of organic molecules on metal surfaces. Unreconstructed (111) and (100) surfaces of Au exist under certain electrochemical conditions [1]. We have extend our work on CH$_3$S/Au(111) in a twofold way: In accordance with other studies [2] at low coverages we found CH$_3$S–radicals to bind as Au(SCH$_3$)$_2$ complexes to the Au(111) surface with a binding energy of 2.38 eV per CH$_3$S. We here present an *ab initio* study of the diffusion barriers for these complexes and bare CH$_3$S. To this purpose, we employ the nudged elastic band method (NEB) as implemented in the VASP code. Furthermore, we compare the diffusion of the bare CH$_3$S–radical on the (100) and (111) surface. On Au(100) the adatom formation and subsequent adsorption of two CH$_3$S–radicals at the adatom is slightly less favorable than chemisorption of individual radicals on the defect free surface. The most stable adsorption position for CH$_3$S is a tilted hollow-bridge geometry (for one radical per (4×4) surface unit cell) with a binding energy of 2.27 eV. The radical is tilted to the surface normal by 54°. Transition states along the minimum energy path with barrier heights of 620 meV and 640 meV have been calculated.

[1] M. A. Schneeweiss, et al., Appl. Phys. A **69**, 537 (1999).

[2] P. Maksymovych, et al., Phys. Rev. Lett. **97**, 146103 (2006).

O 18.31 Mon 18:30 Poster F

The adsorption of PTCDA on coin metal surfaces: a correlation between the adsorption height and the chemisorptive nature of the adsorbate-substrate bonding — •Oliver Bauer[1], Annegret Hauschild[1], Serguei Soubatch[2], Stina K. M. Henze[3], Ruslan Temirov[3], Adam Lassise[3], Frank Stefan Tautz[2], and

Moritz Sokolowski[1] — [1]Institut für Physikalische und Theoretische Chemie, Universität Bonn, Wegelerstr. 12, 53115 Bonn — [2]Institut für Bio- und Nanosysteme 3 (IBN3), Forschungszentrum Jülich GmbH, 52425 Jülich — [3]School of Engineering and Science, Jacobs University Bremen, Campus Ring 1, 28759 Bremen

The vertical bonding distance of the adsorbate to the underlying surface can be regarded as a quantity of the strength and the chemisorptive character of the bond. The Normal-Incidence X-ray Standing Wave (NIXSW) technique has been used to determine the adsorption heights of perylene-3,4,9,10-tetracarboxylic acid dianhydride (PTCDA) on various single-crystalline coin metal surfaces. In addition we have recently investigated the adsorption heights as well as the adsorption geometry of PTCDA in the submonolayer regime on the Ag(100) and Ag(110) surfaces by NIXSW: We find vertical bonding distances of 2.66(4) Å and 2.59(1) Å respectively. For PTCDA/Ag(100), the carboxylic and anhydride oxygen atoms are located 2.57(7) Å and 2.79(10) Å above the substrate surface respectively. Based on the experimental findings bonding models which include a synergetic effect of adsorbate-substrate bonding and back-bonding are discussed for PTCDA adsorption on coin metal surfaces. Supported by the DFG and the ESRF.

O 18.32 Mon 18:30 Poster F

STM/STS Analysis of Molecular Chains Consisting of Mn$_6$Cr Single Molecule Magnets and Single Molecules on Highly Ordered Pyrolytic Graphite (HOPG) — •Aaron Gryzia[1], Armin Brechling[1], Wiebke Hachmann[1], Marc D. Sacher[1], Ulrich Heinzmann[1], Maik Heidemeier[2], and Thorsten Glaser[2] — [1]Molecular and Surface Physics, Bielefeld University — [2]Anorganic Chemistry I, Bielefeld University

We report on the preparation and characterization of Mn$_6$Cr-Single Molecule Magnets on a HOPG(0001) surface.

The Mn$_6$Cr-molecules show 1D molecular arrangements with many interesting features, such as the occurrence of discrete kink angles in the molecular chains of 30 deg., only two different molecular orientations, the orientation of the chains along the main crystal axis of HOPG and much larger molecule-molecule distances than expected from the van der Waals radii of the molecules. By STS we characterized Mn$_6$Cr, thus gaining information on the electronic levels of the molecule and the shift of the levels whether it is part of a chain or not. One of our goals is to obtain data about the exact orientation of the molecule in respect to the surface; thus we can make a statement for the physical interaction why the molecules are assembling in chains. First results of these measurements will be presented.

O 18.33 Mon 18:30 Poster F

High-Density Zig-Zag Dimer-Chain of Trimesic Acid at Graphite-Phenyloctane Interface — Ha N. T. Nguyen[1,3], •Thiruvancheril G. Gopakumar[1], Markus Lackinger[2], and Michael Hietschold[1] — [1]Institute of Physics, Solid Surfaces Analysis Group, Chemnitz University of Technology, D-09107, Chemnitz, Germany. — [2]Institute of Crystallography and Applied Mineralogy, Ludwig-Maximilians-University Munich, Munich, Germany. — [3]Department of Applied Physics, Faculty of Physics ,University of Natural Science, 227 Nguyen Van Cu, Hochiminh city, Viet Nam.

Trimesic acid (TMA) is well known for its self-assembly via hydrogen bonding, especially in fatty acids at solid-liquid interface. The well known open structures are the planar chicken wire and flower structures[1]. It has never been observed for TMA in any of the studied solvents a high density structure with molecules adsorbing parallel to the substrate at solid-liquid interface. We have observed a stable adsorption of TMA in phenyloctane (C14H22), a non-polar solvent, with high packing density at room temperature. The packing density is 1.3 molecules/nm2, which is the highest observed for any of planar adsorption of TMA structures at solid-liquid interface. The molecules interact through the carboxylic functional groups with a dimer motif leading to dimer-chain. In adjacent rows the molecules have inverted symmetry (3-fold), which provides the molecules to interact and close pack themselves in a zig-zag fashion. The high density is expected due to high concentration of TMA in phenyloctane by sonication.

[1] Markus Lackinger, et al., Langmuir 2005, 21, 4984-4988.

O 18.34 Mon 18:30 Poster F

FT IRRAS Studies of Potential-Controlled Transformations of a Monolayer of Dibenzylviologen adsorbed on a Cu(100) Electrode Surface — •Melanie Röefzaad, Duc Thanh Pham, Peter Broekmann, and Klaus Wandelt — Institut für Physikalische und Theoretische Chemie, Universität Bonn

Fourier transform infrared reflection absorption spectroscopy (FT IRRAS) has been combined with cyclic voltammetry (CV) to monitor the potential induced transformations of a monolayer formed by the redox-active 1,1′-dibenzyl-4,4′-bipyridinium (dibenzyl-viologens or DBV) on a chloride pre-covered Cu(100) electrode surface. Both the dication (DBV^{2+}) and the radical cation ($DBV^{+\cdot}$) could be detected. The DBV^{2+} has been found to adsorb at positive electrode potentials with its main molecular axis parallel to the surface in a nearly face-on orientation. Lowering the potential beyond the thermodynamic reduction potential results in a phase transition with the $DBV^{+\cdot}$ molecule in a more side-on orientation. These results are well consistent with previous in situ STM studies [1] where a distinct phase transition from a "cavitand" phase to a polymeric stacking phase has been observed. Spectra of this polymeric phase showed also the same characteristic bands as were detected after dibenzyl-viologen adsorption at potentials where isolated dimers $(DBV^{+})_2$ on the surface have been observed. This indicates that the formation of both phases is based on the same π-π- and spin paring interactions so that dimers and polymers can be hardly distinguished by IR-spectroscopy only.

[1] Pham et al., New J. Chem., 30 (2006), 1439

O 18.35 Mon 18:30 Poster F

Potential induced phase transition of a Cu monolayer on a Au(1 0 0) surface — •Christian Schlaup, Peter Broekmann, and Klaus Wandelt — Institut für Physikalische und Theoretische Chemie, Universität Bonn, Wegelerstr. 12, D-53115 Bonn

Underpotential deposition of Cu on Au(h k l) electrodes has been studied extensively over the past. For underpotential deposition of Cu on Au(1 0 0) electrodes in sulfuric acid electrolytes, these in situ STM studies revealed a commensurate Cu(1 × 1) structure in which Cu adatoms occupy 4-fold hollow sites [1]. Additional quasi-hexagonal Cu adlayer structures with an intermediate coverage identified by STM were traced back to chloride contaminations caused by the reference electrode [1]. However, our own experiments revealed a reversible phase transition between the commensurate Cu(1 × 1) structure at potentials near to Cu bulk deposition and a stripe structure at more positive potentials, near to the dissolution of the Cu upd layer. This phase transition of the Cu adlayer was also observed after exchanging the deposition electrolyte for a blank sulfuric acid solution, pointing to a constant Cu coverage during the phase change. Within a single stripe of the anodic phase, the Cu-Cu distances are shortened perpendicular to the stripe direction whereas between different stripes the Cu-Cu distances are elongated. The potential depended appearance of the two phases points to a stabilisation of the reconstructed phase by (bi)sulfate anions.

[1] F.A. Möller, O.M. Magnussen, R.J. Behm, *Phys. Rev. B* **1995**, *51*, 2484.

O 18.36 Mon 18:30 Poster F

SXPS studies of viologens adsorbed on a halogenide precovered Cu(100) electrode — •Stephan Breuer[1], Thanh Pham Duc[1], Sascha Hümann[2], Peter Broekmann[3], Ralf Hunger[4], Thomas Mayer[4], and Klaus Wandelt[1] — [1]Institut für Physikalische und Theoretische Chemie, Universität Bonn, Wegelerstr. 12, 53115 Bonn — [2]Max-Planck-Institut für Eisenforschung GmbH, Max-Planck-Str. 1, 40237 Düsseldorf — [3]BASF AG, G-CAE/WED - M320, 67056 Ludwigshafen — [4]Institut für Materialwissenschaften, TU Darmstadt, c/o BESSY, Albert-Einstein-Str. 15, 12489 Berlin

We have studied the redox-chemistry of Dibenzyl(DBV)- and Diphenyl(DPV)-Viologenes adsorbed on a chloride and iodide precovered Cu(100) single crystal electrode using cyclic voltametry (CV), in-situ electrochemical scanning tunneling microscopy (ECSTM) and ex-situ X-ray photoelectron spectroscopy with synchrotron radiation at BESSY II (SXPS). From ECSTM it is known, that DBV undergoes a structural phase transition on the anion modified Cu(100) surface as a function of electrode potential. While a checkerboard like cavitand-structure at positive potentials is formed by DBV^{2+}- dications a stripe-phase at negative potentials consists of DBV$^{+\cdot}$-radical cations. This assignment is supported by the N1s-electron binding energies of 402 eV (dications) and 400,7 eV (radical cations) as measured by SXPS. DPV forms only a stripe-phase of radical-cations consistent with a N1s energy of 400,6 eV. No additional chloride or iodide anions are intercalated within the respective viologene layer, as concluded from the Cl2p and I4d signals, respectively.

O 18.37 Mon 18:30 Poster F

Adsorbate-adsorbate interactions at electrochemical interfaces: S/Cu(001) in HCl solution — •Andriy Taranovskyy, Tunay Tansel, and Olaf Magnussen — Institut für Experimentelle und Angewandte Physik, Universität Kiel, D-24098 Kiel, Germany

Following up our previous high-speed scanning tunneling microscopy study of sulfide tracer diffusion on Cu(001) in 0.01M HCl solution [1], we here present an analysis of the mutual motion of sulfide dimers in this system at room temperature. From the experimental video data histograms of the changes of the atomic configurations in subsequent frames were obtained. By fitting those to a theoretical model of dimer motion, based on solution of master equations, the hopping rates of S_{ad} in the presence of a neighboring S_{ad} were extracted. The pair interaction potential obtained from these rates shows an oscillatory distance dependence indicating anisotropic interactions. Also an influence of the electrode potential on the adsorbate interactions was observed.

[1] T. Tansel and O. Magnussen, Phys. Rev. Lett. 96, 026101 (2006).

O 18.38 Mon 18:30 Poster F

In-situ atomic-scale studies of the mechanisms and dynamics of bismuth electrodeposition by Video-STM — •Hisayoshi Matsushima[1], Erwin S. Lin[2], Sylvie Morin[2], and Olaf M. Magnussen[1] — [1]Institut für Experimentelle und Angewandte Physik, Universität Kiel, Kiel, Germany — [2]Chemistry Department, York University, Ontario, Canada

We present direct studies of mechanisms and dynamics of underpotential (UPD) and overpotential (OPD) electrodeposition of bismuth on Au(111) in 0.1 M HClO4 solution by in-situ high-speed scanning tunneling microscopy (Video-STM). Nucleation of Bi second layer islands in the OPD regime occurs heterogeneously at domain boundaries of the UPD layer, starting by trapping of isolated Bi adatoms. High-resolution images of the anisotropic (needle-like) growth [1] reveal the motion of bilayer kinks along the needle edges, indicating parallel growth of both layers.

[1] C. A. Jeffrey, D. A. Harrington and S. Morin, Surf. Sci., 512, L367 (2002)

O 18.39 Mon 18:30 Poster F

X-ray reflectivity studies of the liquid mercury-vapor and the liquid mercury-electrolyte interface — •Annika Elsen, Bridget Murphy, Jochim Stettner, and Olaf Magnussen — Institut für experimentelle und angewandte Physik der Universität Kiel, Leibnizstraße 19, 24118 Kiel

Although the liquid mercury-electrolyte interface is one of the most studied electrochemical systems, almost no structural data on this interface exists up to now. We recently started first investigations of this interface by synchrotron x-ray reflectivity. Here we discuss a new liquid mercury electrochemical cell design, for combined reflectivity and electrochemical measurements on the mercury surface covered with an electrolyte solution. The cell allows the insertion of a degassed mercury sample as well as dearated electrolyte solution under a high purity inert gas atmosphere. Preliminary electrochemical data and results of x-ray-reflectivity measurements on the liquid mercury-vapor and the liquid mercury-electrolyte interface using a laboratory source will be presented

O 18.40 Mon 18:30 Poster F

Au model anodes for Li-ion batteries studied by in-situ X-ray diffraction — •Frank Uwe Renner[1,2] and Hiroyuki Kageyama[2] — [1]MPI für Eisenforschung, Düsseldorf, Germany — [2]AIST, UBIQEN, Ikeda, Osaka, Japan

We present first results of experiments on the electrochemically-driven alloying and de-alloying of Au substrates with Li-ions from organic electrolytes studied by in-situ X-ray diffraction employing Synchrotron radiation. Au(111) single crystals, 111-textured thin Au films and nanometer-sized Au particles on HOPG have been examined using a specially designed in-situ X-ray cell. Starting from single crystalline Au systems we could follow the structural degradation and pulverization under different electrochemical conditions. Reciprocal lattice space maps show the occurrence of powder-like intensity associated with different Li-Au alloy phases. The diffraction data from the bulk Au crystals is compared with the Au(111) thin films and the behavior of the Au nano-particles on HOPG.

O 18.41 Mon 18:30 Poster F

Confined electronic state in small Co islands on Cu(100) — •Timofey Balashov[1], Albert F. Takacs[1], Markus Däne[2], Arthur Ernst[2], Patrick Bruno[2], and Wulf Wulfhekel[1] — [1]Physikalisches Institut, Universität Karlsruhe, Wolfgang-Gaede Strasse 1, 76131 Karlsruhe, Germany — [2]Max-Planck-Institut für Mikrostrukturphysik, Weinberg 2, 06120 Halle, Germany

We investigated the electronic structure of 3ML Co islands on Cu(100) with scanning tunneling microscopy and spectroscopy. A standing wave pattern was observed on the islands in the energy region from -50 to 100 meV with respect to the Fermi energy. We were able to extract the dispersion curve for this state by comparing the state energy on islands of different sizes, with different wavelengths of the standing wave pattern. The observed dispersion corresponds well to a minority Co band in theoretical band structure calculations.

O 18.42 Mon 18:30 Poster F

Mn/Cu(111): alloying, electronic and magnetic properties — Marko Kralj[1], Christian Breinlich[2], Sanja Krajinovic[1], Petar Pervan[1], Conrad Becker[2], and •Klaus Wandelt[2] — [1]Institute of Physics, Bijenicka 46, HR-10000 Zagreb — [2]Institut für Physikalische und Theoretische Chemie, Universität Bonn, Wegelerstr. 12, 53115 Bonn

Spin-split two-dimensional (2D) states which can, for instance, be realized in magnetically stabilized surface alloys, are of immense technological interest for new spintronic devices. For example, Mn/Cu(100)-c(2x2) is considered as a prototypical 2D magnetic alloy [1]. We have studied the interaction of manganese with a Cu(111) surface using different surface sensitive techniques. While the electronic structure and perfectness of a periodic root-3 alloy were characterized by ARPES and LEED, the electronic characteristics of the surface occupied by single Mn atoms were studied by STM and STS. STS at low temperature indicates no observable Kondo-effect for single Mn atoms. Increasing the temperature, leads to incorporation of Mn atoms into and below the surface layer and the appearance of very specific surface defect structures. Formation of this surface alloy first leads to the quenching of the Cu(111) surface state. Only after annealing higher than 500 K, when Mn atoms are incorporated several layers deep, leading to complex changes in the LEED pattern, ARPES indicates the appearance of a modified surface state. All this seems to indicate none or very weak magnetic and spin-splitting effects for Mn/Cu(111).

[1] M. Wuttig, Y. Gauthier, S. Blügel, Phys.Rev.Lett. 70 (1993) 3619.

O 18.43 Mon 18:30 Poster F

Co multilayers on diamond surfaces: Results from ab-initio studies — •Bernd Stärk, Peter Krüger, and Johannes Pollmann — Institut für Festkörpertheorie, Universität Münster

In recent years there has been an ever increasing interest in the development and understanding of metal-semiconductor hybrid systems. They may feature novel functionalities which are not feasible with metals or semiconductors alone combining, e.g., the high conductivity and spin-polarization of ferromagnets with the controllability of semiconductors.

In our work structural, electronic and magnetic properties of Co multilayers on diamond surfaces are investigated within the framework of density functional theory employing the local-spin-density approximation together with Gaussian orbital basis sets and norm-conserving pseudopotentials.

For one Co monolayer on a C(111)-(1×1) surface we find that Co adsorption in on-top positions is energetically most favorable. The attached Co monolayer has a weak magnetic moment of $0.69\,\mu_B$, much smaller than that of an isolated Co(0001) monolayer, which we find to be $1.88\,\mu_B$. This behavior can be attributed to the strong covalent bond forming between Co and C atoms. Adsorption of further Co(0001) layers results in a monotonous increase in the magnetic moment M_{top} of the topmost Co layer. In the case of four Co adlayers M_{top} is already close to the magnetic moment at the clean Co(0001) surface. The evolution of the magnetic moment with increasing number of Co adlayers will be discussed on the basis of the respective electronic structure.

O 18.44 Mon 18:30 Poster F

Crystal-induced surface state of Ni(111) modified by a h-BN overlayer — •Karen Zumbrägel[1], Christian Eibl[1], Kathrin Wulff[1], Matthias Hengsberger[2], and Markus Donath[1] — [1]Physikalisches Institut, Westfälische Wilhelms-Universität, Münster, Germany — [2]Physik-Institut, Universität Zürich, Switzerland

The physics of electronic states at surfaces and interfaces is a highly relevant topic in the context of miniaturised electronic devices. We have studied the influence of a monolayer boron nitride (BN) on Ni(111) with spin-resolved inverse photoemission. While interface states have already been identified and thoroughly studied with respect to their dispersion and spin polarization [1], the behaviour of the crystal-induced surface state of clean Ni(111) [2] upon BN adsorption remains controversial. Our spin-resolved results will be discussed along with theoretical and experimental work available in the literature.

[1] K. Zumbrägel, K. Wulff, Ch. Eibl, M. Donath and M. Hengsberger (to be published) [2] M. Donath, F. Passek, and V. Dose, Phys. Rev. Lett. **70**, 2802 (1993).

O 18.45 Mon 18:30 Poster F

Potential der Mehr-Elektronen-Einfang-Spektroskopie zur Untersuchung des Oberflächenmagnetismus — •Marco Busch, Stephan Wethekam und Helmut Winter — Humboldt-Universität zu Berlin, Institut für Physik, Newtonstraße 15, D-12489 Berlin

Unipan et al. [PRL 96 (2006) 177601; PRA 74 (2006) 062901] haben eine Methode zum Studium des Oberflächenmagnetismus vorgestellt. Sie beruht auf dem Zerfall autoionisierender He**-Zustände, die bei der Streuung von He^{2+}−Ionen an Oberflächen durch resonanten Elektroneneinfang formiert werden. Die relative Besetzung von Singulett- und Triplett-Zuständen wird zur Bestimmung der lokalen Spin-Polarisation von Ni(110) verwendet. Ausgehend von $T = 300$ K wird bei Erhöhung der Temperatur bis zu T_C auf eine Verringerung der Spin-Polarisation von -90% (bei 300 K) auf 0% geschlossen. In vergleichbaren Experimenten beobachten wir an Ni(110) eine ausschliessliche Besetzung von Singulett-Zuständen, die etwa 0,7 eV unterhalb E_F liegen, während der Triplett-Zustand (2,4 eV unterhalb E_F) nur sehr geringfügig besetzt wird. Eine signifikante Triplett-Population konnte am sauberen Ni(110) nicht nachgewiesen werden, sondern erst nach Adsorption von O_2 ($\ll$1 L) bei 300 K verbunden mit einer Erhöhung der Austrittsarbeit um bis zu 0,5 eV. Bei anschliessender Erhöhung der Temperatur bis zu T_C desorbiert der Sauerstoff vollständig und die Besetzung des Triplett-Zustandes nimmt wieder ab. Unsere Befunde legen daher nahe, dass die von Unipan et al. beobachteten Effekte auf Verunreinigungen des Ni(110) sowie deren thermische Desorption zurückzuführen und nicht mit dem Oberflächenmagnetismus korreliert sind.

O 18.46 Mon 18:30 Poster F

Magnetic properties of thin Fe films grown on GaAs(110) in a two-step process — Lars Winking, Martin Wenderoth, •Swante Sievers, Jan Homoth, and Rainer G. Ulbrich — IV. Phys. Inst., Georg-August-Universität Göttingen

Thin Fe films grown on GaAs at room-temperature (RT) or above in general suffer from As outdiffusion and the formation of nonmagnetic compounds at the heterointerface [1]. To avoid such a interdiffused interface we deposited thin Fe films of up to 5 ML thickness on in-situ cleaved GaAs(110) at 130 K and subsequently annealed them within 2 hours to RT in the second step. At RT we studied the in-plane magnetic anisotropy (IPMA) of the Fe films in UHV by means of the Magneto-Optical Kerr Effect (MOKE). Most noticeable and in contrast to Fe films grown at RT or above is the presence of a clear hysteresis already at 3.5 ML film thickness as well as an IPMA in [001] [2]. Recent results on the LT growth of thin Fe films on GaAs(001) suggest that these properties are due to the suppression of As outdiffusion [1]. This is substantiated by the square hysteresis loops. The absence of gradual magnetization reversals indicates single domain Fe films nearly free of defects or precipitates [3]. From these experimental results we deduce that reactions at the heterointerface can be efficiently suppressed by the two-step growth process. This work was supported by the DFG-SFB 602 TP A7

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O 18.47 Mon 18:30 Poster F

Mechanochemistry of thiolates on gold surfaces — •Jordi Ribas, Nisanth N. Nair, and Dominik Marx — Lehrstuhl fuer Theoretische Chemie, Ruhr Universitaet Bochum, 44780 Bochum

The capability to manipulate molecules on the atomic scale by Atomic Force Microscopy techniques has recently made it possible to induce and control chemical reactions and to construct new nanoscale architectures by applying external mechanical forces. The system consisting of thiolate molecules adsorbed on gold surfaces is not only well accessible to such experiments but previous theoretical work [1] has shown that it is possible to draw gold nanowires when alkylic thiolates are pulled off a stepped gold surface or off small gold clusters.

In this contribution we will present the results of the computational studies we have carried out to explore which nanostructures are generated and which chemical phenomena take place when other more complex thiolates rather than the alkylic ones are pulled off a gold surface. Specifically, we will compare the mechanochemical behavior of alkylic and aromatic thiolates and we will explore the mechanochemistry of bidentate and tridentate thiolates. These simulations have been performed by means of DFT static calculations and *ab initio* molecular dynamics calculations. Overall, our results have implications for the stability and degradation of molecule/metal junctions as used, for instance, in coatings and molecular electronics.

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O 18.48 Mon 18:30 Poster F

Optically monitored wet chemical preparation of SEIRA active metallic nanostructures — •Dominik Enders[1,2], Tadaaki Nagao[1,2,3], Tomonobu Nakayama[1,2], and Masakazu Aono[1,2,3] — [1]National Institute for Materials Science (NIMS), 1-1 Namiki, Tsukuba, Ibaraki, 305-0044, Japan — [2]Nanoscale Quantum Conductor Array Project, ICORP, JST, 4-1-8 Honcho, Kawaguchi, Saitama, 332-0012, Japan — [3]WPI Center for Materials Nanoarchitectonics (MANA), 1-1 Namiki, Tsukuba, Ibaraki, 305-0044, Japan

The use of wet chemical methods for the preparation of surface enhanced infrared absorption (SEIRA) active nanostructures has gained much interest in the last years because of its easiness, simplicity, and the low time consumption compared to the known ultra high vacuum based methods. We present a two-step wet-chemical preparation method of plasmonic SEIRA active nanostructures. While in the first step spherical Au nanoparticles are deposited on the SiO_2/Si surface, these nanoparticles are grown in the second step to form elongated tabular islands close to the percolation threshold. In situ monitoring of the preparation process by IR spectroscopy ensures the control of film morphology during the preparation process and enables the reproducible fabrication of highly sensitive SEIRA films [1].

A comparison of our Au films with SEIRA inactive Au films shows, that in IR spectra of octadecanethiol, the CH stretching vibrational peaks are enhanced by several orders of magnitude.

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O 18.49 Mon 18:30 Poster F

Microscale structure formation at the surface of the intercalation system $TaS_2 : Rb$ — Jens Buck[1], •Eric Ludwig[1], Florian Kronast[2], Kai Rossnagel[1], Hermann Dürr[2], and Lutz Kipp[1] — [1]IEAP, Uni Kiel — [2]BESSY, Berlin

Several effects at the surface of the transition metal dichalcogenide TaS_2 occuring under deposition of Rubidium have already been studied in the past, among them nanowire network formation and the well-known metal-insulator transition. Results from spatially resolved experiments such as PEEM reveal a variety of new surface structures at the microscale. The evolution of such structures at increasing Rb concentration was examined stepwise with regard to chemical composition and topography. In contrast to preliminary results, no creation of surface cracks could be observed. It is therefore suggested that crack formation strongly depends on the preparation conditions and the sample history. The PEEM measurements were performed at beamline UE49-PGMa at BESSY,Berlin.

O 18.50 Mon 18:30 Poster F

Electron confinement in nanostructures on Cu(111) — •Sebastian Wedekind, Guillemin Rodary, Dirk Sander, and Jürgen Kirschner — Max-Planck-Institut für Mikrostrukturphysik, Weinberg 2, D-06120 Halle(Saale)

The deposition of 0.7 ML Co onto the clean Cu(111) surface at room temperature leads to the formation of various nanostructures such as hexagonal and triangular vacancy islands on Cu(111), triangular Co islands and elongated rectangular stripes of Cu bounded by parallel dislocation lines. We study the electron confinement within these nanostructures by the means of scanning tunnelling microscopy (STM) and spectroscopy (STS) at 7 K and observe pronounced spatial modulation patterns in the electron local density of states (LDOS) of the nanostructures. We extract the wave-vector (k) of these LDOS modulation patterns in the electron energy range from -1 to $+1$ eV to obtain the electron dispersion relation. We obtain a discontinuous, step-like dispersion relation, which indicates wave-vector quantization according to $k_n = n\pi/d$, where d is the characteristic length of the nanostructure, and n integer [1]. A parabolic fit through the discrete k-states gives the surface state band edge $E_0 = -0.43 \pm 0.01$ eV and the electron effective mass $m^*/m_e = 0.39 \pm 0.01$, where m_e is the electron mass. For the Co islands we find $E_0 = -0.08 \pm 0.02$ eV and $m^*/m_e = 0.42 \pm 0.01$. The step-like dispersion relation also identifies the complete eigenstate-spectrum of the confined system.

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O 18.51 Mon 18:30 Poster F

Direct Writing of Nanostructures with an Electron-Beam in Ultra High Vacuum: Concepts, Results and Rerspectives — Michael Schirmer, Thomas Lukasczyk, Marie-Madeleine Walz, Florian Vollnhals, Miriam Schwarz, Hans-Peter Steinrück, and •Hubertus Marbach — Universität Erlangen-Nürnberg, Lehrstuhl für Physikalische Chemie II, D-91058 Erlangen

The engineering of nanostructures with controlled shape and chemical composition is of pivotal importance for a large number of technological applications as well as for fundamental research. In this work we discuss the generation of nanostructures by using an electron-beam in an ultra high vacuum (UHV) environment. The presented approaches are based on the capability of a high energy electron beam to locally modify adsorbed precursor molecules or the properties of the substrate. Our main method is the electron-beam induced deposition (EBID). The novel aspect is to work in an ultra clean environment, i.e., UHV, which allows us to overcome a hitherto existing limitation concerning the rather poor cleanliness of the deposits and the size limitation due to electron-beam spread in bulk substrates. The successful generation of clean metallic and oxidic nanostructures with lithographic controlled shapes and with lateral dimensions partially smaller than 10 nm on different substrates are reported. The underlying processes, the perspectives and applications of EBID in UHV as well as alternative methods to exploit an electron-beam for lithographic nanostructuring will be discussed. Supported by DFG grant MA 4246/1-1.

O 18.52 Mon 18:30 Poster F

Investigation of the low dimensional surface system Pt(110) by angle-resolved UV-photoemission — •Peter Amann, Mariana Minca, Michael Cordin, Alexander Menzel, and Erminald Bertel — Institute of Physical Chemistry, University of Innsbruck, Innrain 52a, A-6020 Innsbruck, Austria

Photoemission of low dimensional systems is of major importance for the investigation of correlation. The Pt(110) system provides quasi one dimensional d-derived surface resonances which bear a divergent DOS at the Fermi level due to a 2D saddle point topology. Therefore one can expect maxima in the response function at wave vectors connecting the saddle points. Furthermore a strong temperature anomaly of the adsorbate covered system Br/Pt(110) is observed. As the c(2x2) phase is cooled down from RT to 50K it undergoes a phase transition and two new phases, the (3x2) and the p(2x1), additionally appear [1]. The various surface systems as well as possible driving mechanisms (e.g. Fermi-surface nesting) for the transitions are discussed. Additionaly a detailed investigation of the saddle point topology is done by temperature dependent Fermi-surface measurements.

[1] E. Dona et. al. Phys. Rev. Lett. 89, 186101 (2007)

O 18.53 Mon 18:30 Poster F

Leed spot profile analysis of a quasi-one-dimensional system as a function of temperature — •Michael Cordin, Peter Amann, Enrico Doná, and Erminald Bertel — Institute of Physical Chemistry, University of Innsbruck, Innrain 52a, A-6020 Innsbruck, Austria

We employ low-energy electron diffraction (LEED) to investigate phase transition on the quasi-one-dimensional c(2x2)-Br/Pt(110) surface. Lowering the temperature yields a transition from a fluctuating, long range ordered phase at room temperature into an inhomogeneous state. From the LEED spot profile analysis we determine the temperature dependence of the fluctuations and the unusual reduction of the long range order parameter with falling temperature. Furthermore we observe the appearance of additional LEED spots corresponding to a primitive (2x1) and a (3x2) overstructure. The transition from the long-range ordered c(2x2) room temperature state to the inhomogeneous low-temperature state is completely reversible. The correlation length in the system is strongly anisotropic. The results agree with STM data showing the formation of striped disorder and local (2x1) and (3x2) domains at 60 K. DFT calculations yield a degeneracy of the three structures at 0 K. The formation of a long-range ordered state at 300 K out of a low-temperature disordered state seems in apparent contradiction with entropy considerations, but can be rationalised by assuming temperature-dependent interactions in the system. A possible explanation is a Peierls interaction in a surface resonance.

O 18.54 Mon 18:30 Poster F

Fundamental concepts for the structure formation of metalorganic networks based on oligopyridines and copper — •Achim Breitruck[1], Harry E. Hoster[1], Christoph Meier[2], Ulrich Ziener[2], and R. Jürgen Behm[1] — [1]Institute of Surface Chemistry and Catalysis, Ulm University, D-89069 Ulm — [2]Institute of Organic Chemistry III, Ulm University, D-89069 Ulm

We studied the structures of metalorganic coordination networks formed by Cu co-deposited with Bis-terpyridine (BTP) molecules on graphite (HOPG). BTP molecules have been shown to form highly ordered adlayers stabilized by C-H···N type hydrogen bonds.[1] Using these adlayers as precursors, subsequent deposition of Cu leads to a partial lift of the hydrogen bonds to allow for the formation of even more stable Cu···N-pyridine interactions.[2] Depending on the deposited amount of Cu and BTP and also on the sample temperature during and after Cu deposition we find a high variety of ordered metalorganic 2D structures. Despite this large variety, similar characteristic building blocks were observed, in which Cu centers are surrounded by BTP molecules to form chiral units like Cu$_n$BTP$_m$ (n = 1, 2; m= 3, 4)[2] out of achiral BTP's.

[1] H.E. Hoster, M. Roos, A. Breitruck, C. Meier, K. Tonigold, T. Waldmann, U. Ziener, K. Landfester, R.J. Behm, Langmuir 23, 11570-11579 (2007)

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O 18.55 Mon 18:30 Poster F

Electron-Beam Induced Deposition (EBID) for the Generation of Nanostructures on Inert Metal Single Crystal Surfaces — •Marie-Madeleine Walz, Michael Schirmer, Thomas Lukasczyk, Hans-Peter Steinrück, and Hubertus Marbach — Universität Erlangen-Nürnberg, Lehrstuhl für Physikalische Chemie II, D-91058 Erlangen

Nanoelectronic devices, quantum computing and the generation of specific catalytically active structures are some applications in the fast growing field of nanotechnology. The prerequisite in this field is the generation of nanostructures of high purity and defined shapes. For this purpose electron-beam induced deposition was applied under ultra high vacuum (UHV) conditions. With this method, adsorbed precursor molecules are locally cracked, mainly by secondary electrons resulting from the impact of a high energy primary electron-beam from a scanning electron microscope (SEM). After the successful generation of clean metallic and oxidic nanostructures on semiconductor and reactive metal substrates, this contribution focuses on inert metal surfaces as substrates. Thereby, unwanted processes, like the catalytic decomposition of the precursor molecules without electron exposure, should be reduced. The generation of metallic or oxidic nanostructures was performed with various organometallic precursor molecules. One example is the fabrication of titanium oxide nanostructures on a Au(111) surface using Ti(^{i}OPr)$_4$ as precursor molecule. The chemical composition was studied by local Auger electron spectroscopy (AES). The work is supported by DFG grant MA 4246/1-1.

O 18.56 Mon 18:30 Poster F

Deviation from pure s-wave scattering of surface-state electrons from adatoms — •Tobias Sonnleitner and Jascha Repp — Institute of Experimental and Applied Physics, University of Regensburg, 93040 Regensburg

Surface state electrons on the close-packed surfaces of noble metals form a two-dimensional nearly-free electron gas. The scattering of the electrons off adatoms generates standing wave patterns in the electron density, which can be directly observed with the scanning tunneling microscope. Analysis of the standing wave patterns provides a direct way to determine the scattering properties of the adatoms. So far it has been widely accepted that metal adatoms act as s-wave scatterers due to the efficient screening of the adatom potential by bulk electrons. However, a deviation from a pure s-wave scattering would only express itself in the fraction of the standing wave pattern arising from multiple scattering events. This fraction is rather small since adatoms act as ideal absorbing black scatterers. Therefore, it is not obvious from the experimental point of view, that the assumption of a pure s-wave scattering is justified. To this end we have studied isolated pairs of copper adatoms on a clean Cu(111) substrate surface. The standing-wave patterns around these pairs have been analyzed in numerous different arrangements in order to average out effects from other scattering centers far away. In comparison to calculated patterns the fraction of these patterns arising from multiple scattering events has been extracted.

O 18.57 Mon 18:30 Poster F

Non-linear Optical Properties of Nanostructured Metal Surfaces — •Heike Arnolds[1], Natalia Garcia[1], Simon J. Henley[2], and J. David Carey[2] — [1]Surface Science Research Centre, University of Liverpool, Oxford Street, Liverpool, L69 3BX, UK — [2]Nano-Electronics Centre, Advanced Technology Institute, School of Electronics and Physical Sciences, University of Surrey, Guildford GU2 7XH, UK

Nanosecond pulsed-laser irradiation of Ag and Ni thin films was employed to produce nanostructured Ag/SiO$_2$ and Ni/SiO$_2$ substrates. By tailoring the laser fluence, it is possible to controllably adjust the mean diameter of the resultant near-spherical metal droplets [1]. We have investigated the nonlinear optical properties of these nanostructured films and find a strong enhancement of femtosecond infrared-visible sum and difference frequency yields by two to three orders of magnitude, depending on the exact size and shape of the metal droplets. The likely cause of the enhancement is the excitation of plasmons in the infrared and visible regions of the spectrum and the concomitant electric field enhancement near the metal droplets. We discuss the use of these films for plasmon-enhanced photochemistry.

[1]S.J. Henley, J.D. Carey, and S.R.P. Silva, Appl. Phys. Lett. 88, 081904 (2006)

O 18.58 Mon 18:30 Poster F

STM analysis of the fluctuations at 2D phase boundaries between ordered and disordered organic adlayers — •Thomas Waldmann, Harry E. Hoster, and R. Jürgen Behm — Institute of Surface Chemistry and Catalysis, Ulm University, D-89069 Ulm, Germany

The dynamic equilibrium between distinct 2D phases of organic molecules on Ag(111)-oriented films on Ru(0001) at room temperature are studied by time resolved STM. As recently found, the parallel chain structure (PCS) [2] formed by a bis(terpyridine) derivative (2,4'-BTP)[1] can be produced coexistent with a disordered 2D molecular adlayer [2]. At the boundaries between both phases a continuous exchange of molecules takes place with equal rates. At room temperature, these fluctuations are too fast for direct STM-observation, even at scan rates of 5 images s^{-1}. Adapting the approach previously applied to analyse the step dynamics at metal surfaces [3], we evaluated the displacement of the phase boundary in single scan lines as a function of time. The results are discussed in comparison with 2D phase equilibria observed at other coverages [4] and with metal step fluctuations.

[1] C. Meier, U. Ziener, K. Landfester, P. Weihrich, J. Phys. Chem. B 109, 21015 (2005)

[2] M. Roos, H.E. Hoster, A. Breitruck, R.J. Behm, Phys. Chem. Phys. 9, 5672 (2007)

[3] M. Giesen, S. Baier, Atomic transport processes on electrodes in liquid environment, J. Phys.: Condens. Matter 13, 5009 (2001)

O 18.59 Mon 18:30 Poster F

Modes in dielectric loaded surface plasmon polariton waveguides — •Jan Renger[1], Maria Ujué González[1], Sukanya Randhawa[1], Romain Quidant[1], Sébastien Massenot[2], Jonathan Grandidier[2], Alexandre Bouhelier[2], Gerard Colas des Francs[2], Laurent Markey[2], Jean-Claude Weeber[2], and Alain Dereux[2] — [1]ICFO-Institut de Ciencies Fotoniques, 08860 Castelldefels (Barcelona), Spain — [2]Institut Carnot de Bourgogne, UMR 5209 CNRS-Université de Bourgogne, F-21078 Dijon Cedex, France

Surface plasmon polaritons (SPPs) existing at metal/dielectric interfaces feature a high confinement of the electromagnetic field, which make them very promising for small photonic devices and biochemical sensors. Dielectric loading of the metal surface by thin dielectric layers, such as SiO$_2$, can be used to alter the SPP effective mode index n$_{eff}$. In this way, optical elements can be designed by patterning the dielectric layer to get areas with different n$_{eff}$. In particular, SPP waveguides can be obtained by depositing thin SiO$_2$ stripes on top of gold films. We analysed the SPPs on dielectric loaded waveguides having a width down to 100 nm by leakage radiation microscopy. The imaginary part of n$_{eff}$ - therewith the propagation length - was measured in the object plane; the real part of n$_{eff}$ was determined in the Fourier plane. The measured propagation length for very narrow dielectric stripes is close to the SPP propagation length at the bare metal interface. For increasing width of the dielectric stripes, the additional modes contribute and the propagation length is reduced to the value at an infinite extending dielectric loaded metal film.

O 18.60 Mon 18:30 Poster F

Ab initio study of oxygen adsorption and initial incorporation in Pd-Pt alloy — •Arezoo Dianat, Manfred Bobeth, and Wolfgang Pompe — Institut fuer Werkstoffwissenschaft, Technische Universitaet Dresden, Germany

In order to get insight into the catalytic behavior of the bimetallic alloy Pd-Pt, the adsorption of oxygen on the alloy surface as well as the initial oxygen incorporation have been studied by means of density-functional theory. Due to segregation processes the composition of the near-surface layers of the alloy is in general different from the bulk composition. In this work, ordered bulk phases (L1$_0$,L1$_2$) of Pd$_x$Pt$_{1-x}$ with compositions $x = 0.25$, 0.5, 0.75 as well as different compositions and atom configurations of the two outermost layers have been investigated. Adsorption energies for oxygen adsorbed *on* the (111) alloy surface and for oxygen in sub-surface position have been calculated for different oxygen coverages (0.25 to 1 ML). In the case of oxygen adsorption *on* the surfaces, the highest adsorption energy at low oxygen coverage ($\leq$ 0.25 ML) has been found for the Pd$_{0.5}$Pt$_{0.5}$ composition o f the two outermost layers, whereas at higher coverage the oxygen binding energy is highest for a Pd-rich first monolayer and Pt-rich second monolayer. Interestingly, on the latter layer system the oxygen adsorption energy is higher than on pure Pd(111). Oxygen occupation of sub-surface sites starts at a coverage of 0.5 ML for all alloy models considered. The calculated oxygen adsorption energy depends only weakly on the bulk composition. It increases slightly with Pt bulk concentration, but it differs less than 50 meV.

O 18.61 Mon 18:30 Poster F

Growth and characterization of single-wall carbon nanotubes for electronic and optical applications — •Hans Kleemann, Philipp Zeigermann, Michael Blech, Mathias Steglich, and Bernd Schröter — Universität Jena, Institut für Festkörperphysik, Max-Wien-Platz 1, 07743 Jena, Deutschland

A controlled growth of carbon nanotubes with particular structural and electronic properties at predefined positions on solid substrates is a prerequisite to utilize them in electronic or nanooptical devices. We grow single-wall nanotubes by thermal chemical vapour deposition (CVD) on various substrates like silicon, fused silica and sapphire as well as on silicon carbide. Metal films are vacuum-evaporated to catalyze the growth of high-purity single-wall nanotubes by CVD using methane as precursor gas. The quality of nanotubes is tested by raman and x-ray spectroscopy: residual catalyst amount and contamination is in general lower than the detection limits of these techniques. The morphology and orientation of the nanotubes is characterized by scanning electron and atomic force microscopy. A preferred orientation is observed on the (single-crystalline) surface of sapphire.

O 18.62 Mon 18:30 Poster F

Self-selection and Error Correction in Multi-ligand Supramolecular Networks at Surfaces — •Steven L. Tait[1], Alexander Langner[1], Nian Lin[1], Chandrasekar Rajadurai[2], Mario Ruben[2], and Klaus Kern[1,3] — [1]Max-Planck-Institut für Festkörperforschung, Stuttgart — [2]Forschungszentrum Karlsruhe GmbH — [3]Ecole Polytechnique Fédérale de Lausanne, Switzerland

Supramolecular networks stabilized by metal–organic coordination can be designed to self-organize in regular, two-dimensional lattices at surfaces, whose dimensions and properties can be controlled by selection of the organic ligand components. This approach offers a natural and highly efficient alternative to current nano-fabrication methods and provides a model system for (bio-)molecular assembly. With high-resolution scanning tunneling microscopy of such networks, we demonstrate structural error correction during assembly achieved by active molecular self-selection. Experiments were made by deposition of Fe atoms and organic ligands at the Cu(100) surface. Binary mixtures of complementary ligands allow for constructions of highly-ordered 2D arrays of compartments, whose shape and size can be predictably programmed by modular ligand replacement. Redundant mixtures of ligands of different sizes demonstrate the ability of the system to correct structural errors and achieve a high degree of order by sorting themselves into rows according to molecule size. We contrast this with a ligand mixture where the energy landscape of the intermolecular interactions does not activate an error correction mechanism, but rather provides a route for structural error tolerance.

O 18.63 Mon 18:30 Poster F

Growth of SiGe nanoislands on prestructured silicon substrates — •Marlen Schulze, Anne-Kathrin Gerlitzke, and Torsten Boeck — Institute for Crystal Growth in the Forschungsverbund Berlin e. V.

Coherently strained and highly ordered silicon-germanium nanoscale pyramids on silicon, grown by liquid phase epitaxy (LPE) via the Stranski*Krastanov growth mechanism are very interesting objects to reduce the size of semiconductor devices. Generally, LPE is very well appropriate to study fundamental atomistic processes at the liquid-solid interface because it operates very close to thermodynamical phase equilibrium.

A patternlike array of SiGe nanostructures has been realised on prestructured silicon substrates. Si (100) substrates have been patterned by squarelike oxide stripes using local oxidation nanolithography in an atomic force microscope (AFM). The width of the stripes is precisely controlled by progress of the lateral oxidation. Subsequently, LPE was employed to grow SiGe nanoislands on the prepatterned substrates. The truncated pyramids are arranged within the oxide-free cavities directly along the stripes. The final island size significantly probes an effectively lowered lattice mismatch, i.e. a locally expanded crystal lattice in noncovered areas of the silicon substrate.

O 18.64 Mon 18:30 Poster F

Surface- induced handedness in adsorbed layers — •Philipp Schmidt-Weber[1], Thorsten Kampen[1], Arantzazu Mascaraque[2], Rocio Cortez[2], Jan-Hugo Dil[1], and Karsten Horn[1] — [1]Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin — [2]Universidad Autonoma de Madrid, Spain

Molecules that are achiral in the gas phase may acquire a chiral character through the loss of symmetry elements, which has a strong influence on their arrangement in long-range ordered structures. We have studied stilbene and its derivates, using STM, LEED and photoemission with the aim of identifying such ordering processes. Dicarboxystilbene (DCSB) loses its carboxyl hydrogen atom when adsorbed on Cu(110), and acquires a handedness on the surfaces which is readily seen in STM images. The two enantiomers then arrange in different long-range ordered structures (”herringbone” and ”parquet” patterns), which themselves possess a handedness, i.e. they exist in a dextro- and laevo- form. Using STM images in which both the substrate and the adsorbate are imaged with atomic resolution, we were able to identify two distinct types of adsorption sites as basic building blocks of the long-range structures. One of these (the ”parquet” pattern) is enantiomerically pure, while the other (”herringbone”) is a racemic structure. The fact that the latter is the thermodynamically stable one can be understood from general thermodynamic principles.

O 18.65 Mon 18:30 Poster F

Comparative study of the structure formation by two different bis(terpyridine)derivates (BTP) on HOPG — •Michael Roos[1], Christoph Meier[2], Daniel Caterbow[2], Harry E. Hoster[1], Ulrich Ziener[2], and R. Jürgen Behm[1] — [1]Institute of Surface Chemistry and Catalysis, Ulm University, D-89069 Ulm, Germany — [2]Institute of Organic Chemistry III, Ulm University, D-89069 Ulm, Germany

Depostition of BTP molecules on HOPG by evaporation in UHV or from solution leads to large domains of highly ordered structures, which are stabilized by C-H···N type hydrogen bonds [1-3]. The energetically most favorable molecule-molecule configuration can be modified by varying the position of the N-atoms within the BTP molecules. Furthermore, depending on the deposited amount and the deposition conditions (solvent and concentration), a large variety of ordered structures is obtained. The possibility to describe these structures as a sum of localized molecule-molecule and molecule-substrate interactions is discussed. In addition, the role of dynamic effects like molecule mobility and rotation for the stability of the different phases is considered.

1. H. E. Hoster et al., Langmuir 23, 11570 (2007).
2. A. Breitruck et al., Surf Sci 601, 4200 (2007).
3. C. Meier et al., J Phys Chem B 109, 21015 (2005).

O 18.66 Mon 18:30 Poster F

SERS and single-molecule SERS in metallo-dielectric structures — •Manuel Rodrigues Gonçalves, André Siegel, and Othmar Marti — Ulm University, Institute of Experimental Physics, Albert-Einstein-Allee 11, D-89081 Ulm, Germany

Surface enhanced Raman scattering (SERS) refers to a technique to enhance the Raman scattering cross section of few molecules adsorbed on metallic surfaces, in order to achieve high enhanced spectra. Despite its success as a chemical identification technique at very low molecular concentrations, its main drawbacks are the extreme sensitivity to the electromagnetic enhancements of the metallic structures, the poor reproducibility, and the fabrication of structures with defined strong field enhancements at specific wavelengths.

Single-molecule SERS requires very high field enhancements, of the order of 10^{14}. The Raman spectra of very few, or single molecules present a blinking behaviour. It is commonly accepted that the blinking is characteristic of the Raman spectra of single molecules, adsorbed at metallic clusters or structures with extreme enhancements.

We have fabricated metallo-dielectric structures suitable for SERS using colloidal crystals as templates. The fabrication of the structures is reproducible. FEM and FDTD calculations indicate that very high field enhancements can be expected. Experiments using a confocal Raman microscope find blinking SERS at the predicted locations. This is an indication of a low number of molecules in the detection volume.

O 18.67 Mon 18:30 Poster F

Nanosecond-laser interference pattering at 266nm wavelength — •Mike Hettich, Stephen Riedel, Paul Leiderer, and Johannes Boneberg — University of Konstanz, Departement of Physics, D-78457 Konstanz, Germany

Direct laser interference patterning by ns-laser pulses allows producing periodic surface structures in a single illumination step. For that purpose thin metallic films (Au, Ta) or Si wafers are irradiated by two or more interfering laser beams. The local intensity variations achieved in this way induce lateral flow of material. We show that this enables achieving structures with a periodicity down to 150nm, if the fourth harmonic of a ns-Nd:YAG-laser is used. Upon moving the substrate laterally between the first and subsequent illumination steps, structure periods below $\lambda/2$ can be realized.

O 18.68 Mon 18:30 Poster F

SERS on micro-fabricated sharp-etched nanostructures — •Henrik Schneidewind[1], Uwe Hübner[1], Dana Cialla[2], Roland Matthes[1], Jörg Petschulat[3], Siegmund Schröter[1], and Jürgen Popp[1,2] — [1]Institute of Photonic Technology (IPHT), Albert-Einstein-Straße 9, 07745 Jena, Germany — [2]Friedrich-Schiller-University Jena, Department of Physical Chemistry, Jenaer Biochip Initiative (JBCI), Helmholtzweg 4, 07743 Jena, Germany — [3]Friedrich-Schiller-University Jena, Institute of Applied Physics, Center for Ultra-Optics, Max-Wien-Platz 1, 07743 Jena, Germany

We introduce highly reproducible metallic nanostructure arrays which can be used as active substrates for the Surface Enhanced Raman Spectroscopy (SERS). The arrays were prepared by means of e-beam lithography, vacuum deposition, and ion-beam etching. The sharp-edged gold nanostructures with corner radii smaller than 20 nm are arranged in arrays with a periodicity of 200 nm. Sharp-edged structures were chosen instead of round dots, which are easier to prepare, in order to achieve large enhancement factors by using the lightning rod effect. The resonance frequency of the arrays was determined by using UV-Vis-spectrometry in order to select the excitation wavelength for SERS experiments. The arrays showing uniform SERS-signals across the whole field size of 0.2 mm in edge length are ready for practical use, which will be shown using a dye as test substance.

O 18.69 Mon 18:30 Poster F

In-situ Etching of self-organized InAs/GaAs (001) Quantum Dots — •Theresa Lutz[1], Takayuki Suzuki[1], Lijuan Wang[1], Suwit Kiravittaya[1], Armando Rastelli[2], Oliver G. Schmidt[2], Giovanni Costantini[1], and Klaus Kern[1,3] — [1]Max Planck Institute for Solid State Research, Stuttgart — [2]Leibniz Institute for Solid State and Materials Research, Dresden — [3]Ecole Polytechnique Fédérale de Lausanne, Switzerland

It is well known that the epitaxial growth of InAs on GaAs(001) leads to the development of strain induced nanoscale islands with high crystalline quality. Because of the enormous potential for device applications there is a great interest in understanding the growth process in detail. Even though there are a lot of experimental results concerning the growth of quantum dots, the physics behind it is not completely understood yet. Recently, it has been shown that during growth a transition takes place from small shallow faceted pyramidal islands to bigger and steeper islands, so-called domes. We use selective InAs in-situ etching to systematically modify the island size. The result is a backward transition of the islands as a function of the etching time. The details of the shape transition are discussed taking into account the non-uniform composition of the islands. This demonstrates that the shape of the quantum dots depends on their size and composition, which is typical for processes close to thermodynamic equilibrium.

O 18.70 Mon 18:30 Poster F

Fabrication of Cobalt clusters by pulsed laser deposition — •Markus Trautmann, Christian Pansow, Matthias Büenfeld, Veit Grosse, Frank Schmidl, and Paul Seidel — Institut für Festkörperphysik, Friedrich-Schiller-Universität Jena, Helmholtzweg 5, D-07743 Jena

Besides Fe and Ni (and different Fe-/Ni-compounds) Co is a catalyst material used in synthesis of carbon nanotubes (CNTs). Clusters can be formed for example by annealing of thin Co films which are usually produced by sputtering technique or electron beam evaporation. To get applicable clusters for the growth of CNTs thin films of about 1 nm are required. In this work we use pulsed laser deposition (PLD). This method enables low deposition rates of less than 0,04 monolayers per pulse using a 99,99 % Co target and a KrF excimer laser. We present our experimental set up for PLD under different vacuum conditions to produce Co layers on SiO_2-coated Si-substrates. First results of surface and film analysis using different methods as atomic force microscopy (AFM), x-ray diffraction (XRD), scanning electron microscopy (SEM) and Auger electron spectroscopy (AES) will be presented.

O 18.71 Mon 18:30 Poster F

Production of patterned metal clusters using Focused Ion Beams (FIB) — •Farhad Ghaleh[1], Niklas Grönhagen[1], Heinz Hövel[1], Lars Bruchhaus[2], Sven Bauerdick[2], Jürgen Thiel[2], and Ralf Jede[2] — [1]Technische Universität Dortmund, Exp. Physik I, Dortmund — [2]Raith GmbH, Dortmund

Nanometer sized pits on HOPG substrates can be used as nucleation centers to produce clusters with a narrow size distribution. In previous experiments [1] nanometer sized pits were produced by sputtering and oxidizing the sample. As a result we get nanopits which are a few nanometers wide and only one monolayer deep, distributed at random locations on the surface.

In the present study a focused beam of gallium ions is used to produce nanopits in a given pattern on the substrate. The FIB instrument (Raith ionLiNE) is capable of a resolution below 10 nm [2]. Using the nanopits as nucleation centers we are able to produce patterned gold islands as well as patterned silver clusters by depositing metal atoms.

Furthermore the nanopit distribution on the surface in combination with Monte Carlo simulations helps investigating the ion beams, e.g. ion distribution, recoils as well as the penetration depth of the ions [3]. In this respect the oxidation of HOPG-samples provides a method to study the ion impact effects.

[1] H. Hövel, Appl. Phys. A 72, 295 (2001)

[2] J. Gierak et al.: Appl. Phys. A 80, 187 (2005)

[3] F. Ghaleh, R. Köster, H. Hövel, L. Bruchhaus, S. Bauerdick, J. Thiel, R. Jede: J. Appl. Phys. 101, 044301 (2007)

O 18.72 Mon 18:30 Poster F

In-situ Scanning Tunneling Microscope studies of the ripening process of InAs Quantum Dots on GaAs during Growth in the MOVPE — •M. Guderian, R. Kremzow, M. Pristovsek, and M. Kneissl — TU Berlin, Institut für Festkörperphysik, EW 6-1, Hardenbergstr. 36, D-10623 Berlin, Germany

Quantum dots (QD) are highly interesting for a number of different applications, like single photon emitters or semiconductor lasers. For industrial applications these optoelectronic devices are mainly grown by metal organic vapour phase epitaxy (MOVPE) systems which allows mass fabrication. QD growth has been studied intensely, but the understanding of the mechanisms responsible for the formation of the QDs and especially of the ripening process is still poor. In order to investigate the dynamics of the ripening process and to clarify the theory of QD ripening we employed our novel in-situ scanning tunnelling microscope (STM) technique which allows measurements directly during MOVPE growth. In this presentation we will discuss the ripening process of InAs QDs on GaAs(001):Si at 475°C where the development of the surface was analysed directly with the in-situ STM. Ex-situ AFM measurements showed a big scattering of the data, due to different substrates and varying cooling rates, while the in-situ measurements showed clear trends in RMS roughness and size distributions. E.g. the dot density decreased proportional to e^{-1} while the average dot size increased. In comparison of different ripening theories our experimental result follows the classical Ostwald ripening theory for the InAs on GaAs(001):Si system.

O 18.73 Mon 18:30 Poster F

Melting behaviour of metallic nanostructures — •Daniel Benner, Anja Habenicht, Paul Leiderer, and Johannes Boneberg — Universität Konstanz, Fachbereich Physik, LS Leiderer, 78457 Konstanz

Triangular flat metallic nanostructures and metallic films of identical thickness on inert substrates (e.g. glass, silicon) are illuminated by single intensive nanosecond laser pulses with fluences at and above the melting threshold and the melting behaviour of these two systems is compared.

For the metallic thin films we determine the melting threshold by nanosecond time-resolved reflectivity measurements which can be used to deduce the melting time. Upon melting of the nanostructures a dewetting process sets in which also reduces the reflected intensity. Our measurements show that the dewetting process of the nanostructures sets in at laser intensities well below the melting threshold of the films. For the dimensions of the nanostructures used here (thickness ˜50nm, lateral dimensions ˜ 200nm) reduced melting temperatures are not expected. Therefore we assign that behaviour to the increased absorption cross section of the nanostructures.

O 18.74 Mon 18:30 Poster F

Preparation and Characterization of Gold Nanocrystals on the native Oxide Layer of Si-Surfaces — •Jawad Slieh, Andreas Winter, Aaron Gryzia, Armin Brechling, Wiebke Hachmann, and Ulrich Heinzmann — Molecular and Surface Physics, Bielefeld University

We report on the fabrication of gold crystals in the size range between one hundred nm and several μm, using a combination of a sputter and an annealing technique. Gold was deposited on the native oxide layer of freshly cleaned silicon wafer pieces (10×10 mm^2) in an inert gas sputtering chamber at a rate of 5 nm/min. Subsequently the samples were transferred into a UHV chamber and annealed for several hours at temperatures between 800°C and 1000°C. The deposited gold layer thickness and the annealing temperature and time have been studied systematically. After preparation, the gold crystals were characterized by means of different techniques such as Atomic Force Microscopy (AFM), Transmissions Electron Microscopy (TEM), Scanning Electron Microscopy (SEM), X-Ray Diffraction (XRD) and Laue Diffraction.

These different sized gold crystals will be used in a diffraction experiment (Laue configuration) with a micro focus x-ray tube (Oxford Instruments UltraBright) in order to estimate the minimal crystal size for the observation of diffraction spots of individual gold crystals. First results of these experiments will also be discussed.

O 18.75 Mon 18:30 Poster F

Mass selected Co clusters in contact with semiconductor surfaces — •Viola v. Oeynhausen, Kristian Sell, Ingo Barke, and Karlheinz Meiwes-Broer — Institut für Physik, Universität Rostock, Universitätsplatz 3, 18051 Rostock

Metal-semiconductor structures are of substantial technical relevance since Schottky-barrier based devices are fundamental elements of high-speed electronic applications. Metal nanoparticles on semiconductor surfaces can be seen as a model system for such devices. The Scanning Tunneling Microscope (STM) provides insight in transport properties on nanometer scale and at low temperature. Furthermore, it reveals the geometric structure and shape of clusters, an important prerequisite for understanding the detailed electronic and magnetic properties. We produce mass-selected Co clusters with an Arc Cluster Ion Source (ACIS) and deposite them onto Si(111)7x7 and Ge(001) under UHV conditions. These are ideal substrates due to their well-known electronic structure and simple preparation under UHV conditions. They serve as a reference in STS measurements, thus minimizing tip-induced artefacts. Macroscopic Cobalt surfaces show dominant, highly localized d-states near the Fermi level . Such states are proposed to cause interesting effects like Kondo interaction and spin modulation of captured surface state electrons.

O 18.76 Mon 18:30 Poster F

Study of supported metal Clusters and nano Dots with time and energy resolved PEEM — •Martin Rohmer[1], Christian Schneider[1], Michael Bauer[2], Heinz Hövel[3], Farhad Ghaleh[3], and Martin Aeschlimann[1] — [1]Technische Universität Kaiserslautern, 67663 Kaiserslautern — [2]Institut für Experimentelle und Angewandte Physik, Universität Kiel, 24118 Kiel — [3]Experimentelle Physik I, Universität Dortmund, 44221 Dortmund

The ultrafast dynamics associated with collective (plasmon) excitations as well as single electron excitations in supported clusters is addressed with high lateral resolution by means of the time- and energy resolved two-photon Photoemission Electron Microscopy (TR-2PPEEM). Experiments performed at different cluster and nanostructured systems show that this setup is capable to map even very small particle to particle variations in the hot electron lifetime of the order of a few femtoseconds [1]. The high temporal sensitivity of time-resolved PEEM to these inhomogenities arises from the parallel data acquisition mode intrinsic to this technique. It significantly reduces the resolution limiting influence of systematic error arising from temporal fluctuations in the experimental parameters. Here we report about the potential and our progress in measuring electron live times in silver clusters and nano dots.

[1] Mapping the femtosecond dynamics of supported clusters with nanometer resolution, M. Rohmer, F. Ghaleh, M. Aeschlimann, M. Bauer, H. Hövel; Eur. Phys. J. D, Online First

O 18.77 Mon 18:30 Poster F

Image-potential states at (001) surfaces of alkaline-earth metal oxides — •Björn Baumeier, Peter Krüger, and Johannes Pollmann — Institut für Festkörpertheorie, Universität Münster, Wilhelm-Klemm-Str. 10, 48149 Münster

We present the results of a comparative *ab initio* study of the atomic and electronic structure of MgO, CaO, SrO and BaO and their relaxed (001) surfaces. Based on density functional theory, we use self-interaction-corrected pseudopotentials which permit a reliable description of electronic properties, in particular. The calculated bulk and surface geometric structures are consistent with well established literature data. The bulk electronic structure turns out to be in very good agreement with the results of quasiparticle calculations and experiment. Concerning surface electronic properties, the calculations reveal, in particular, that MgO(001), CaO(001) and SrO(001) exhibit negative electron affinity while BaO(001) does not. As a consequence, not only bound surface states which are localized at the surface occur in the former three cases but also a salient band of image-potential states appears in sections of the surface Brillouin zone which reside in vacuum in front of the surface. Such image-potential states do not arise at the BaO(001) surface.

The image-potential states at MgO(001) are compared to traditional image-potential states at Cu(001) and to traditional surface states at MgS(001), respectively. This exemplary comparision reveals details of the peculiar nature of the image-potential states at (001) surfaces of alkaline-earth metal oxides.

O 18.78 Mon 18:30 Poster F

Tensor LEED study of the surface relaxation of SrF$_2$(111) — •Stephan Härtel, Jochen Vogt, and Helmut Weiss — Chemisches Institut der Otto-von-Guericke-Universität Magdeburg, Universitätsplatz 2, D-39106 Magdeburg

The knowledge about the surface relaxation of other insulators than the alkali halides is comparatively weak yet. Experimental work was carried out for instance for CaF$_2$(111) and BaF$_2$(111) [1] which both crystallize in the fluorite structure. Very often those two compounds are treated together with the homologous material SrF$_2$ but up to now there are no quantitative experimental results available for the surface relaxation of this alkaline earth fluoride. In the present work the SrF$_2$(111) surface was investigated by means of LEED in an energy range from 80 to 320 eV. The recorded I(E) data were analyzed using the tensor LEED approach. The topmost F$^-$ layer in the first F-Sr-F triple layer is shifted inward by 0,13±0,07 Å whereas the Sr^{2+} layer does not exhibit a significant shift. The following F$^-$ layer is also relaxed towards the bulk by 0,07±0,07 Å which is in the range of the measuring accuracy. No significant changes of the ion positions in the deeper triple layers were observed. The results are in qualitative good agreement with a theoretical calculation [2] for SrF$_2$(111).

[1] Vogt, J. et al., Surf. Sci. **578** (2005)

[2] Jockisch et al., J. Phys.: Cond. Matt. **5** (1993)

O 18.79 Mon 18:30 Poster F

Exploring Optical Properties of MgO Films with an STM — •Hadj Mohamed Benia, Philipp Myrach, Niklas Nilius, and Hans-Joachim Freund — Fritz-Haber-Institut, Berlin, Germany

Electron injection from the tip of an STM is used to stimulate local photon emission from the surface of a thin MgO film on Mo(001). Depending on the excitation energy, several emission regimes are identified on the basis of the energy and the spatial distribution of the emitted photons. At low excitation bias, tip-induced plasmons are preferentially excited in the tip-sample gap, carrying little information on the oxide. With increasing tip bias, radiative electron transitions between field-emission resonances dominate the optical response. Their dependence on the local work function allows mapping of this quantity across the oxide film. Intrinsic optical modes of the MgO, e.g. radiative decays of excitons, are only observed when operating the STM in the field emission regime.

O 18.80 Mon 18:30 Poster F

Diffraction of fast atoms and molecules during grazing scattering from a LiF(001) Surface — •Andreas Schüller, Stephan Wethekam, and Helmut Winter — Humboldt-Universität zu Berlin, Institut für Physik, Newtonstraße 15, 12489 Berlin

Neutral atoms and molecules with energies from 300 eV up to some 10 keV are scattered under a grazing angle of incidence from a clean and flat LiF(001) surface. For scattering along low index directions in the surface plane ("axial surface channeling") we observe defined patterns in the intensity distributions for scattered atoms which can be attributed to diffraction effects [1, 2]. The data can be understood by diffraction of fast atoms at the surface where the symmetry of the crystal lattice and of the interaction potential between atom and surface determine the diffraction pattern. The periodicity of the surface potential follows the geometrical arrangement of surface atoms and determines the angular position of diffraction peaks. The corrugation of the surface potential determines the characteristic intensity modulations of these diffraction peaks which can be observed also for fast and for heavy atoms, where diffraction based on the periodicity of the crystal lattice can not be resolved. Such so called "supernumerary rainbows" allows one to derive the corrugation of atomic interaction potentials in the eV regime with high accuracy.

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[2] P. Rousseau, H. Khemliche, A.G. Borisov, and P. Roncin, Phys. Rev. Lett. 98, 016104 (2007).