O 59: Poster Session II (Nanostructures at surfaces: Dots, particles, clusters; Nanostructures at surfaces: arrays; Nanostructures at surfaces: Wires, tubes; Nanostructures at surfaces: Other; Plasmonics and nanooptics; Metal substrates: Epitaxy and growth; Metal substrates: Solid-liquid interfaces; Metal substrates: Adsoprtion of organic / bio molecules; Metal substrates: Adsoprtion of inorganic molecules; Metal substrates: Adsoprtion of O and/or H; Metal substrates: Clean surfaces; Density functional theory and beyond for real materials)

Time: Wednesday 17:45–20:30 Location: Poster B1

O 59.1 Wed 17:45 Poster B1

Monte Carlo simulations of nucleation processes on prepatterned surfaces — •Stefan Frieder Hopp and Andreas Heuer — Institut für Physikalische Chemie, Universität Münster, 48149 Münster, Germany

The properties of template-directed nucleation are studied on a microscopic level by applying the kinetic Monte Carlo method. In this context, the conditions for full nucleation control as well as the progression of cluster growth with increasing coverage are investigated. The shape and the height of the clusters are discussed for 1D and 2D patterns with reference to the experimental observations.

It is shown that the simulation results of a continuous Monte Carlo algorithm can be approximated quite well using a discrete Monte Carlo technique based on the lattice gas model. In the course of this approach the latter algorithm is modified by the introduction of barriers depending on the particular diffusion process on the surface. Furthermore, the underlying discrete pair potential is adjusted to the Lennard-Jones potential. The application of the discrete method leads to a dramatic reduction of simulation time and thus allows in particular a more detailed comparison with experimental data.

O 59.2 Wed 17:45 Poster B1

Analysis of surface nucleation processes with a coarse-grained Monte Carlo (CGMC) method — •Tanja Mues and Andreas Heuer — Institut für physikalische Chemie, WWU Münster, 48149 Münster, Germany

The properties of template-directed growth on surfaces are the topic of this work. The theoretical study of the nucleation process has been performed via a particle based method (Monte Carlo (MC)) and with the help of a concentration field (finite-difference scheme (FD)) in our working group. We introduce a new CGMC method, combining four sites of a square lattice to one coarse-grained cell. Thereby we connect the MC method with the FD method, which differ in time and length scale. In other CGMC methods [1] boundary effects, which are necessary in the simulation of nucleation processes, are neglected. Therefore, we use fine-grid simulations to compute the average jump rate between two neighbouring cells by numerical sampling (before the MC-simulation) regarding boundary effects of every cell. With this new method, we analyse the nucleation behaviour via the radial distribution function g(r) and the nucleation density.

[1] Markos A. Katsoulakis and Dionisios G. Vlachos. Coarse-grained stochastic processes and kinetic monte carlo simulators for the diffusion of interacting particles. The Journal of Chemical Physics, 119(18):9412-9427, 2003.

O 59.3 Wed 17:45 Poster B1

The height of size selected Ag clusters on C_{60} films — •Natalie Miroslawski[1], Niklas Grönhagen[1], Kolja Mende[1], Stefanie Duffe[1], Bernd von Issendorff[2], Michael Moseler[2,3,4], and Heinz Hövel[1] — [1]TU Dortmund, Experimentelle Physik I — [2]Universität Freiburg, Fakultät für Physik — [3]Fraunhofer Institut für Werkstoffmechanik, Freiburg — [4]Freiburger Materialforschungszentrum

Mass selected clusters from Ag_{55}^+ to $Ag_{138\pm2}^+$ were soft landed at 77 K on C_{60}/Au(111) and imaged with STM at 77 K. We observed extremely narrow cluster height distributions. The cluster heights are constant up to Ag_{80}^+ which can be explained assuming an icosahedrical shape for Ag_{55}^+ and the formation of caps of silver atoms at the rim of the clusters for larger sizes. A remarkable change in height occurs between Ag_{80}^+ and Ag_{88}^+ clusters. An additional monolayer formed at the top cluster facet might be responsible. Ag_{88}^+ and Ag_{95}^+ have the same height, $Ag_{138\pm2}^+$ is larger and corresponds to the height of the closed shell icosahedral cluster $Ag_{147\pm2}^+$. It was possible to deposit different cluster masses onto one sample. Although the deposition spots were deposited in close proximity, we were able to separate them clearly. Experiments with scanning tunnelling spectroscopy (STS) at 5 K hint to notable differences between our measurements on C_{60}/Au(111) and previous measurements on C_{60}/HOPG.

O 59.4 Wed 17:45 Poster B1

Deposition of silver nanoparticles on to thin films of ionic liquid on SiO2 — •E. Pachomow[1], O. Höfft[2], M. Marschewski[1], W. Maus-Friedrichs[1], and F. Endres[2] — [1]Intitut für Physik und Physikalischen Technologien, Technische Universität Clausthal, Leibnizstr. 4, 38678 Clausthal-Zellerfeld — [2]Institut für Mechanische Verfahrenstechnik, Technische Universität Clausthal, Arnold-Sommerfeld-Str. 6, 38678 Clausthal-Zellerfeld

Ionic liquids(IL) are a highly interesting group of solvents for electrochemical processes - mainly due to the combination of their high electrical conductivity, their electrochemical stability and their ability to dissolve a wide range of compounds[1]. Due to the low vapor pressure ionic liquids can be used in UHV. In this work the influences of ionic liquid films on the growth of silver nanoparticles on SiO2 were investigated. Here, monolayers of 1-ethyl-3-methylimidazolium bis(trifluoromethylsulfonyl)amide [EMIM]Tf2N on SiO2 were produced by vapor deposition. On these layers silver was evaporeted. The chemical composition and electronic strucrure of the silver-IL-SiO2 interface was characterized by metastable induced electron spectroscopy(MIES) and photoelectron spectroscopy(XPS, UPS(HeI)). The particles size distribution was determined with AFM. We compare these resultes with measurements on silver deposited on pure SiO2. We find that due to the ionic liquid films the particles size is increased. [1] F. Endres, S. Zein El Abedin, Phys. Chem. Chem. Phys., 8(2006)2101

O 59.5 Wed 17:45 Poster B1

THECLA - Setup of a THErmal CLuster Apparatus — •Sabrina Hennes, Stefanie Duffe, and Heinz Hövel — TU Dortmund, Experimentelle Physik I, Otto-Hahn-Str. 4, 44221 Dortmund, Germany

THECLA is a THErmal CLuster Apparatus which produces clusters by supersonic nozzle expansion [1,2]. It enables optical spectroscopy of clusters in a free jet and of the same clusters deposited on substrates or in a matrix material. A hot-cathode plasma ionisation [3] and a moveable Faraday cup for ion-current measurement are installed for an in-situ determination of the cluster mass. Using the cluster velocity of the supersonic expansion, the ion-displacement by an electric field perpendicular to the cluster beam can be used to determine the cluster mass. In addition time-of-flight measurements can be used to analyse the cluster velocity and mass [1]. In first experiments we studied the plasmon resonance of Ag clusters deposited on SiO_2 in vacuum and exposed to air. Using the same samples it is planned to perform XANES measurements of the L-absorption edge at the synchrotron radiation source DELTA to gain detailed information about the structure, the chemical environment and changes of the unoccupied density of states of those clusters [4,5].

[1] O. F. Hagena, Z. Phys. D 20, 425 (1991). [2] H. Hövel et al., Phys. Rev. B 48, 18178 (1993). [3] I. M. Goldby et al., Rev. Sci. Instrum. 68, 3327 (1997). [4] O. Sipr et al., J. Synchrotron Rad. 6, 770 (1999). [5] A. Bzowski et al., Phys. Rev. B 49, 13776 (1994).

O 59.6 Wed 17:45 Poster B1

Photoconductivity of metal nanoparticle ensembles supported by localized surface plasmon polariton resonances (LSPPRs) — •Elena Vashchenko[1], Tigran Vartanyan[2], Frank Träger[1], and Frank Hubenthal[1] — [1]Universität Kassel, 34132 Kassel, Germany — [2]SPbSU ITMO, 197101 Saint-Petersburg, Russia

Owing to their specific properties, various kinds of dispersive systems attract great interest of researchers. Intriguing examples of such systems are metal nanoparticle ensembles (MNEs), which exhibit superior optical properties. Recently, the electric properties of such MNEs have found increasing attention. MNEs represent interlinked systems, which can be used as light driven electric devices.

In this contribution we demonstrate a LSPPR driven photoconductivity in silver and sodium nanoparticle ensembles. For this purpose MNEs were prepared on dielectric substrates and afterwards characterized by extinction spectroscopy and atomic force microscopy. The extinction spectra of the MNEs showed pronounced LSPPRs at wavelengths below the threshold of the external photo effect in the corresponding bulk metal. Subsequently a voltage has been applied to the MNEs and the current has been measured. We found that the current through the illuminated MNEs is more than one order of magnitude higher compared to the current without illumination. The strongest increase is obtained for wavelengths that are in resonance with the LSPPR of the MNEs. A theoretical interpretation of the observed phenomena based on the reduction of the tunneling barrier for the photoexcited electrons is provided.

O 59.7 Wed 17:45 Poster B1

Photochemical particle growth in ordered two-dimensional arrays

— •Axel Seidenstücker[1], Thomas Härtling[2], Alfred Plettl[1], Phillip Olk[2], Paul Ziemann[1], and Lukas Eng[2] — [1]Universität Ulm, Institut für Festkörperphysik, 89069 Ulm (Germany) — [2]TU Dresden, Institut für Angewandte Photophysik, 01062 Dresden (Germany)

A novel procedure is reported which allows the controlled manipulation of the size of metal nanoparticles. The technique is demonstrated here on two-dimensional particle arrays of gold nanoparticles (diameter 10 nm), fabricated by means of diblock copolymer micelle lithography (BCML), but can in principle be applied to any kind of ordered structures. The particles are used as nucleation centers in seed-mediated photochemical metal deposition, whereby the particle diameter increases. Repeatedly combining photochemical growth with annealing steps facilitates controlling the particle shape as well as their uniformity.

O 59.8 Wed 17:45 Poster B1

Characterization of Fe_2O_3-Nanotubes prepared by ALD

— •Markus Sproll[1], Ulf Wiedwald[1], Christian Pfahler[1], Alfred Plettl[1], Paul Ziemann[1], and Julien Bachmann[2] — [1]Institut für Festkörperphysik, Universität Ulm, D-89069 Ulm — [2]Institut für Angewandte Physik, Universität Hamburg, D-20355 Hamburg

Metallic nanoparticles from a micellar technique or colloidal polystyrene (PS) particles with diameters of 100 nm are used to generate nanomasks on Si and SiO_2. Dip-coating the latter ones onto a pre-treated substrate permits the deposition of monolayers over areas up to 20 mm^2. Anisotropic separation and subsequent isotropic etching in an oxygen plasma reduces the size of the PS-particles down to the desired diameter. In case of the metallic Nanoparticles, the diameter can be varied by photoseeding [1]. Using both types of particles as a mask for anisotropic reactive ion etching (RIE), arrays of nano-pores can be fabricated with variable depth and diameter [2].
An Atomic Layer Deposition (ALD) process with ferrocene is used to refill the pores. After removing the top layer on the substrate, the remaining magnetic nanotubes can be investigated. In a furnace or a hydrogen plasma the Fe_2O_3 tubes are reduced to Fe_3O_4 or even metallic Fe. SQUID measurements of all these states will be presented.

[1] A. Seidenstücker - poster at this conference,
[2] A. Plettl et al., Adv. Funct. Mater. **19**, 3279 (2009).

O 59.9 Wed 17:45 Poster B1

Enhanced LED emission by ordered metallic nanoparticle arrays

— •Tino Göhler[1], David Gottwald[1], Stefan Grafström[1], Jürgen Moosburger[2], and Lukas M. Eng[1] — [1]Institut für Angewandte Photophysik, Technische Universität Dresden, D-01062 Dresden — [2]OSRAM Opto Semiconductors GmbH, D-93055 Regensburg

The external quantum efficiency of light-emitting diodes (LEDs) based on AlGaAs is limited by the total internal reflection because of the high refractive index (typically between 3 and 4) of the semiconductor. Metal nanoparticles (MNPs) can be used as dipole scatterers in order to enhance this LED emission. We investigated arrays of MNPs, produced by Fischer pattern nanolithography [1] on top of both high-index substrates and on the LED itself. Light that would otherwise remain trapped inside the substrate is coupled out by both grating coupling and resonant plasmonic scattering. Here, we present 2D and 3D calculations based on the multiple-multipole method [2] of the light output produced by an array of MNPs of different sizes and distances, and then compare these findings with our experimental results.

[1] U.Ch. Fischer and H.P. Zingsheim, J. Vac. Sci. Technol. 19 (1981) 881

[2] C. Haffner, Post-modern Electrodynamics: Using Intelligent MaXwell Solvers. Wiley, (1999)

O 59.10 Wed 17:45 Poster B1

Exploring the CoPc@HOPG interface: STM and STS study

— •Lars Smykalla, Marius Toader, Pavel Shukrynau, and Michael Hietschold — Chemnitz University of Technology, Institute of Physics, Solid Surfaces Analysis Group, D-09107 Chemnitz, Germany

Using an UHV VT-STM, we report results obtained on a submonolayer of cobalt(II)-phthalocyanine (CoPc) grown on Highly Oriented Pyrolytic Graphite (HOPG) by OMBD. The very low deposition rate has allowed the formation of large defect-free self-assembled organic domains, mainly governed by the molecule-molecule interaction, where sometimes different orientation of the molecules with respect to each other leads to the development of relatively new type of structure. Nevertheless, the reported coexistence of molecular multi-phases has to be discussed in terms of the epitaxial relation between the organic adlayer structure and substrate surface orientation. Tip-sample distance-dependent scanning tunneling spectroscopy studies have been addressed in order to understand the electronic properties at the organic-inorganic interface. The observed shift in the molecular levels induced by the current set point variation is discussed and compared with the energy level diagram obtained by single molecule DFT calculations.

O 59.11 Wed 17:45 Poster B1

Exploration of critical parameters in production of nano structures with Focused Ion Beams

— •Stefan Balk[1], Lukas Patryarcha[1], Karl Bauer[1], Axel Rudzinski[2], Lars Bruchhaus[2], and Heinz Hövel[1] — [1]TU Dortmund, Experimentelle Physik I — [2]Raith GmbH, Dortmund

Surface defects on highly orientated polycrystalline graphite (HOPG) were produced with Focused Ion Beams (FIB) in a pattern of squares with varying ion doses using the ionLiNE FIB-Tool (Raith GmbH). Thereafter the sample was oxidized at 500 °C for a duration of 200 minutes with 2% O_2. Only defect-rich areas oxidize completely and form nanocavities, which are nanopits deeper than 10 mono layers (ML). The gallium ions have a dose independent maximum penetration depth of about 50 nm at 25 keV. STM and AFM measurements show the existence of a critical ion dose at 20 $\mu As/cm^2$ where the transition from nanopit to nanocavity appears. Below 20 $\mu As/cm^2$ only a few ML deep nanopits are formed. Above 20 $\mu As/cm^2$ nanocavities with an increasing depth up to 50 nm were detected. The results have a good match with TRIM simulations of the produced defect density. The critical defect density is $6,25 \cdot 10^{-3}$ defects/$\AA^3$. We plan to use these results to realize isolated nano structures of HOPG by treatment of thin films of HOPG on insulator materials.

O 59.12 Wed 17:45 Poster B1

Electrodeposition of free-standing regular arrays of metallic nanowires using template synthesizing technique

— •Nina Winkler, Yong Lei, and Gerhard Wilde — Institut für Materialphysik, Westfälische Wilhelms-Universität Münster, Wilhelm-Klemm-Str. 10, 48149 Münster

The fabrication of free-standing metallic nanowires with a template synthesizing method is investigated.

Magnetic nanowires may serve as high density perpendicular recording hard disks to avoid the superparamagnetic limit of nanometer-sized metallic structures.

Due to the high pore regularity of porous anodic alumina membranes, they serve as templates for the electrochemical growth of metallic nanowires. The alumina membranes were fabricated by a two-step anodization process of aluminum foils in oxalic and sulfuric acids. The insulating alumina barrier layer should be removed for electrodeposition of metallic nanowires. A method for perforating this barrier layer is presented in this work. A voltage pulse profile is applied for the electrodeposition processes with a potentiostat to achieve regular nanowires. The total time for the deposition is depending on the desired length of the nanowires.

After the deposition of the metals, the alumina membranes are removed by acidic etching to realize free-standing metallic nanowires.

Their magnetic properties are investigated.

O 59.13 Wed 17:45 Poster B1

One-dimensional ZnO nanostructures and their property investigation — •Peter Hess, Yong Lei, and Gerhard Wilde — Institut für Materialphysik, Westfälische Wilhelms-Universität Münster

One-dimensional (1-D) ZnO nanostructures were systematically investigated concerning their micro-structures and properties. The main focus of this work is on the assembly of thin and well-aligned nanowires to investigate their optical properties. The ZnO 1-D structures were prepared using a Chemical Vapour Deposition (CVD) system with ZnO/C mixtures as sources, Au-coated silicon or sapphire as substrates, and an argon and oxygen gas flow as a distributor and oxidation source. Depending on the conditions during the CVD process, different kinds of ZnO nanostructures were obtained. The morphology of the ZnO nanostructures was checked by SEM while the optical properties (photoluminescence) were investigated using a spectrometer. Additionally, the crystalline structures, the growth direction, and the lattice spacing of ZnO nanostructures were characterized using TEM. First experiments were also conducted using porous alumina membranes as templates to obtain very thin and well-aligned ZnO nanowires.

O 59.14 Wed 17:45 Poster B1

Growth and photoluminescence of carbon-nanotubes laying on silicon substrates — •Peter Löptien[1,2], Shigeru Moritsubo[1], Tomoaki Murai[1], and Yuichiro K. Kato[1] — [1]Institute of Engineering Innovation, University of Tokyo, Tokyo 113-8656, Japan — [2]Institute of Applied Physics, University of Hamburg, Jungiusstr. 11, 20355 Hamburg, Germany

Carbon nanotubes are self-assembled one-dimensional systems with exceptional electronic properties. Depending on their structure they are either metallic or semiconducting. In this project, semiconducting carbon nanotubes were investigated with photoluminescence spectroscopy. Starting with a bare silicon wafer, islands were defined by e-beam-lithography. Cobalt acetate with silica nanoparticles were deposited as islands acting as catalysts in the chemical vapor deposition growth process. The obtained nanotubes on and in between the islands were revealed by scanning electron microscope images and Raman spectroscopy. According to our photoluminescence data and previous results, there is a signal from air-suspended carbon nanotubes, but no signal from carbon nanotubes laying on the wafer in between the islands. The samples were treated with surfactants in an attempt to obtain micelle-encapsulated nanotubes showing photoluminescence even when they are in contact with the surface.

O 59.15 Wed 17:45 Poster B1

Structural and electronic properties of Au induced nanowires on Ge(001) — •Tijs Mocking, Daan Kockmann, Arie van Houselt, Bene Poelsema, and Harold Zandvliet — MESA+ instute for Nanotechnology and University of Twente, Enschede, The Netherlands

The structural and electronic properties of Au induced self-organized nanowires on Ge(001), prepared by different procedures, are investigated with scanning tunnelling microscopy and spectroscopy at room temperature and 77 K [1]. The Au induced nanowires are comprised of dimers that have their bond aligned in a direction perpendicular to the nanowire. The dimers are buckled, leading to a 2x periodicity along the nanowires. Dimers located at anti-phase boundaries are dynamic and flip back and forth between two buckled configurations. The troughs between the nanowires have a depth of several atomic layers. Finally, the differential conductivities of the nanowires and the troughs are very comparable in magnitude.

[1]. D. Kockmann, A. van Houselt, T.F. Mocking, B. Poelsema and H.J.W. Zandvliet, Journal of Physical Chemistry C 113, 17156 (2009).

O 59.16 Wed 17:45 Poster B1

Investigation of the geometric structure of one-dimensional Au nanowires on the Ge(001) surface with STM and LEED — •Sebastian Mietke[1], Melanie Klinke[1], Tatjana Podlich[1], René Matzdorf[1], Christian Blumenstein[2], Jörg Schäfer[2], Sebastian Meyer[2], and Ralph Claessen[2] — [1]Fachbereich Naturwissenschaften, Experimentalphysik II, Universität Kassel, 34132 Kassel, Germany — [2]Physikalisches Institut, Universität Würzburg, 97074 Würzburg, Germany

The deposition of Au on a clean Ge(001) surface yields one-dimensional (1D) structures, so-called nanowires. Using the techniques of low-temperature scanning tunneling microscopy (LT-STM) and low-energy electron diffraction (LEED), it could be demonstrated that the resulting surface reconstruction exhibits excellent $c(8\times2)$ long-range order. Since the wires are confined to atomic dimension, this system renders an ideal playground for the study of 1D physics, such as the charge density wave (CDW) or a Luttinger liquid. Experimentally, we find in addition to the $c(8\times2)$ structure that a fourfold superstructure along the wire direction exists over a wide temperature range. As the origin of the superstructure, the appearance of a CDW could be excluded by using scanning tunneling spectroscopy. By studying occupied and unoccupied states with the STM it could be shown that the nanowires consist of Au chains of single atom dimension.

O 59.17 Wed 17:45 Poster B1

Micromanipulation of individual InAs nanowires — Kilian Flöhr[1], •Marcus Liebmann[1], Kamil Sladek[2], Hilde Hardtdegen[2], Thomas Schäpers[2], Detlev Grützmacher[2], and Markus Morgenstern[1] — [1]II. Institute of Physics, RWTH-Aachen University and JARA-FIT, 52074 Aachen, Germany — [2]Institute of Bio- und Nanosystems (IBN-1), Jülich Aachen Research Alliance (JARA), Forschungszentrum Jülich, 52425 Jülich, Germany

We investigated methods to manipulate InAs nanowires using micromanipulators, an optical microscope as well as atomic force microscopy with the goal to produce InAs tips for scanning tunneling microscopy. Within the optical microscope, the InAs wires with diameters of approximately 100 nm and length up to 12 μm can be identified as colored stripes (1000 magnification) due to the diffraction of light. The wires, which have been grown by metalorganic vapor phase epitaxy (MOVPE) on a GaAs wafer without catalyst, could be picked up individually using the sharp corner of a doubly cleaved wafer exploiting adhesion forces. Later, the wires are placed onto a desired position at the edge of another wafer. Contacting of the wires is accomplished using indium microsoldering [1], which leads to a two-point resistance down to 1.5 kΩ. First STM measurements, however, did not reveal a tunneling current probably due to oxidation of the tip. Different etching procedures have been tested in order to remove the oxide of the wire.

[1] C. Ö. Girit and A. Zettl, Appl. Phys. Lett. 91, 193512 (2007).

O 59.18 Wed 17:45 Poster B1

Nanoline templates for single atom wires on Si(001) — •Sigrun A. Köster[1], James H. G. Owen[1], François Bianco[1], Daniel Mazur[1], Alvaro Rodriguez-Prieto[2], David R. Bowler[2], and Chrisoph Renner[1] — [1]Université de Genève, Section Physique/DPMC, Quai Ernest-Ansermet 24, 1211 Genève 4, CH — [2]London Centre for Nanotechnology (LCN), University College London, UCL 17-19 Gordon Street, WC1H 0AH, London, UK

Low dimensional structures are of wide scientific and technological interest. The physics of single atom metallic wires is already described in detail by theory, but a more systematic experimental verification is still desirable. The experimental problems are mainly caused by the difficulties of growing electronically isolated wires which is necessary to test the expected properties from existing theories. Here we introduce templates on a Si(001) surface which enable the growth of self-assembled single atom wires on top of them. The main template consists of a Si reconstruction called the Haiku structure[1] which develops underneath self-assembled Bi nanowires[2]. By hydrogenation the Si surface can be passivated and additionally the Bi dimers are stripped off while the underlying reconstruction of the Si surface remains intact. In addition the Bi nanowire by itself can be considered as a template[3].

[1] J.H.G.Owen, K.Miki, H.Koh, H.W.Yeom and D.R.Bowler, Phys. Rev. Lett. 88, 226104 (2002) [2] J. H. G. Owen, K. Miki, and D. R. Bowler, J. Mater. Sci. 41, 4568 (2006) [3] J. H. G. Owen and K. Miki, Nanotechnology 17, 430 (2006)

O 59.19 Wed 17:45 Poster B1

Iron-Induced Reconstructions on the Ge(001) Surface: a Scanning Tunneling Microscopy Study — •Michael Lochner[1,2], Christian Blumenstein[1], Jörg Schäfer[1], and Ralph Claessen[1] — [1]Physikalisches Institut, Universität Würzburg, 97074 Würzburg — [2]Fachbereich Naturwissenschaften, Universität Kassel, 23132 Kassel

Low-dimensional systems can be realized by self-organized arrays of adatoms on semiconductor surfaces. In the last years, significant advances have been made in the growth and spectroscopy of nanowire systems, especially on Ge(001). A fascinating and still open question is whether one can grow such structures with magnetic atoms, which might lead to spin-ordered chains.

Here we study the growth of Fe atoms on Ge(001) by scanning tunneling microscopy (STM). Deposition of Fe at $\sim 400^\circ$C substrate temperature leads to formation of two different Fe-induced reconstructions: A (2×1) reconstruction exhibiting chain-like character, and a c(4×2) reconstruction that shows a two-dimensional architecture. The structural features for both phases as seen in STM, as well as their occurence in the phase diagram will be discussed in detail.

O 59.20 Wed 17:45 Poster B1

Conductive AFM on Supramolecular Assemblies — •Carsten Hentschel[1], Daniel Ebeling[1], Lin Jiang[1,2], Harald Fuchs[1], and Lifeng Chi[1] — [1]Center for Nanotechnology (CeNTech) and Physikalisches Institut, Westfälische Wilhelms-Universität Münster, Germany — [2]present address: School of Materials Science and Engineering, Nanyang Technological University, Singapore

Based on the continuous reduction of electronic device sizes there is an increasing interest in conductors of molecular dimensions. As a result of these molecular dimensions the atomic force microscope (AFM) has developed for a suitable standard tool for surface analysis in this range.

However, among the mechanical characterisation it is possible to measure electrical properties of samples by this technique. Therefore, a conductive cantilever tip is scanned over a sample surface while a bias voltage is applied between tip and sample. With an external current amplifier the local current between tip and surface is measurable [1-2].

Here we will present a method to perform conductivity measurements with nanoscopic resolution on supramolecular assemblies. Therefore, the topographical images and current maps are simultaneously recorded in order to study the electrically behaviour on a length of about several micrometers.

[1] H. Dai, E. W. Wong, C. M. Liebert, Science 272 (1996)

[2] P. J de Pablo et al., Phys. Rev. Lett. 88 (2002) 036804

O 59.21 Wed 17:45 Poster B1

Pentacene on insulators and the growth of nanocrystals: an STM study with submolecular resolution — •Alexander Kabakchiev[1], Klaus Kuhnke[1], Theresa Lutz[1], and Klaus Kern[1,2] — [1]Max Planck Institut für Festkörperforschung, Stuttgart, Germany — [2]Ecole Polytechnique Fédérale de Lausanne, Lausanne, Switzerland

Pentacene has become the drosophila of single molecule imaging. Molecular orbital maps in conjunction with tunneling spectroscopy provide new insight in the local electronic structures of model adsorbates. We use the dewetting of Pentacene films on thin insulating layers to grow nanocrystals a few nm high and base dimensions of several 100 square nanometers. Scanning tunneling microscopic (STM) topography reveals steep crystal edges reaching down to the bare insulator. Submolecular spatial resolution allows to image molecular orbitals on top of the crystal and to determine the local molecular structure. We demonstrate that in contrast to thin film structures so far found on insulators, the crystallites forming on KCl layers below room temperature exhibit a bulk-like phase with the long molecular axis oriented parallel to the surface. Comparison of scanning tunneling spectroscopy for the crystal phase with isolated molecules on the insulator layer indicates a shift of the molecular orbitals to lower binding energies.

O 59.22 Wed 17:45 Poster B1

Ion induced surface topography evolution of Cu — •Maria Lenius[1], Reiner Kree[2], and Cynthia A. Volkert[1] — [1]Institut für Materialphysik, Georg-August-Universität Göttingen — [2]Institut für Theoretische Physik, Georg-August-Universität Göttingen

Ion beam sputtered surfaces develop complex patterns that depend on crystal and ion beam parameters. The patterns are controlled by the interplay of various mechanisms such as surface curvature dependent sputtering, channelling effects, anisotropic and temperature dependent diffusion as well as ion induced diffusion processes and are not fully understood.

This work systematically considers the influence of crystal orientation dependent surface energy as a driving force. The sputter erosion profiles of Cu grains with various crystal orientations have therefore been investigated as a function of dose and ion beam incidence using a focused ion beam microscope. The resulting patterns with amplitudes up to 150 nm and wavelengths of about 0.5 um were characterized using SEM, AFM, and EBSD. Those investigations provide indications that surface energy minimization has an impact on pattern formation.

O 59.23 Wed 17:45 Poster B1

Focused electron beam induced processing in UHV: "nanowriting" with an electron-beam as a pen and precursor molecules as ink — Florian Vollnhals, Marie-Madeleine Walz, Michael Schirmer, Thomas Lukasczyk, Hans-Peter Steinrück, and •Hubertus Marbach — Lehrstuhl für Physikalische Chemie II and Interdisciplinary Center for Molecular Materials (ICMM), Friedrich-Alexander-University Erlangen-Nuremberg, Egerlandstr. 3, 91058 Erlangen

In this contribution we aim towards the generation of arbitrarily shaped naonostructures with well defined chemical composition by focused electron beam induced processing (FEBIP) of either adsorbed precursor molecules or the substrate itself. The electron beam irradiation of adsorbed precursor molecules results in the local decomposition and thus the deposition of non-volatile fragments (electron beam induced deposition, EBID). In our distinct "surface science approach" to EBID we could show that working in an ultra clean environment, i.e. in ultra high vacuum (UHV), is advantageous in terms of cleanliness and partially size of the generated deposits. Recently we could also explore the localized activation of an oxide surface by an focused electron beam, such that $Fe(CO)_5$ dosed after the exposure is decomposed at the irradiated area, resulting in clean iron deposits. Results and principles of the described techniques will be presented and discussed as an engineering tool to generate or modify nanosized objects. This work was supported by the Deutsche Forschungsgemeinschaft under grant MA 4246/1-1.

O 59.24 Wed 17:45 Poster B1

Characterization of Plasmonic Nanoantennas for Enhanced High Harmonic Generation by 2P-TOF-PEEM — •Soo Hoon Chew[1], Adrian Wirth[2], Frederik Süssmann[2], Nils Weber[3], Matthias Escher[3], Sergey Zherebtsov[2], Jürgen Schmidt[1], Michael Hofstetter[2], Matthias Kling[2], Mark Stockman[4], Ferenc Krausz[1,2], and Ulf Kleineberg[1] — [1]Department of Physics, University of Ludwig-Maximilians, Garching, Germany — [2]Max Planck Institute of Quantum Optics, Garching, Germany — [3]Focus GmbH, Hünstetten Kasselbach, Germany — [4]Georgia State University, Altanta, USA

Metallic bowtie nanostructures have recently been demonstrated to enhance high harmonic generation from noble gases attributing to resonant plasmon field enhancement in the vicinity of nanostructures driven by femtosecond laser pulse excitation. Two-photon photoelectron emission microscopy (2P-PEEM) is a powerful tool to image the near field enhancement and "hot spot" photoemission from plasmonic nanostructures. Besides imaging the spatial electron distribution, the photoelectrons kinetic energy distribution within the nanostructures can be mapped using a time-of-flight (TOF) detector coupled to the 2P-PEEM. We have characterized various plasmonic nanoantennas by means of 2P-TOF-PEEM using a ps diode laser. Our ultimate goal is to characterize the nanoplasmonic fields not only on a nm spatial scale but also on $\sim$100 as temporal scale. Therefore, the concept of as field microscope utilizing a TOF-PEEM in combination with fs optical-pump/as XUV-probe experiment will be discussed.

O 59.25 Wed 17:45 Poster B1

Excitation of plasmonic gap waveguides by nano antennas — •Jing Wen[1,2], Peter Banzer[1,2,3], Daniel Ploss[1,2], Arian Kriesch[1,2], and Ulf Peschel[1,2,3] — [1]Institute of Optics, Information and Photonics, University Erlangen-Nuremberg — [2]Max Planck Institute for the Science of Light — [3]Cluster of Excellence 'Engineering of Advanced Materials' at the University of Erlangen-Nuremberg

We experimentally demonstrate the excitation of plasmonic gap waveguides by nano antennas. The excitation is shown to be both spatially and spectrally dependent which can potentially be used for the selective excitation of plasmonic nanostructures. Due to its small size the antenna can be easily integrated into plasmonic circuits.

The simulated optimized coupling efficiency of exciting with antenna is 10.6% which is 129 times as large as the case without antenna. In experiments, the coupling of the far field to the plasmonic waveguide can only be successfully achieved when the optical beam is on the antenna and at resonant wavelength with the right polarization direction. The measured sum of the coupling efficiency and antenna absorption reaches up to 20% compared to the simulated optimum value of coupling efficiency of 10%. The offset between the simulated coupling efficiency and the experimentally determined lack of power is quite likely due to absorption in the antenna or a higher coupling efficiency than expected.

O 59.26 Wed 17:45 Poster B1

Near field and far field excitation of plasmonic waveguide arrays — •Arian Kriesch[1,2,3], Jing Wen[1,2], and Ulf Peschel[2,3,4] — [1]MPI für die Physik des Lichts, Erlangen, Germany — [2]Friedrich-Alexander-Universtität Erlangen-Nürnberg, Erlangen, Germany — [3]Erlangen Graduate School in Advanced Optical Technologies (SAOT) — [4]Cluster of Excellence Engineering of Advanced Materials (EAM)

Recently it was demonstrated that highly birefringent materials can show negative refraction and self-imaging with sub-wavelength resolution. An array of metallic stripes with sub-wavelength periodicity can serve as such kind of metamaterial. It provides a negative permittivity for electric fields pointing along the stripes and a positive polarisability perpendicular to the lines. It also forms a system of coupled plasmonic waveguides thus transferring the concept of optical discreteness to the nano-world. Here we report results on the pointwise excitation of nanoscale plasmonic waveguide arrays with nanoantennas. We fabricated respective structures, using nanostructuring techniques. We found much stronger coupling between the waveguides than it is achievable and reported for arrays made from dielectrics, thus allowing for a much faster energy transport. Using a scanning near field optical microscope (SNOM) and highly focused beams propagating, waves were excited in the arrays. The experimental examination of coupling between neighbouring waveguides promises new insights into the processes of discrete diffraction and negative refraction on previously unmatched small spatial scales. A further goal is to achieve the formation of discrete spatial solitons in such a nanoarray.

O 59.27 Wed 17:45 Poster B1

Interactions in electrically and magnetically coupled stereometamaterials — •Lutz Langguth[1], Ralf Vogelgesang[2], and Harald Giessen[1] — [1]4th Physics Institute, University of Stuttgart, Germany — [2]Max Planck Institut für Festkörperforschung, Stuttgart, Germany

We consider metallic metamaterials which consist of stacked split-ring resonators. Upon twisting of two vertically adjacent split rings, the resonance frequencies of the coupled system change [1]. In split-ring resonators, both electric as well as magnetic interactions are present. Besides dipole interactions, also higher-order modes such as quadrupoles or octupoles play a significant role. We take an analytical model for the electric and magnetic dipole interactions and analyze the spatial dependence of both interactions in the quasistatic limit as well as in the dynamic case. We investigate the distance and the angle dependence of the coupled split-ring modes and find an intriguing behavior, especially at points in space where one or both of the dipole interactions are extremal. Our work explains this behavior in a dipole approximation, points out how to evaluate the strength of higher-order modes and will lead to a better theoretical modelling of the optical properties of stereometamaterials. [1] N. Liu et al., Stereometamaterials, Nat. Phot. 3, 157 (2009)

O 59.28 Wed 17:45 Poster B1

Nanoparticle-based Photothermal Control of the Catalytic Activity of the Enzyme HRP — Jan Bretschneider[1], Maximilian Reismann[2], •Malte Linn[2], Gero von Plessen[2], and Ulrich Simon[1] — [1]Institute of Inorganic Chemistry, RWTH Aachen University, Germany — [2]I. Inst. of Physics (IA), RWTH Aachen University, Germany

The optical excitation of particle plasmons in a gold nanoparticle by laser irradiation induces a temperature rise in the nanoparticle and its immediate surroundings. This effect can be exploited to control temperature-sensitive chemical reactions in a contactless and highly localized manner. In this work, this photothermal effect is utilized to control the catalytic activity of an enzyme. For this purpose, the enzyme horseradish peroxidase (HRP) is bound to the surface of gold nanoparticles which are suspended in water. The HRP catalyses the oxidation of the diazonium compound ABTS to $ABTS^{+}$. A resonant excitation of the HRP-functionalized nanoparticles by cw-laser light with a wavelength of 532 nm leads to a heating of the nanoparticle environment.

We show that this photothermal heating reduces the rate of the catalytic conversion process. For this purpose, the reaction kinetics is spectroscopically monitored via a color change of the colorless reactant (ABTS) transformed into the greenish product ($ABTS^{+}$).

O 59.29 Wed 17:45 Poster B1

Optical Properties of Plasmonic Planar Septamer Nanostructures — •Mario Hentschel[1,2], Na Liu[1], and Harald Giessen[1] — [1]4. Physikalisches Institut, Universität Stuttgart — [2]Max-Planck-Institut für Festkörperforschung, Stuttgart

Planar septamer nanostructures are supposed to show interesting coupling effects. Mirin et al. [1] predicted a plethora of symmetry-dependent spectral features. For instance, the symmetric mode takes in-phase oscillations of all particle plasmons into account, whereas the antisymmetric mode allows for phase shifts of pi.

We fabricated a variety of septamer structures by high-resolution electron beam lithography and varied coupling as well as symmetry parameters. Coupling distances as small as 12 nm have been achieved.

We are going to discuss the optical spectra as a function of structure sizes, geometry, and neighbor-neighbor distance and find interesting coupling effects. A simple dipole-dipole coupling picture between the electric dipole moment of particle plasmons can be utilized to visualize the energy levels as well as the oscillator strength of the optical spectra.

[1] Nikolay A. Mirin et al., J. Phys. Chem. A 113, 4028-4034 (2009)

O 59.30 Wed 17:45 Poster B1

Calculation of the up-conversion efficiency of Er^{3+} ions near noble-metal nanoparticles — Florian Hallermann[1], Jan Christoph Goldschmidt[2], Stefan Fischer[2], Philipp Löper[2], •Christian Maasem[1], and Gero von Plessen[1] — [1]Institute of Physics (1A), RWTH Aachen University, 52056 Aachen, Germany — [2]Fraunhofer Institute for Solar Energy Systems, Heidenhofstr. 2, 79110 Freiburg, Germany

In conventional silicon solar cells, the near-infrared part of the solar spectrum could possibly be exploited by making use of up-conversion processes. For instance, electrons could be excited from the ground state to a final state via intermediate states through sequential absorption of infrared photons. The radiative relaxation of the electrons from the final state generates photons whose energy is high enough to be absorbed in the silicon.

In this work, we show on the basis of model calculations how the up-conversion efficiency of Er^{3+} ions can be enhanced using spherical gold nanoparticles. The changes of the excitation rate in the vicinity of nanoparticles are computed for Er^{3+} ions homogeneously distributed around a single gold nanoparticle using Mie theory and a rate equation system. In addition, the relaxation rates of all involved excited states of the ions are changed due to additional radiative and nonradiative decay channels provided by the metallic nanoparticle. Using experimentally accessible transition rates of Er^{3+} ions, we semi-analytically calculate the effects these changes have on the up-conversion efficiency.

O 59.31 Wed 17:45 Poster B1

Near-field phase and flux controllability in the near-field — •Giovanni Piredda, Caroline Gollub, Regina de Vivie-Riedle, and Achim Hartschuh — Physikalische Chemie, Department Chemie und Biochemie, Ludwig-Maximilians-Universität München

Ultrafast nanooptics is an emerging field that combines the concepts and tools of ultrafast spectroscopy with those of near-field optics [1]. A basic form of coherent control in the near-field is the ability to concentrate the linear optical flux at a desired location with sub-diffraction resolution. This task requires polarization pulse shaping of the incident electric field [2]. We show, using simple examples, that the presence of quick spatial variations of the phase ("near-field phase") is an essential ingredient for the controllability of linear flux in the near-field. The near-field phase, that does not depend on propagation, is almost always present when light interacts with a nanostructure [3]. We analyze a nanoparticle and incident field configuration in which near-field spatial variations of the phase are almost completely absent to highlight the fact that without them control of flux localization cannot succeed. In addition we present our first results of control of second-harmonic generation from rough gold films in a near-field optical setup.

[1] M.I. Stockman et al., Phys. Rev. Lett., **88**, 067402 (2002).
[2] T. Brixner et al., Phys. Rev. B, **73**, 125437 (2006).
[3] R. Carminati, Phys. Rev. E **55**, R4901 (1997).

O 59.32 Wed 17:45 Poster B1

Acousto-Plasmonic Properties of Single Metal Nanoparticles — •Kai Kratzer[1,2], Thorsten Schumacher[1,2], and Markus Lippitz[1,2] — [1]Max-Planck-Institut für Festkörperforschung, Stuttgart — [2]4. Physikalisches Institut, Universität Stuttgart

Acoustic vibrations of a single metal nanoparticle are detectable via the particle's plasmonic properties because mechanical oscillations cause a periodical variation of the electron density and thus a periodically changing plasmon resonance. Ultrafast pump-probe spectroscopy allows us to measure these small variations and to characterize a single nanoparticle by analyzing the acoustic breathing mode on a picosecond timescale.

Metal nanoparticles show a diverse behavior as they vary in shape, size and coupling to the substrate. To overcome this inhomogeneity it is necessary to measure single particles. We demonstrate these variations by a series of experiments on the single particle level and show the influence of deviations from spherical shape and the coupling to the substrate.

O 59.33 Wed 17:45 Poster B1

Temperature dependence of antenna-like plasmon resonances of gold nanowires in the Infrared — •Jörg Bochterle[1], Frank Neubrech[1], Hoang Vu Chung[1], Dominik Enders[2], Tadaaki Nagao[2], and Annemarie Pucci[1] — [1]Kirchhoff-Institute for Physics, Heidelberg University, Germany — [2]National Institute for Material Science, Tsukuba, Japan

Quantitative knowledge about conductivity parameters in metal nanostructures is of high practical interest in nanotechnology. Since contacts for direct current measurements mostly are problematic, contact-free spectroscopic measurements would be preferable. In fact, plasmonic resonance spectra are determined by the conductivity parameters. Unfortunately, except few special cases, the relation between metal conductivity and plasmonic particle resonance is complicated and it is important to get systematic experimental data.

We therefore study infrared plasmonic excitation of lithographic gold nanowires at various temperatures between 30 K and 600 K. The experiments were performed under UHV conditions to realize LHe cooling down to 30 K without formation of thick adsorbate layers. Electron impact heating was used to control the amount of energy transferred to the sample holder, thus being able to approach various temperatures in the desired range. With decreasing temperature a decreasing number of phonons in the gold nanowires is expected and therefore a lower relaxation rate of conducting electrons and accordingly a change in the plasmonic resonance curve.

O 59.34 Wed 17:45 Poster B1

Third harmonic generation from gold nanostructures using a femtosecond laser scanning microscope — •Siegfried Weisenburger[1,2], Tobias Utikal[1,2], Harald Giessen[2], and Markus Lippitz[1,2] — [1]Max Planck Institute for Solid State Research, Stuttgart — [2]4th Physics Institute, University of Stuttgart

There are different competing mechanisms of third harmonic generation from gold nanostructures on a dielectric substrate: First of all third harmonic light generated at the dielectric-air interface is Rayleigh scattered at the metal structure. Furthermore the strong field enhancement in the vicinity of the plasmonic nanostructure increases the dielectric bulk third harmonic generation. Last but not least there is third harmonic generation from the particle itself due to a nonlinear potential of the metal's conduction electrons caused by the finite size of the structure. We look into the question, which of these mechanisms dominates in which size regime the third harmonic generation from the nanostructures.

We use a titanium-sapphire laser system producing 8 fs pulses that are strongly focussed onto the samples by a reflective Cassegrain objective. The third harmonic signal at 4.6 eV is collimated by an immersion glycerin quartz objective and detected by an UV photomultiplier. The focussing properties of the Cassegrain objective and the influence of the Cassegrain on the ultrashort laser pulses are investigated experimentally and by numerical simulations. We will show the principle of a femtosecond laser scanning microscope setup as well as first experimental results on the third harmonic generation from gold nanostructures.

O 59.35 Wed 17:45 Poster B1

Second-harmonic generation at thin gold films: Comparison of experiment and theory — •Philipp Reichenbach, Andreas Hille, Stefan Grafström, and Lukas M. Eng — Technische Universität Dresden, Institut für Angewandte Photophysik, George-Bähr-Str. 1, 01062 Dresden

The existence of optical second-harmonic generation (SHG) at metallic surfaces has been well known for a many years in experiment [1] as well as in theory, where several electron gas models exist [2-4]. Further investigations have dealt with SHG at thin metallic films [5, 6], for which these models have been compared with experimental measurements. In our work the SHG signal from thin gold films of various thicknesses was measured. The experimental results are compared with a simple and fundamental classical model: an extended Lorentz model taking second-order corrections into account. The model was implemented into a discontinuous Galerkin algorithm [7], which provides higher spatial resolution in time domain than other common methods such as FDTD and FVTD.

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[4] J. E. Sipe et al., Phys. Rev. B 21, 4389 (1980)
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O 59.36 Wed 17:45 Poster B1

Controlling the Third-Harmonic Generation in a Metallic Photonic Crystal Coupled to a Waveguide — •Reinold Podzimski[1], Matthias Reichelt[1], Torsten Meier[1], Tobias Utikal[2], and Harald Giessen[2] — [1]Department Physik und CeOPP, Universität Paderborn, Warburger Str. 100, D-33098 Paderborn, Germany — [2]Physikalisches Institut, Universität Stuttgart, D-70550 Stuttgart, Germany

The behavior of waveguide plasmon polaritons is studied employing ultrafast coherent control like schemes for a gold lattice coupled to a photonic waveguide, see Ref. [1] for the structure. Different models to describe the third-harmonic generation are presented and the resulting equations are solved numerically. [2] The calculations are compared to recent experimental data and show good agreement for the most prominent features in the time-integrated third order intensity. [3]

[1] T. Utikal *et al.*, Phys. Rev. B. **76** , 245107 (2007).
[2] T. Meier, P. Thomas, and S.W. Koch, *Coherent Semiconductor Optics*, Springer (2007).
[3] R. Podzimski, *Modellrechnungen zur Erzeugung und Kontrolle der dritten Harmonischen*, Bachelor Thesis, University of Paderborn (2009).

O 59.37 Wed 17:45 Poster B1

Coupled surface plasmon polariton - exciton modes for absorbing and pumped excitons — •Stephan Schwieger, David Leipold, and Erich Runge — Institut für Physik and Institut für Mikro- und Nanotechnologien, Technische Universität Ilmenau, 98693 Ilmenau, Germany

The coupling of surface plasmon polaritons (SPPs) at metal gratings and excitons in optically excitable media can potentially be used to compensate the large SPP-losses found at metal gratings [1,2]. This coupling leads to very much increased propagation lengths and new device concepts such as SPASERS proposed by Bergman and Stockman [3]. The coupled modes are investigated theoretically for a model system that consists of a gold-nanowire array and a semiconductor quantum-well (QW) structure. Properties of the coupled modes as, e.g., their dispersion relations, their group velocities, and the coupling to propagating far-field modes are discussed. The cases of absorbing QW and optically pumped QW are compared.

[1] P. Vasa, R. Pomraenke, S. Schwieger, Yu. I. Mazur, Vas. Kunets, P. Srinivasan, E. Johnson, J. E. Kihm, D. S. Kim, E. Runge, G. Salamo, and C. Lienau, *Phys. Rev. Lett.* **101**, 116801 (2008).
[2] S. Schwieger, P. Vasa, and E. Runge, *Phys. Stat. Sol. (b)* **245**, 1071(2008).
[3] D. J. Bergman and M. I. Stockman, *Phys. Rev. Lett.* **90**, 027402 (2003).

O 59.38 Wed 17:45 Poster B1

Surface plasmon polaritons in a gold double-grating structure — •Steve Lenk, Stephan Schwieger, and Erich Runge — Institut für Physik und Institut für Mikro- und Nanotechnologien, Technische Universität Ilmenau, 98693 Ilmenau, Germany

We investigated theoretically the near- and the far-field distribution of a gold double-grating structure with two overlapping lattice periods. Under illumination by a plane wave, surface plasmon polaritons (SPPs) can be excited at the resonance angle and the resonance frequency. For single-grating structures, the detection signal is a mixture of directly reflected and re-radiated light from the SPPs. The double-grating structure allows the detection of the SPPs at novel angles compared to the angles of the single-grating. Thus, detection angles may be found where the SPP character dominates the signal and information on the SPP (lifetime, intensity, ...) can be obtained in the far field. For our calculation, we solved Maxwells equations in time-domain (FDTD) and frequency-domain (FEM). We compared our results with recent experimental studies.

O 59.39 Wed 17:45 Poster B1

Simulation of the behaviour of surface plasmon polaritons on C_3 symmetric nano-holes arranged as C_4 symmetric arrays — •David Leipold, Stephan Schwieger, and Erich Runge — Institut für Physik und Institut für Mikro- und Nanotechnologien, Technische Universität Ilmenau

Surface plasmon polaritons (SPPs) can couple to propagating light, e.g., via a grating. We perform FDTD simulations to obtain insight into the coupling via arrays of nano-holes cut into a silver film. In particular, we investigate the influence of nano-holes with three-fold symmetry, which is incompatible with the four-fold symmetry of the whole array. These studies are motivated by earlier experiments[1] that revealed unexpected dependencies of the reflectivity on the direction and the polariziation of the incident light. Our simulations reproduce many aspects of these findings and give insight into the behaviour of the near fields and, in particular, their relation to the excitation of SPPs.

[1] B. Ashall, M. Berndt, and D. Zerulla, *App. Phys. Lett.* **91**, 203109 (2007)

O 59.40 Wed 17:45 Poster B1

Goos-Hänchen-Effect for a SPP — •Felix Huerkamp[1,2], Alexei Maradudin[2], and Tamara Leskova[2] — [1]Westfälische Wilhelms-Universität, Münster — [2]Univerity of California, Irvine

When a beam of finite cross section is incident from an optically more dense medium on its planar interface with an optically less dense medium,and the angle of incidence is greater than the critical angle for total internal reflection, the reflected beam undergoes a lateral displacement, as if it is being reflected from a plane in the optically less dense medium parallel to the physical interface. This lateral displacement of the reflected beam is the *Goos-Hänchen effect* .

We show that a surface plasmon polariton beam can also display a Goos-Hänchen effect. The system we consider consists of vacuum in the region $x_3 > 0$, a metal whose dielectric function is $\epsilon_1(\omega)$ in the regions $x_1 < 0$, $x_3 < 0$,and $x_1 > L$, $x_3 < 0$, and a metal whose dielectric function is $\epsilon_2(\omega)$ in the region $0 < x_1 < L$, $x_3 < 0$ ($|\epsilon_1(\omega)| < |\epsilon_2(\omega)|$). By means of an impedance boundary condition, and solution of the integral equations for the scattering amplitudes to which its use gives rise, by a purely numerical approach and by the *Wiener-Hopf method*, we determine the reflected surface plasmon polariton beam when a surface plasmon polariton beam is incident from the region $x_1 < 0$ on the interface $x_1 = 0$ at an angle that is greater than the critical angle for total internal reflection. The system where L tends to infinity is also studied in this way. In both of these systems the reflected beam undergoes a lateral shift along the x_2 direction whose magnitude is a few times the wavelength of the incident beam.

O 59.41 Wed 17:45 Poster B1

Influence of C_{60}-Adsorption on Surface Plasmon Polariton Properties — •Pierre Kirschbaum, Niemma M. Buckanie, Michael Horn-von Hoegen, and Frank-J. Meyer zu Heringdorf — Universität Duisburg-Essen, Fakultät für Physik, Lotharstraße 1, 47057 Duisburg

Surface Plasmon Polaritons (SPP) are collective excitations of the free electron gas in metallic systems that propagate along nanoparticle surfaces. In our experiments, SPPs are optically excited at the edges of Ag-Islands. These SPPs can be imaged by nonlinear Photoemissions Electron Microscopy (PEEM), using ultra short femtosecond laser pulses for illumination. The observed periodic pattern in PEEM relates to a time integrated superposition of the exciting laser pulse and the excited SPP-wave (beating pattern). Defects and adsorbates manipulate the observed pattern.

Here, the influence of C_{60}-adsorption on the properties of surface plasmon polaritons is discussed. Under illumination with femtosecond laser pulses we observe a decrease of the photoemission yield with increasing coverage. Furthermore, the beating pattern wavelength changes because of a modified effective surface dielectric function. Our findings imply that the SPP-wavelength becomes shorter as a result. Finally, we observe a decrease of the intensity of the beating pattern maxima compared with the intensity of the first maximum with increasing C_{60} coverage. Accordingly the damping becomes stronger, which means the propagation length decreases.

O 59.42 Wed 17:45 Poster B1

Acoustic surface plasmons on Au(111) and Au(788) — •U. Krieg[1], L. Vattuone[2], M. Smerieri[2], M. Rocca[2], H. Pfnür[1], and C. Tegenkamp[1] — [1]Institut für Festkörperphysik, Leibniz Universität Hannover, Appelstrasse 2, D-30167 Hannover, Germany — [2]Dipartimento di Fisica and IMEM-CNR, Università di Genova, I-16146 Genova, Italy

The Acoustic Surface Plasmon (ASP), was predicted theoretically long ago but due to its relatively low cross section it eluded observation until it was firstly observed on Be(0001) and eventually also on Cu(111). We show here that the ASP exists also on Au(111) and on its vicinal surface Au(788). The experiment was performed using ELS-LEED which allows for a high momentum resolution and easy investigation of azimuthal anisotropy of Plasmon dispersion. Interestingly, we find for Au(111) two dispersion branches for ASP. One is nearly isotropic in k-space with slope of 3.8 eVÅ, whereas the other has roughly twice the slope and is visible only along the ΓM direction. Although Au(788) exhibits a quasi one-dimensional partially occupied surface state, the plasmonic dispersion for ASP measured here is two-dimensional and even nearly isotropic. The periodic step structure, however, leads to strong Umklapp scattering so that the multiple branches seen here can actually all be derived from only one dispersing ASP. These results will be discussed taking into account the Rashba split surface bands as well as the role of the reconstruction on flat and regularly stepped Au surfaces. Theoretical ab initio calculations are needed to achieve a full understanding of this complex behaviour.

O 59.43 Wed 17:45 Poster B1

Probing Exciton Propagation and Localization in Single-Walled Carbon Nanotubes — •Carsten Georgi, Miriam Böhmler, and Achim Hartschuh — Department Chemie und Biochemie & CeNS, Ludwig-Maximilians-Universität München, Germany

Tip-enhanced near-field photoluminescence (PL) microscopy providing nanoscale spatial resolution has been mainly used to image localized emitters, such as single molecules [1,2]. Semiconducting single-walled carbon nanotubes are photoluminescent 1D-nanostructures with highly mobile excited states (excitons). We study exciton propagation by combining near-field PL measurements and numerical simulations describing exciton diffusion and the imaging process. Hereby, we can extract e.g. the exciton diffusion range [3]. In some cases, highly confined and exceptionally bright PL is observed and attributed to exciton localization. This localization results from strong exciton energy gradients exceeding 2 meV/nm, evidenced by energy-resolved PL imaging. Numerical simulations of exciton diffusion in the presence of energy variations support this interpretation predicting strongly enhanced PL at local energy minima. Our results indicate that the PL intensity along a single nanotube is determined by the complex interplay between exciton mobility, localization and quenching sites.

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[2] T. Taminiau et al., Nature Photon. 2, 234 (2008)
[3] C. Georgi et al., phys. stat. sol. (b) 246, 2683 (2009)

O 59.44 Wed 17:45 Poster B1

FDTD Simulations of Near-field Mediated Semiconductor Molecular Optical Properties — Dai Zhang, Marcus Sakrow, •Josip Mihaljevic, and Alfred J. Meixner — Institute of Physical and Theoretical Chemistry, University Tübingen, Auf der Morgenstelle 8, Tübingen

The optical properties of molecules can be dramatically altered when they are in a close proximity of an excited metal antenna. In order to get insight into how the antenna generated near-field influences the optical properties of low quantum yield molecules, we carried out FDTD simulations of a sharp laser-illuminated Au tip approaching to a semiconductor thin film. The time-averaged field distribution between the semiconductor thin film and the tip antenna is calculated regarding to different distances. Our calculation demonstrates that the coupling between the localized plamon at the tip apex and semiconductor polariton can be achieved building up a distance-dependent high field enhancement. Our experimental results show that such a high field strength enhances not only the excitation process by a factor of 104, but alters the radiative : non-radiative decay rate giving approx. 15 times stronger photoluminescence emission.

O 59.45 Wed 17:45 Poster B1

One-dimensional analytical model for strong-field photoelectron emission from metal nanostructures — •Sergey Yalunin, Reiner Bormann, Alexander Weismann, Max Gulde, and Claus Ropers — University of Göttingen, Courant Research Center Nano-Spectroscopy and X-Ray Imaging, Friedrich-Hund-Platz 1, 37077 Göttingen, Germany

Ultrashort electron pulse generation from nanostructures has attracted significant interest, due to its potential for time-resolved electron experimentation. Alongside numerical models of the associated nonlinear emission processes, an analytical model can provide important insight in the physical principles.

Here, we present an analytical quantum mechanical model for nonlinear photoelectron emission that takes into account multiple emission channels. The model describes both multiphoton and optical field (i.e. tunneling) emission in the presence of arbitrary static and laser fields. Several limiting cases are correctly reproduced. In the multiphoton regime and without a static field, the model yields the usual power law for the emission current. In the absence of a laser field, the Fowler-Nordheim equation is obtained. For the optical tunnel regime, the results coincide with the adiabatic approximation.

O 59.46 Wed 17:45 Poster B1

Modeling the Optical Response of Metallic Nanostructures in the Discontinuous Galerkin Time-Domain Method — •Christopher Prohm^1, Michael König^{1,2}, Jens Niegemann^{1,2}, and Kurt Busch^{1,2} — ^{1}Institut für Theoretische Festkörperphysik, Karlsruher Institut für Technologie — ^{2}DFG Forschungszentrum Center for Functional Nanostructures (CFN), Karlsruher Institut für Technologie

The discontinuous Galerkin time-domain method (DGTD) combines the highly flexible spatial discretization of finite-element methods with the possibility to investigate nanophotonic systems in the time-domain. Here, we investigate the interaction of three-dimensional metallic nanostructures with an incoming light field. In particular, we discuss the linear modeling of the dielectric function of metals via a combination of Drude and Lorentz terms. Furthermore, we present some results on the nonlinear modeling of the metallic response by using a hydrodynamic model.

O 59.47 Wed 17:45 Poster B1

Ultrafast optical response of metal surfaces — •Mathias Wand, Arno Schindlmayr, Yevgen Grynko, Torsten Meier, and Jens Förstner — Department Physik and CeOPP, Universität Paderborn, 33098 Paderborn, Germany

We present a numerical method for calculating the dynamics of surface electrons in metals. This will enable us to simulate the linear or nonlinear response of complex plasmonic nanostructures, e.g., metamaterials built from split-ring resonators. As shown by Rudnick and Stern [Phys. Rev. B 4, 12 (1971)], the motion of electrons perpendicular to the surface requires a quantum-mechanical treatment due to nonlocal effects. As we aim to incorporate the ultrafast material response into a Maxwell solver, it is highly desireable to have a time-domain description of the surface electron dynamics. This can be achieved by using the time-dependent density-functional theory (TDDFT), which is able to describe the time evolution of the charge density of a quantum-mechanical many-body system. The charge density along the normal direction of the metal surface is resolved on an Ångström scale and propagated in time on a secondary grid. The current density can be extracted from the TDDFT simulation and incorporated into Maxwell's equations as a nonlinear source current. To illustrate the capabilities of TDDFT we further present optical conductivities of selected simple and noble metals extracted from ab initio calculations of the linear response function.

O 59.48 Wed 17:45 Poster B1

Time-Domain Simulations of Semiclassical Radiation Dynamics in Photonic Nanostructures — •Paolo Longo, Jens Niegemann, and Kurt Busch — Institut für Theoretische Festkörperphysik, Karlsruhe Institute of Technology

Versatile numerical techniques have become indispensable in the field of photonics. In particular, the Discontinuous Galerkin Time-Domain Method (DGTD) [1] combines key benefits from both classical finite element and finite-difference approaches such as adaptive meshing, a local coupling of neighboring elements and an explicit time-stepping scheme.

Within this framework, we go beyond the widely spread purely classical models of light-matter-interaction and investigate radiation dynamics in photonic systems by simultaneously evolving Maxwell's equations and quantum mechanical equations of motion in time. In a first step, matter is modeled as an ensemble of two-level systems which results in the well-known Maxwell-Bloch equations [2]. Such semiclassical models automatically incorporate back-action effects, e.g., the non-Markovian radiation dynamics of emitters in photonic band-gap media.

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O 59.49 Wed 17:45 Poster B1

Cantilever based Scanning Near Field Optical Microscopy probes as platform for optical antenna sensors — •Bernhard Schaaf^1, Marc Salomo^1, Jennifer Linden^1, Daniela Bayer^1, Jens Niegemann^2, Michael König^2, Christopher Prohm^2, Martin Aeschlimann^1, Kurt Busch^2, and Egbert Oesterschulze^1 — ^{1}Technische Universität Kaiserslautern, 67663 Kaiserslautern, Germany — ^{2}Institut für Theoretische Festkörperphysik, Universität Karlsruhe, 76128 Karlsruhe, Germany

Scanning Nearfield Optical Microscopy (SNOM) is a powerful tool to investigate the electron dynamics in metallic nanostructures. An AFM cantilever based SNOM probe is presented exploiting a hollow pyramidal tip as platform for the integration of an nano-antenna onto the very tip. As a prerequisite, various types of antennas were fabricated on planar substrates to investigate their spectral resonance behavior. In the next step antennas are placed onto the pyramidal tips using FIB milling as well as e-beam lithography as high precision fabrication tools. The probes aim at the investigation of the excitation of e.g. collective electron oscillations like localized surface plasmons (LSPs). For this purpose, metallic nanostructures are prepared on planar glass or silica substrates. Measurements on the farfield and nearfield performance of the probes and samples as well as coupling of both regimes are presented as function of the impinging field amplitude distribution and the polarization state. Simulations of the spatial as well as temporal field distribution were conducted to get insight in the probe performance and in future also into the coupling of probe and sample.

O 59.50 Wed 17:45 Poster B1

Lateral manipulation of surface plasmons by hollow structures — •Michael Lutz, Stephen Riedel, Paul Leiderer, and Johannes Boneberg — Universität Konstanz

A frequency doubled Nd:YAG pulse (10ns,532nm) is splitted into three beams of equal intensity. The beams are recombined on a thin goldfilm under specific angles which define the periodicity of the resulting interference pattern. We observe the formation of hollow structures with diameters between few microns and few hundred nanometers.

The structures originate from thermal expansion upon melting of the surface which occurs only in regions of high intensity. This generates a shift of the centre of mass off the surface. The motion of the centre of mass causes the liquid lamella to lift off. After resolidification a nanostructured surface with hollow bumps has formed.

We show how these structures can be used to manipulate surface plasmons laterally.

O 59.51 Wed 17:45 Poster B1

Golden Nanocones for Near-Field Optical Applications — •Christian Schäfer^1, Bastian Zeeb^1, Peter Nill^1, Alexander F. F. Weber-Bargioni^2, Stefano Cabrini^2, Monika Fleischer^1, and Dieter P. Kern^1 — ^{1}University of Tübingen, Auf der Morgenstelle 10, 72076 Tübingen — ^{2}Molecular Foundry, 1 Cyclotron Road, Berkeley, CA94720, USA

Manipulating light by means of the enhanced electromagnetic field of metallic nanoparticles has become an interesting and well developed method for microscopic imaging in several branches of study. Through external electromagnetic excitation particle plasmons can be generated, and the resulting field enhancement can be used for near-field imaging as well as for tip enhanced Raman-Spectroscopy. Here two different processes for the fabrication of sharp-tipped golden nanocones are presented. In the first process we use electron beam lithography to structure a layer of hydrogen silsesquioxane (HSQ) coated on a gold surface, which can be evaporated thermally on different kinds of substrates. The structured layer of HSQ is then used as mask in the following Argon-ion etch step which forms the golden nanocones. In this way fields of nanocones with tip radii of less than 10 nanometers can be produced in parallel. In the second method, which is particularly useful for non-planar surfaces, we use electron beam induced deposition to structure an etch mask. For that purpose the precursor tetra-ethyl-ortho silicate is brought next to the gold surface. Silicon oxide is deposited via decomposition by the focused electron beam and serves as etch mask in the following Argon-ion etch step.

O 59.52 Wed 17:45 Poster B1

Signal-to-background ratio in scattering-type Scanning Near-Field Microscopy (s-SNOM) — •Jón Mattis Hoffmann[1], Jon Schuller[2], Mark Brongersma[2], Stefanie Bensmann[3], and Thomas Taubner[1,3] — [1]I. Physikalisches Institut (IA), RWTH Aachen — [2]Stanford University — [3]Fraunhofer-Institut für Lasertechnik

The scattering-type Scanning Near-Field Optical Microscopy (s-SNOM) surpasses the diffraction-limit and provides the possibility of non-destructive microscopy and the analysis of material properties at the nanometer scale [1]. This allows, for example, the identification of different polymers [2] or the analysis of viruses [3]. Furthermore, the combination of s-SNOM with a broadband light source gives the possibility to record a full spectrum with a single measurement [4].

One limiting factor of the s-SNOM is the signal-to-background ratio. This is getting more crucial for the probing of weakly-absorbing samples and especially for the the use of broadband lasers, which offer less power. In our current research project, the possibility of increasing the sensitivity of s-SNOM by using resonant probing-tips will be worked out. Therefore, as a first step, commercially available tips will be characterized with respect to their scattering properties, in the far-field and the near-field.

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[2] T. Taubner et al., Appl. Phys. Lett. 85, (2004)
[3] M. Brehm et al., Nano Lett. 6, 1307-1310 (2006)
[4] S. Amarie et al., Opt. Express 17, 21794-21801 (2009)

O 59.53 Wed 17:45 Poster B1

Shadow nanosphere lithography of nanospirals — •Bettina Frank, Jun Zhao, and Harald Giessen — Universität Stuttgart, Deutschland

We fabricated a hexagonal densely packed monolayer of polystyrene nanospheres (Langmuir-Blodgett film) with $450nm$ diameter. Coating a $1cm^2$ glass substrate with such a monolayer resulted in a good evaporation mask for nanopinhole lithography [1] of high quality. We deposited planar gold nanospirals inbetween the nanosphere mask by polar and azimuthally stepper-motor controlled sample rotation during the evaporation process. Large-area samples of very high quality were obtained. Measuring reflectance spectra by FTIR-spectroscopy yields good agreement with FDTD simulations. We modified gap width and wire length of the spiral structure and studied the dependence of the optical spectra on these parameters. Such structures are useful for broadband optical nanoantennas that radiate preferentially into the third dimension.

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O 59.54 Wed 17:45 Poster B1

Pump-probe apertureless near-field microscopy - a Tool for time resolved Nanooptics — •Marcus Rommel[1,2], Stephanie Essig[1,3], Ralf Vogelgesang[1], and Markus Lippitz[1,3] — [1]Planck Institute for Solid State Research, Stuttgart, Germany — [2]Department of Experimental Physics 5, University of Würzburg, Würzburg, Germany — [3]4th Physics Institute, University of Stuttgart, Stuttgart, Germany

We develop a pump-probe apertureless scanning near-field optical microscope (PPaSNOM) to analyze plasmonic structures. This setup allows us to detect the temporal and spatial dependence of localized surface plasmon resonances (LSPR) as well as propagating SPRs. One of the first applications of this instrument will be the investigation of acoustic vibrations in single plasmonic particles of different shape.

As LSPR's depend sensitively on the electron density, the changes in volume due to GHz acoustic oscillations can be tracked with time-resolving pump-probe experiments [1]. The optical near-field indirectly contains information on the structure's acoustic oscillation. This allow us to extract nanoscale Chladni figures, i.e., maps of the acoustic vibration amplitude on the particle surface.

[1]M. A. van Dijk, M. Lippitz, M. Orrit, Detection of acoustic oscillations of single gold nanospheres by timeresolved interferometry, Phys. Rev. Lett. 2005, 95, 267 406.

O 59.55 Wed 17:45 Poster B1

LEEM/LEED investigation of Fe_3O_4 thin film growth on a Pt(111) substrate: morphology, growth and atomic termination — •Alessandro Sala, Helder Marchetto, Thomas Schmidt, and Hans-Joachim Freund — Fritz Haber Institut der Max Planck Gesellschaft, Berlin, Germany

Iron oxide is widely used as a catalyst and as a support for catalytically active systems. Although the system has been intensively studied with various techniques, controversies arise in the literature regarding the surface termination and structural inhomogeneities. This clearly hinders the direct linking of surface electronic and structural properties to chemical properties. Our aim is therefore a comprehensive and consistent characterization of the Fe_3O_4 film growth on a Pt(111) substrate with well defined preparation conditions by using the unique SMART instrument. This Low Energy and Photo-Emission Electron Microscope (LEEM/PEEM) is specially designed to obtain chemical and structural information with high lateral resolution.

O 59.56 Wed 17:45 Poster B1

Growth of nanostructures on fcc(110) metal surfaces at the atomic scale — •Oleg V. Stepanyuk[1,2,3], Nikolay N. Negulyaev[2], Pavel A. Ignatiev[3], Wolfram Hergert[2], and Alexander M. Saletsky[1] — [1]Faculty of Physics, Moscow State University, 119899 Moscow, Russia — [2]Fachbereich Physik, Martin-Luther-Universität, D06099 Halle, Germany — [3]Max-Planck-Institut für Mikrostrukturphysik, D06120 Halle, Germany

We report on an unusual mechanism of atomic-scale structures growth on fcc(110) metal surfaces, which is promoted by interface intermixing of deposited and substrate atoms. We investigate a self-assembly of 1D and 2D nanostructures during thermal deposition of 3d atoms on Pd(110) [1] and Cu(110) [2] surfaces at different temperatures. Diffusion barriers of basic atomic events are calculated by means of density functional theory. Incorporation of deposited 3d atoms into the topmost substrate layer is found to be energetically and kinetically feasible in the examined interval of temperatures (120-350 K). Kinetic Monte Carlo model for atomic self-organization demonstrates that surface nanostructures consist mainly of expelled substrate atoms, while deposited 3d magnetic atoms are embedded into the topmost surface layer [1, 2]. Recently our theoretical predictions have been confirmed by experiments [3]. Magnetic properties of novel nanostructures are also discussed.

[1] Stepanyuk O.V., et al., Phys. Rev. B 78, 113406 (2008). [2] Stepanyuk O.V., et al., Phys. Rev. B 79, 155410 (2009). [3] Wei D.H., et al., Phys. Rev. Lett. 103, 225504 (2009).

O 59.57 Wed 17:45 Poster B1

Adatoms with character: Co and Pt atoms on Pt (111) — •Andreas Garhofer[1,2], Zuzana Bortlova[1], Michael Schmid[1], Peter Varga[1], and Josef Redinger[1,2] — [1]Institut f. Angewandte Physik, TU Wien — [2]Center for Computational Materials Science, TU Wien

Surface diffusion of Co adatoms on Pt(111) has been studied by first principles DFT methods, implemented in the program package VASP and STM. A diffusing Co adatom jumps over bridge sites between two surface Pt atoms from stable fcc to hcp sites and vice versa. The calculated barrier of 0.194 eV is in good agreement with recent experiments (0.200 eV) [1]. Adding a second Co adatom at the largest separation possible on a (5x5) surface unit cell reveals a repulsive interaction between the Co adatoms, presumably due to unfavorable relaxations imposed on the Pt substrate, while magnetic interactions could be ruled out. Only if the two Co atoms come close together a stable dimer is formed. Both theoretical findings agree well with our STM observations. Mimicking the onset of growth of Co layers, calculations for three Co adatoms confirm our STM experiments by predicting a triangular Co adatom configuration to be most stable. Surprisingly, the results for three (four) Pt adatoms on Pt(111) are different. In contrast to Co, Pt adatoms behave "strange" and prefer linear configurations instead of maximizing the number of nearest neighbor bonds.

[1] P. Buluschek, thesis No. 3944, Ecole Polytechnique federale de Lausanne (2007)

O 59.58 Wed 17:45 Poster B1

Ultrathin Epitaxial Molecular C_{60} Layers on Bi(111): Morphology, Strain State, and Order-Disorder Phase Transition — •Hichem Hattab, Dennis Meyer, Giriraj Jnawali, and

Michael Horn-von Hoegen — Faculty of Physics, University of Duisburg-Essen, Lotharstr.1, 47048 Duisburg, Germany

Using Spot Profile Analyzing Low Energy Electron Diffraction (SPA-LEED) we have studied the order-disorder structural phase transition [1] of C_{60}(111) films on a Bi(111) surface. Initially a smooth Bi(111) base film was prepared on Si(001) [2]. Sub-monolayer coverages of C_{60} were adsorbed at 80 K and annealed to 450 K. These molecular adsorbate layers exhibit a moiré pattern with a periodicity of 5 nm which is determined by the lattice mismatch of the C_{60} adlayer and the Bi(111) virtual substrate. The coverage of the C_{60} film was subsequently increased by additional deposition of C_{60} at 450 K. For each step LEED spot profiles were recorded at 80 K. Comparing these profiles, we conclude that the initial (1×1) phase changes into the disordered (2×2) phase as soon as the coverage is increased beyond a single layer of C_{60}. The formation of the second molecular C_{60} layer is accompanied by a sudden relaxation of the lateral lattice parameter of the C_{60} adlayer. We have additionally confirmed that C_{60} films thicker than 1 BL show the temperature dependent surface orientational-disordering phase transition from (2×2) to (1×1) at 235 K in analogy to previous studies [1].

[1] A. Goldoni *et al.*, Phys. Rev. B **54**, 2890 (1996)
[2] G. Jnawali *et al.*, Phys. Rev. B **74**, 195340 (2006)

O 59.59 Wed 17:45 Poster B1

Properties of ultrathin In layers on the Ni(001) face

— •Aleksander Krupski, Maciej Góral, and Wojciech Pawłowski — Institute of Experimental Physics, University of Wroclaw, pl. Maksa Borna 9, 50-204 Wroclaw, Poland

The atomic structure and morphology of ultrathin In layers on the Ni(001) face deposited in ultrahigh vacuum at the substrate temperature ranging from 145 K to 900 K were investigated with the use of Auger electron spectroscopy (AES) and low-energy electron diffraction (LEED).

O 59.60 Wed 17:45 Poster B1

Properties of Ultrathin Pb Layers on the Ni(001) Face

— •Katarzyna Miśków, Maciej Góral, Wojciech Pawłowski, Tomasz Kraśnicki, Tomasz Kosmala, Zbigniew Jankowski, and Aleksander Krupski — Institute of Experimental Physics, University of Wroclaw, PL.Maksa Borna 9, Pl 50-204 Wroclaw, Poland

The atomic structure and morphology of ultrathin Pb layers deposited on the Ni(001) face in ultrahigh vacuum at the substrate temperature ranging from 145 K to 900 K were investigated with the use of Auger Electron Spectroscopy (AES) and Low-Energy Electron Diffraction (LEED). AES results indicate that the growth of lead layer on the Ni(001) face depends on substrate temperature. The analysis of AES measurements shows that the two-dimensional growth of the first Pb monolayer takes place for the substrate temperature from 145 K to 900 K. After the completion of the first lead monolayer, the three-dimensional growth of Pb is observed. Over the range the Stransky - Krastanov growth was observed. The Pb-Ni alloy formation was not observed. Above $T > 600$K, desorption of lead atoms is observed. The ordered LEED patterns corresponding to p(1x1) and c(2x2) structures have been observed.

O 59.61 Wed 17:45 Poster B1

General aspects of surface alloy formation

— •Andreas Bergbreiter[1], András Berkó[2], Albert K. Engstfeld[1], Ralf T. Rötter[1], Harry E. Hoster[1], and R. Jürgen Behm[1] — [1]Institute of Surface Chemistry and Catalysis, Ulm University, D-89069 Ulm, Germany — [2]Permanent address: Institute of Nanochemistry and Catalysis, of CRC-HAS, University of Szeged, H-6720 Szeged, Hungary

Surface confined alloys are excellent model systems for studies of structure-property relationships of bimetallic surfaces. They are formed by deposition of a guest metal B onto a substrate A, followed by annealing to a temperature, where place exchange between adatoms and atoms from the underlying surface layer becomes possible and diffusion into the bulk is sufficiently slow. We exemplarily confirmed by scanning tunneling microscopy and Auger electron spectroscopy for PtRu/Ru(0001) [2], PdRu/Ru(0001) [3,4], AuPt/Pt(111), AgPt/Pt(111), and AgPd/Pd(111), surface alloys are obtained for systems where metal B has a negative surface segregation energy within metal A [1]. By exchanging A and B, however, AB surface alloys are most likely overgrown by metal B, which we will demonstrate for RuPt/Pt(111) [5,6] in comparison to PtRu/Ru(0001) [2].

[1] A. Christensen et al., *Phys.Rev.B* 56(10), **1997**, 5822.
[2] H.E. Hoster et al., *Phys.Chem.Chem.Phys.* 10, **2008**, 3812.
[3] H. Hartmann et al., *Surf.Sci.* 603, **2009**, 1439.
[4] N. Rougemaille et al., *Phys.Rev.Lett.* 99, **2007**, 106101.
[5] A. Bergbreiter et al., *Vacuum* 84(1), **2009**, 13.
[6] A. Berkó et al., *Surf.Sci.* 603, **2009**, 2556.

O 59.62 Wed 17:45 Poster B1

Temperature-induced modifications of PdZn surface alloys on Pd(111) and first results for Ga on Pd(111)

— •Werner Stadlmayr, Christoph Rameshan, Simon Penner, Berhard Klötzer, and Norbert Memmel — Institut für Physikalische Chemie, Universität Innsbruck, Innrain 52a, 6020 Innbruck, Austria

Pd-Zn and Pd-Ga alloy films on Pd(111) are model systems aiming for a microscopic understanding of the mechanisms in Pd-Zn and Pd-Ga based catalysis for methanol steam reforming. The temperature-induced compositional and structural changes of these films are investigated in the catalytically relevant temperature range. We find that upon heating from 550 K to 630 K the alloy films change from a multilayer PdZn system to a "monolayer" situation due to diffusion of subsurface Zn into the Pd bulk. The change in subsurface stoichiometry triggers an inversion of the surface corrugation from Zn-out/Pd-in to Pd-out/Zn-in. This modification in surface geometric (and electronic) structure provides an explanation for the recently observed drastic changes in catalytic selectivity.

Furthermore, first results for Ga on Pd(111) are presented. Similar to Zn/Pd(111) we observe, that in the temperature window around 500 K an alloy with a 1:1 surface composition is formed. However in contrast to the Zn/Pd system no long-range order is observed in the alloyed state, while the short range order is preserved.

O 59.63 Wed 17:45 Poster B1

Transport-measurements of electro-chemically fabricated metallic contacts under laser illumination

— •Bastian Kopp[1], Markus Schmotz[1], Daniel Benner[1], Christian Obermair[2], Fangqing Xie[2], Thomas Schimmel[2], Paul Leiderer[1], and Elke Scheer[1] — [1]Universität Konstanz — [2]Universität Karlsruhe

Aim of this work is to study the effects of laser illumination on metallic point contacts. So far lithographically fabricated Mechanically Controllable Breakjunctions (MCBs) [E. Scheer, Phys. Rev. Lett. **78**, 3535 (1997)] as well as Gate-Controlled Atomic Quantum Switches (GQS) [F.-Q. Xie, Phys. Rev. Lett. **93**, 128303 (2004)] were used to create atomic point-contacts. MCBs operate at ambient conditions whereas GQS use the electrochemical deposition and dissolution of metal atoms to create these contacts.

Previous work on illumination effects on MCBs showed dependences on the wavelength, the position, the size of the contacts [D. C. Guhr, Phys. Rev. Lett. **99**, 086801 (2007)] and the optical properties of the substrate material [unpublished]. The latter result points to the possible influence of thermal expansion besides the photo-assisted transport due to the excitation of high-energy quasiparticles [J.K. Viljas, Phys. Rev. **B 75**, 075406 (2007)] and the excitation of surface plasmons.

In order to minimize the influence of thermal expansion we now investigate the effect of light on GQS. We will present first results obtained under light irradiation on GQS and discuss possible mechanisms including photochemical reactions.

O 59.64 Wed 17:45 Poster B1

Dealloying below the critical potential: Cu-Au and Cu-Pd

— Frank Uwe Renner, •Shilan Meimandi, and Aparna Pareek — MPI Eisenforschung, Düsseldorf

Corrosion causes a loss of more than 3% of GDP to society. Dealloying is an important corrosion process occurring at alloy surfaces immersed in electrolyte, and which are composed of elements with a large difference in Nernst potentials. The dealloying behaviour of the model system Cu3Au in 0.1M H2SO4 was previously investigated using in-situ X-ray diffraction [1] and we will present here recent ex-situ measurements using scanning Auger electron spectroscopy with a lateral resolution of less than 10 nm. We reported the formation of an ultra-thin epitaxial passive Au layer at lower overpotentials with a reversed stacking sequence, which transforms to thicker Au islands and finally to porous Au at higher overpotentials (critical potential for dealloying). For the in-situ X-ray diffraction studies we developed recently an UHV compatible electrochemical chamber in order to study more reactive samples and electrolytes which we recently adapted for use with ionic liquids as electrolytes [2]. The research on dealloying is now extended to the system of Cu-Pd alloys and we will present first results by in-situ XRD, scanning Auger electron spectroscopy and atomic force microscopy (AFM).

[1] Renner et al., Phys. Rev. B 77 (2008) 235433 [2] Borrisov et al., submitted to PCCP

O 59.65 Wed 17:45 Poster B1

Atomic structures of absorbed Zn(ll) phthalocyanine on an iodide modified Cu(1 0 0) electrode — •Thanhhai Phan[1], Hahn Uwe[2], Thomas Torres[2], and Klaus Wandelt[1] — [1]Institute of Physical and Theoretical Chemistry, University of Bonn, Wegelerstr.12, 53115 Bonn, Germany — [2]Departamento de Quimica Organica c-i-305, Universidad Autonoma de Madrid, Campus de Canoblanco, 28049 Madrid, Spain

Combined Voltammetric and in-situ STM studies were employed to gain information about the structures of partially water-soluble Zn-PcPyMe molecules covered on an iodide template. The flat-lying molecules form a square-lattice on a $c(p \times 2)$–I superstructure modified Cu(1 0 0) within the double layer regime. The distance between molecules was estimated to be (1.95 ± 0.2) nm based on line-profile measurements. This molecular lattice is rotated by $(62 \pm 2)^\circ$ with respect to the [0 1 1] direction of the substrate, i.e. the commensurate direction of the iodide under layer. This clearly excludes a template effect of the substrate surface, but rather hints to a molecular self-assembly. Detailed molecular models are also proposed for two phases obtained in perfect agreement with the experimental observation.

O 59.66 Wed 17:45 Poster B1

Competitive Adsorption of Viologen Species on a Chloride Modified Copper (100) Surface — •Martino Saracino[1], Nguyen Thi Minh Hai[2], Peter Broekmann[2], and Klaus Wandelt[1] — [1]Institut of Physical and Theoretical Chemistry, University of Bonn, Wegelerstr. 12, 53115 Bonn, Germany — [2]Interfacial Electrochemistry Group, Department of Chemistry and Biochemistry, University of Berne, Freiestr. 3, 3012 Berne, Switzerland

A number of technological relevant processes involve charge transfer reactions at electrified solid\liquid-interfaces. Their microscopic understanding requires the study of the electrode surface under in situ reactive conditions, for instance STM and cyclic voltammetry. The competitive adsorption of Diphenyl- (DPV) and Dibenzylviologen (DBV) on a Cl^- modified Cu(100) surface was chosen as model system for similar N-containing aromatic molecules, which play a significant role as additives in metal plating. Upon adsorption DPV^{2+} is reduced even at most anodic potentials to the monocationic radical DPV^{+*} and forms a full monolayer of a hydrophobic π-stacked stripe phase which, however, does not prevent further redox reactions to take place. Lowering the electrode potential to the DBV^{2+} reduction potential at -250mV [RHE] leads to the replacement of the DPV^{+*} phase by a π-stacked stripe phase consisting of the produced monocationic DBV^{+*}. Conversely, returning to the DPV^{+*} oxidation potential at -100mV [RHE] leads to a re-substitution of the DBV^{+*}- by the initial DPV^{+*}-stripe phase. In contrast to mono-viologen systems no stable dicationic phases have been observed at all.

O 59.67 Wed 17:45 Poster B1

Deposition of thin films of Ionic Liquids - Access to the IL/Solid-interface — •Michael Stark[1], Till Cremer[1], Claudia Kolbeck[1], Florian Maier[1], Peter Wasserscheid[2], and Hans-Peter Steinrück[1] — [1]Lehrstuhl für Physikalische Chemie II — [2]Lehrstuhl für Chemische Reaktionstechnik, University of Erlangen-Nuremberg, Egerlandstr. 3, 91058 Erlangen

Ionic Liquids (ILs), salts with melting points below 100° C, have attracted a great deal of interest in the last few years due to their promising physico-chemical properties. Important phenomena such as surface passivation, charge transfer and wetting behavior are determined by the IL/solid interface.

To access such interfaces by means of XPS, ultra thin IL films are prepared by physical vapor deposition (PVD) under ultra high vacuum conditions, as has been shown earlier.[1]

In this study, thin layers of selected ILs were deposited on well defined Au (111) single crystal surfaces in order to obtain a more detailed understanding of IL/substrate interactions. The main aspects thereby are the electronic interactions between the gold surface and the IL and the growth behavior of the films.

This work was supported by the DFG through SPP 1191 "Ionic Liquids" and by the "Cluster of Excellence 'Engineering of Advanced Materials'".

Literature: [1] T. Cremer, ChemPhysChem, 2008, 9, 2185-2190

O 59.68 Wed 17:45 Poster B1

Structural transitions of heptyl viologen adlayers on Cu(1 0 0) – an electrochemical and in situ STM study — •Min Jiang, Knud Gentz, and Klaus Wandelt — Institute for Physical and Theoretical Chemistry, University of Bonn, Wegelerstr. 12, 53115 Bonn

The redox behaviour and potential dependent adsorption structure of heptyl viologen (abbreviated as DHV^{2+}) on a Cu(1 0 0) electrode have been investigated in a chloride-containing electrolyte solution by in situ electrochemical scanning tunneling microscopy (EC-STM). After injecting DHV^{2+} molecules into the KCl electrolyte solution, a highly ordered 2D dot-array structure in STM images emerges on a $c(2 \times 2)$ chloride modified Cu(1 0 0) electrode surface. DHV^{2+} molecules spontaneously arrange themselves with their molecular planes facing to the electrode surface and their long molecular axis parallel to a step edge. Such adsorption structure can be described by mirror domains and rotational domains which stably exist between 200mV and −100mV. One-electron reduction of dication DHV^{2+} around −150mV causes a phase transition from a dot-array assembly to a stripe pattern in STM images which has a bilayer structure. With a decrease of the applied electrode potential, the structure of $DHV^{\bullet+}$ adlayer undergoes a change from a loose stripe phase to a more compact stripe phase, and a subsequent decay of the compact structure, and then a formation of new dimer phase. A further electron transfer reaction at −400mV causes the appearance of an amorphous phase on the electrode surface.

O 59.69 Wed 17:45 Poster B1

Chemical Charaterization of Porphyrin Adsorbed on Anion Modified Copper Electrodes: An SXPS Study — •Stephan Breuer[1], Knud Gentz[1], Duc Thanh Pham[1], Thanh Hai Phan[1], Thomas Mayer[2], Peter Broekmann[3], and Klaus Wandelt[1] — [1]Universität Bonn, Institut für Physikalische und Theoretische Chemie, Wegelerstraße 12, D-53115 Bonn — [2]Technische Universität Darmstadt, FB Materialwissenschaft, Petersenstraße 23, D-64284 Darmstadt — [3]Universität Bern, Departement für Chemie und Biochemie, Freiestraße 23, CH-3012 Bern

Several Anions adsorb specifically from aqueous solution on copper electrodes. In case of copper single crystals, the electrode acts as a template for the anion adsorption and well ordered superstructures are observable. These, negatively charged, anion layers are used as secondary templates for the adsorption of cationic organic molecules.

The adsorption of TMPyP (Tetramethylpyridiniumporphyrin) has been extensively studied by in-situ EC-STM [1] which provides structural and electrochemical data, but there are less data about the chemical composition of the adsorbate layer. We have characterized (ex-situ) the chemical composition of the adsorbed TMPyP molecules on halide and sulfide modified Cu(100) and Cu(111) using XPS at the synchrotron radiation facility BESSY II.

[1] N.-T.M. Hai, B. Gasparovic, P. Broekmann, K. Wandelt, Surf. Sci. 601, 2007, 2597-2602.

O 59.70 Wed 17:45 Poster B1

Electrospray Ion Beam Deposition of Molecules and Nanoparticles — •Gordon Rinke[1], Nicha Thontasen[1], Zhitao Deng[1], Nikola Malinowski[1], Stephan Rauschenbach[1], and Klaus Kern[1,2] — [1]Max Planck Institute for Solid State Research, Heisenbergstrasse 1, 70569 Stuttgart, Germany — [2]Institut de Physique de la Matiere Condensee, Ecole Polytechnique Federale de Lausanne, 1015 Lausanne, Switzerland

The vacuum deposition of complex molecules and nanoparticles is an important technological step towards applications, for instance in molecular devices or as surface functionalization. Vacuum based processing assures well defined and clean structures in contrast to deposition under ambient conditions or from solution. A possibility to deposit non-volatile particles is given by electrospray ion beam deposition (ES-IBD) [1]. In-situ sample preparation, beam preparation, and sample analysis by scanning tunneling microscopy (STM) allows full control over all deposition parameter [2]. Here, we present recent results of the deposition of molecules and nanoparticles by ES-IBD. We demonstrate the control of coverage, cleanliness, deposition energy, and beam composition and give examples for the in-situ characterization by STM.

[1] Small 2 (2006), 540-547

[2] ACS Nano 3 (2009), 2901

O 59.71 Wed 17:45 Poster B1

Electronic properties of metal-organic coordination bonding — •Christoph Limbach[1], Robert Drost[1], Nils Henningsen[1], Riccardo Rurali[2], Katharina J. Franke[1], and Nacho Pascual[1] — [1]Freie Universität Berlin, Berlin, Germany — [2]Institut de Ciència de Materiales de Barcelona (ICMAB), Barcelona, Spain

Metal organic networks are a promising system for tuning the electronic and magnetic properties of single metal atoms. Using low temperature scanning tunneling microscopy and spectroscopy (STM/STS) we investigate the coadsorption of di-metacyano azobenzene (DMC) molecules and cobalt atoms on a Au(111) surface leading to metal-organic chains. dI/dV spectroscopy and conductance maps plotting the distribution of unoccupied resonances are used to localize and characterize the coordination bonds between Co adatoms and DMC. We find that Co-molecule coordination bonds are formed distinguishably at different intramolecular sites, i.e. at the lone-pair electrons at the cyano termination and the di-azo bridge (-N=N-). Density functional theory simulations find a different degree of charge transfer and hybridization of the atomic and molecular orbitals for the two different sites, thus sustaining the experimental observations.

O 59.72 Wed 17:45 Poster B1

Ab initio investigation of surface adsorption phenomena: from pyridine gold complexes to larger system — Doreen Mollenhauer, Johannes Floss, •Elena Voloshina, and Beate Paulus — Institut für Chemie und Biochemie - Physikalische und Theoretische Chemie, Freie Universität Berlin, Takustraße 3, 14195 Berlin, Germany

The investigation of the adsorption of organic molecules on metal substrates plays an important role for the understanding of multivalent interactions. Due to the enhancement of the adsorption new architectures of multivalent molecules can appear on metal surfaces. Taking into account recent molecular electronic experiments involving molecules linked via N-heterocycles to gold electrodes and nanoclusters[1], pyridine derivates are seen to be interesting objects for theoretical studies. The interaction of the parent compound pyridine and some substituted derivates with a single gold atom has been investigated. Different quantum-chemical methods and basis sets have been used to find a reliable description. We plan to extend our studies to gold clusters, gold nanoparticles and para-linked pyridine derivates. The main purpose is to analyze the nature of multivalent bonding in comparison to monovalent interaction.

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O 59.73 Wed 17:45 Poster B1

What encodes the diversity and ordering of self-organized monolayers? — •Carsten Rohr[1], Marta Balbás Gambra[2], Kathrin Gruber[1], Edwin C. Constable[3], Erwin Frey[2], Thomas Franosch[2], and Bianca A. Hermann[1] — [1]Walther-Meissner-Institute (WMI) of Low Temperature Research of the Bavarian Academy of Science and Center for Nano Science (CeNS), Germany Walther-Meissner-Strasse 8, 85748 Garching b. München — [2]Arnold Sommerfeld Center for Theoretical Physics (ASC) and Center for Nano Science (CeNS), Department of Physics, LMU München, Theresienstraße 37, 80333 München, — [3]Department of Chemistry, University of Basel, Spitalstrasse 51, 4056 Basel, Switzerland

The a priori prediction of patterns formed by molecular self-organization is of crucial importance for the deliberate application of monolayers in functionalizing surfaces. We used scanning tunneling microscopy (STM) to image self-organized monolayers of Fréchet dendrons, which display a large variety of 2D ordering motifs. The ordering of the different phases was simulated by molecular mechanics (MM) energy optimizations. We conceived a coarse-grained interaction-site model, which condenses the essential molecular properties determined by MM modeling. In a Monte Carlo (MC) approach based on this interaction site model placed on a lattice allowing discrete $\pi/3$ rotations the various ordering motifs were successfully predicted. With this model we could confirm that geometry as well as a few salient interaction sites encode the observed variety of structural motifs.

O 59.74 Wed 17:45 Poster B1

Hydrocarbon contamination of different ruthenium surface orientations — •Thanh-Nam Nguyen[1], Sina Gusenleitner[1], Marius Ernst[1], Holger Wetzstein[1], Dirk Ehm[2], and Friedrich Reinert[1] — [1]University of Würzburg, Experimental Physics VII, Am Hubland, 97074 Würzburg — [2]Carl Zeiss SMT AG, Rudolf-Eber-Str. 2, 73447 Oberkochen

Multilayer mirrors for Extreme Ultraviolet (EUV) Lithography applications are threatened by various damaging processes. During exposure, the dominating contamination processes are carbonization and oxidation due to adsorption of hydrocarbons and oxygen and their reaction with the mirror surface, reducing the mirror lifetime. One possibility to limit these lifetime risks is to coat the mirror with a dedicated capping material, such as Si, Ti, Mo, Pd, Ru, or their oxides. To study the general interaction mechanisms of adsorbates with the capping materials, organic model molecules are used. In this work, the interaction of 3,4,9,10-perylene tetracarboxylic dianhydride (PTCDA) with single crystalline Ru(0001) and Ru(1-100) surfaces as well as evaporated thin Ru films is presented. PTCDA molecules are deposited on the Ru surfaces by organic molecular beam epitaxy. The structural and electronic properties of the resulting interfaces are investigated by various surface analytical techniques, including low energy electron diffraction (LEED), scanning tunnelling microscopy (STM), X-ray photoelectron spectroscopy (XPS) and ultraviolet photoelectron spectroscopy (UPS).

O 59.75 Wed 17:45 Poster B1

A Nanocalorimeter for Adsorption Studies of Organic Molecules — •H.-J. Drescher, F. Bebensee, O. Lytken, H.-P. Steinrück, and J. M. Gottfried — Lehrstuhl für Physikalische Chemie II, Egerlandstraße 3, 91058 Erlangen

Surface nanocalorimetry (SNC) is an UHV based technique for the measurement of adsorption enthalpies on well defined substrates. It is the only technique that provides access to adsorption enthalpies in cases of non-reversible adsorption, i.e., if decomposition occurs at lower temperature than desorption. Typical examples are large organic molecules on metal substrates. SNC relies on the direct measurement of very small temperature changes induced by the adsorption of molecules on single-crystal surfaces. Its outstanding sensitivity in the nanojoule and picomole regimes is achieved by pyroelectric detectors in combination with pulsed molecular beams and highly accurate flux, sticking probability and reflectivity measurements. The adsorption enthalpy is a direct measure for the strength of the adsorbate-substrate interaction and thus one of the most important parameters for the quantitative characterization of chemical bonds at surface and interfaces. We focus especially on metal/organic interfaces, which occur in organic electronic devices. The character of the interfacial bond determines crucial parameters for the device performance, such as the charge injection rate. A setup of an advanced adsorption calorimeter is presented, which is optimized for the studies of π-conjugated molecular semiconductors on metal single-crystal surfaces. It features several new technical developments, which lead to improved sensitivity and accuracy.

O 59.76 Wed 17:45 Poster B1

Electron Spectroscopy of Organic Heterointerfaces: SnPc/PTCDA/Ag(111) — •Michael Greif[1], Marc Häming[1], Michael Wiessner[1], Achim Schöll[1], and Friedrich Reinert[1,2] — [1]Universität Würzburg, Experimentelle Physik VII, D-97074 Würzburg — [2]FZK Karlsruhe, Gemeinschaftslabor für Nanoanalytik, D-76021 Karlsruhe

Heterointerfaces between different organic molecules are an issue of great technologic relevance. However, structurally well-defined ultrathin interfaces which are suited for the investigation with surface sensitive techniques are difficult to prepare. In order to exploit its potential as a model system in this respect we have investigated hetero-layers consisting of tin-phthalocyanine (SnPc) and perylene-tetracarboxylic acid dianhydride (PTCDA) deposited on clean Ag(111) surfaces with photoelectron spectroscopy (XPS and UPS), x-ray absorption and low energy electron diffraction (LEED). The spectroscopic signatures of the two compounds can be distinguished unambiguously in the core and valence spectra. For ultra-thin SnPc layers deposited on a single layer of PTCDA on Ag(111) structural information can be derived from angle resolved XPS and NEXAFS. The data indicates that a closed monomolecular layer of flat lying SnPc is established. This is corroborated by the UPS spectra which show a characteristic splitting of the SnPc HOMO signal due to dimer formation only for SnPc coverages beyond one layer. Moreover, LEED was applied in order to investigate the lateral ordering.

O 59.77 Wed 17:45 Poster B1

Self-assembled metal-organic networks of tripyridyl-triazine on Au(111) and Cu(111) surfaces — •Hendrik Mohrmann, Christian Lotze, Katharina J. Franke, and Jose I. Pascual — Institut für Experimentalphysik, Freie Universität Berlin

Self-assembled metal-organic networks have lately attracted a lot of interests since they possibly provide arrays of spins which have promising properties for applications in molecular electronics. We investigate the coadsorption of tripyridyl-triazine (t4pt) and Cobalt on noble metal surfaces by low and variable temperature scanning tunnelling microscopy and spectroscopy (STM/STS) in ultrahigh vacuum.

On Au(111), several highly ordered structures with a wide range of Co-N bond lengths and packing densities, depending on the Co/t4pt deposition rates and annealing temperatures, are observed. We also observe double layer islands in which Co atoms are coordinated in a 3-dimensional complex.

When deposited on Cu(111) t4pt forms a long-range ordered honey comb nanomesh. This structure is stabilized by coordination bonds of the lone-pair electrons of the pyridil groups to Cu adatoms as evidenced by conductance maps.

O 59.78 Wed 17:45 Poster B1

Surface assisted oxidation of flat lying organic molecules - a real-time STM study — •Thomas Waldmann[1], Daniela Künzel[2], Michael Roos[1], Achim Breitruck[1], Harry E. Hoster[1], Axel Gross[2], and R. Jürgen Behm[1] — [1]Institute of Surface Chemistry and Catalysis, Ulm University, D-89069 Ulm, Germany — [2]Institute of Theoretical Chemistry, Ulm University, D-89069 Ulm, Germany

Using time resolved scanning tunneling microscopy (STM), we tested the interaction of O_2 from gas-phase with ordered adlayers of the Bis(terpyridine) derivative 2,4'-BTP [1,2] on Au(111) [3], Ag(111) [3,4] and graphite (HOPG) [1-3,5] surfaces at T = 300 K. At an O_2 pressure of 10^{-5} mbar, the adlayers on Ag(111) undergo chemical and structural changes. These include modifications of the 2-pyridyl rings of individual 2,4'-BTP adsorbates and rearrangements of the hydrogen bonded adlayer. Since we do not observe similar changes on HOPG and Au(111), we assume that Ag(111) acts as catalyst for the underlying processes. Based on our STM data in combination with DFT calculations, we conclude that the observed reaction is pyridyl-N-oxide formation. Furthermore, we derive reaction yields, enantiomeric excess, reaction rates and reaction orders from the time-resolved STM data.

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[3] H.E. Hoster et al., *Langmuir* 23, **2007**, 11570.
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[5] M. Roos et al., *Phys.Chem.Chem.Phys.*, DOI:10.1039/b920481d

O 59.79 Wed 17:45 Poster B1

Multi-molecular networks on Ag(111) displaying a novel bonding scheme — •Wolfgang Krenner[1], Dirk Kühne[1], Florian Klappenberger[1], Svetlana Klyatskaya[2], Mario Ruben[2], and Johannes V Barth[1] — [1]Physikdepartment E20, TU München, München, Germany — [2]Institute of Nanotechnology, Forschungszentrum Karlsruhe, Karlsruhe, Germany

The combination of different types of molecular building blocks provides a wide range of possibilities for the hierarchic construction of molecular networks on metallic surfaces via self-assembly. We present a UHV, low-temperature scanning tunneling microscopy study of the formation of multi-molecular networks constructed with two different bonding schemes.

After deposition of the two building blocks, namely dicarbonitrile polyphenyl (A) and diphenyl oxalic amide (B), at room temperature onto Ag(111), hydrogen-bonded networks formed by molecular self-assembly can be observed. The shape of the molecular networks depends on coverage and stoichiometry.

By tuning the growth conditions highly regular molecular networks can be achieved providing rhombic cavities of an approximate size of 8 nm^2. The elementary binding motif features a hydrogen bond from a carbonitrile group of molecule A to the amine group of molecule B. This type of hydrogen bond has not been observed so far for surface confined self-assembly.

O 59.80 Wed 17:45 Poster B1

A photoelectron diffraction investigation of vanadyl phthalocyanine on Au(111) — David Duncan[2], •Werner Unterberger[1], Tsenolo J. Lerotholi[2], Kirsty Hogan[3], Christine Lamont[3], and Phillip Woodruff[1,2] — [1]Fritz-Haber-Institute — [2]Physics Department, University of Warwick — [3]Deptartment of Chemical and Biological Sciences, University of Huddersfield

Scanned-energy mode photoelectron diffraction (PhD) is a well-established method to determine quantitatively the local structure of adsorbates at surfaces. Here we describe its application to adsorption of vanadyl phthalocyanine (VOPc) on Au(111) which was used as a model system for vanadyl species (V=O) on the clean V_2O_3 surface.

VOPc was dosed at 130°C on the clean Au(111) surface and a coverage of approximately 0,015ML was reached which is half of that found by STM experiments (Hipps et. al.). O 1s and V 2p scanned-energy mode photoelectron diffraction has been used to investigate the adsorption structure of VOPc. The V=O vanadyl bond is found to point out of the surface with a bondlength of 1.60+-0.04 A. Relative to bulk VOPc, the V atom is pulled down into the approximately planar region defined by the N and C atoms by 0.52 (+0.14/-0.10) A.

O 59.81 Wed 17:45 Poster B1

Thin vacuum deposited films of charge transfer compounds on the Au(111) surface investigated by SPA-LEED — •Benjamin Fiedler, Oliver Bauer, and Moritz Sokolowski — Institut für Physikalische und Theoretische Chemie der Universität Bonn

Thin films of different charge transfer compounds were prepared on the Au (111) surface and studied by spot profile analysis LEED (SPA-LEED). For tetrathiafulvalene / tetracyanoquinone (TTF/TCNQ) the films were obtained via two different routes. In the first, we prepared the films by vacuum sublimation from a single crucible containing the charge transfer compound. In the second, the single components (TTF and TCNQ) were evaporated from two different crucibles. Findings of both preparation methods are compared with each other. From the LEED patterns a unit cell of the monolayer was derived and is compared with those unit cells concluded from earlier STM investigations [1,2]. We also studied the larger molecule tetrathiatetracene (TTT) as donor component in combination with dimethyl-dicyanoquinondiimine (DCNQI) and TCNQ as acceptors. First results are presented.

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[2] J. I. Pasqual, Phys. Rev. Lett. 100, 156805 (2008)

O 59.82 Wed 17:45 Poster B1

Investigation of self-sustained molecular wires — •Kerrin Dössel[1], Maya Lukas[1], Alexandrina Stuparu[1], Christophe Stroh[1], Karin Fink[1], Marcel Mayor[1,2], and Hilbert von Löhneysen[3,4] — [1]Institut für Nanotechnologie, KIT, D-76021 Karlsruhe — [2]Department of Chemistry, University of Basel, CH-4056 Basel — [3]Physikalisches Institut, KIT, 76128 Karlsruhe — [4]Institut für Festkörperphysik, KIT, 76021 Karlsruhe

In recent years the conductance of organic molecules has been investigated in a growing number of scanning tunneling microscopy (STM) experiments since STM is capable of characterising the investigated system with (sub)molecular resolution. However, conductance measurements with the current along the long axis of a wire-like molecule are difficult to achieve by STM because the molecules have the tendency to "lie" with their long axis parallel to the surface. We investigate the electronic properties of taylor-made organic molecules: While one wire-like part of the molecule is lying with the long axis parallel to the surface another identical wire is sticking out freely from the surface, accessible by the tip of our STM. We used scanning tunneling microscopy and scanning tunneling spectroscopy to investigate the molecules' position and surrounding on the surface and the electronic properties at low temperature (30K). Due to the special geometry of our molecules we are able to investigate and compare the transport across the wire as well as along the wire in the same experiment without altering further parameters which might otherwise influence the conductance behaviour.

O 59.83 Wed 17:45 Poster B1

Cobalt porphyrin and phthalocyanine complexes on Ag(111) and Au(111): Interfacial coordination interactions — •Yun Bai, Martin Schmid, Michael Sekita, Thomas Bischof, Hans-Peter Steinrück, and Michael Gottfried — Universität Erlangen-Nürnberg, Lehrstuhl für Physikalische Chemie II

Metalloporphyrins and metallophthalocyanines are of increasing technological interest due to their potential applications in heterogeneous catalysis, sensor systems, photovoltaics and organic electronics. In most of these applications the interfacial electronic interactions and the chemical bonds between the metal complexes and a solid substrate (metal or oxide) plays an important role. To obtain fundamental insight especially into the contributions of the coordinated metal centers to the surface chemical bond, we studied monolayers of cobalt(II)-phthalocyanine (CoPc), cobalt(II)-octaethylporphyrine (CoOEP), and cobalt(II)-tetraphenylporphyrine (CoTPP), adsorbed on Ag(111) and Au(111), using XPS and UPS. On Ag(111), uniform core level shifts and the appearance of a new valence state indicate that the Co ions interact strongly with the substrate and that the interactions are laterally homogenous, i.e., virtually all Co ions interact in a same way with the Ag substrate. On Au(111), however, a split Co $2p_{3/2}$ signal suggests the presence of two different cobalt species in the monolayer. This observation is discussed in the context of the herringbone reconstruction of the Au(111) surface, which leads to lateral variations of geometric and electronic structure and thus potentially different adsorption sites. Supported by the DFG through SFB 583.

O 59.84 Wed 17:45 Poster B1

Substrate- and temperature-dependent adsorption studies of azobenzene molecules. — •Alex Krüger[1], Marten Piantek[1], Matthias Bernien[1], Felix Hermanns[1], Jorge Miguel[1], Klaus Hermann[2], and Wolfgang Kuch[1] — [1]Freie Universität Berlin, Institut für Experimentalphysik — [2]Theory Department, Fritz-Haber-Institut der Max-Planck-Gesellschaft

The adsorption of dimetacyano-azobenzene (DMC) evaporated onto Cu(100) and Au(111), as well as on CoO/Ag(100), was studied at different substrate temperatures in order to ascertain the influence of substrate and coverage. Angle-dependent NEXAFS spectroscopy was used to resolve the adsorption geometry of the molecules. By XPS the formation of additional bonds between the molecules and surface was investigated. For the adsorption on Au(111) at room temperature (RT), and on Cu(100) at 150 K, we find the molecules physisorbed in a planar conformation parallel to the surface. In the case of molecules adsorbed at 100 K on CoO/Ag(100), we observe a change in the angle dependence of the π^* resonances of the N-K edge NEXAFS. After annealing the Cu(100) substrate to RT, the angle dependence and intensity of the π^* resonances change significantly. From the peak assignment derived from DFT-based simulation of the NEXAFS spectra, we conclude that chemisorption takes place at the azo-nitrogen on Cu(100) at RT, whereas a mixed phase of physisorbed and chemisorbed molecules is found on CoO/Ag(100) at 100 K, and on Cu(100) at 150 K. In contrast, only the physisorbed phase was found for DMC on Au(111) at RT. This work has been supported by Sfb 658.

O 59.85 Wed 17:45 Poster B1

Binding chemistry and interface dipole formation of dithiol-based monolayers on gold — •Philip Schulz[1,2], Christopher D Zangmeister[2], Dominik Meyer[1], Matthias Wuttig[1], and Roger D Van Zee[2] — [1]Institute of physics (IA), RWTH Aachen University of Technology, 52062, Aachen, Germany — [2]Chemical Science and Technology Laboratory, National Institute of Standards and Technology, Gaithersburg, Maryland 20899, USA

The conditioning of metal surfaces via self-assembled monolayers (SAM) of molecules anchored by a sulfur endgroup is a widely studied issue in the field of organic electronics. In particular the electronic properties of the interface between electrode and subsequent functional organic layer in organic light emitting diodes (OLED), thin film transistors (OTFT) and photovoltaic devices (OPV) can be altered in order to promote charge transfer and improve the overall device efficiency. In our study we investigated the growth and electronic structure of dithiol-based monolayers on a Au(111) surface. We focus on the influence of this linker chemistry on the energy level alignment of the SAM and the workfunction change of the gold substrate. FTIR measurements were employed to verify the film formation while the electronic structure was further investigated by photoelectron spectroscopy. Not only did we derive the coverage and film perfection from XPS measurements but could also show a distinct charge rearrangement in the molecular layer while UPS measurements revealed a considerable lowering of the workfunction. DFT calculations have been employed in order to describe these phenomena.

O 59.86 Wed 17:45 Poster B1

L-tyrosine on Ag(111): universality of the amino acid 2D zwitterionic bonding scheme? — •Joachim Reichert[1,3], Agustin Schiffrin[2], Willi Auwärter[1], Alexander Weber-Bargioni[3], Matthias Marschall[1], Martina Dell'Angela[4], Dean Cvetko[4], Gregor Bavdek[4], Albano Cossaro[4], Alberto Morgante[4], and Johannes V. Barth[1,3] — [1]Physik Department E20, TU München, Germany — [2]Max-Planck-Institut für Quantenoptik, Garching, Germany — [3]Department of Physics & Astronomy, University of British Columbia, Vancouver, Canada — [4]C.N.R.-INFM, Laboratorio Nazionale TASK, Trieste, Italy

We present a combined study of the adsorption and ordering of the L-tyrosine amino acid on close-packed noble-metal surfaces in ultra-high vacuum by means of low-temperature STM, XPS and NEXAFS spectroscopy. Our high resolution topographical STM data reveal noncovalent molecular dimerization within the highly ordered one-dimensional nanostructures, which recalls the geometrical pattern already seen in the L-methionine/Ag(111) system and supports a universal bonding scheme for amino acids on the Ag(111) surface. XPS measurements reveal a zwitterionic adsorption, whereas NEXAFS experiments show a tilted adsorption configuration of the phenol moiety. This enables the interdigitation between aromatic side-chains of adjacent molecules via parallel-displaced Pi-Pi interactions which, along with the hydrogen-bonding capability of the hydroxyl functionality, could provide an explanation for the emergence of the self-assembled supramolecular nanoribbons.

O 59.87 Wed 17:45 Poster B1

Coordination networks of the charge transfer compounds TTF and TCNQ on Pb(111) — •Mario Konschake, Isabel Fernandez-Torrente, Katharina Franke, and Jose Ignacio Pascual — Freie Universität Berlin, Berlin, Germany

The charge transfer complex TTF-TCNQ has recently attracted considerable interest due to its electronic and magnetic properties when adsorbed on a Au(111) surface [1]. Here, we use low-temperature scanning tunnelling microscopy and spectroscopy to investigate the influence of a different substrate, i.e. Pb(111), on the adsorption properties.

As individual components, TTF and TCNQ exhibit very distinct bonding properties with the substrate. TTF adsorbs with its molecular skeleton perpendicular to the surface, giving rise to domains of π-stacked molecular islands. TCNQ, on the other hand, remains in a flat adsorption configuration and leads to an intriguing network, which is stabilized by Pb adatoms and their coordination bonding to the lone-pair electrons of the cyano terminations.

The coadsorption of TTF-TCNQ gives rise to a variety of phases with or without lead adatoms. Indications of a negative charging of the TCNQ molecules can be found in those forming metal-organic coordination networks.

[1] I. Fernández-Torrente et al. PRL 101(21):217203, 2008

O 59.88 Wed 17:45 Poster B1

Porphyrin based molecular switches and quantum corrals — Felix Bischoff, •Willi Auwärter, Knud Seufert, Daniel Heim, and Johannes V. Barth — Physik Department, E20, Technische Universität München, James-Franck Str. 1, D-85748 Garching, Germany

Porphyrin molecules exhibit an intriguing variety of functional properties, which are exploited in both biological and artificial systems. Hereby, particular interest lies on the porphyrin macrocycle, which can act as a chemical pocket and host either two hydrogen atoms or a metal ion. Here, we present first results on the tautomerization of free-base tetraphenylporphyrin molecules (H2-TPP) anchored on a Ag(111) surface. STM experiments proof that the switching of the two H's in the porphyrin pocket can be induced by voltage pulses. This process is directly monitored by current versus time (I-t) spectra, which exhibit two characteristic current levels. In addition, a tip induced process can be applied to remove one H atom from the porphyrin pocket. As a result, the remaining H atom can be switched between four possible positions (the four nitrogen atoms of the macrocycle).

In a different set of experiments, we show that the TPP's chemical pocket plays a non-neglibible role for the interaction of the porphyrin with the electronic structure of the supporting surface. By STM manipulation, individual TPP molecules are removed one-by-one from highly ordered TPP arrays on Ag(111), to construct artifical structures confining the Ag(111) surface state electrons. Hereby, the chemical nature of the corral walls, i.e. the use of either H2-TPP or Co-TPP arrays, affects the electron confinement and the coupling of resonators.

O 59.89 Wed 17:45 Poster B1

Diffusion of 1,4-butanedithiol radicals on Au(111) and Au(100): A DFT-based comparison — Andreas Franke and •Eckhard Pehlke — Institut für Theoretische Physik und Astrophysik, Universität Kiel, 24098 Kiel, Germany

Organic molecules chemisorbed on surfaces hold the perspective of surface functionalization. The 1,4-butanedithiol radical chemisorbed at the Au(111) or Au(100) surface serves as a model system for the S-Au molecule-substrate bond. Density functional total-energy calculations have been carried out for the chemisorption of the radical on the unreconstructed Au surfaces, which are both known to be stabilized under electrochemical conditions [1]. Local minima with close-by energies indicate multi-valley potential-energy surfaces, which originate from the interplay between the two S-Au adsorbate-substrate bonds and the internal degrees of freedom of the butanedithiol radical. Diffusion paths of the radical on both Au surfaces have been calculated within DFT using VASP [2]. The diffusion barriers for translation and rotation of the radical differ. They can be fine-tuned by varying the applied potential in the electrochemical cell. This is considered theoretically by inspecting the variation of the dipole moment along the reaction paths. Consequences for the dynamics of succeeding diffusion hops are discussed.

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[2] http://cms.mpi.univie.ac.at/vasp

O 59.90 Wed 17:45 Poster B1

STM study of the structual formation of C_{60} on a thiol tethered Au(111) surface — •Patrick Mehring, Axel Beimborn, and Carsten Westphal — Fakultät Physik - Technische Universität Dortmund, Otto-Hahn-Str. 4, D 44221 Dortmund, Germany

Since the discovery of fullerenes and their unique properties a large variety of potential applications was predicted. Different structures of fullerenes including ring, ball, and tube variations attracted attention especially in the fields of molecular electronics and nanotechnology. The understanding of the structural formation on different substrates is important for future applications of these carbon molecules. The influence of a methylthiol tethered Au(111) surface on the self assembly of C_{60} buckyballs was investigated by means of scanning tunneling microscopy. Methylthiol arranges in several structures on Au(111) depending on the monolayer coverage. C_{60} was prepared by evaporator deposition on two different striped phases of CH_3S. Both exhibit domains with 3 distinct orientations but different line spacing between single molecule rows. Instead of the typical hexagonal orientation of C_{60} on noble metals, domains of a striped phase can be found. Single domains show 6 possible orientations on the CH_3S monolayer. The spacing between C_{60} molecules varied depending on the orientation of the methylthiol layer. They are clearly located on top of the CH_3S rows.

O 59.91 Wed 17:45 Poster B1

Scanning Tunneling Microscopy and Spectroscopy of Phthalocyanine Molecules on Insulating Films — •Christof Uhlmann, Ingmar Swart, Tobias Sonnleitner, and Jascha Repp — Institute of Experimental and Applied Physics, University of Regensburg, 93040 Regensburg, Germany

Ultrathin insulating films on metal substrates can be used to electronically decouple individual molecules from the metallic substrate. As electrons can still tunnel through the films, scanning tunneling microscopy can be used to characterize these molecules. This geometry represents a double-barrier tunneling junction, in which at the resonances in conductance spectra, an electron is temporarily added to or removed from the molecule. Here we present a study of Cu-phthalocyanine molecules on different substrate systems. For a neutral Cu-phthalocyanine molecule the lowest unoccupied molecular orbital (LUMO) and the LUMO+1 are degenerate. By varying the substrate system, and thereby also varying the work-function, it is possible to permanently charge the molecules. Consequently, either the former LUMO or the former LUMO+1 is occupied with one electron. Due to the Jahn-Teller effect, the degeneracy of these orbitals is lifted. This manifests itself in a lowering of the symmetry as deduced from STM images.

O 59.92 Wed 17:45 Poster B1

Morphology, geometric and electronic structure of ultra thin films of perylene bisimide dyes on Ag(111) — •Markus Scholz[1], Rüdiger Schmidt[2], Achim Schöll[1,3], Frank Würthner[2], and Friedrich Reinert[1,3] — [1]Universität Würzburg, Experimentelle Physik VII, 97074 Würzburg — [2]Universität Würzburg, Institut für Organische Chemie, 97074 Würzburg — [3]Gemeinschaftslabor für Nanoanalytik, Forschungszentrum Karlsruhe, 76021 Karlsruhe

Perylene tetracarboxylic acid bisimides dyes (PBI) are among the best n-conducting organic materials. The molecular structure and electronic properties of these molecules can be tailored by halogen substituents attached to the perylene core which induces a twist angle in the planar perylene backbone. We studied the morphology, geometric and electronic structure of ultra thin epitaxial films of the planar $PBI - H_4$, the slightly twisted $PBI - F_2$ and the strongly twisted $PBI - Cl_4$ on Ag(111) substrates. At coverages below one molecular layer a long range order was observed at room temperature. From the characteristic LEED patterns we deduced real space models for each sample. Incommensurate superstructures were found were the size of the unit cell increases from $PBI - H_4$ to $PBI - Cl_4$. Moreover, the bonding at the interface and consequently the electronic structure is significantly influenced by the molecular conformation thus providing a possible route for tailor the properties of metal-organic interfaces.

O 59.93 Wed 17:45 Poster B1

Impact of central metal atoms and F-substituents on the adsorption geometry of phthalocyanine molecules on Cu(111) — •Christoph Bürker[1], Takuya Hosokai[1], Alexander Gerlach[1], Steffen Duhm[2], Norbert Koch[3], Hiroyuki Yamane[4], and Frank Schreiber[1] — [1]Universität Tübingen — [2]Chiba University — [3]HU Berlin — [4]Institut for Molecular Science

The adsorption geometry of large organic molecules on metal surfaces is essential for understanding and controlling the interface electronic structure, thin film structure and growth mechamism. The X-ray standing wave (XSW) technique is one of the most precise methods to determine the vertical positions of specific atoms relative to the substrate and can therefore establish the adsorption geometry of organic molecules.

Metal Phthalocyanines (MPc) as typical organic semiconductors are one of the most suitable systems for XSW experiments due to their chemical stability, high structural symmetry and variability of both the central metal atom and substituents. Using the XSW technique we show how fluorination and a central metal atom affect the adsorption geometry of Pc molecules. We compare the structural differences of metal-free Pc (H_2Pc), zinc-Pc (ZnPc) and perfluorinated ZnPc (F_{16}ZnPc) on Cu(111). The XSW data reveal significant deviations for both the bonding distance and molecular distortion. These results indicate an interaction strength of each atom with the surface depending on its chemical vicinity.

O 59.94 Wed 17:45 Poster B1

"Unbinding" an adsorbed organic molecule: K plus PTCDA on Ag(110) — •Oliver Bauer[1], Giuseppe Mercurio[2], Sergey Subach[2], Christoph H. Schmitz[1], Benjamin Fiedler[1], Frank Stefan Tautz[2], and Moritz Sokolowski[1] — [1]Institut für Physikalische und Theoretische Chemie, Universität Bonn — [2]Institut für Bio- und Nanosysteme 3, Forschungszentrum Jülich

We have doped the well-known brick-wall structure of pristine PTCDA which is present in the monolayer on the Ag(110) surface with potassium (K) and investigated the induced structural and electronic changes at the interface. SPA-LEED measurements reveal that the structural order of the PTCDA molecules is strongly altered upon K dosing: A variety of co-existing binary phases is observed within the monolayer. In addition we have conducted XPS and NIXSW measurements on K + PTCDA / Ag(110). The photoemission experiments indicate that the K atoms preferentially interact with the carboxylic groups of the co-adsorbed PTCDA molecules. This interpretation is further supported by the NIXSW results: The adsorption geometries of the carboxylic and the anhydride oxygen (O) atoms are highly influenced by the presence of K on the surface, the bonding distances are extended. The adsorption height of the perylene core is also increased by K doping. Hence we conclude that the local Ag-O bonds at the interface are partially lifted by the co-adsorbed K and that K and Ag atoms compete for the interaction with the carboxylic groups of PTCDA while the bonding across the interface is weakened. Supported by the DFG and the ESRF.

O 59.95 Wed 17:45 Poster B1

Kondo effect on a mixed Na-TCNQ layer — •Tobias R. Umbach, Isabel Fernández-Torrente, Robert Drost, Jose I. Pascual, and Katharina J. Franke — Institut für Experimentalphysik, Freie Universität Berlin, Animallee 14, 14195 Berlin, Germany

Mixing organic molecules with dopant atoms is a key issue in the field of organic electronics, as charge transfer processes may be used to tune the electronic properties of the compound. Here we report, by means of low-temperature scanning tunneling microscopy and spectroscopy measurements (LT-STM, STS), the doping of TCNQ by Na on a Au(111) surface. The addition of NaCl to previously formed TCNQ domains breaks the hydrogen network structure of the pure molecular island, leading to the formation of a new ordered Na-TCNQ phase with a bidimensional *wind-mill*-like structure. This self-assembling provokes a lateral electron transfer from the alkali metal to the organic molecule, inducing the localization of an unpaired spin on TCNQ. This free radical state can be demonstrated by the observation of a Kondo resonance arising in the Na-TCNQ unit cell. By STS we can plot the Kondo intensity of this unpaired spin: the Kondo resonance exhibits a different height along the Na-TCNQ layer, being largest at the center of the *wind-mill*structure and smaller at the center of the molecule.

O 59.96 Wed 17:45 Poster B1

DFT Studies on the Interaction of Sulfur with Transition Metal Surfaces — •Porntip Seema, Jörg Behler, and Dominik Marx — Lehrstuhl für Theoretische Chemie, Ruhr-Universität Bochum, D-44780 Bochum, Germany

The interaction of sulfur atoms with transition metal surfaces plays an important role for example in the poisoning of heterogeneous catalysts and the formation of self-assembled monolayers of thiolates. In the present work, the sulfur adsorption on Cu(111), Ag(111) and Au(111) surfaces has been studied within the framework of density-functional theory (DFT). Calculations have been carried out for a variety of adsorbate phases, and the sulfur binding sites and binding energies have been investigated systematically as a function of coverage at ideal surfaces as well as at defects. We find that the order of the adsorption energies of the sulfur atoms on the different defect-free metal slabs is Cu(111) $>$ Ag(111) $>$ Au(111). This result is independent of the coverage of the surface.

O 59.97 Wed 17:45 Poster B1

Vibrational Spectroscopy of Adsorbate Molecules on Roughened Cu(111) — Heiner Maslosz, •Jan Pischel, Olaf Skibbe, and Annemarie Pucci — Kirchhoff-Institut für Physik, Im Neuenheimer Feld 227, D-69120 Heideberg

In order to close the so-called material gap between pristine low-index single crystal surfaces and rough surfaces we study slightly roughened copper surfaces. The roughness is introduced by evaporation of small amounts of copper to the cooled Cu(111) surface. Vibrational spectroscopy (HREELS and IRRAS) has shown in the past several interesting findings regarding the interaction of the roughened surface with adsorbed molecules (e.g. [1,2]). In this study, we present high-resolution electron energy loss spectroscopy (HREELS) measurements of the system O_2/Cu/Cu(111). We found already at oxygen exposures of 0.01 Langmuir spectral features that we attribute to atomically adsorbed oxygen. Since the sticking probability for oxygen on the smooth Cu(111) surface is quite low, this system provides a sensitive tool to quantify the introduced roughness.

[1] O. Skibbe, M. Binder, A. Otto, and A. Pucci. J. Chem. Phys., 128:194703, 2008.

[2] O. Skibbe, D. Vogel, M. Binder, A. Pucci, T. Kravchuk, L. Vattuone, V. Venugopal, A. Kokalj, and M. Rocca. J. Chem. Phys., 131:024701, 2009.

O 59.98 Wed 17:45 Poster B1

Interaction of Fe and Fe_2O_3 with H_2O and CO — •Kai Volgmann[1], Anselm Hahn[1], Florian Voigts[1], and Wolfgang Maus-Friedrichs[1,2] — [1]Institut für Physik und Physikalische Technologien, TU Clausthal, Leibnizstr. 4, 38678 Clausthal-Zellerfeld — [2]Clausthaler Zentrum für Materialtechnik, TU Clausthal, Leibnizstr. 4, 38678 Clausthal-Zellerfeld

Basic investigations have been done on the interaction of Fe and Fe_2O_3 with molecular oxygen[1]. MIES/UPS and XPS measurements revealed that a passivating oxide layer has been formed and inhibits a further oxidation. The scope of this work is to examine the interaction of Fe and Fe_2O_3 with water and CO. This is a further step towards a basic data set for further research on the photocatalytical processes on hematite surfaces found under Martian conditions.

Iron and Iron(III) oxide films are investigated by means of their interaction with H_2O and CO. These reactions have been studied with photoelectron spectroscopy. X-ray photoelectron spectroscopy is used to determine stoichiometry of the samples, while Ultraviolet photoelectron spectroscopy and Metastable Induced Electron Spectrocopy are used to analyse the valence band region and to gain information about changes in workfunction due to reactions on the surfaces.

[1] K.Volgmann, F. Voigts, W. Maus-Friedrichs, *The interaction of oxygen molecules with iron films studied with MIES, UPS and XPS*, Surface Science, submitted

O 59.99 Wed 17:45 Poster B1

Adsorption of CO on clean and oxidized Pt3Ti(111) — •Marco Moors[1], Séverine Le Moal[2,3], Jan Markus Essen[1], Conrad Becker[2], and Klaus Wandelt[1] — [1]Institut für phys. und theoret. Chemie, Universität Bonn — [2]Centre Interdisciplinaire de Nanoscience de Marseille — [3]Technische Universität München

The adsorption of CO on Pt3Ti(111) before and after its oxidation has been investigated by AES, TDS, LEED and HREELS. The adsorption of CO has clearly been evidenced on clean Pt3Ti(111). The LEED patterns exhibit either a diffuse or a sharp c(4x2) structure (stable up to 300 K) attributed to CO depending on the adsorption temperature. Remarkably, the adsorption / desorption behavior of CO on clean Pt3Ti(111) exhibits similarities to that previously reported for CO on Pt(111). Our results clearly evidence a partial CO decomposition on Ti sites and molecular adsorption of CO on on-top Pt sites. Therefore, the clean surface can not be terminated by a pure Pt plane as previously discussed in the literature. Lowly oxidized Pt3Ti(111) surfaces ($<$ 135 L O2 exposure at 1000 K) exhibit a CO adsorption / desorption behavior similar to that of the clean surface with again a c(4x2) structure (stable up to 250 K) attributed to CO adsorption. These results indicate that some areas of the substrate remain non-oxidized upon low oxygen exposures. Highly oxidized and therefore completely oxide covered Pt3Ti(111) surfaces ($>$ 220 L O2 exposure at 1000 K) allow no CO adsorption at sample temperatures over 100 K.

O 59.100 Wed 17:45 Poster B1

Electron beam induced effects in ice on Pt(111) — •Daniel Schwarz, Herbert Wormeester, and Bene Poelsema — Solid State Physics, IMPACT, University of Twente, The Netherlands

The interactions at the water-solid interface determine a wide range of physical and chemical properties, relevant in nature and technology. The growth of a thin water layer on Pt(111) is considered a model system for studying this interaction. A series of complex crystalline structures were found as a function of the thickness of a thin ice film on this metal surface when grown at temperatures above 135K [1]. Below this temperature strongly amorphous ice growth is found. The thin ice layers (1-50ML) form a delicate structure. A fast restructuring of the film under the influence of an electron beam was found [2]. These energetic electron induced changes prohibit a detailed structural analysis with LEED. Although some lateral lattice structure determination is reported, an IV analysis is beyond the capabilities of a standard LEED system.

Electron induced phenomena can be reduced by using MCP-LEED which allows to use much lower electron current densities compared to conventional LEED. This does not only allow to measure in detail the development of the lattice parameter parallel to the interface with ice thickness, but also opens the possibility for a more detailed analysis via IV-LEED. A quadrupole is used to identify kinetics and composition of the desorbed species after prolonged electron bombardment.

[1] A. Glebov et al., J. Chem. Phys. 106 (1997) 9382

[2] J. Harnett et al., Surface Science. 528 (2003) 15

O 59.101 Wed 17:45 Poster B1

Particle Size Dependent Heat of Adsorption for CO on supported Pd Nanoparticles — •Jan-Henrik Fischer-Wolfarth[1], Jose Manuel Flores-Camacho[1], Jason Farmer[2], Charles Campbell[2], Jens Hartmann[1], Swetlana Schauermann[1], and Hans-Joachim Freund[1] — [1]Fritz-Haber-Institute of the Max-Planck-Society, Faradayweg 4-6, 14195 Berlin, Germany — [2]Department of Chemistry, University of Washington, Seattle, USA

The particle size dependence of the heat of adsorption for carbon monoxide on supported Pd nanoparticles has been investigated at 300 K with a new single crystal microcalorimeter and compared to the heat of adsorption on Pd(111). The average Pd particle size was varied systematically in the range of 100 to 4900 Pd atoms, i.e. 2 to 8 nm diameter. All nanoparticles were supported on Fe_3O_4(111)/Pt(111). The initial heat of adsorption was found to decrease monotonically with decreasing particle size below 4 nm. The correlation of the heat of adsorption with a particle size dependent reduction of the particle lattice constant [1] will be discussed.

Further, the microcalorimetry technique used to determine the adsorption energies and its performance will be presented.

[1] Nepijko *et al.* Langmuir 15 **1999** 5309

O 59.102 Wed 17:45 Poster B1

Manipulation of the wetting layer of H_2O on Pt(111) —

•Sebastian Standop[1], Alex Redinger[1], Markus Morgenstern[2], Thomas Michely[1], and Carsten Busse[1] — [1]II. Physikalisches Insitut, Universität zu Köln, Zülpicher Straße 77, D-50937 Köln — [2]II. Physikalisches Institut (IIB), RWTH Aachen, D-52056 Aachen

Previous LEED experiments unveiled strong effects of electron exposure on the structure of the adsorbed water layer on Pt(111) [1]. A transition from the $\sqrt{39} \times \sqrt{39}$ R16.1° structure to the simple commensurate $\sqrt{3} \times \sqrt{3}$ R30° arrangement was observed. Upon electron beam induced restructuring also exposure of bare Pt was found.

Using scanning tunneling microscopy we investigated the influence of electron dose, energy and scanning parameters on the $\sqrt{39} \times \sqrt{39}$ R16.1° overlayer. Our results show that above a threshold electron energy of about 4 eV the high order commensurate phase transforms into the $\sqrt{3} \times \sqrt{3}$ R30° overlayer through partial dissociation of water molecules. This superstructure has a higher molecular density than the initial domains with a $\sqrt{39}$ arrangement which explains the occurrence of uncovered substrate areas after electron beam manipulation. We could rule out that the tip electrical field is of relevance for the structural transition.

[1] J. Harnett, S. Haq and A. Hodgson, Surface Science 528 (2003) 15

O 59.103 Wed 17:45 Poster B1

Formation of copper oxide surface structures via pulse injection of air onto Cu(111) surfaces — •Carmen Pérez León[1], Michael Marz[1], Christoph Sürgers[1], and Hilbert v. Löhneysen[1,2] — [1]Karlsruher Institut für Technologie (KIT), Physikalisches Institut and DFG-Center for Functional Nanostructures (CFN), D-76131 Karlsruhe — [2]Karlsruher Institut für Technologie (KIT), Institut für Festkörperphysik, D-76131 Karlsruhe

The pulse-injection method is widely used for deposition of molecules in solution onto clean surfaces. A potential source of contamination of the solution in the valve can be the ambient air. Therefore we have investigated the clean Cu(111) surface after injection of air by Auger electron spectroscopy and scanning tunneling microscopy (STM). The results show that mainly oxygen is adsorbed on the copper surface. The initial stages of oxidation of Cu(111) are governed by the restructuring of the surface, since Cu atoms from the step edges and terraces are incorporated into the growing surface oxide. The nucleation and growth of the oxide is strongly influenced by the substrate temperature during deposition as well as by the oxygen coverage. At submonolayer coverage three different kind of oxide islands are observed, whereas at monolayer coverage these are reduced to two. High resolution STM images reveal that oxidation at room temperature produces poorly ordered oxide structures. In contrast, surface oxides produced at higher temperature ($\sim 200\,^\circ$C) exhibit additional highly ordered structures corresponding to the strained Cu$_2$O(111) lattice that coincides with the Cu(111) substrate.

O 59.104 Wed 17:45 Poster B1

Electronic structure of oxygen/W(110): photoemission study — Martin Weser[1], Alexander Generalov[1,2], Karsten Horn[1], and •Yuriy Dedkov[1] — [1]Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, Germany — [2]St. Petersburg State University, Russia

The study of oxygen interaction with W(110) has been a focus of many surface-science studies. Thermodinamics of the oxygen adlayer, including the phase diagram and critical behavior [1], have been investigated in series of LEED studies [2] and in later STM study [3]. Because of the relative simplicity in adsorption behavior, the W(110) surface provides an ideal surface to study the electronic structure of the initial stages of the interaction of oxygen with tungsten metal, and this system can be considered as a model for the consideration of catalysis effects on the heavy *d*-metal surfaces. Here we present the results of angle-resolved photoemission studies of the clean and oxidized W(110) surface. The both systems are examined via analysis of the electron dispersions at the particular regions of the Brillouin zone and the effect of the oxygen chemisorption on the electronic structure of W(110) is discussed.

[1] G. C. Wang et al., J. Chem. Phys. 69, 479 (1978).
[2] M. C. Tringides, Phys. Rev. Lett. 65, 1372 (1990).
[3] K. E. Johnson et al., Phys. Rev. Lett. 71, 1055 (1993).

O 59.105 Wed 17:45 Poster B1

DFT studies on the hydrogen adsorption on Pt(111) and Pt(111)-hydride surfaces — •Fedir Strygunov and Timo Jacob — Universität Ulm, Albert-Einstein-Allee 47, D-89069 Ulm, Germany

The catalytic reaction of hydrogen on Pt electrodes is one of the simplest, most fundamental and important reactions in electrochemistry. However, despite the apparent simplicity of the hydrogen oxidation and evolution reactions (HOR/HER) and a large numbers of studies, there is still no consensus about adsorption states of hydrogen on Pt electrodes.

Using periodic density functional theory in combination with the extended *ab initio* atomistic thermodynamics approach [1, 2] the structure and stability of clean Pt(111) and Pt(111)-hydride electrodes have been investigated. We find that at low coverages hydrogen prefers surface positions, but above 2 ML hydrogen also occupies subsurface tetrahedral positions, leading to the formation of a surface hydride. The electrochemical surface phase diagram showed that such a surface hydride might be stabilized with negative electrode potentials. On the basis of the most relevant surface hydride structures, further studies will aim on the electrocatalytic hydrogen reactions.

[1] M. Scheffler, J. Dabrowski, *Phil. Mag.*, **A 58**, 107 (1988).
[2] T. Jacob, *J. Electroanal. Chem.*, **607**, 158, (2007).

O 59.106 Wed 17:45 Poster B1

DFT Studies on the Oxygen Adsorption at Copper Surfaces — •Björn Hiller, Nongnuch Artrith, and Jörg Behler — Lehrstuhl für Theoretische Chemie, Ruhr-Universität Bochum, D-44780 Bochum, Germany

Oxide-supported copper clusters are important catalysts used for example in methanol synthesis. The surface structures and the morphologies of the copper clusters strongly depend on the composition of the surrounding gas phase [1], which therefore must have a significant influence on the catalytic activity and the reaction mechanisms. Using density-functional theory, we determine the stability of a variety of possible oxygen adsorbate phases and discuss the consequences for the equilibrium shape of the clusters under different catalytic conditions. [1] P.L. Hansen et al., Science, 295 (2002), 2053.

O 59.107 Wed 17:45 Poster B1

Surface oxidation of planar and stepped Pt(111) surfaces studied by DFT — •Jochen Bandlow and Timo Jacob — Universität Ulm, Albert-Einstein-Allee 44, 89069 Ulm, Germany

The surface oxidation of Pt(111) seems to be a rather basic and quite simple reaction but nevertheless plays an important role for a wide range of catalytic reactions in gas-phase surface science and electrochemistry. Despite the fact that many experimental studies are focused on single crystal systems with (almost) perfect surfaces, realistic catalysts always contain stepedges, kinks, vacancies and other imperfections on the surface. Especially these lower coordinated sites are believed to play a decisive role for surface reactions and the catalytic performance.

In the present work we investigated the adsorption of oxygen on perfect and stepped Pt(111) using density functional theory and the extended *ab initio* thermodynamics approach. By comparing the (p,T) phase diagram for the system in contact with a gaseous O$_2$ atmosphere with the corresponding electrochemical (p,T,ϕ) phase diagram, characteristics of the surface morphology under specific conditions were evaluated. It turned out that the model of a pure and perfect Pt(111) surface, which is often used to study this reaction, is clearly incomplete.

O 59.108 Wed 17:45 Poster B1

Quantum kinetics of electrons at plasma boundaries — •Franz Xaver Bronold, Holger Fehske, Rafael Leslie Heinisch, and Johannes Marbach — Institut für Physik, Ernst-Moritz-Arndt-Universität Greifswald, 17489 Greifswald, Germany

Macroscopic objects in contact with an ionized gas are usually negatively charged. They accumulate electrons more efficiently than ions leading to the build-up of a quasi-stationary electron film at the plasma boundary. The plasma is strongly affected by surface charges, via sheath formation, electron-ion recombination, and secondary electron emission. A kinetic description of surface charges on par with the kinetic modeling of the bulk plasma is however still missing. As a first step in this direction, we propose a physisorption-inspired model for the formation of surface charges at plasma boundaries and their interaction with the bulk plasma [1]. Besides identifying key issues of the electronic microphysics at plasma boundaries we also discuss results of exploratory calculations for clean metallic boundaries focusing in particular on the electron sticking coefficient s_e, the thermal electron desorption rate $1/\tau_e$, and the secondary electron emission coefficient due to de-excitation of metastable molecules in front of the boundary γ_e^m.

[1] F. X. Bronold et al., Eur. Phys. J. D 54, 519-544 (2009).

O 59.109 Wed 17:45 Poster B1

Electron-induced emission of correlated electron pairs from Fe(001) — •Franz Giebels[1,2], Herbert Gollisch[1], and Roland Feder[1,2] — [1]Theoretische Festkörperphysik,Universität Duisburg-Essen, 47048 Duisburg, Germany — [2]Max-Planck Institut für Mikrostrukturphysik, Weinberg 2, 06120 Halle, Germany

As an essential prerequisite we have calculated the electronic structure of the ground state of a thick Fe(001) film by means of an ab initio Full-Potential Linear Augmented-Plane-Wave method. On the basis of the ground state spin densities we constructed effective quasi-particle potentials, which in particular incorporate a spin-dependent mean free path for the primary electron and the two outgoing electrons. Using these potentials and a screened Coulomb interaction model, we calculated (e,2e) equal-energy angular distributions from Fe(001) by means of a Green function formalism involving Coulomb-correlated two-electron states. For primary spin up and down these distributions are resolved according to parallel and antiparallel alignment of the spins of the primary electron and the relevant valence electron. For parallel spins the outgoing two electrons are thus correlated by exchange and Coulomb interaction, whereas for antiparallel spins there is only the Coulomb correlation. The central depletion zones, which we find in the angular distributions, may therefore – with the proviso of some modification by matrix element effects – be viewed as manifestations of an exchange-correlation hole or a correlation hole in momentum space. Like in the well-known real-space case, the former is significantly larger than the latter.

O 59.110 Wed 17:45 Poster B1

Theoretical investigation of the InN/In2O3 interface — •Giancarlo Cicero[1,2], Antonio Aliano[1], and Alessandra Catellani[2] — [1]Chemical Engineering and Materials Science Department, Politecnico of Torino, Torino, Italy. — [2]CNR-IMEM, Parma, Italy

Contribution has been withdrawn by the author.

O 59.111 Wed 17:45 Poster B1

A quantum-mechanical study of ZnO and TiO2 based Dye Sensitized Solar Cells — •Giancarlo Cicero[1], Giuseppe Mallia[2], Leandro Liborio[2], and Nicholas M Harrison[2,3] — [1]Chemical Engineering and Materials Science Department, Politecnico of Torino, Torino, Italy. — [2]Imperial College London - Thomas Young Centre - Chemistry Department, London UK — [3]STFC, Dares- bury Laboratory, Daresbury, Warrington WA4 4AD, UK

Since the pioneering work of Regan and Graetzel [1], a great attention has been paid to dye sensitized solar cell (DSC) as cheap, effective and environmentally benign candidates for a new generation solar power devices. Optimization of the DSC is still a challenging task as it is a highly complex interacting molecular system. Surface properties of the oxide and in particular proper sensitization with dye molecules may highly affect the efficiency of these cells. Aim of this study is to address the binding of cathecol and isonicotinic acid to oxide surfaces usually employed in DSC, namely ZnO and TiO2, in terms of geometry, stability, electronic structure and band alignment. To this end, we employ quantum mechanical simulations based on hybrid density functional theory. Our analysis helps understanding whether the difference between ZnO and TiO2 in photoeletricity generation efficiency is due to the changes in the bonding geometry of the dye anchoring groups or to electronic effects.

[1] B. O. Regan and M. Graetzel Nature, 353, 737 (1991).

O 59.112 Wed 17:45 Poster B1

Calculation of GW electronic structure for large systems : application to amorphous silica — •David Waroquiers[1,2], Matteo Giantomassi[1,2], Gian-Marco Rignanese[1,2], and Xavier Gonze[1,2] — [1]Unité de Physico-Chimie et de Physique des Matériaux (PCPM), Université Catholique de Louvain, B-1348 Louvain-la-Neuve, Belgium. — [2]European Theoretical Spectroscopy Facility (ETSF)

For accurate ab initio electronic structure calculations, many-body perturbation theories such as GW approximation or Bethe-Salpeter equation are essential. Up to recently, these methods could only be applied to small systems because of the large computational cost of these techniques. New theoretical and algorithmic developments (extrapolar method to reduce the number of empty states needed in GW calculations [1], band parallelism [2], and PAW formalism [3]) now enable us to perform GW calculations in supercells with more than 50 atoms within a reasonable amount of CPU time.

We applied these methods [4] to study the electronic structure of amorphous silica. More than twenty different configurations have been considered, each of them being obtained by relaxing 72-atom supercells at fixed volume. Then, different charged states of atomic hydrogen have been incorporated and relaxed in the larger voids of the systems. Defect energy levels have been calculated within the GW approximation.

[1] F. Bruneval and X. Gonze, Phys. Rev. B **78** (2008) 085125.

[2] X. Gonze *et al.*, Comput. Phys. Comm. **180** (2009) 2582.

[3] M. Torrent *et al.*, Comput. Mater. Sc. **42** (2008) 337.

[4] As implemented in the version 6 of ABINIT (http://www.abinit.org).

O 59.113 Wed 17:45 Poster B1

Optical switching of sodium nitroprussides — •Mirco Pötter, Mirco Imlau, and Michael Rohlfing — Fachbereich Physik, Universität Osnabrück, Barbarastraße 7, 49069 Osnabrück

The optical switching of the NO ligand groups in sodium nitroprussides (e.g. $Na_2[Fe(CN)_5NO]\cdot 2H_2O$) constitutes a prototypical photoactivation process in solid-state optics. The key issue is the existence of several (local) minima in the electronic ground-state total-energy landscape, separated by barriers that do not occur in the photoexcited states, thus allowing switching via the excited state. Here we present theoretical investigations aiming at a detailed understanding of the total-energy landscapes and the transitions between them. Based on density-functional (DFT) calculations, the excitations are described by constraint-DFT, as well as by a simplified version of many-body perturbation theory. Our results show that in the excited state the energy landscape is rather flat, thus facilitating the configurational changes leading to the switching of the NO groups.

O 59.114 Wed 17:45 Poster B1

Influence of the XC Functional on Band Parameters of AlN, GaN and InN — •Luiz Claudio de Carvalho, Andre Schleife, Frank Fuchs, and Friedhelm Bechstedt — Institut für Festkörpertheorie und -optik, Friedrich-Schiller-Universität, Max-Wien-Platz 1, 07743 Jena, Germany

The group III-nitrides have a great potential for optoelectronic devices operating in the visible spectrum and deep ultraviolet. Therefore, a detailed knowledge of their structural, electronic and optical parameters is necessary for the interpretation of experimental data and theoretical results. The most successful theoretical method is the DFT, but its accuracy depends on the choice of the functional of the exchange-correlation (XC) energy. Different choices yield slightly varying results for the structural properties. However, this effect is usually believed to be small, when comparing the results of ab-initio calculations using different XC functionals. In this work we investigate the influence of the structural deviations, introduced by different XC functionals, on the quasiparticle-band structure. We present our results for AlN, GaN, and InN, comparing the XC functionals LDA, PBE, and AM05. DFT as implemented in the VASP code is used to calculate the lattice constants, bulk moduli, band-gap energies, volume deformation potentials and hydrostatic pressure coefficients. The quasiparticle band structures are obtained by GW calculations, using the hybrid XC functional HSE03 as a starting point. We compare our results with experimental data reported in the literature, and discuss the influence of the XC induced structural changes on the band parameters.

O 59.115 Wed 17:45 Poster B1

Non adiabatic effects in photo excited electronic states from ab initio Green's function method — •Marcin Kaczmarski, Yuchen Ma, and MIchael Rohlfing — University of Osnabrueck, Department of Physics, Barbarastrasse 7, 49076 Osnabrueck, Germany

In this work we apply a universal diabatization method by Baer [Chem. Phys. Lett. 35, 112 (1975)] for the description of electronic excited states. A diabatization denotes a unitary transformation which allows for incorporating non adiabatic effects into the quantum Hamiltonian expressed in the adiabatic representation. A typical example is the occurrence of avoided crossings in the potential energy surface as a result of the Born-Oppenheimer approximation, for instance in the case of the retinal chromophore. We present analytical and numerical calculations for the diabatic states in the context of Green's function based ab initio many body perturbation theory (density functional theory plus GW method plus Bethe-Salpeter equation, DFT-GW-BSE). We present the calculation of the adiabatic and diabatic lowest excited electronic states of HeH^+ and the retinal chromophore molecule.

O 59.116 Wed 17:45 Poster B1

Optical spectra of AlN and CaO from first principles — •Arthur Riefer, Frank Fuchs, André Schleife, and Friedhelm Bechstedt — Institut für Festkörpertheorie und -optik, Friedrich-Schiller-Universität, Max-Wien-Platz 1, 07743 Jena, Germany

Modern ab-initio calculations can nowadays reliably predict the optical and electronic properties of semiconductors and insulators, also for non-equilibrium crystal structures. Recently, AlN has been grown and characterized by optical ellipsometry also in the unfavored zincblende structure. Therefore, we compute the electronic and optical properties for the zincblende and wurtzite polytype from first principles. Further we investigate the experimentally well studied CaO employing the same approach. More precisely we compute the band structure and its key quantities by applying quasiparticle corrections to the results of a self-consistent calculation using the nonlocal hybrid HSE03 functional as approximation to exchange and correlation. Based on the so obtained electronic structure the optical properties including electron-hole attraction and local field effects are calculated. The so computed optical spectra and exciton-binding energies are analyzed and compared to available experimental data.

O 59.117 Wed 17:45 Poster B1

Ab initio study of structural stability of InAs nanowires — •Leila Salimi[1], Nahid Ghaderi[2], Seyed Javad Hashemifar[1], and Hadi Akbarzadeh[1] — [1]Department of Physics, Isfahan University of Technology, 84156-83111 Isfahan, Iran — [2]Theory@Elettra Group, INFM-CNR DEMOCRITOS, c/o Sincrotrone, I-34012 Trieste, Italy

We have studied the structural stability of InAs nanowires with different diameters by using density functional theory - pseudopotential computations. The stable structure of bulk InAs is Zinc Blende (ZB) although under special experimental conditions Wurtzite (WZ) InAs has also been observed. Due to the high symmetry and low ratio of dangling bonds, we have considered hexagonal and triangular WZ nanowires in [0001] direction and hexagonal ZB nanowires in [111] direction. In order to select facets of the nanowires, we calculated formation energy of nonpolar surfaces of both structures and found that ZB(110) and WZ($10\bar{1}0$) surfaces are more stable than others. All nanowires were calculated in the optimized and relaxed supercells. Calculating the cohesive energy of nanowires with small diameters, we found WZ structure more stable than ZB, in good agreement with experimental results. The obtained cohesive energy of the small diameter nanowires were fitted by a phenomenological model to obtain dangling bond energies and then extrapolate the cohesive energy of large diameter nanowires. The extrapolated results indicate that for diameters up to 50 Angstrom, the WZ nanowires are more stable than ZB nanowires while for larger diameters, the contribution of dangling bonds reduces and the results converge to that of bulk InAs.

The poster O 59.118 has been withdrawn.