O 60: Poster Session IV (Solid/liquid interfaces; Semiconductors; Oxides and insulators; Graphene; Plasmonics and nanooptics; Electronic Structure; Surface chemical reactions; Heterogeneous catalysis)

Time: Wednesday 17:30–21:00 Location: P4

O 60.1 Wed 17:30 P4

Investigation of the growth of thin Ionic Liquid films on Au(111) and HOPG — •Marcel Marschewski[1], Evgenij Pachomov[1], Oliver Höfft[2], Wolfgang Maus-Friedrichs[1], and Frank Endres[2] — [1]Institut für Energieforschung und Physikalische Technologien, TU Clausthal, Leibnizstr. 4, 38678 Clausthal-Zellerfeld, Germany — [2]Institut für Mechanische Verfahrenstechnik, TU Clausthal, Arnold-Sommerfeld-Str. 6, 38678 Clausthal-Zellerfeld, Germany

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 vapour pressure ionic liquids can be used in ultra high vacuum. We present our results on the growth of thin films imidazolium - based ionic liquids on Au(111) and HOPG. These were studied by electron spectroscopy using ultraviolet photoelectron spectroscopy (UPS, HeI) and metastable atom induced electron spectroscopy (MIES). We have prepared monolayers of [RMIm]Tf2N; (R stands for Ethyl- and Octyl-chains) on the substrates by vapour deposition. For Au(111) we find hints for a reorientation of [OMIm] cation during the growth of the first two monolayers. In addition we have investigated the behaviour of evaporated silver on [EMIm]Tf2N monolayers on HOPG. We find that due to the ionic liquid films the silver particles size is increased compared to silver on clean HOPG. [1] F. Endres, S. Zein El Abedin, Phys. Chem. Chem. Phys., 8 (2006) 2101

O 60.2 Wed 17:30 P4

Potential dependent structural transition of heptyl viologen on Cu(100) studied by in situ STM and IRRAS — •Melanie Röefzaad[1], Min Jiang[2], and Klaus Wandelt[1] — [1]Institute for Phys. Chem., University of Bonn, Germany — [2]Inst. Bioenergy and Bioprocess Technology,Chinese Academy Sciences, P.R. China

The potential dependent adsorption structure of heptyl viologen (1,1*-Diheptyl-4,4*-bipyridinium, DHV) on a chloride precovered Cu(100) electrode has been investigated by Cyclic Voltammetry (CV), in situ electrochemical STM and IR-Reflection Absorption Spectroscopy (IRRAS). The redox-active DHV molecule exhibits pairs of current waves in CV measurements which are ascribed to two typical one-electron transfer steps and phase transformation processes. Between +200 and -100 mV, an ordered 2D dot-array structure in STM images emerges on the Cl- modified Cu(100) electrode surface. One-electron reduction of the dication around -150 mV causes a phase transition from a dot-array assembly to a stripe pattern in STM images which has a double layer structure. With a decrease of the applied electrode potential, the structure of the adlayer undergoes a subsequent change from the double layer phase to a closed packed monolayer of stripes. Orientation analysis with IRRAS of the bipyridine moiety reveals a slight tilt of the long molecular axis to the surface in the dicationic phase and a parallel orientation in the mono cationic striped phases. Calculation of the average angle of the alkyl chains hints to an orientation along the surface within the dot structure while protruding out of the more closely packed stripe phase.

O 60.3 Wed 17:30 P4

Phase transitions of adsorbed viologen monolayers in the presence and absence of specifically adsorbed halides — •Knud Gentz, Min Jiang, and Klaus Wandelt — Institute for Physical und Theoretical Chemistry, Uni Bonn

The structure and stability of self-assembled organic monolayers are scientifically and technologically very timely research subjects. In those cases where larger organic molecules may not be intact volatile and therefore not be deposited by vapor deposition, adsorption from solution may be an alternative route. Here we present results on heptylviologen layers on HOPG and Cu(1 0 0) surfaces as obtained with cyclic voltametry and in-situ scanning tunneling microscopy in solution. Heptylviologen was adsorbed on the HOPG- and Cu(1 0 0) electrode surfaces from a supporting electrolyte. In the CV spikes characteristic of surface phase transitions of HV monolayers on HOPG were observed. The STM images clearly show a stripe structure on the surface in the regime negative of the spike peaks indicating the presence of the radical cationic phase $HV^{\bullet +}$ stabilized by π–π-interaction of the individual molecules. On HOPG a single row and a double row structure were found showing a herringbone-like arrangement of the molecules. Additionally, on copper a second layer adsorption of HV molecules was observed the concentration and structure of which depending on the applied electrode potential. In the regime positive of the spike peak an ordered viologen layer was observed only on copper, where chloride is specifically adsorbed on the surface, which stabilizes the dicationic species on the positively charged electrode.

O 60.4 Wed 17:30 P4

Tunneling Current Driven Electrodeposition of Metals onto n-Si(111):H — •Sebastian Jakob and Werner Schindler — Physikdepartment, Lehrstuhl E20, Technische Universität München, James-Franck-Straße, D-85748 Garching bei München

Electrochemical (EC) metal deposition onto Silicon surfaces should be impossible at potentials of the n-Si(111):H electrode lying above the flatband potential due to the electron depletion at the Silicon suface. Here, we show in sophisticated *in-situ* EC-STM experiments in great detail that electrodeposition onto n-Si(111):H occurs at potentials positive with respect to the flatband potential, although obviously not found in conventional STM experiments at the solid/ liquid interface. By STM imaging and in high-resolution cyclic voltammetry we observe a deposition/ dissolution of metal, determined by the corresponding Nernst potential of the metal. We explain this behaviour by electrodeposition originating from tunneling currents through the electron depletion zone at the n-Si(111):H surface.

O 60.5 Wed 17:30 P4

Ionic Liquid on Cu(100) studied by X-ray Photoelectron Spectroscopy — •Ellen Fischermeier and Thomas Fauster — Lehrstuhl für Festkörperphysik, Universität Erlangen-Nürnberg, Staudtstr. 7, D-91058 Erlangen, Germany

Room temperature Ionic Liquids have attracted a lot of attention during the last years due to their extraordinary physical and chemical properties. As a number of important processes depend on the properties of the interface between Ionic Liquid and substrate, it is crucial to gain a deeper insight into the Ionic Liquid/surface interactions.

In this study films of [EMIm][Tf_2N] of different thickness were deposited under UHV-conditions by physical vapor deposition on well defined Cu(100) single crystal surfaces using a home-built evaporator. These samples were studied by X-ray Photoelectron Spectroscopy under different emission angles.

We focus on the growth behavior of the films and the radiation induced changes observed in the Ionic Liquid and compare the results obtained at different layer thickness.

O 60.6 Wed 17:30 P4

Copper electrodeposition and additives: from underpotential deposition to bulk growth — •Yuriy Yanson, Joost Frenken, and Marcel Rost — Leiden University, Leiden, the Netherlands

Cu electrodeposition at different stages on Au(111) surface is accessed in-situ on atomic scale by means of our newly developed fast electrochemical STM. We show the effect of industrially used additives, such as bis-(3-sodiumsulfopropyl) disulfide (SPS) and polyethylene glycol (PEG), on the Cu deposit. The EC-STM results are complemented by electrochemical measurements and discussed in the light of current state of knowledge on electrodeposition and molecular processes involving the additives.

O 60.7 Wed 17:30 P4

EC-STM investigation of self-organized Porphyrin layers on an iodide-modified Au(111) surface — •Tomasz Kosmala[1,2], Michael Schneider[2], Aleksander Krupski[1], and Klaus Wandelt[1,2] — [1]Institute of Experimental Physics, University Wroclaw, plac Maksa Borna 9, 50-204 Wrocław, Poland — [2]Institute of Physical and Theoretical Chemistry, University Bonn, Wegelerstr.

12 , 53115 Bonn, Germany

The self-assembly of Tetra(N-methyl-4-pyridyl)-porphyrin molecules (TMPyP) on an iodide- modified Au(111) surface has been studied by means of Cyclic Voltametry (CV) and in-situ Electrochemical Scanning Tunneling Microscopy (EC-STM).

The iodine precovered Au(111) surface was found to be a good substrate for the self-assembly of highly ordered layers of porphyrin cations from solution [1,2].

Unlike the Itaya group [1,2], however, we have prepared the iodine precoverage on Au(111) in situ and found the iodine layer to be stable at potential even below the first reduction potential of adsorbed TMPyP. As a consequence we were able to monitor interesting structural phase transitions as a consequence of the molecular redox-processes, which could not be seen in the previous work [1,2].

[1] M. Kunitake, N. Batina, and K. Itaya, Langmuir, vol. 11, no. 7, pp. 2337 - 2340, (1995).

[2] M. Kunitake, U. Akiba, N. Batina, and K. Itaya, Langmuir, vol. 13, no. 6, pp. 1607 - 1615, (1997).

O 60.8 Wed 17:30 P4

Fast switching of the electrochromism in thin films of a perfluoroalkyl-substituted phthalocyanine — Stefanie Nagel[1], Martin Lener[1], •André Dragässer[1], Robert Gerdes[2], Sergiu Gorun[2], and Derck Schlettwein[1] — [1]Institute of Applied Physics, Justus-Liebig-University Giessen, Germany. email:schlettwein@uni-giessen.de — [2]Department of Chemistry and Environmental Science, New Jersey Institute of Technology, Newark, NJ 07102, USA

Thin films of metal complexes of octakisperfluoro(isopropyl)-phthalocyanine ($F_{64}Pc$) vapour-deposited on indium tin oxide electrodes were studied at negative potentials in contact to LiCl aqueous electrolyte solutions. In situ monitoring of the absorption spectra of the films during electrochemical reduction revealed electrochromic characteristics which are of possible interest for applications in displays or as smart windows. Electroneutrality of the films was preserved by intercalation of Li^+ ions. The technically relevant speed of switching the absorbance characteristics by an applied potential depends on both electron conduction and ion diffusion in the matrix. The switching speed was studied by a variation of the scan rate in cyclic voltammetry and by potential step experiments. The observed charge flow and spectral changes are discussed both in view of relevance of the decisive sample parameters and a possible technical application.

O 60.9 Wed 17:30 P4

Density functional calculation of electronic surface structure and Fe adsorption on ZnO (0001) and (000$\bar{1}$) — •Sougata Pal, Torben Jasper-Toennies, Michael Hack, and Eckhard Pehlke — Institut für Theoretische Physik und Astrophysik, Universität Kiel, Germany

The structure and electronic properties of the ZnO(0001) and ZnO(000$\bar{1}$) surfaces as studied by density functional calculations will be presented. The stability of the surface has already been investigated by various groups [1,2,3]. The electronic surface band structure, however, in particular the existence of surface states and the differences between experimental band dispersion for both terminations, still appears to pose open problems [4,5]. To address these issues, we compare Kohn Sham band structures and electrostatic potentials close to the surface for the relaxed (1x1)-surface, (2x2) vacancy reconstructions, and surfaces with pits. In particular the effect of the bending of the electrostatic potential at the surface on the eigenstates is quantified.

Comparing the adsorption energies of Fe atoms for various adsorption sites on ZnO(000$\bar{1}$), the fcc hollow position turned out to be energetically favorable. The oxidation state of the Fe atom is derived from the projected density of states.

[1] G. Kresse *et al.*, Phys. Rev. B **68**, 245409 (2003).

[2] M.-H. Du *et al.*, Phys. Rev. B **78**, 155424 (2008).

[3] M. Valtiner *et al.*, Phys. Rev. Lett. **103**, 065502 (2009).

[4] K. Ozawa *et al.*, Phys. Rev. B **79**, 075314 (2009).

[5] J. Dumont *et al.*, Appl. Phys. Lett. **95**, 132102 (2009).

O 60.10 Wed 17:30 P4

Different bandstructures of for- and backward buckled π-bonded chains of the Si(111)-2×1 surface reconstruction revealed by STS-measurements — •Karolin Löser, Martin Wenderoth, Thomas K. A. Spaeth, and Rainer G. Ulbrich — IV. Physikalisches Institut, Georg-August Univ. Göttingen, Germany

According to the Pandey model, the π-bonded chains of the Si(111)-2×1 surface reconstruction might be buckled either for- or backward but it is extremely hard to distinguish the buckling types as the energetic difference is very small [1] and the projection of the atomic positions is exactly the same seen from above the surface. Because of this, STM cannot be used to determine the buckling type directly.

To gain access to information on the buckling type we exploit the boundaries between domains of differently reconstructed π-bonded chains as a tool to reveal displacements of the chains. Thus, with high-resolution STM and STS measurements of π-bonded chains on cleaved Si(111)-2×1 samples in the UHV, we can not only proof the co-existence of for- and backward buckled π-bonded chains but also study the local Density of States (LDOS) of differently buckled π-bonded chains. We find that two different LDOSs for the two buckling types, one of them has a smaller bandgap than the other, which fits well with calculations [2] that predict the backward buckled π-bonded chains to have a slightly smaller bandgap. We acknowledge financial support by the DFG via project WE 1889/3.

[1] A. A. Stekolnikov, et al. Phys. Rev. B 65 (11), 115318 (2002)

[2] S. H. Lee and M. H. Kang. Phys. Rev. B 54 (3), 1482(1996)

O 60.11 Wed 17:30 P4

STM characterization of MOVPE-prepared silicon surfaces — Peter Kleinschmidt, Sebastian Brückner, •Johannes Luczak, Oliver Supplie, Anja Dobrich, Henning Döscher, and Thomas Hannappel — Helmholtz-Zentrum Berlin für Materialien und Energie, Hahn-Meitner-Platz 1, 14109 Berlin, Germany

The clean Si(100) surface reconstructs by forming dimers, thus reducing the number of dangling bonds at the surface. In the MOVPE environment hydrogen is commonly used as process gas, which leads to a monohydride silicon surface with a 2×1 unit cell consisting of H-Si-Si-H dimers. Even so, the quality of the surface can vary dramatically depending on process conditions. In general, annealing in hydrogen leads to a two-domain surface structure with monoatomic steps, where the resulting structure also strongly depends on misorientation. We find process conditions for preparation of Si(100) surfaces with 0.1°, 2° and 6° offcut where a strong preference for one domain is obtained, making the resulting surfaces ideal substrates for III-V-on-Si epitaxy. A process consisting of deoxidation, homoepitaxial buffer layer growth and annealing is found to result in D_A-type double layer steps for 0.1°, and D_B-type double layer steps for 6° offcut. The identical process leads to single layer steps for 2° offcut. Here, we obtain D_A-type double layer steps by a modified process which includes a slow cooling phase after the annealing step. Our results, verified by scanning tunneling microscopy, low energy electron diffraction and Fourier-transform infrared spectroscopy, are in sharp contrast to the clean and the hydrogenated Si(100) surface prepared in UHV.

O 60.12 Wed 17:30 P4

Thermal stability of thin HfO_2 films on plasma nitrided Si(100) — •Katharina Skaja[1,2], Frank Schönbohm[1,2], Daniel Weier[1,2], Ulf Berges[1,2], and Carsten Westphal[1,2] — [1]Fakultät Physik - Technische Universität Dortmund, Otto-Hahn-Str. 4, D 44221 Dortmund, Germany — [2]DELTA - Technische Universität Dortmund, Maria-Goeppert-Mayer-Str. 2, D 44227 Dortmund, Germany

Thin dielectric films such as HfO_2 grown on Si(100) are interesting for metal-oxide semiconductor MOS devices, because HfO_2 has a high dielectric constant. Up to 750 °C HfSi increases in the HfO_2/Si layer stack, which creates unwanted conductive states. To avoid the formation of HfSi an amorphous Si_3N_4 diffusion barrier can be grown between the HfO_2 film and the silicon substrate. The ultrathin Si_3N_4 films were grown on the Si(100) surface by nitrogen plasma which was provided from a special plasma source. Different thicknesses of Si_3N_4 interlayers were prepared in-situ and the HfO_2 films were grown on top of the sample by electron beam evaporation. The film thicknesses were determined by ARXPS meassurements. The samples were flash heated for 1 minute at several temperatures. After each annealing step the chemical properties of the system HfO_2/Si_3N_4/Si(100) were checked by photoelectron spectroscopy (PES). For temperatures up to 750 °C the HfO_2 layer remains unchanged. For higher temperatures a further signal could be observed in the spectra, due to the chemical shift in the Hf 4f signal to higher kinetic energies. This new component could be identified as $Hf_{x_1}Si_{x_2}O_{x_3}N_{x_4}$. The $Hf_{x_1}Si_{x_2}O_{x_3}N_{x_4}$ appears to be stable up to 850 °C.

O 60.13 Wed 17:30 P4

Adsorption of metalorganic molecules on metal-

semiconductor systems — •Christian Brand, Jędrzej Schmeidel, Wei Chen, Christoph Tegenkamp, and Herbert Pfnür — Institut für Festkörperphysik, Leibniz Universität Hannover, Germany

The controlled implementation of single molecules in appropriate contact assemblies is the ultimate realization of an ultra-small device structure. Besides extremely high integration densities the functionalities of the devices are adjustable by chemical synthesis. However, the interaction of the molecule with its environment is decisive.

The adsorption of ferrocene-1,1'-dithiol (FDT) on Ag-$\sqrt{3}$ reconstructions on nominally flat and vicinal Si(111) substrates has been studied. The FDT was chosen because of its large conductance and high structural flexibility with respect to rotation of the two cyclopentadienyl (Cp) rings. The reconstruction is a prototype of a highly conductive low dimensional electron gas on a technologically relevant substrate. The adsorption of intact molecules takes place predominantly at defect sites, e.g. vacancy and step structures. Submolecular resolution showing the Cp-ring structure was obtained at perfect terrace sites. Due to chemisorption of the S-atoms at hollow sites the molecule axis is oriented parallel to the substrate. The initial rotational flexibility is frozen and only tow different rotated configurations were found. The adsorption geometry is confirmed by VASP calculations. Recently, Ag reconstructions on Si(557) substrates have been used. The effect of the uniaxial step configuration towards the adsorption of the FDT molecules will be discussed.

O 60.14 Wed 17:30 P4

Investigation of Bis(phthalocyaninato)lutetium(III) on HOPG by STM, STS and DFT — •Lars Smykalla, Pavel Shukrynau, Marius Toader, and Michael Hietschold — Chemnitz University of Technology, Institute of Physics, Solid Surfaces Analysis Group, D-09107 Chemnitz, Germany

We report results obtained on ordered layers of Bis(phthalocyaninato)-lutetium(III) (LuPc$_2$) on highly oriented pyrolytic graphite (HOPG) by using a variable temperature scanning tunneling microscope (STM) at 30K in UHV. These double decker phthalocyanine molecules were deposited by OMBE at low rates. Through slight annealing self-assembled highly ordered islands of LuPc$_2$ were formed which show a close packed square structure governed by molecule-molecule interactions. Experiments with submonolayer coverage and multilayer coverage were carried out to investigate the epitaxy of the molecular layers on the substrate, the stacking behaviour and tilting of molecules relative to the layer. Very high resolved STM-images at negative bias voltage show intra-molecular features which are in very good agreement with the appearance of the highest occupied molecular orbital (HOMO) of LuPc$_2$ gained by density functional theory (DFT). Tip-sample-distance-dependent tunneling spectroscopy was applied to study the electronic properties of the ordered molecular layers of LuPc$_2$ on HOPG and the influence of the tip and the electric field. To identify the peaks in the normalized conductance spectra DFT calculations were performed and a comparison of the energy levels with STS shows a good agreement of the HOMO-LUMO-gap.

O 60.15 Wed 17:30 P4

Surface photovoltage investigation of gold chains on Si(111) by two-photon photoemission — •Sebastian Otto, Kerstin Biedermann, and Thomas Fauster — Lehrstuhl für Festkörperphysik, Universität Erlangen-Nürnberg, Staudtstr. 7, D-91058 Erlangen, Germany

We present surface photovoltage measurements on Si(111)-(7×7) with monoatomic gold chains. The gold coverage was varied between zero and 0.6 ML, where the Si(111)-(5×2)-Au reconstruction covers the surface completely.

During the two-photon photoemission experiments the p- or n-doped samples were illuminated by infrared (IR, $E_{IR} = 1.55$ eV) and ultraviolet (UV, $E_{UV} = 4.65$ eV) laser pulses. For all coverages the photovoltage was determined for sample temperatures of 90 K and 300 K by variation of the IR and UV laser power.

P-doped as well as n-doped Si(111) wafers show a linear dependence of the photovoltage on gold coverage. This stands in contrast to scanning tunneling spectroscopy measurements [1], which show a coverage-independent photovoltage over a wide coverage range for n-doped wafers. While for p-doped wafers our experimentally determined photovoltage is in agreement with previous reports, for n-doped wafers the observed values are lower than expected.

[1] K. Sell et al., phys. stat. sol. (b) **1087**, 247 (2010)

O 60.16 Wed 17:30 P4

C_2 inclusion by C_{60} in thin films deposited on HOPG — Seyithan Ulas, Dmitry Strelnikov, Daniel Löffler, Patrick Weis, •Artur Böttcher, and Manfred M. Kappes — Karlsruher Institut für Technologie, Institut für Physikalische Chemie, Fritz-Haber-Weg 2, 76131 Karlsruhe, Germany

The deposition of hyperthermal C_2^- anions onto C_{60} films has been studied by means of mass spectrometry, thermal desorption spectroscopy (MS), ultraviolet photoionization spectroscopy (UPS), atomic force microscopy (AFM) and Raman spectroscopy. The inclusion of C_2 dimers by C_{60} cages manifests itself by the sublimation of the C_{62}, C_{64} and C_{66} cages as well as by pronounced modifications of the thermal, electronic and vibronic properties of the C_{60} films. The most efficient reaction channel: the formation of volatile C_{62} species depends on the deposition conditions. Its yield, y(C_{62}), does not overcome 10^{-2} per C_2. UPS and Raman spectra of the C_2/C_{60} layers supported by DFT calculations indicate the formation of polymeric network based on -C_{60}-C_2-C_{60}- chains as well as C_{62} (and -C_{62}-C_{62}- chains) as two prevailing inclusion channels. Thermal desorption spectra reveal coherent sublimation of C_{60} and C_{62} what implies that thermal decomposition of the -C_{60}-C_2-C_{60}- oligomeric chains is the common dissociative reaction step. In temperature range 750 - 975 K the thermal decomposition of the -C_{60}-C_2-C_{60}- oligomeric chains competes with the thermally activated inclusion of the C_2 into C_{60} cages resulting in non-IPR C_{62} cages arranged in semiconducting network. At higher temperatures the network becomes converted predominantly into conducting carbon chains of fused C_{62} cages.

O 60.17 Wed 17:30 P4

Karlsruher Institut für Technologie, Institut für Physikalische Chemie, Fritz-Haber-Weg 2, 76131 Karlsruhe, Germany — Seyithan Ulas, Dmitry Strelnikov, Daniel Löffler, Patrick Weis, •Artur Böttcher, and Manfred M. Kappes — Karlsruher Institut für Technologie, Institut für Physikalische Chemie, Fritz-Haber-Weg 2, 76131 Karlsruhe, Germany

Thin monodisperse films consisting of non-IPR C_{58} fullerene cages have been deposited onto HOPG by exploiting the soft-landing of mass-selected C_{58}^+ ions. The ions have been created by performing the electron-impact induced fragmentation/ionization of IPR C_{60} cages. In analogy to IPR fullerenes the doping of the C_{58} films by alkali metals (e.g. Cs) leads to the formation of alkali-metal-based fullerides. The mass spectra taken during the sublimation of CsxC58 phase reveal well distinguishable three components, C_{56}, C_{58} and C_{60}. Both new components, C_{56} and C_{58}, indicate the transfer of the C_2 unit from a C_{58} to the adjacent one, $C_{58} + C_{58} \rightarrow C_{56} + C_{60}$ as a process competing with the breakage of the intercage bonds constituted by non-IPR sites (e.g. 2AP-2AP). The doping Cs atoms located in vicinity of the intercage bonds weaken them significantly and consequently facilitate the high-temperature C_2 transfer. The yield of the $C_{58} \rightarrow C_{60}$ conversion depends on the doping degree x and reaches a level of 10^{-2} per C_{58} deposited.

O 60.18 Wed 17:30 P4

Photocatalytic CO_2 reduction on dye sensitized TiO_2 — •Leo Pöttinger[1] and Thomas Bürgi[2] — [1]Im Neuenheimer Feld 253, D-69117 Heidelberg — [2]30 Quai Ernest-Ansermet, CH-1211 Genève 4

Reducing the greenhouse gas CO_2 and substituting fossil fuels are challenging tasks for the future. The photocatalytic recycling of CO_2 to hydrocarbons with sunlight as renewable energy is therefore investigated. Attenuated total reflection infrared (ATR-IR) spectroscopy was used to probe a thin layer of porous TiO_2. In the first step "in-situ" adsorption experiments of CO_2 and dyes with exposure to UV and visible light were performed. Furthermore metal co-catalysts were added to enhance the photocatalytic activity. The ATR-IR measurements show stable carbonates on the TiO_2 nanoparticles after purging the CO_2 saturated aqueous solution with pure water. After irradiation with UV light the carbonate bands vanish. The same characteristics can be observed with dye sensitized TiO_2 and visible light exposure. The increase of new bands could be a hint of intermediate products in the multiple electron process towards methanole.

O 60.19 Wed 17:30 P4

III-V semiconductors for photoelectrochemical applications: surface preparation and characterization — •Dominic Fertig, Birgit Schächner, Wofram Calvet, Bernhard Kaiser, and Wolfram Jaegermann — TU Darmstadt, Fachbereich Materialwissenschaft, Fachgebiet Oberflächenforschung

III-V semiconductors are promising reference systems for photoelectrochemical energy conversion. Therefore we have studied the influence of different acids and acidic solutions on the etching of p-doped gallium-arsenide and gallium-phosphide single crystal surfaces. From our experiments we conclude, that etching with HCl and subsequent annealing up to 450°C gives the best results for the removal of the carbonates and the oxides without affecting the quality of the sample. By treating the surfaces with "piranha"-solution ($H_2SO_4 : H_2O_2 : H_2O/7{:}2{:}1$), the creation of an oxide layer with well defined thickness can be achieved. For the creation of an efficient photoelectrochemical cell, Pt nanoparticles have been deposited from solution. These surfaces are then characterized by photoelectron spectroscopy and AFM. Further electrochemical measurements try to correlate the effect of the surface cleaning and the Pt deposition on the photoactivity of the GaAs- and GaP-semiconductors.

O 60.20 Wed 17:30 P4

The growth of ultra thin Praseodymia oxide films on boron-passivated Si(111) surfaces — •Henrik Wilkens, Alexander Knobeler, Sebastian Gevers, Nina Jeppesen, Daniel Bruns, Thomas Weisemoeller, and Joachim Wollschläger — FB Physik, Universität Osnabrück, Barbarastr. 7, 49069 Osnabrück, Germany

Silicon on insulator (SOI) CMOS technology already have an enormous commercial impact with Si dioxide as insulating material. Alternative insulating materials are in the focus of investigation to integrate semiconductors for system on chip (SOC) solutions that cannot be built on Si alone.

Due to its good insulations characteristics and a high dielectric constant, praseodymium oxide is an interesting candidate for such applications. To prevent the formation of silicate at the substrate-oxide interface it is essential to use passivated silicon substrates. In this work the influence of boron-passivation is investigated. Prior to praseodymium oxide evaporation by molecular beam epitaxy the Si substrate surface was passivated by boron via evaporation of boric acid and subsequent annealing of the substrate to 900°C. In situ Spot Profile Analysis Low Energy Electron Diffraction (SPA-LEED) and Auger Electron Spectroscopy (AES) were used to characterize the surface structure and morphology. Additional Ex-situ X-Ray Reflectivity (XRR) and X-Ray Diffraction (XRD) analyses were performed. The results show that at a substrate temperature of 500°C a single crystalline oxide film is formed.

O 60.21 Wed 17:30 P4

Optical Second-Harmonic Generation at the GaP/Si(001) interface — •Kristina Klass, Johannes Reimann, Gerson Mette, Wolfgang Stolz, Kerstin Volz, and Ulrich Höfer — Fachbereich Physik und Zentrum für Materialwissenschaften, Philipps-Universität Marburg, D-35032 Marburg

Due to similar lattice constants ($a = 0.54$ nm) GaP as a compound semiconductor can be grown on Si without significant lattice mismatch. The combination of Silicon with GaP-based direct III/V semiconductors is of great interest for the realization of optoelectronics based on this well understood substrate. We have employed optical second-harmonic generation (SHG) as a non-invasive and contactless method to characterize the GaP/Si(001) interface. Femtosecond laser pulses are focused on a thin sample which can be rotated around its z-axis. Irradiation and detection of different polarizations as well as variation of the angle of incidence yield access to different tensor elements of the second-order nonlinear susceptibility tensor. The investigated samples show surprisingly strong variation of the SHG response depending on growth condition and the Si(001) substrate structure. In particular, we find a strong 2-fold symmetric SHG-component which is correlated to the presence of double height steps and an almost single-domain Si(001) substrate.

O 60.22 Wed 17:30 P4

Electron pair emission from NiO(100) — •Changhui Li, Lucie Behnke, Frank O. Schumann, and Jürgen Kirschner — Max-Planck-Institut für Mikrostrukturphysik, 06120 Halle, Germany

The study of electron pair emission from surface upon electron or photon impact allows to study the electron-electron correlation, which plays an important role to determine the electronic and magnetic properties of materials, especially for strongly correlated systems. We present a first electron pair emission study from a strongly correlated system, namely NiO. We have grown ultrathin NiO(100) films on Ag(100) following standard procedures. We excite the sample with a primary electron beam in the energy range energies (E_p=35-85 eV). Compared with Ag, the coincidence count rate of NiO is about 7 times larger and the secondary electrons make much larger contributions in the electron pair emission. The sum energy spectra of the pairs shows structure which we can relate to the valence band structure. The way the available energy is shared among the electrons depends strongly on the primary energy. For E_p in the range 35-54 eV, the electrons prefer unequal energy sharing, whereas equal energy sharing is adopted for higher primary energies.

O 60.23 Wed 17:30 P4

The chemisorption of hydrogen molecules on CaO films — •Sebastian Dahle[1], Henning Munkert[1,2], and Wolfgang Maus-Friedrichs[1,3] — [1]Institut für Physik und Physikalische Technologien, TU Clausthal, Leibnizstr. 4, 38678 Clausthal-Zellerfeld, Germany — [2]Institut für Metallurgie, TU Clausthal, Robert-Koch-Str. 42, 38678 Clausthal-Zellerfeld, Germany — [3]Clausthaler Zentrum für Materialtechnik, TU Clausthal, Leibnizstr. 4, 38678 Clausthal-Zellerfeld, Germany

The oxide and hydroxide species of Calcium and the underlying reaction processes are of great technological interest. Even the hydration of burnt limestone is just barely predictable. Our investigations start with the preparation of the Calcium oxide and hydroxide species in a clean ultra high vacuum (UHV) environment. During the development of in-vacuo preparation methods of Calcium hydroxide, the adsorption of hydrogen molecules has been investigated. We have found that hydrogen leads to the formation of hydroxide groups, which appears to be unlikely due to thermodynamics at the first glance. Furthermore, hydrogen apparently acts as catalyst for the hydroxidation of a complete Calcium oxide film through water impinging on the surface out of the residual gas. These effects have been studied with Metastable Induced Electron Spectroscopy (MIES), Ultraviolet Photoelectron Spectroscopy (UPS) and X-ray Photoelectron Spectroscopy (XPS).

O 60.24 Wed 17:30 P4

Ab initio calculations on the adsorption energy of NO on TiO_2(110) — •Marie Arndt and Thorsten Klüner — Theoretische Chemie, Carl von Ossietzky Universität Oldenburg, PO Box 2503, 26111 Oldenburg

Catalytic surface reactions are an essential section in the technical industries. Especially photocatalytic reactions on metaloxide surfaces became more and more important since the last decade. The focus of theoretical and experimental analysis lies on the adsorption- and desorption-processes going on onto the substrate surface. In this context, the semiconductor titaniumdioxide has proved as an outstanding photocatalyst. In this study we use *ab initio* calculations to characterize the adsorption of NO on a rutile(110) surface. We use an embedded cluster model of type $\mathrm{Ti_9O_{18}Mg_7^{14+}}$ to describe the electronical ground state of this open-shell system. Using the *Molcas* quantum chemistry package, the aim lies in finding the global minimum of the adsorption energy. Within our model we are able to regard six degrees of freedom, the desorption coordinate z, the polar angle θ, the azimuth angle ϕ, the two lateral coordinates x and y and the inner NO distance r. On RMP2-level an BSSE corrected adsorption energy of -0.57 eV at a distance from NO to rutile of 3.0 Å was found. The result affords first insight to the NO-TiO_2-system and this study serves as a basis for further studies concerning excited states involved in the desorption processes within this interesting adsorbate-substrate complex.

O 60.25 Wed 17:30 P4

Organic Molecules on Wide-Gap Insulating Surfaces from First-Principles — •Wei Chen, Karthiga Kantasamy, Christoph Tegenkamp, and Herbert Pfnür — Institut für Festkörperphysik, Leibniz Universität Hannover, 30167 Hannover, Germany

We investigate the adsorption of benzoic acid and its various phenolic derivatives on wide-gap insulators (e.g. NaCl and KCl surfaces) from first-principles, in an effort to demystify the contact charging effect between salt mines mixed with organic molecules. While Kohn-Sham density functional theory (KS-DFT) becomes a *de facto* standard for the predictions of ground-state properties, it is far from being perfect and the standard semi-local density functional approximations suffer from several limitations, such as the notorious *gap problem* and the neglect of the prevalent long-range *van der Waals* interaction in the weakly bonded systems. Moreover, the problem of electronic excitations are beyond the scope of KS-DFT. In this work, a variety of *ab initio* methods are adopted at the respective level of theory, from

KS-DFT (with hybrid functionals and dispersion force corrections) to Hedin's *GW* approximation and ultimately the two-particle Bethe-Salpeter equation. The important roles of the long-range correlations, *surface defects* and the *excitonic effect* are presented in the context of the molecule-insulator interfaces.

O 60.26 Wed 17:30 P4

LEED I(V) analysis of CO and N_2 physisorption on the NaCl(100) surface — •Jochen Vogt and Helmut Weiss — Chemisches Institut der Otto-von-Guericke-Universität Magdeburg, Universitätsplatz 2, 39106 Magdeburg, Germany

Carbon monoxide and N_2 physisorbed on the NaCl(100) surface have been considered in the past as model systems for orientational order-disorder phase transitions in two dimensions [1,2]. Although CO and N_2 are isoelectronic, the lateral intermolecular potential of adsorbed CO is governed by dipole-dipole interaction, while in the case of N_2 quadrupole-quadrupole interaction is the leading electrostatic term. Low-energy electron diffraction experiments (LEED) prove, that upon cooling below 35 K the lattice symmetry in the system CO/NaCl(100) changes from a (1×1) to a (2×1). However, few is known about the adsorbate structure from an experimental point of view. We report a LEED I(V) structure analysis of CO/NaCl(100) and N_2/NaCl(100), guided by density functional theory (DFT-D/PBE) calculations. Although predicted by theory [2], our experiments do not support a disorder/order phase transition (1×1)→(2×1) for N_2/NaCl(100) above 18 K.

[1] W. Rzysko, A. Patrykiejew, K. Binder, Phys. Rev. B 76 (2007), 195409

[2] A. K. Sallabi, D. Jack, Phys. Rev. B 62 (2000), 4841

O 60.27 Wed 17:30 P4

LEED and FTIR spectroscopy studies of CO_2 adsorption at NaF(100) — •Stephan Härtel, Anne Möller, Jochen Vogt, and Helmut Weiss — Chemisches Institut der Otto-von-Guericke-Universität Magdeburg, Universitätsplatz 2, 39106 Magdeburg

In the present work the adsorption system CO_2-NaF(100) was investigated by means of low-energy electron diffraction (LEED) and Fourier transform infrared (FTIR) spectroscopy. According to LEED I(V) analysis the clean NaF(100) surface shows hardly any deviation from the ideal bulk structure but enlarged vibrational amplitudes [1]. Different from other alkali halide cleavage planes such as NaCl(100) or KCl(100) up to now there are few data available dealing with the adsorption behaviour of molecules on this surface. The LEED patterns of CO_2-covered NaF(100) show no evidence for a superstructure but just a decreased intensity of the substrate spots. Apparently the adsorbed molecules do not form a long range order. This result is comparable to that for CO_2 adsorption on LiF(100) and KBr(100). However there are also alkali halide surfaces such as e.g. NaCl [2] where a superstructure could be observed. The adsorption/desorption behaviour was also studied by recording isotherms and isobars by FTIR spectroscopy from which the heat of adsorption was calculated to be $28.6 \pm 2.9\,\mathrm{kJ/mol}$ which is comparable to the corresponding values in the above mentioned homologous systems.

[1] S. Härtel, J. Vogt, and H. Weiss, Surf. Sci., **604**, 1996 - 2001 (2010)

[2] J. Vogt and H. Weiss, J. Chem. Phys., **119**, 1105 (2003)

O 60.28 Wed 17:30 P4

Luminescence of PTCDA on epitaxial KCl films on Ag(100) — M. Müller, •A. Paulheim, C. Marquardt, and M. Sokolowski — Institut für Physikalische und Theoretische Chemie der Universität Bonn, Wegelerstraße 12, 53115 Bonn, Germany

On surfaces of the wide gap dielectric materials the luminescence of organic molecules can be studied in great detail. Thin films of the molecule perylence-3,4,9,10-tetracarboxylic acid dianhydride (PTCDA) were vacuum deposited on epitaxial KCl films on Ag(100). The structural and optical properties were investigated by spot-profile-analysis low energy electron diffraction (SPA-LEED) and by photoluminescence- (PL) and PL excitation spectroscopy (PLE). We investigated molecules in the limit of isolated entities and of a completed monolayer. The SPA-LEED measurements reveal the know quadratic unit cell of the monolayer with the molecules arranged in a brickwall-structure [1]. The optical spectra exhibit a dominating 0-0 transition and well resolved vibronic modes. The transition energy of molecules embedded in a completed monolayer phase is redshifted with respect to that of isolated molecules. In addition, we analyzed the polarization of the emitted light and were able to determine the azimuthal orientation of the organic molecules in both phases with respect to the KCl(100) surface. From these data we achieve detailed information on the role of the intermolecular coupling on the optical properties of the layers. Supported by the DFG through the research group 557. [1] T. Dienel, C. Loppacher, S. C. B. Mannsfeld, R. Forker, and T. Fritz, Advanced Materials 20, 959 (2008)

O 60.29 Wed 17:30 P4

FUNCTIONALIZATION OF THE TIO_2 (110) SURFACE BY TEREPHTHALIC ACID TOWARD THE MOF GROWTH — •Michael Naboka, Alexei Nefedov, and Christof Wöll — Institute of Functional Interfaces, Karlsruher Institute of Technology, D- 76344 Eggenstein-Leopoldshafen, Germany

Chemically functionalized surfaces play an important role in many nanotechnological applications. A functionalization of TiO2 surface by adsorption of TPA (C6H4(COOH)2) molecules has already been studied previously. It was shown that TPA has a flat orientation at low coverages and up-standing carboxyl-terminated orientation at high coverages. This up-standing orientation at the coverage of one monolayer means that the this system may found similar application to carboxyl-terminated self assembling monolayers. Metal Organic Frameworks (MOFs) is a class of material where metal ions are bound together with organic ligands forming the 2D or 3D porous structure. In addition to the use of MOFs as powders there is currently a significant interest to anchor and grow them on functionalized surfaces. The first steps in this direction were made on the TPA-functionalized TiO2(110) surface. For this purposes the stability of the TPA/TiO2 (110) system was tested by exposing it to the nitrogen atmosphere and subsequent NEXAFS measurements. After that the sample was immersed in the copper trifluoroacetate solution. The obtained structure was studied by NEXAFS and XPS.

O 60.30 Wed 17:30 P4

FUNCTIONALIZATION OF THE TIO_2 (110) SURFACE BY TEREPHTHALIC ACID TOWARD THE MOF GROWTH — •Michael Naboka, Alexei Nefedov, and Christof Wöll — Institute of Functional Interfaces, Karlsruher Institute of Technology, D- 76344 Eggenstein-Leopoldshafen, Germany

Chemically functionalized surfaces play an important role in many nanotechnological applications. A functionalization of TiO_2 surface by adsorption of TPA ($C_6H_4(COOH)_2$) molecules has already been studied previously. It was shown that TPA has a flat orientation at low coverages and up-standing carboxyl-terminated orientation at high coverages. This up-standing orientation at the coverage of one monolayer means that the this system may found similar application to carboxyl-terminated self assembling monolayers. Metal Organic Frameworks (MOFs) is a class of material where metal ions are bound together with organic ligands forming the 2D or 3D porous structure. In addition to the use of MOFs as powders there is currently a significant interest to anchor and grow them on functionalized surfaces. The first steps in this direction were made on the TPA-functionalized TiO_2(110) surface. For this purposes the stability of the TPA/TiO_2 (110) system was tested by exposing it to the nitrogen atmosphere and subsequent NEXAFS measurements. After that the sample was immersed in the copper trifluoroacetate solution. The obtained structure was studied by NEXAFS and XPS.

O 60.31 Wed 17:30 P4

Growth of Co-Salen on NiO(001) at submonolayer coverages: A non-contact atomic force microscopy study — •Josef Grenz, Alexander Schwarz, Johannes Hattendorff, and Roland Wiesendanger — Institute of Applied Physics, University of Hamburg, Jungiusstr. 11, 20355 Hamburg

Co-Salen is a planar metal-organic Schiff base complex and known for its oxygen affinity. In a previous study we investigated the adsorption of this molecule on NaCl(001) [1,2]. The observed island growth mode indicates a rather weak molecule-surface interaction. As a result the molecular ordering within the islands is the same as in bulk Co-Salen, where the building blocks are dimers, which form a monoclinic unit cell.

Interestingly, on NiO(001), which also crystallizes in the rocksalt structure, a layer-by-layer growth is observed. Such a growth mode suggests a larger molecule-substrate interaction than on NaCl(001), most likely due to the above-mentioned oxygen affinity of Co-Salen. The measured island heights at submonolayer coverages indicate also dimers as building blocks. However, the shapes of the islands are rather irregular. In this presentation the influence of the substrate temperature on the island shape as well as the molecular ordering within the island will be discussed.

[1] S. Fremy *et al.*, Nanotechnology **20**, 405608 (2009).

[2] K. Lämmle *et al.*, Nano Lett. **10**, 2965 (2010).

O 60.32 Wed 17:30 P4

Distinction of the $SrTiO_3/NdGaO_3$ surface termination by phase resolved Second Harmonic Generation — •Thomas Fink[1], Andrea Rubano[1], Tim Günter[1], Domenico Paparo[2], Carmela Aruta[2], Fabio Miletto Granozio[2], Umberto Scotti Di Uccio[2], Lorenzo Marrucci[2], and Manfred Fiebig[1] — [1]HISKP, University of Bonn, Germany — [2]CNR-INFM Coherentia, Università Frederico II, Napoli, Italy

The development of new oxide heterostructures, like $LaAlO_3/SrTiO_3$, requires to control the substrate surface termination. Under normal conditions, a TiO_2 termination of $SrTiO_3$ is favored. However, recent experiments demonstrated that a SrO termination can be achieved by epitaxially growing the $SrTiO_3$ on a $NdGaO_3$ substrate.

Second Harmonic Generation (SHG) is an ideal tool for studying surface phenomena, since it is sensitive to surface-induced symmetry breaking. Furthermore, it allows to directly image the sample surface. Here, we report on SHG imaging of the $SrTiO_3$ /$NdGaO_3$ surface using amplified femtosecond laser pulses. For 24 unit cells of $SrTiO_3$ epitaxially grown on $NdGaO_3$, two distinct types of domains with a length scale of about 500 μm, are observed. By interference with a reference signal, we measured a 180° SHG phase shift and an additional intensity difference between both of them. The phase shift can be directly assigned to the termination of $SrTiO_3$. Thus, phase-resolved SHG is an ideal tool in order to distinct different surface terminations, opening new possibilities to control the oxide interface electronic property.

O 60.33 Wed 17:30 P4

Growth mode, morphology, and reducibility of $CeO_2(111)$ thin films on Cu(111) — Filip Dvořák[1], Oleksandr Stetsovych[1], Michael Steger[2], El Miloudi Cherradi[2], Iva Matolínová[1], Natalya Tsud[1], Michal Škoda[1], Tomáš Skála[3], •Josef Myslivеček[1], and Vladimír Matolín[1] — [1]Charles University, Faculty of Mathematics and Physics, V Holešovičkách 2, Praha 8, Czech Republic — [2]Heinrich-Heine-Universität, Institut für Experimentelle Physik der kondensierten Materie, Universitätsstrasse 1, Düsseldorf, Germany — [3]Sincrotrone Trieste SCpA, Strada Statale 14, km 163.5, Basovizza-Trieste, Italy

We investigate morphology and degree of reduction in model oxide system CeO_2 (ceria) on Cu(111) using scanning tunneling microscopy and photoelectron spectroscopy. We identify growth mechanisms of ceria on Cu(111) - formation of incomplete oxide interfacial layer and formation of three-dimensional ceria pyramids by stacking of monolayer-high islands. Using these mechanisms we control the coverage, the number of open monolayers, and the step density of ceria thin films on Cu(111). Annealing in vacuum allows us to control besides the morphology also the degree of ceria surface reduction. We find a correlation between surface reduction and morphological stability in annealed ceria layers. Oriented and stoichiometric thin films of ceria on Cu(111) can be prepared at temperatures as low as 150 °C and 250 °C. Both the morphology and the degree of reduction of these films readily change with increasing temperature, which must be accounted for in evaluating temprature-programmed experiments with ceria on Cu(111).

O 60.34 Wed 17:30 P4

Growth and electronic structure of $MgO_{1-x}N_x$ on Mo(001) investigated by scanning tunneling microscopy/spectroscopy — •Martin Grob, Christian Pauly, Mike Pezzotta, Marco Pratzer, and Markus Morgenstern — II. Physikalisches Institut B, Otto-Blumenthal-Straße, RWTH Aachen University and JARA-FIT, 52074 Aachen

Theoretical calculations [1] predict nitrogen-doped MgO being a ferromagnetic half metal. Therefore we investigated $MgO_{1-x}N_x$ films on Mo(001) by scanning tunneling microscopy (STM) and spectroscopy (STS) at room temperature. The films were prepared by evaporation of magnesium in oxygen/nitrogen atmosphere. A concentration of up to $x = 6\,\%$ has been achieved in films up to 11 monolayers. Similarities and differences of pristine MgO and $MgO_{1-x}N_x$ were observed by STM. The electronic structure measured by STS differs in a significant way, showing additional states appearing in the band gap of MgO. The influence of the Mo substrate taking affect as a catalizer for N-dissociation is discussed as well as possible solutions in order to prepare N-doped MgO bulk for further magnetic investigations.

[1] P. Mavropoulos, M. Ležaić, and S. Blügel, Phys. Rev. B **80**, 184403 (2009).

O 60.35 Wed 17:30 P4

Photoelectron spectroscpoy of ultrathin epitaxial rare earth oxides on silicon — •Dominik Schwendt and Hans Jörg Osten — Institut für Materialien und Bauelemente der Elektronik, Leibniz Universität Hannover, Hannover, Deutschland

Thin crystalline rare earth oxide layers are a promising candidate as future high-k materials replacing silicon dioxide in various MOS applications. In order to integrate these new materials into CMOS technology, a good knowledge of the silicon - oxide interface and growth behaviour of the rare earth oxides is mandatory. Epitaxial growth not only avoids recrystallization during post-growth annealing steps but also provides good interface engineering options.

Here, we present an in situ study of the molecular beam epitaxy of rare earth oxides on silicon substrates. The growth process was monitored using reflection high-energy electron diffraction. Photoelectron spectroscopic measurements of the layers were taken at different growth stages showing the change of the electronic state of the oxide. Thus we can estimate the way the oxide layer is bound to the silicon and also draw conclusions on the successful suppression on interfacial layers.

O 60.36 Wed 17:30 P4

PTCDA monolayer growth on epitaxial graphene — •Matthias Meissner, Bernd Schröter, and Torsten Fritz — Institute of Solid State Physics, University of Jena, 07743 Jena, Germany

As a model system for organic epitaxy on graphene we have investigated the epitaxy of 3,4,9,10-perylenetetracarboxylic dianhydride (PTCDA) on epitaxial graphene (EG) with Low Energy Electron Diffraction (LEED), Angle-Resolved Ultraviolet Photoelectron Spectroscopy (ARUPS) and Scanning Tunneling Microscopy (STM). Graphene was grown by thermal decomposition of 6H-SiC(0001) in an argon atmosphere at ambient pressure [1]. For a PTCDA monolayer on EG, a new point-on-line phase has been discovered, beside that phase known already from the epitaxy of PTCDA on graphite(0001) [2]. ARUPS measurements coincide well with theoretical and experimental UPS data on thick PTCDA films [3] and show additionally a complete lack of dispersion in the PTCDA bands within experimental accuracy, confirming a weak intermolecular overlap of wave functions.

[1] K. V. Emtsev et al., Nature Materials **8**, 203 (2009).

[2] C. Ludwig et al., Physik B Condensed Matter **86**, 397 (1992).

[3] I. G. Hill et al., Chemical Physics Letters **317**, 444 (2000).

O 60.37 Wed 17:30 P4

EELS study of epitaxial graphene/Ni(111) and graphene/Au/Ni(111) — •Alexander Generalov[1], Konstantin Simonov[2], Karsten Horn[1], and Yuriy Dedkov[1] — [1]Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, Germany — [2]V.A. Fock Institute of Physics, St. Petersburg State University, St. Petersburg, Russia

Due to its surface sensitivity, the electron energy loss spectroscopy in reflection mode (REELS) with electron beam of low primary energy is very suitable for investigation of true and quasi two-dimensional (2D) systems. The goal of the present work is the comparative study of strongly bonded graphene/Ni(111) and quasi free standing graphene/Au/Ni(111) systems by means of REELS spectroscopy.

The graphene/Ni(111) system was prepared via thermal decomposition of ethylene C_2H_4 on the Ni(111) single crystal surface. The 2 ML Au layer was intercalated underneath graphene on Ni(111) via thermal annealing of the Au/graphene/Ni(111) system. After intercalation of gold under graphene the features in EELS spectrum which are characteristic of graphene/Ni(111) interface disappear and shift of π plasmon to the lower loss energy is observed indicating the transition of initial system of strongly bonded graphene on Ni(111) to a graphite like state. Application of the free-electron model for the dependence of surface plasma frequency on density of free carriers to our experimental results gives the value of graphene doping from Ni(111) substrate to be about of 0.05e per carbon atom relative to quasi free standing graphene on Au/Ni(111).

O 60.38 Wed 17:30 P4

Electronic scattering at defects in graphene investigated by scanning tunneling microscopy — •Marco Pratzer, Alexander Georgi, Viktor Geringer, Christian Pauly, Dinesh Subramaniam, Torge Mashoff, Marcus Liebmann, and Markus Morgenstern — II. Physikalisches Institut B, Otto-Blumenthal-Straße, RWTH Aachen University and JARA-FIT, 52074 Aachen

We investigated the electronic scattering pattern appearing at different types of defects in monolayer graphene by scanning tunneling microscopy (STM) at 5 K. The graphene sample has been prepared by exfoliation on a SiO_2-substrate and electrically contacted by indium microsoldering.
First the electronic scattering pattern appearing at a monolayer-bilayer step edge has been investigated. Using FFT-filtering a $\sqrt{3} \times \sqrt{3}$ interference pattern could be separated from the atomic corrugation, which is characteristic for the graphene intervalley scattering. The amplitude of the interference pattern decreases with increasing energy. This is caused by the growth of the equipotential lines in k-space leading to the overlap of more wave vectors and partially to a destructive interference. Further we could identify different types of point defects and their characteristic local density of states. In addition to adsorbates on top of the graphene lattice and carbon vacancies we found defects located below the graphene flake at the SiO_2 substrate. The interference pattern caused by this type of defects could be suppressed by lifting up the graphene flake from the substrate using tip induced forces.

O 60.39 Wed 17:30 P4

Vibrational spectroscopy of atomic hydrogen adsorbed on graphene — •Hyunil Kim, Thorsten Balgar, and Eckart Hasselbrink — Fakultät für Chemie, Universität Duisburg-Essen, D-45117 Essen, Germany

Graphene is a promising candidate as an alternative material for future electronic devices. Thus, graphene is an very interesting system to study its properties.

Our research is focused on vibrational excited absorbates on solid state surfaces by means of VIS/IR sum frequency generation (SFG). Here we present studies on the vibrational stretching mode of atomic hydrogen on graphene. We compare our results with DFT calculations, done by Sakong et al. SFG spectroscopy offers high interface sensitivity and allows for analysing such adsorbat systems.

We generate the graphene by the chemical vapor deposition process (CVD) of ethylene on Ir(111) in an ultra high vacuum chamber. The vibrational spectroscopy is realized by a ps-lasersystem with an optical parametric generator/difference frequency generator (OPG/DFG).

S. Sakong and P. Kratzer, J. Chem. Phys. 133, 054505 (2010).

X. Han, T. Balgar and E. Hasselbrink, J. Chem. Phys. 130, 134701 (2009).

J. Coraux et al., New J. Phys. 11 (2), 023006 (2009).

O 60.40 Wed 17:30 P4

Micro Four-Point-Probe Conductivity Measurements on Graphene — •Edward Perkins, Bjarke Jørgensen, Liv Hornekaer, and Philip Hofmann — Institut for Fysik og Astronomi, Aarhus Universitet, Ny Munkegade 120, Aarhus 8000C, Denmark

Four-point-probe measurements are a well-known technique for measuring conductivity independent of contact resistances. In these experiments, we apply this method at the micrometer scale to investigate surface transport. By varying the separation and geometry of the contacts it is possible to distinguish between two-dimensional and three-dimensional conductivity. This technique thus allows us to study the details of transport at surfaces in a wide range of materials.

Measurements from epitaxial graphene on silicon carbide at room temperature and 77 K are presented. The characteristic two-dimensional transport is analysed and compared to transport in other materials. Simulations of the potential are also considered with a view to understanding the details of the conductivity profile.

O 60.41 Wed 17:30 P4

Growth of uniaxial graphene nanostructures by self-assembly — •Jens Baringhaus, Thomas Langer, Herbert Pfnür, and Christoph Tegenkamp — Institut für Festkörperphysik, Leibniz Universität Hannover, Appelstrasse 2, 30167 Hannover, Germany

Graphene nanostructures such as ribbons and dots are building blocks for any graphene based device architecture. Furthermore, the controlled fabrication of nanostructures allows to study the feedback of defects towards the peculiar transport properties seen in perfect 2d templates. Among others the epitaxial growth of graphene on prepatterned SiC is a promising strategy for growing such nanostructures on insulating substrates.
Using vicinal 4H-SiC(0001) substrates (4°miscut) the in-situ graphitization process has been monitored by spot profile analysis LEED and angle resolved electron energy loss spectroscopy (ELS). At first for temperatures above 1200° step bunching sets in. The flat terrace sites are in the order of 20 nm, thus, the initial structural anisotropy in not reflected in the plasmon dispersion of graphene. In a second approach uniaxial mesa structures of 6H-SiC(0001) ($1\mu m$ in width) were fabricated by means of photolithography and reactive ion etching (RIE). Heating of the substrate induces step flow and the development of inclined nano-facets. At high temperatures silicon desorbs predominantly from these nano-facets leading to the formation of graphene ribbons. The structure and plasmon properties are analyzed by SEM, STM and EELS. In addition, also first transport properties will be presented.

O 60.42 Wed 17:30 P4

Growth of Graphene on Ir(100) — •Pascal Ferstl, Matthias Gubo, Lutz Hammer, and M. Alexander Schneider — Lehrstuhl für Festkörperphysik, Universität Erlangen-Nürnberg, Staudtstr. 7, 91058 Erlangen

Graphene monolayers have been grown on a variety of different metal substrates with hexagonal symmetry. In contrast, the growth on substrates with square symmetry remains rather unexplored so far. Therefore, we have studied graphene growth on a Ir(100) surface by means of LEED and STM. Both, temperature programmed growth (TPG) and chemical vapour deposition (CVD) at various temperatures were tested with C_2H_4 as reacting gas. For TPG we find as a function of the reaction temperature a sequence of different superstructures indicative of the stepwise hydrocarbon decomposition towards surface carbide. Randomly oriented graphene islands are formed for temperatures above 700°C. By CVD at 700 - 900°C graphene forms domains oriented along the [001] direction, with an angular tolerance below ±4°. There are no indications for a Moiré structure from the LEED pattern. In contrast, ethylene deposition at higher temperatures (900 - 1300°C) leads to a preferential alignment of the graphene layer 5° off [001]. Also, a complex Moiré pattern is observed in LEED. In STM we find two graphene phases for all deposition temperatures: one being essentially flat, while the other shows a linear corrugation with an amplitude of up to 3 Å and a lateral spacing of about 22 Å. Possible structural models will be discussed.

O 60.43 Wed 17:30 P4

Inhomogeneous electronic properties of monolayer graphene on Ru(0001) — •Mike Gyamfi, Thomas Eelbo, Marta Waśniowska, and Roland Wiesendanger — Institute of Applied Physics, University of Hamburg, Jungiusstr. 11, 20355 Hamburg

Understanding properties of the interface between graphene and a metal surface has recently gained considerable attention. In case of Ru(0001) the linear dispersion of monolayer graphene is not preserved due to the hybridization between C and Ru orbitals at the interface [1]. In order to get access to the electronic structure inside the Moiré pattern of graphene we performed spatially resolved STS at low temperature. We report on direct evidences for variations of the electronic properties regarding the exact position of the carbon atoms with respect to Ru atoms and the corrugation within the subunit cell. The shape of dI/dU spectra is quite similar on all parts of the Moiré pattern, the spectra differ only by a slight shift, $\Delta E = 30$ meV, of the peak position at -0.4 eV and its intensity. This small energy difference is related to the carbon and Ru atoms' hybridization upon growth of graphene on the Ru surface. A detailed analysis revealed that the dominant peak at -0.4 eV originates from a *d*-like Ru bulk state.

[1] T. Brugger *et al.*, *Phys.Rev.B* **79**, 045407 (2009)

O 60.44 Wed 17:30 P4

Controlled fabrication of nanocrystalline graphene films on insulating substrates — •Nils-Eike Weber[1], Rainer Stosch[2], Armin Gölzhäuser[1], and Andrey Turchanin[1] — [1]Physik supramolekularer Systeme und Oberflächen, Fakultät für Physik, Universität Bielefeld — [2]Physikalisch-Technische Bundesanstalt, Braunschweig

We report on the fabrication and characterization of nanocrystalline graphene films on insulating substrates. Graphenoid (graphene like) carbon nanosheets with a thickness of 1 nm were made by the electron beam induced cross-linking of aromatic self-assembled monolayers. When transferred onto insulating substrates, the graphenoid sheets were converted into nanocrystalline graphene by thermal annealing. We used thermal annealing in an argon atmosphere to produce large area (cm square or larger) films of nanocrystalline graphene with a well defined thickness on silicon oxide wafers and quartz glass.

The electrical conductivity was measured at room temperature by four point probe measurements. The structure and chemical composition were studied by X-ray photoelectron and Raman spectroscopies. Since the electrical conductivity, thickness and optical properties of the graphene films can be well controlled, the suggested method opens broad prospects for the fabrication of transparent conductive coating.

O 60.45 Wed 17:30 P4

Mechanically stacked 1 nm thick carbon nanosheets: 2D layered materials with tunable optical, chemical and electrical properties — Christoph Nottbohm[1], Andrey Turchanin[1], André Beyer[1], Rainer Stosch[2], •Matthias Büenfeld[1], Andreas Winter[1], and Armin Gölzhäuser[1] — [1]Physik supramolekularer Systeme und Oberflächen, Fakultät für Physik, Universität Bielefeld — [2]Physikalisch-Technische Bundesanstalt, Braunschweig

Carbon nanosheets are mechanically stable free-standing two-dimensional materials with a thickness of ~1 nm and well defined physical and chemical properties. They are made by radiation induced cross-linking of aromatic self-assembled monolayers. Here we present a route to the scalable fabrication of multilayer nanosheets with tunable electrical, optical and chemical properties. Stacks up to five nanosheets with sizes of ~1 cm2 on oxidized silicon were studied. Their optical characteristics were investigated by optical microscopy, UV/Vis reflection spectroscopy and model calculations. Their chemical composition was studied by X-ray photoelectron spectroscopy. The samples were then annealed in ultra high vacuum at various temperatures up to 1100 K. A subsequent investigation by Raman, X-ray photoelectron and UV/Vis reflection spectroscopy as well as by electrical four-point probe measurements demonstrates that the layered nanosheets transform into nanocrystalline graphene. This structural transformation is accompanied by changes in the optical properties and electrical conductivity and opens up a new path for the fabrication of ultrathin functional conductive coatings.

O 60.46 Wed 17:30 P4

An analytical approach to the spectrum of π electrons in bilayer graphene nanoribbons and nanotubes — •Julius Ruseckas[1], Gediminas Juzeliunas[1], and Igor Zozoulenko[2] — [1]Institute of Theoretical Physics and Astronomy, Vilnius University, A. Goštauto 12, LT-01108 Vilnius, Lithuania — [2]Solid State Electronics, ITN, Linköping University, 601 74 Norköping, Sweden

We present an analytical description of π electrons of a finite size bilayer graphene within a framework of the tight-binding model. The considered bilayered structures are characterized by a rectangular geometry and have a finite size in one or both directions with armchair- and zigzag-shaped edges. An exact analytical description of the spectrum of π electrons in the zigzag and armchair bilayer graphene nanoribbons and nanotubes is provided. The exact solution of the Schrödinger problem, the spectrum and wave functions, has been obtained and used to analyze the density of states and the conductance quantization.

O 60.47 Wed 17:30 P4

Electronic and structural properties of hydrogen-intercalated monolayer graphene on SiC(0001) — •Stiven Forti[1], Camilla Coletti[1], Konstantin Emtsev[1], Dong Su Lee[1], Alexei Zakharov[2], Jurgen H. Smet[1], and Ulrich Starke[1] — [1]Max-Planck-Institute for Solid State Research, Heisebergstr. 1, 70569 Stuttgart, Germany — [2]MAX-lab, Lund University, Lund, S-22100, Sweden

The growth of epitaxial graphene on SiC is one of the most promising techniques to provide large area, homogeneous graphene. In this work we demonstrate the possibility to combine the growth of epitaxial graphene under Ar atmosphere [1] with the capability of decoupling the carbon interface layer from the substrate by means of hydrogen intercalation [2] to obtain large area, homogeneous, free standing and undoped graphene on top of SiC(0001). The quality of the graphene samples is demonstrated by a variety of surface science experiments. AFM shows a morphology with regular steps and large terraces. Low defect concentration is revealed by Raman spectroscopy. LEEM highlights the homogeneity of the electronic structure on a micrometer scale with nanometer resolution. High-resolution ARPES shows extremely sharp bands with the dispersion of a free-standing monolayer graphene, confirming the good quality of the graphene obtained via this process and therefore demonstrating the effective decoupling of the carbon layer from the SiC substrate. [1] K.V. Emtsev et al., Nat. Mat. 8, 203(2009), [2] C. Riedl et al., PRL 103, 246804(2009).

O 60.48 Wed 17:30 P4

Kelvin probe and atomic force microscopy of pristine and irradiated graphene sheets — •Oliver Ochedowski, Benedict Kleine Bussmann, Sevilay Akcöltekin, and Marika Schleberger — Universität Duisburg-Essen, Lotharstr. 1 47048 Duisburg

We have prepared graphene by mechanical exfoliation on SrTiO3 and TiO2 single crystalline surfaces and transferred them into an Ultra-Hgih-Vacuum system. By using an atomic force microscope and the Kelvin probe technique the contact potential differences (CPD) of graphene are mapped. The CPD is directly linked to the work function and is used to study doping effects induced by the substrate, adsorbates, water as well as laser and particle irradiation.

We show that graphene on SrTiO3 exhibits an accumulation of carriers corresponding to n-type doping and that water underneath the graphene decreases this effect. Irradiating graphene with laser light at a wavelength of 514,5 nm (5 mW, spot size: 1 micrometer^2), leads to a cleaning effect already after 5 minutes, followed by the formation of defects after about 10 minutes. Furthermore, we present KPFM measurements of graphene irradiated with swift heavy ions under glancing angles of incidence.

O 60.49 Wed 17:30 P4

Graphene and graphene nanodots on Ir(111) — •Andreas Zusan[1], Philipp Leicht[1], Muriel Sicot[1], Mikhail Fonin[1], Yuriy S. Dedkov[2], and Karsten Horn[2] — [1]Fachbereich Physik, Universität Konstanz, 78457 Konstanz — [2]Fritz-Haber-Institut der Max-Planck Gesellschaft, 14195 Berlin

The investigation of the electronic properties of graphene nanostructures is one of the most fundamental requirement on the route towards graphene based nanoelectronics. Within these studies a weak chemical bonding between the carbon monolayer and the substrate is required. For this purpose we used an Ir(111) substrate for the preparation of quasi-freestanding graphene and graphene nanodots by the decomposition of hydrocarbons. The topographic properties as well as the local electronic properties were studied by means of scanning tunneling microscopy and scanning tunneling spectroscopy. The nanodots exhibit a typical size of about 15 to 25 nm and show the well known Moiré superstructure. The edges of the nanodots are predominantly running along the main crystallographic directions of the Ir(111) substrate and the edge structure was determined to be of a zigzag type.

O 60.50 Wed 17:30 P4

Local electronic structure of graphene on SiC(0001) studied by scanning tunneling microscopy and spectroscopy — •Thomas Druga, Martin Wenderoth, and Rainer G. Ulbrich — IV. Physikalisches Institut, Georg-August-Universität Göttingen

In this work we present a low temperature (6K) scanning tunneling microscopy study of mono- and bilayer graphene on the silicon-terminated 6H-SiC(0001) surface. The untreated crystals were electrically contacted exsitu by tantalum foils. After annealing at base pressure of $1 * 10^{-10}$ mbar at 500°C for several hours the samples were graphitized between 1350°C and 1450°C by direct current heating. This preparation technique results in graphitized surfaces of mainly mono- and bilayer graphene up to a few hundred nm. Atomically resolved topographies of monolayer graphene show the honeycomb structure of the graphene layer, the 6x6 periodicity and disordered adatom features induced by the underlying interface layer [1]. These features have a strong influence on lateral resolved differential conductivity maps dI/dV(x,y) measured by scanning tunneling spectroscopy (STS) and demonstrate the necessity of a high lateral resolution to study the electronic properties of graphene. On bilayer graphene dI/dV - spectra show in addition to spectral features observed by other groups [e.g. 2] atomic scale modulations according to the 6x6 periodicity. This work was supported by the DFG as part of SFB 602 Tp A7.

[1] Rutter et al. Phys. Rev. B 76, 235416 (2007) [2] Lauffer et al. Phys.Rev. B 77, 155426 (2008)

O 60.51 Wed 17:30 P4

Production Nitrogen Doped Graphene on Ni(111) Surface — •Wei Zhao, Junfa Zhu, Oliver Höfert, Karin Gotterbarm, Christian Papp, and Hans-Peter Steinrück — Lehrstuhl für Physikalische Chemie II, Universität Erlangen-Nürnberg, Egerlandstr. 3, 91058 Erlangen

Graphene, the 2D-carbon network is considered as one of the most promising candidates for the post-silicon semiconductor materials.[1] Referring to the classic semiconductor research route, introducing hetero-atoms to the graphene sheet will modify the electronic properties and make it possible to use it in realistic applications. Therefore, nitrogen doped graphene sheets on a Ni(111) surface were prepared by low energy nitrogen sputtering of graphene below 150 K and also directly by exposure of the Ni(111) surface to pyridine at elevated temperatures. Applying in-situ high resolution X-ray photoelectron spectroscopy, the structure and thermal stability of N-doped graphene sheets on Ni(111) were investigated. It is found that at 900 K the graphitic-N and the pyridinic-N dominate the nitrogen doped parts in the sputtered graphene layers, of which the nitrogen concentration is $\sim$ 1.5%. For the graphene sheet prepared from exposure to pyridine pyridinic-N is the main structure element found. Here we achieve a doping of with $\sim$ 1.7% of nitrogen. Moreover a closer examination of the thermal stability of these layers was conducted.

Support is acknowledged from the BMBF (05 ES3XBA/5) and the Cluster of Excellence "Engineering of Advanced Materials". [1]Novoselov, K.S., et al. Science, 2004. 306(5696).

O 60.52 Wed 17:30 P4

Ambipolar doping in quasi-free epitaxial graphene on SiC(0001) controlled by Ge intercalation — •Konstantin Emtsev[1], Alexei Zakharov[2], Camilla Coletti[1], Stiven Forti[1], and Ulrich Starke[1] — [1]Max-Planck Institute for Solid State Research, Stuttgart, Germany — [2]MAX Lab, Lund University, Lund, Sweden

Growth of graphene on single crystals of SiC is considered among the most promising routes for large scale graphene fabrication [1]. Recently we have shown that the electronic structure of graphene on SiC(0001) can be tailored by controlling the atomic structure of the interface [2]. In the present work we utilized the intercalation phenomenon to introduce atomically thin layers of germanium at the interface between the graphene-like $(6\sqrt{3}\times6\sqrt{3})$R30°-reconstructed buffer layer and the SiC surface. The expanded interface decouples the graphene from the SiC surface structurally and electronically. A quasi-free standing graphene monolayer develops and shows moderate p- or n-doping depending on the amount of Ge intercalated. We present a detailed study of the structural and electronic properties of such films. The samples were characterized by high resolution ARPES and XPS. In addition, microscopic properties of Ge-intercalated graphene films were investigated in detail by means of low-energy electron microscopy (LEEM). Importantly, relatively low temperatures required for the intercalation have enabled us to capture the transformation process by LEEM in situ in real-time. [1] P.N. First et al., MRS Bulletin, 35, 296 (2010). [2] C. Riedl et al., Phys. Rev. Lett. 103, 246804(2009)

O 60.53 Wed 17:30 P4

YIELD and Kelvin probe study of graphene — •Samir Mammadov, Jürgen Ristein, and Thomas Seyller — Lehrstuhl für Technische Physik, Universität Erlangen-Nürnberg, Germany

Subject of this study is the investigation of the work function and photo-YIELD of epitaxial graphene(EG) films. Two types of samples were investigated: regular EG films and H-intercalated EG films, referred to as quasi-freestanding graphene (QFG). EG films were formed by thermal decomposition on the Si-face of n-type 6H-SiC substrates and QFG samples were formed by subsequentially intercalating EG samples by hydrogen.

The work function was determined precisely for each type of samples.The YIELD spectra of the different samples display significant variation which will be discussed in details.

O 60.54 Wed 17:30 P4

Self-assembly of Pt, Ru and bimetallic PtRu clusters on Ru(0001) supported monolayer graphene — •Albert K. Engstfeld[1], Christoph U. Lorenz[1], Ottavio B. Alves[1], Harry E. Hoster[1,2], and R. Jürgen Behm[1] — [1]Institute of Surface Chemistry and Catalysis, Ulm University, D-89069 Ulm, Germany — [2]Current address: Technische Universität München, Centre for Electromobility, 50 Nanyang Drive, Singapore 637553

The Moiré-type nm-scale patterns of graphene monolayers on metal single crystals were recently shown to allow facile fabrication of ordered arrays of virtually monodisperse metal nanoclusters by simple metal vapour deposition in UHV [1-3]. In view of a potential utilization as structurally well defined model systems in electrocatalysis, with extremely small metal clusters, we have tested the possibility of preparing Ru and bimetallic PtRu clusters by an analogous procedure. Based on statistically evaluated STM images, we will report on the nucleation behaviour of Ru and Pt clusters respectively and its consequences on bimetallic PtRu cluster growth, depending on the evaporation sequence of the two metals.

[1] A.T. N'Diaye et al., New J.Phys. 11, 2009, 103045.
[2] Yi Pan et al., Appl.Phys.Lett. 95, 2009, 093106.
[3] K. Donner and P. Jakob, J.Chem.Phys. 131, 2009, 164701.

O 60.55 Wed 17:30 P4

Intrinsic Voltage Rectification in a Graphene Nano Device — •Robert Göckeritz[1], Jörg Pezoldt[1], and Frank Schwierz[2] — [1]FG Nanotechnology, Institute for Micro- and Nanotechnology, Ilmenau University of Technology, PF 100565, 98684 Ilmenau, Germany — [2]FG Solid State Electronics, Institute for Micro- and Nanotechnology, Ilmenau University of Technology, PF 100565, 98684 Ilmenau, Germany

Recently, voltage rectification effects at GHz frequencies have been observed in three-terminal junctions (TTJ) based on III-V heterojunctions. In the present work, such effects at DC voltages are reported for the first time in TTJs made of epitaxially grown graphene. Most notably, our T-shaped TTJ devices show a pronounced rectification behavior already at room temperature.

The graphene was grown on SiC using a high temperature process at 1800°C under atmospheric pressure applying a carbon capping technique prior to growth. The 50 nm wide and 500 nm long graphene devices were patterned by electron beam lithography. Raman spectroscopy revealed the fingerprint of graphene and AFM, XPS and electrical measurements have been performed.

The reported room-temperature rectification in graphene TTJs may pave the way for new applications of graphene in electronics.

O 60.56 Wed 17:30 P4

Raman spectroscopy of quasi-freestanding monolayer graphene — •Felix Fromm, Florian Speck, Martin Hundhausen, and Thomas Seyller — Universität Erlangen-Nürnberg, Lehrstuhl für Technische Physik, 91058 Erlangen, Germany

The epitaxial growth of graphene on silicon carbide (SiC) by thermal sublimation of silicon in an argon atmosphere is a promising method to produce high quality graphene layers. We focus here on the mechanical properties of graphene samples produced by converting the $(6\sqrt{3} \times 6\sqrt{3})R30^\circ$ reconstructed surface into a quasi-freestanding graphene monolayer on hydrogen terminated SiC. Raman spectroscopy of graphene is well suited to determine mechanical strain by measuring the frequency shifts of phonon modes. We evaluate the strain from the shift of the 2D peak in the Raman spectrum. Intercalation of the $(6\sqrt{3} \times 6\sqrt{3})R30^\circ$ surface reconstruction at 550°C results in tensile strained graphene. The size of strain however is reduced with prolonged intercalation time. After intercalation at higher temperature the obtained graphene layers show much smaller tensile strain.

O 60.57 Wed 17:30 P4

Gas permeation in graphenoid nanomembranes — •Nils Mellech[1], Xianghui Zhang[1], Elina Oberländer[1], André Beyer[1], Edgar Hansjosten[2], Roland Dittmeyer[2], and Armin Gölzhäuser[1] — [1]Faculty of Physics, Bielefeld University, Postfach 10 01 31, 33501 Bielefeld, Germany — [2]Karlsruhe Institute of Technology, Institute for Micro Process Engineering (IMVT), Karlsruhe, Germany

Permeation and selectivity measurements with helium and argon are carried out on freestanding nanomembranes of cross-linked self-assembled mono- and multilayers. The monolayers of 1,1'-biphenyl-4-thiol and 4'-nitro-1,1'-biphenyl-4-thiol are prepared on gold on mica and cross-linked by electron irradiation which results in layer thicknesses of approximately 1 nm. Afterwards the nanomembranes are transferred either onto millimeter-sized polished sintered porous steel substrates or onto a micron-sized opening in a silicon nitride window on silicon substrates. The latter samples are investigated with an ultra-high vacuum permeation measurement system based on a quadrupole mass spectrometer. The nanomembranes seal the UHV chamber from the high pressure feed gas side of the system and remain stable for days under pressures up to 30 kPa. The nanomembranes on the porous substrates are characterized by a gas flow measurement system. The membranes cover the pores and substantially reduce the gas flow. Permeation properties of the nanomembranes are discussed based on the measured data.

O 60.58 Wed 17:30 P4

Experimental indication of quantum mechanical effects in surface enhanced IR-spectroscopy? — •Jörg Bochterle[1], Frank Neubrech[1], Annemarie Pucci[1], Dominik Enders[2], and Tadaaki Nagao[2] — [1]Kirchhoff-Institute for Physics, Heidelberg, Germany — [2]Institute for Material Science, Tsukuba, Japan

The conduction electrons of metal nanoparticles can be collectively excited by incident electromagnetic radiation. Their resonance frequency strongly depends on the geometric dimensions of the particles and can be tuned from the classical radio frequencies up to the visible range. Such resonantly excited localized surface plasmon-polaritons are accompanied by an electromagnetic nearfield enhancement at the surface. In the infrared spectral range these huge local fields can be applied to the enhancement of infrared vibrations of molecules. Using this technique with gold nanostripes, attomol sensitivity has been achieved.

In this contribution we look at the signal enhancement of the carbon monoxide (CO) stretching vibration of physisorbed CO ice on gold nanoantennas on silicon substrates under ultrahigh vacuum conditions. The signal changes with increasing CO layer thickness are measured in situ and exhibit a behavior differing from the classical expectations. While in the classical description the nearfield is monotonically increasing with decreasing distances to the surface, the quantum description of the localized plasmon resonance exhibits such monotonic increase only down to a certain distance and then decreases for smaller distances to the surface.

O 60.59 Wed 17:30 P4

Infrared optical properties of gold nanoantenna arrays — •Daniel Weber[1], Frank Neubrech[1], Han Gui[2], Dominik Enders[2], Tadaaki Nagao[2], and Annemarie Pucci[1] — [1]Kirchhoff Institute for Physics, Heidelberg, Germany — [2]National Institute for Materials Science, Tsukuba , Japan

Antenna-like gold nanoparticles are proven to be well-suited for spectroscopic applications due to their tuneable plasmonic properties. Excited resonantly by electromagnetic radiation, they are able to strongly enhance the local electromagnetic field. This effect can be exploited for example for surface-enhanced infrared (IR) spectroscopy, making the detection of very small amounts of molecules possible. Although the investigation of single particles is possible, well-arranged arrays of nanoantennas promise to have greater potential for possible sensor applications since the overall sensitivity can be increased if several nanoantennas interact. In this paper, we report on the IR optical properties of gold nanoantenna arrays and show the dependence of characteristic resonance parameters from the geometrical arrangement of the antennas on the substrate. The stripe-like, polycrystalline gold nanoantennas with rectangular cross-sections were produced by electron beam lithography on silicon wafers. The resonance characteristics were extracted from spectroscopic measurements with our IR microscope. Special focus herein is on interaction between nanoantennas in direction perpendicular to the long particle axis. It is shown that beginning from a crucial distance, the optical properties change dramatically if the gap between the nanoantennas is further decreased.

O 60.60 Wed 17:30 P4

Cutting gold nanoantennas by focused ion beams — •Daniel Weber[1], Frank Neubrech[1], Han Gui[2], Dominik Enders[2], Tadaaki Nagao[2], and Annemarie Pucci[1] — [1]Kirchhoff Institute for Physics, Heidelberg, Germany — [2]National Institute for Materials Science, Tsukuba , Japan

Gold nanowires (nanoantennas) are plasmonic particles of great interest due to the possibility of tuning their ability to strongly enhance the local electromagnetic field from the THz to the visible range by mainly changing the length. Furthermore, coupling of nanoparticles can lead to even higher enhancement of the local field compared to invidual particles. One very promising approach is an arrangement of two nanoantennas which are separated by a very small gap (few nm) between their tip ends. We tried to prepare such nanosized gaps by applying focused ion beam (FIB) milling. Stripe-like, polycrystalline gold nanoantennas were produced by electron beam lithography on silicon wafers and subsequently cut in the middle by FIB. It turned out that the question if the nanoantennas are really separated cannot be answered by scanning electron microscopy or FIB imaging. However, measuring the infrared optical response of such prepared dimers provides a non-contacting, non-destructive, and easy method to prove the successful cut. Alternative methods like cross-sectional transmission electron microscopy and energy dispersive spectroscopy were also applied to confirm the findings from IR spectroscopic measurements.

O 60.61 Wed 17:30 P4

Modelling of Optical Nanoantennas for Nonlinear Spectroscopy — •Daniela Ullrich[1,2], Thorsten Schumacher[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

The null-field method (also known as the T-Matrix approach) is a powerful tool to simulate the light scattering by single and compound particles. Here, we demonstrate that our nonlinear transient transmission measurements on single as well as antenna-coupled gold nanoparticles can be modelled numerically using the null-field method. This allows us to further optimize the optical nanoantennas with the help of the simulations. Additionally, other materials such as aluminium or silver can be included. We compare the predicted behavior to our measurements on the optimized antenna structures. Finally we show that the numerical model can be adapted to describe plasmon-enhanced sensing using dielectric nanoparticles.

O 60.62 Wed 17:30 P4

Optical properties of gold nanorings prepared by different lithography methods — •Yuliya Fulmes[1], Kai Braun[2], Christian Schäfer[1], Andreas Horrer[1], Dominik Gollmer[1], Dai Zhang[2], Alfred Meixner[2], Dieter Kern[1], and Monika Fleischer[1] — [1]Institute of Applied Physics, University of Tuebingen, 72076 Tuebingen, Germany — [2]Institute of Physical and Theoretical Chemistry, University of Tuebingen, 72076 Tuebingen

Gold nanorings feature a variety of optical phenomena and exhibit a size- and shape-dependent resonance wavelength tuneable over a wide range in the visible and near-infrared spectrum. Different approaches have been pursued for the preparation of gold nanorings. In the first one, the individual rings are fabricated from a thin gold layer by HSQ e-beam lithography followed by angular argon ion milling. In the second one, Au rings are produced using colloidal lithography. A gold film is evaporated onto polystyrene particle coated substrates. During argon ion milling secondary sputtering of material creates a gold shell around the sides of the particles, which are removed afterwards. In the third approach, the patterns are defined in PMMA by e-beam lithography. Gold rings are obtained after a standard lift-off process of a gold layer which was deposited after development of PMMA. Using the above-mentioned methods it is possible to structure gold nanorings of many desirable sizes and geometries. The optical properties of the structures under excitation with an electromagnetic field are simulated by means of finite element methods and investigated in a parabolic mirror confocal microscope.

O 60.63 Wed 17:30 P4

SEIRS with gold nanoantennas towards health diagnostics — Frank Neubrech[1], Daniel Weber[1], Jörg Bochterle[1], Wolfgang Petrich[1], •Annemarie Pucci[1], Javier Aizpurua[2], Enzo Di Fabrizio[3], and Marc Lamy De La Chapelle[4] — [1]Kirchhoff Institute for Physics, Heidelberg, Germany — [2]Donostia International Physics Center, Donostia-San Sebastian, Spain — [3]Italian Institute of Technology, Genoa, Italy — [4]University Paris 13, Bobigny, France

It is well established, that plasmonic oscillations in metal nanorods efficiently enhance near-field under resonant conditions. In the infrared, fundamental antenna-like resonance can be used for surface-enhanced infrared spectroscopic (SEIRS) studies. In the project NANOANTENNA we optimize such system for application of SEIRS to the detection of rare biomolecular disease indicators in the human blood. Accordingly, as first step, a biocompatible material combination was identified and secondly, the resonance condition is optimized.

O 60.64 Wed 17:30 P4

Volume plasmon modes in Ag@Au core-shell nanoparticles — Katja Höflich[1], Aliaksei Dubavik[2], Nikolei Gaponik[2], Silke Christiansen[1], Alexander Eychmüller[2], Lukas M. Eng[3], and •Thomas Härtling[4] — [1]Max-Plack-Institut für Mikrostrukturphysik, 06120 Halle, Germany — [2]Physikalische Chemie und Elektrochemie, TU Dresden, 01062 Dresden, Germany — [3]Institut für Angewandte Photophysik, TU Dresden, 01062 Dresden, Germany — [4]Fraunhofer Institut für Zerstörungsfreie Prüfverfahren, 01109 Dresden, Germany

In the case of special nanoparticle geometries like e.g. spherical nanoshells and cylindrical core-shell structures, classical light can not only excite surface plasmons, but also volume plasmon modes [1, 2]. We investigate the properties of such a volume mode in core-shell Au@Ag nanoparticles which we find manifested as an UV extinction peak in the plasmonic spectrum. Analytical calculations with varied dielectric functions for the particle shell demonstrate that the mode occurs if the permittivity of the shell vanishes. We furthermore provide both theoretical and experimental proof that in contrast to surface plasmon modes the spectral position of the volume mode is independent of the core-shell geometry. To this end, we calculated and prepared Au@Ag particles with different geometries and compare their extinction spectra. [1] K. Höflich, U. Gösele, C. Christiansen, Phys. Rev. Lett. 103, 087404 (2009) [2] K. Höflich, U. Gösele, C. Christiansen, J. Chem. Phys. 131, 164704 (2009)

O 60.65 Wed 17:30 P4

Fabrication and Application of Nanostructured Substrates for Surface Enhanced Raman Spectroscopy — •Sabrina Darmawi, Limei Chen, Torsten Henning, and Peter J. Klar — I. Physikalisches Institut, Justus-Liebig-Universität, Heinrich-Buff-Ring 16, 35392 Giessen

Detecting single nanoparticles or small concentrations of particles within a chemical complex has become more and more important. With the application of manufactured nanoparticles, such as oxides, in our daily products, concerns about our safety and their impact on us increase. In order to detect metal oxides, such as ZnO or TiO_2, a greatly sensitive approach of detection is necessary. With surface enhanced Raman Spectroscopy (SERS) the weak Raman signal can be amplified considerably. This can be achieved by a pattern of rhomb arrays that are transferred on a silicon substrate via electron beam lithography. As an alternative pathway to the subtractive method, the additive technique (lift-off) is used by evaporating silver or gold layers on the developed structure. Interactions between the analyte and the metallic lateral tip nanostructured surface lead to plasmonic excitations which cause a high electromagnetic field enhancement at the tips of the rhombs. For purposes of testing, engineered nanoparticles such as ZnO are deposited on the structured substrate. The resulting system is investigated by SERS and we will report on the dependence of the Raman signal on the tip parameters.

O 60.66 Wed 17:30 P4

Quantum-size effects on the dielectric response of metal clusters — •Koray Koksal[1,2], Yaroslav Pavlyukh[2], and Jamal Berakdar[2] — [1]Physics Department, BitlisEren University, Bitlis, 13000, Turkey — [2]Institüt für Physik, Martin-Luther-Universitat Halle-Wittenberg, Heinrich-Damerow-Strasse 4, 06120 Halle, Germany

We present analytical and numerical techniques and calculations for the quantum, dielectric response of metal clusters and elucidate the dependencies on the clusters size and topology. The calculations have been performed for Al, Ag and Cu clusters. We will discuss possible ways for the experimental verification on the basis of scanning tunneling spectroscopy [1] and electron energy loss spectroscopy [2] and also point out the relevance to nano-plasmonics.

[1] L. Limot, E. Pehlke, J. Kröger, and R. Berndt, Phys. Rev. Lett. 94, 036805 (2005)

[2] J. W. L. Eccles, U. Bangert, M. Bromfield, P. Christian, A. J. Harvey and P. Thomas, J. Phys.: Conf. Ser. 241, 012090 (2010)

O 60.67 Wed 17:30 P4

Observing optical transitions inside an STM junction: a study on field emission resonances and molecular wires — •Gunnar Schulze, Thomas Sirtl, Marten Piantek, Jingcheng Li, Katharina Franke, and Jose Ignacio Pascual — Institut für Experimentalphysik, Freie Universität Berlin, Berlin, Germany

Light emitted from direct optical transitions of tunneling electrons in a scanning tunneling microscope (STM) junction can provide rich information about electronic systems. Resulting spectra reflect the interaction of plasmonic and electronic degrees of freedom and can reveal an energy resolved picture of dipole active inelastic transitions during tunneling. Our STM light emission (STM-LE) experiments aim to get closer insights into the nature of these effects. In our study on field emission resonances (FER) on a metal surface we demonstrate the observation of direct optical electron transitions. A second study deals with the activation of inelastic transitions inside a single molecular wire and their effects on the STM-LE spectra.

O 60.68 Wed 17:30 P4

Leakage radiation microscopy of surface plasmons — •Jörg Schmauder, Michael Lutz, Stephen Riedel, Paul Leiderer, Elke Scheer, and Johannes Boneberg — Universität Konstanz

We excite surface plasmons on metal layers (Ag, Au) using an ATR (attenuated total reflection) setup in Kretschmann-configuration with a laserdiode at the wavelenght of 980 nm. A small fraction of the surface plasmons is scattered at the surface into the half space above the prism. The natural roughness of the metal film is sufficient for this scattering process.

We observe the light emitted from the scattered surface plasmons by optical microscopy in dark field mode (leakage radiation microscopy). We report on the decay of the surface plasmons as well as on interference patterns around step structures and optical elements like mirrors, curved mirrors and diffractive gratings.

O 60.69 Wed 17:30 P4

Calculation of the Equilibrium Electron Density of Plasmonic Nanostructures — •Timo Köllner, Kurt Busch, and Jens Niegemann — Institut für Theoretische Festkörperphysik and DFG-Center for Functional Nanostructures (CFN), Karlsruhe Institute of Technology (KIT), 76128 Karlsruhe, Germany

The hydrodynamic description of plasmonic devices allows the modeling of the nonlocal and nonlinear response of such structures to optical excitation. However, in order to properly conduct numerical calculations of the full hydrodynamic model, one first needs to find the equilibrium electron density of the system. In particular, the behaviour of the density at the surface of a metallic object is suspected to have a significant influence.

Here, we present an efficient and accurate finite-element approach to calculate the equilibrium electron density distribution and the electrostatic fields at the edge of the positively charged jellium background.

O 60.70 Wed 17:30 P4

Kerr-microscopy of magnetic nanostructures — •Christian Dicken[1,2], Klas Lindfors[1,2], Mario Hentschel[1,2], and Markus Lippitz[1,2] — [1]Max-Planck-Institute for Solid State Research, Stuttgart — [2]4th Physics Institute, University of Stuttgart

Merging the fields of micromagnetism and plasmonics promises many new applications in both industry and science. As a first step towards experiments on micromagnetic particles, we use a combination of Sagnac interferometry and an improved sample design to measure the magnetization of isolated nickel-gold particle systems. With the present technique, we were able to observe the Kerr rotation of particles smaller than 90nm in diameter with an SNR of 28. We will show a model that describes the size dependence of the signal and allows us to adapt our sample design for even better performance.

O 60.71 Wed 17:30 P4

Development of a Raman Correlation Spectroscopy Experiment — •Aude Barbara[1,2], Tomas Lopez-Rios[1], Pascal Quémerais[1,3], Martin Helfrich[2], and Lukas Eng[2] — [1]Institut Néel, CNRS-UJF, Grenoble, France — [2]IAPP, TU Dresden, Germany — [3]MPI-PKS, Dresden, Germany

We develop a Raman Correlation Spectroscopy (RCS) experiment. Analogous to Fluorescent Correlation Spectroscopy, we measure the time-dependence of Raman band intensities of particles in solution. The main advantages of Raman spectroscopy is its direct chemical selectivity and its non-dependence to the wavelength while its biggest drawback its cross-section that may be up to 10^{14} times smaller than that of the fluorescence. However, adding metallic colloids may significantly enhance the Raman signal. Taking advantage of this SERS (Surface Enhanced Raman Scattering) effect has two goals: (i) increase the sensibility of the RCS experiments and (ii) establish a direct link between the Raman exaltation and the size of the metallic colloids which can be simultaneously measured. More insight into the SERS mechanism could thus be obtained. We present the preliminary experiments that aim at demonstrating the capabilities of the set-up to perform reliable time-dependent and particle sizing measurements. Experiments done with fluorescent and Raman light on toy-system will also be presented.

O 60.72 Wed 17:30 P4

Surface plasmon polariton induced electronic transport through metallic nanostructures — •Daniel Benner, Matthias Bädicker, Johann Berres, Reimar Waitz, Johannes Boneberg, Paul Leiderer, and Elke Scheer — Universität Konstanz, Fachbereich Physik

We investigate the influence of pulsed and cw laser light onto the electronic transport through a metallic nanoconstriction. Light-matter interaction, in particular when the matter is in the nanometer scale, is an important and steadily growing field of research due to possible applications in opto-nanoelectronics. We use lithographically fabricated Mechanically Controllable Break-junctions (MCBJs) operated at ambient conditions for fabricating atomic-size contacts and atomically-sharp tips of gold. Detailed analysis of light-induced conductance changes has shown photo-assisted transport due to the excitation of high-energetic quasiparticles [1] and collective effects such as surface plasmon excitation. Also optical near fields due to antenna effects as well as thermal expansion contribute to the signal [2, 3, and 4]. We optimize the plasmon-induced effect for the development of opto-electronic devices by studying systematically the effects on different wavelengths, position of the laser spot, and geometries (e.g. design of the nanocontacts and polarization of the laser light). [1]J.K. Viljas et al., Phys. Rev. B 75, 075406 (2007) [2]D. Guhr et al., Phys. Rev. Lett. 99, 086801 (2007) [3]D. Guhr et al., J. of Microscopy 229, 407 (2008) [4]N. Ittah et al., Nano Lett. 9, 4 (2009)

O 60.73 Wed 17:30 P4

Gold nanocones for Raman-based biosensing — •Christian Schäfer, Katharina Broch, Yuliya Fulmes, Dominik Gollmer, Frank Schreiber, Dieter Kern, and Monika Fleischer — Universität Tübingen, Institut für Angewandte Physik, Auf der Morgenstelle 10, 72076 Tübingen

Raman spectroscopy is a powerful tool for detection and analysis of biomolecules because it delivers a specific fingerprint of the tested molecule. In order to develop a highly sensitive biosensor the small cross section of Raman scattering has to be increased. This is usually done by rough metallic surfaces or nanoparticles and their strong plasmon induced near-field. We use gold nanocones, with sharp tips of less than 10 nanometers in diameter [1], for surface enhanced Raman spectroscopy (SERS). The nanocones, which are fabricated by e-beam lithography and Argon ion-milling, have a well-defined plasmon resonance frequency which can be tuned through the size of the cones. Therefore they can be optimized for the applied laser frequency. The Raman enhancement by the cones is demonstrated by the measurement of thin pentacene films on arrays of different-sized gold nanocones.

[1] M. Fleischer et al., Appl. Phys. Lett. 93, 111114 (2008)

O 60.74 Wed 17:30 P4

Parallel methods for the fabrication of gold nanocones — •Andreas Horrer, Christian Schäfer, Yuliya Fulmes, Dominik Gollmer, Monika Fleischer, and Dieter Kern — Institut für Angewandte Physik, Eberhard Karls Universität Tübingen, Auf der Morgenstelle 10, D-72076 Tübingen

When interacting with an electromagnetic field, metallic nanoparticles create a local field enhancement caused by excitation of localized surface plasmons. The resonance frequency depends on the shape, the size and the material of the nanoparticle and its dielectric environment. At the tip of a nanocone the field enhancement is particularly strong. A large array of identical nanocones could be used for biosensing. The fabrication of such large arrays in reasonable time requires parallel methods. Nanosphere lithography is a low cost technique which utilizes highly ordered self-assembled hexagonally close-packed layers of colloids. Different processes were developed using double or monolayers of polystyrene beads. They either directly act as an etch mask, or as a mask for the deposition of an aluminium oxide etch mask for an underlying gold layer, from which the cones are formed in an argon ion milling step.

O 60.75 Wed 17:30 P4

Coupled exciton-plasmon modes in metal-dye hybrid systems — •Sabine Auer, David Leipold, and Erich Runge — Technische Universität Ilmenau, 98693 Ilmenau, Germany

At nano-structured metal surfaces, visible light can be localized to spatial regions well below the diffraction limit by the excitation of surface plasmon polaritons (SPPs). A major challenge for future devices employing SPPs is the fact that SPPs can only travel for very short ranges since they are strongly damped by Ohmic losses in the metal. One idea to overcome this problem is to compensate the damping by coupling of the SPPs to active media (e.g., dyes [1] or quantum wells [2]).

We present calculation results for the coupling of quantum mechanical excitations in a j-aggregated dye with the SPP excitation at a metal grating [1]. The strong coupling (energy transfer) of the SPP and the dye resonance manifests itself as avoided crossing in the dispersion relation. At resonance, the coupled eigenmodes show excitonic as well as plasmonic features.

The good agreement of the calculation with the experiment confirms that our description can be used in future work on the design of devices with SPPs coupled to gain media.

[1] P. Vasa, et al., “Ultrafast control of strong coupling in metal-molecular aggregate hybrid nanostructures”, *ACS Nano*, accepted. [2] P. Vasa, et al., “Coherent exciton–surface-plasmon-polariton interaction in hybrid metal-semiconductor nanostructures”, Phys. Rev. Lett. **110**, 116801 (2008).

O 60.76 Wed 17:30 P4

Low dimensional plasmons in Ag-nanowires grown on Si (557) — •Ulrich Krieg, Christoph Tegenkamp, and Herbert Pfnür — Institut für Festkörperphysik, Leibniz Universität Hannover, Appelstrasse 2, D-30167 Hannover, Germany

A quasi 1-dimensional system was prepared by adsorption of about 1 monolayer Ag on Si(557) at 550° via self assembly. The morphology and metallicity of these uniaxially grown nanowires were studied by the combination of using low electron energy diffraction and high resolution electron energy loss spectroscopy in one instrument (ELS-LEED) . The clean Si(557) surface consists of a periodic sequence of (111) mini-terraces (3 nm width), separated by (112) facets. After adsorption of Ag LEED reveals the same spot splitting along the $[\bar{1}\bar{1}2]$ direction, i.e. the initial alternating facet structure is conserved upon adsorption. A streaky $\sqrt{3} \times \sqrt{3}R30°$ reconstruction suggests further the formation of nanowires along the $[1\bar{1}0]$ direction. An alternating contrast seen by STM with spatial separations similar to those seen on Si(557) indeed confirms the growth of separated nanowires. These findings are fully supported by angle resolved EELS measurements. While along the wires a dispersion of a sheet plasmon has been found, across the wires only a non-dispersing state at around 450 meV has been identified. The localized peak, which is apparent also in the direction along the wires, can be reasonably explained assuming metallic wires with finite width of around 2.5 nm. Similar results were obtained recently for $DySi_22$ wires grown on vicinal Si(111) substrates (PRB 81 (2010) 165407)

O 60.77 Wed 17:30 P4

Plasmon propagation in structural and dieletric controlled gold films probed by phase-resolved PEEM — •Christoph Lemke[1], Till Leissner[1], Christian Schneider[2], Martin Aeschlimann[2], and Michael Bauer[1] — [1]Institut für Experimentelle und Angewandte Physik, Universität Kiel — [2]Fachbereich Physik, Technische Universität Kaiserslautern

In a phase-resolved photoemission electron microscopy experiment, the near field associated with propagating surface plasmon polaritons (SPP) can be locally sensed via interference with the excitation laser field [1]. Here we apply this technique to monitor and analyze SPP propagation in gold films where the plasmonic response is controlled by structural design via e-beam lithography as well as by dielectric loading. Phase resolved simulations based on Huygens principle allow us to reconstruct SPP properties such as group velocity, damping, direction of propagation.

[1] A. Kubo, N. Pontius, and H. Petek, Nano Lett. 7, (2007) 470

O 60.78 Wed 17:30 P4

Plasmonic Nanocones — •Dominik Gollmer, Christian Schäfer, Yuliya Fulmes, Andreas Horrer, Dieter Kern, and Monika Fleischer — Universität Tübingen, Institut für Angewandte Physik, Auf der Morgenstelle 10, 72076 Tübingen

Through external electromagnetic excitation, plasmons can be generated in metallic nanostructures. The resulting enhanced electromagnetic near-field can be used for applications, e. g. near-field imaging or surface enhanced Raman spectroscopy (SERS). The plasmon resonance of nanostructures depends on their geometry and composition [1]. We fabricate well-defined metallic nanocones, with tip radii of less than 10 nm [2]. The cones are fabricated using e-beam lithography, defined aluminium oxide masks and Ar ion-milling. The resonance frequency of these cones can be tuned by variation of material or size. The shift of the plasmon frequency when the height of Au cones is varied is shown in dark field spectra. Both an accurate fabrication process and the tunability of the plasmon resonance are fundamental requirements for applications.

[1] H. Kuwata et al. ; Appl. Phys. Lett. 83 (2003); 4625

[2] M. Fleischer at al.; Nanotechnology 21 (2010); 065301

O 60.79 Wed 17:30 P4

Tuning resonant infrared antennas with phase change materials — •Kathrin Schönauer[1], Jens Richter[1], Xinghui Yin[2], Jón Mattis Hoffmann[1], and Thomas Taubner[1,2] — [1]1st Institute of Physics, RWTH Aachen University, Sommerfeldstraße 14, 52074 Aachen, Germany — [2]Fraunhofer Institute for Laser Technology, Steinbachstraße 15, 52074 Aachen, Germany

In the field of active plasmonics one recent interest lies in tunable resonances, e.g. for the use as optical switches [1]. Tuning of resonances of metallic nanostructures can be done by changing their dielectric environment. Phase change materials show a change of their refractive index between amorphous and crystalline phase. Especially in the mid-infrared spectral region some of these materials show the advantage of having low losses.

Thin films of phase change materials, e.g. $Ge_2Sb_2Te_5$, are deposited by sputtering onto Si-substrates. On top of these films nanostructures are prepared by nanosphere lithography. We use Fourier-Transform Infrared Microscopy for measuring the resonance frequency of these infrared antennas.

A future application of these systems could be their use as tunable sensors for enhanced infrared spectroscopy [2-3].

[1] Z. L. Sámson et al., APL 96, 143105 (2010)

[2] R. Adato et al., PNAS, 106, 19227 (2009)

[3] F. Neubrech et al., PRL 101, 157403 (2008)

O 60.80 Wed 17:30 P4

Time-Resolved Near-Field Microscopy of Acoustic Vibrations — •Matthias Brandstetter[1,2], Ralf Vogelgesang[1], and Markus Lippitz[1,2] — [1]Max Planck Institute for Solid State Research, 70569 Stuttgart, Germany — [2]4th Physics Institute, University of Stuttgart,70550 Stuttgart, Germany

The localized surface plasmon resonance (LSPR) of a metal nanoparticle depends directly on the geometry and the dielectric constant of the nanoobject. The resonance is influenced by the electron density which can be modified locally by acoustic oscillations of the nanostructure. The optical near-field thus contains information on the structure's acoustic oscillation pattern. The combination of an apertureless scanning near-field optical microscope (aSNOM) and ultrafast pump-probe spectroscopy gives an instrument to detect the temporal and spatial dependence of the LSPR. We present our implementation of a pump-probe aSNOM which at the end will allow us to map out nanoscale mechanical oscillation patterns. We show numerical simulation of the field changes caused by local plasma frequency changes, nanoacoustical modes as well as first experimental results.

O 60.81 Wed 17:30 P4

Imprinting the optical near field of single and monolayered micro spheres into phase-change films — •Paul Kühler[1], Jan Siegel[2], Javier García de Abajo[2], Andreas Kolloch[1], Philipp Leiprecht[1], Johannes Boneberg[1], and Paul Leiderer[1] — [1]Fachbereich Physik, Universität Konstanz — [2]Instituto de Optica, CSIC, Madrid

Control over the optical near-field is a crucial prerequisite for several applications of light at the nanoscale, such as material processing, microscopy and biosensing. We present a method that allows for directly imaging the near-field distribution of nanostructures. Our test systems were scattering dielectric micro spheres on a planar substrate. Irradiation with short, infrared laser pulses were performed on particles on a thin, chalcogenide film, which is modified depending on the local fluence and therefore records the scattering field distribution. Single particles as well as monolayers of these particles were used as target. Investigating the single particle patterns with optical microscopy, we demonstrate the influence of polarization and angle of incidence of the incident beam as well as the particle size on the imprints. Due to the monotonicity over a large fluence range of the chalcogenide film's response to irradiation, the experimental results could be shown to be in quantitative agreement with a model based on a rigorous solution of Maxwell's equations. In case of monolayers, high-resolution scanning electron measurements reveal modifications in the chalcogenide film with lateral dimensions down to 1/16 of the irradiation wavelength.

O 60.82 Wed 17:30 P4

Fabrication and application of core-shell nanorod structures — •Vera Hoffmann[1], René Kullock[1], Mathias Böhm[1], Gunther Scheunert[2], and Lukas M. Eng[1] — [1]Institut für Angewandte Physik/Photophysik, TU Dresden, Dresden, Germany — [2]Department of Physics and Astronomy, Queen's University Belfast, Belfast, UK

The fabrication of nanorod arrays made of a single material such as gold, silver, cobalt and others is already an established technique. However, nanorods made of material combinations have hardly been exploited so far, and may lead to novel physical properties of the array. In this study, we present how gold-nickel core-shell nanorod structures are fabricated: An anodised aluminium oxide matrix containing gold nanorods is partly etched to obtain an air shell around the gold rods. Then the resulting gaps are filled with nickel in a subsequent electrodeposition step .

Nanorod arrays can be used for various sensor applications. For example, the interrod distance and the angle of incidence strongly influence the collective surface plasmon resonance (CSP) of the structure [1,2]. Thus, if the structure is prepared on a transparent flexible substrate, application of external mechanical stress affects the optical properties of the device, which can be used to detect strain on a local scale. Furthermore, the magnetic properties of nickel-gold nanorod arrays can be exploited for magnetic sensors with optical read-out.

[1] R. Kullock et al., Optics Express 16, 21671 (2008) [2] R. Kullock et al., J. Opt. Soc. Am. B 27, 1819 (2010)

O 60.83 Wed 17:30 P4

Improving SHG Calculations with 3D Curved Elements in the Discontinuous Galerkin Method — •Andreas Hille, Rene Kullock, Alexander Haussmann, Stefan Grafström, and Lukas M. Eng — Institut für Angewandte Photophysik, Technische Universität Dresden, 01069 Dresden, Germany

The existence of optical second-harmonic generation (SHG) at metallic surfaces has been well known for a long time in experiment as well as in theory, where several electron gas models [1] exist. Further investigations have dealt with SHG at thin metallic films and nanoparticles, for which these models have been checked against experimental data. In order to apply the model not only to films or spheres but also to more complex structures such as nanorods, efficient and powerful numerical methods are needed.

One such method is the Discontinuous Galerkin method (DG) [2], which allows for explicit time stepping and finite-element-like meshing. We demonstrate here that, due to the nonlinear sensitivity of SHG signals, an accurate boundary description by means of curved elements is necessary in order to obtain reliable and non-erroneous results. Furthermore, we apply this DG method to metallic nanorods and show their usefulness as SHG antennas.

[1] J. E. Sipe, "Analysis of second-harmonic generation at metal surfaces", Phys. Rev. B 21, 10, 1980

[2] J. S. Hesthaven and T. Warburton, "Nodal High-Order Methods on Unstructured Grids", J. Comput. Phys. 181, 186-221 (2002)

O 60.84 Wed 17:30 P4

Dependence of the photochromic transformation of TiO_x- and ZrO_x-embedded Ag nanoparticles on the photon energy of the irradiating light — Hendrik Holzapfel[1], Alexander Sprafke[1], Florian Hallermann[1], •Nils Becker[1], Melanie Meixner[2], Matthias Wuttig[1], and Gero von Plessen[1] — [1]Institute of Physics (IA), RWTH Aachen University, 52056 Aachen, Germany — [2]present address: Fraunhofer Institute for Laser Technology ILT, 52074 Aachen, Germany

Photochromic materials change their color under irradiation with light. Uniform TiO_x- and ZrO_x-embedded Ag nanoparticles with photochromic properties can be fabricated through a combination of nanosphere lithography and electron-beam evaporation. In comparison to the dc-sputter deposition technique as employed in our previous work [1], the good reproducibility of this approach and the less inhomogeneously broadened plasmon line of the resulting samples allow us to analyze the photochromic transformation in a more quantitative way.

In this work, we investigate the dependence of the photochromic transformation of TiO_x- and ZrO_x-embedded Ag nanoparticles prepared by nanosphere lithography on the photon energy of the irradiating light. We find a photon energy below which no photochromism is observed, almost independently of the embedding medium. Furthermore, the photochromic effect increases with increasing photon energy.

[1] C. Dahmen et al., Appl. Phys. Lett. 88, 011923 (2006)

O 60.85 Wed 17:30 P4

Calculation of up-conversion signal of Er^{3+} ions near gold nanospheres — •Florian Hallermann[1], Stefan Fischer[2], Jan Christoph Goldschmidt[2], and Gero von Plessen[1] — [1]Institute of Physics (IA), RWTH Aachen University, 52056 Aachen, Germany

— [2]Fraunhofer Institute for Solar Energy Systems, Heidenhofstr. 2, 79110 Freiburg, Germany

In conventional silicon solar cells, photons with energies below the silicon band gap (1.12 *e*V) do not contribute to current generation. The near-infrared part of the solar spectrum could possibly be exploited by use of up-conversion processes. For example, electrons could be excited from the ground state to a final state via intermediate states through sequential absorption of infrared photons. Such electrons subsequently relax from the final state by emitting 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 signal of Er^{3+} ions can be enhanced using spherical gold nanoparticles. In the vicinity of the nanoparticles, the excitation rate of the ions is changed due to the near-field of the particles. These changes are computed using Mie theory and a rate equation system. In addition, also the relaxation times of all involved excited states of the ions are changed by the presence of metal nanoparticles. This is caused by a near-field induced energy transfer from the ions to the nanoparticles, which offer additional radiative and nonradiative decay channels. Here, we semi-analytically calculate the effects that these changes have on the up-conversion signal.

O 60.86 Wed 17:30 P4

Near-and farfield investigations of individual sub-nanometre plasmonic gap resonances — •Florian Schertz[1], Reza Mohammadi[2], Marcus Schmelzeisen[2], Hans-Joachim Elmers[1], Gerd Schönhense[1], and Max Kreiter[2] — [1]Inst. f. Physik, J. Gutenberg-Universität, Mainz — [2]MPI f. Polymerforschung, Mainz

An increasing interest evolved on the mutual interaction of distinct plasmonic resonances during the last years, due to the extremely enhanced and localized electromagnetic fields that are provoked. Prominent examples are nanoparticle (NP) dimers with an ultrasmall gap between them or NPs close to metallic films, the latter can be manufactured with reproducible sub-nm gaps. These coupled plasmons supporting systems act as optical antennae, as they efficiently convert free-propagating radiation into localized electromagnetic energy. Hence, understanding the optical near-field (NF) and far-field (FF) properties is essential for a full understanding of nano-antennae and for application-oriented optimization. We present NF- and FF-spectra and corresponding SEM images of the same individual gap-resonance supporting Au NPs on a Au film with a gap of 0.8nm. Dark-field confocal microscopy is used for detection of the FF response, photoemission electron microscopy for the NF characteristics. Beside the well-known FF gap-resonances, additional dark-mode resonances were observed exclusively in the NF, depending strongly on the NP properties. The experimental findings are analyzed and systematized concerning their correlation to FIT-simulations of the optical NF and FF. Funded by DFG EL172-16.

O 60.87 Wed 17:30 P4

Plasmonic Collimation of near-IR Laser Diodes — •Xinghui Yin[1,2], Thomas Taubner[2,3], and Peter Loosen[1,2] — [1]Institute for Technology of Optical Systems, RWTH Aachen University, Steinbachstr. 15, 52074 Aachen — [2]Fraunhofer Institute for Laser Technology ILT, Steinbachstr. 15, 52074 Aachen — [3]I. Institute of Physics (IA), RWTH Aachen University, Sommerfeldstr. 14, 52074 Aachen

Laser diodes are compact and versatile components for numerous applications. However, they show a strongly asymmetric beam-profile in the far-field due to the confined dimensions of their emitting area (ca. 1 μm × 5 μm). Currently, high-index cylindric lenses are employed to reduce the beam divergence. This is a nonmonolithic, costly approach as lenses have to be manually adjusted.

We investigate beam collimation in one direction by effectively enlarging the emitting area. To do so, we use a plasmonic structure consisting of a slit and a grating structured in a gold layer directly on top of the laser facet. Previous work done by Ebbesen et al [1] confirm the beaming properties of such structures. Capasso et al [2] successfully combined plasmonic collimators and Quantum Cascade Lasers at wavelengths of $\lambda = 9.8\ \mu$m. We optimize the structure parameters for near-infrared wavelengths ($\lambda = 960$ nm). Using the obtained parameters, we fabricate the plasmonic collimator and characterize it.

[1] Ebbesen et al., Beaming Light from a subwavelength Aperture, 2002, Vol 297, Science

[2] Capasso et al., Nature Photonics, 2008

O 60.88 Wed 17:30 P4

Probing subwavelength plasmonic components from the far field — •Jing Wen[1,2], Arian Kriesch[1,2,3], Daniel Ploss[1,2,3], Peter Banzer[1,2], and Ulf Peschel[1,2] — [1]MPI für die Physik des Lichts, Erlangen, Germany — [2]Friedrich-Alexander-Universität Erlangen-Nürnberg, Erlangen, Germany — [3]Erlangen Graduate School in Advanced Optical Technologies (SAOT)

Optical antennas connected to waveguides with subwavelength width enable the investigation of different nanoplasmonic components. An high-NA focal scanning setup exploits the distinctive spectral and polarization selectivity of these antennas. A clever combination of several antennas for receiving and emitting light in mutually orthogonal configurations allows unprecedented signal-to-noise ratio in probing different waveguide configurations. We report the first experimental characterization of an optical antenna connected to a nanoplasmonic gap waveguide. A strongly confined bound mode can not leak to the far field unless it is scattered out at an antenna or a waveguide end. Far-field measurements of the light emitted from those waveguide ends or extra antennas are performed in crossed polarization and enable the detection of extremely weak signals. To allow for highly efficient crossed polarization detection, a 90° waveguide bend is used. Our method allows for the probing nano-structures that were previously only accessible by Scanning Near-field Optical Microscopy, and we therefore circumvent the intrinsic disadvantages of near-field microscopy such as high losses and elaborate operation. Instead of intruding the near field directly, we focus the far field to the nanoscale and vice versa.

O 60.89 Wed 17:30 P4

Plasmonic antennas and wireless interconnects on a subwavelength scale — •Daniel Ploss[1,2,3], Arian Kriesch[1,2,3], Jing Wen[1,2], and Ulf Peschel[1,2] — [1]MPI für die Physik des Lichts, Erlangen, Germany — [2]Friedrich-Alexander-Universität Erlangen-Nürnberg, Erlangen, Germany — [3]Erlangen Graduate School in Advanced Optical Technologies (SAOT)

Wireless transfer of electromagnetic radiation requires antennas with well-designed directivity and high efficiency. In optics those antennas offer particularly interesting applications in the intermediate domain between the far- and near- field; integrating wireless transfer channels with highly confined plasmonic circuitry can significantly decrease losses, thus avoiding the major disadvantage of nanoplasmonics. We report on optical antennas loaded with nanostructures under investigation and which are optimized for low reflection at the connection. Different types of antennas were designed and simulated with Finite Elements Methods (FEM), and their estimated performance finally compared with experimental results. A concept for engineering exceptionally high directionality are Yagi-Uda antennas, well known from the radio-frequency range. We intend to use them as wireless interconnects between highly packed, plasmonic waveguide structures. Hence, carefully designed antennas can not only be used to transfer the far field to the near field, but also for optimizing the arrangement of waveguide structures and for allowing more efficient, less lossy configurations.

O 60.90 Wed 17:30 P4

Towards the realization of an efficient nanoantenna — •Reto Giannini[1], Patrick Leidenberger[2], Christian Hafner[2], and Jörg F. Löffler[1] — [1]Laboratory of Metal Physics and Technology, Department of Materials, ETH Zurich, 8093 Zurich, Switzerland — [2]Laboratory for Electromagnetic Fields and Microwave Electronics, ETH Zurich, 8092 Zurich, Switzerland

Different aspects of nanoantennas, such as radiation pattern or wavelength-dependent near-field enhancement, are being heavily discussed in recent years. Many simulation-based contributions concentrate either on the general usability of simulation methods or use such methods to verify experimental data. Especially in systems that are more complex to realize, estimations concerning performance and its reproducibility are needed before the development of the production process starts. In this study, we present a series of FEM-based simulations carried out using JCMsuite on a nanoantenna consisting of two stacked nanodiscs. The goal was to realize a geometry that delivers first and second order plasmon resonance at the later excitation and emission wavelength of the activated nanoantenna as well as estimations concerning design stability. Besides the most important geometry parameters, such as height, diameter or gap, production-based parameters (diminution of the antenna or round corners) as well as the influence of a later integration (excitation and emission) are considered. The results of the simulations are compared with actual experiments on nanoantennas, produced using guidelines obtained from the simulation studies.

O 60.91 Wed 17:30 P4

Structural changes of percolated metal films by laser irradiation — Christian Maasem, •Daniela Schneevoigt, Florian Hallermann, and Gero von Plessen — Institute of Physics (IA), RWTH Aachen University, 52056 Aachen, Germany

In semi-continuous, percolated metal films, both localised and propagating surface-plasmon modes can be excited by light irradiation over a wide spectral range. This can lead to strong optical field enhancements which are confined to 'hot spots' of a few nanometers in size.

In this work, we show that percolated silver films on glass substrates change their structure upon irradiation with focussed laser light. The irradiated areas exhibit more light scattering and higher light transmission than non-irradiated areas. This could point towards an aggregation of the films to larger structures and thus towards a reduction of the coverage of the substrate surface. Even after an additional coating with SiO_2, changes of the structure of the silver films occur already at low laser intensities.

In contrast, no changes are observed when irradiating percolated gold films. Thus, it can be assumed that the restructuring of the film material is not purely a thermal effect.

O 60.92 Wed 17:30 P4

Investigations on laser-beam immobilised gold nanoparticles — •Falko Brögger[1], Ninet Babajani[2], Malte Linn[1], and Gero von Plessen[1] — [1]Institute of Physics (1A), RWTH Aachen University, 52056 Aachen, Germany — [2]FZ Jülich, Inst. of Solid State Research (IFF-6), 52428 Jülich, Germany

The plasmon lines of chemically synthesized noble-metal nanoparticles of nearly spherical shape and approximately uniform size exhibit surprisingly large particle-to-particle variations of their resonance peak positions and line widths. The reasons for these spectral variations are still unknown. Possible explanations include faceting of the nominally spherical particles, charges and chemical effects within the suspension, and interactions with the substrate.

In this work, single gold nanoparticles suspended in an aqueous environment are trapped by an optical tweezer, and their light-scattering spectra, which are free of substrate effects, are measured. Each of the trapped nanoparticles is subsequently deposited onto a substrate using the optical tweezer and its spectrum is measured again. A comparison of the single-particle spectra shows that the particle-to-particle plasmon line variations in the aqueous suspension and the substrate-induced line changes do not seem to be correlated. Remarkably, additional line changes are observed upon drying the sample surface and covering it again with water.

O 60.93 Wed 17:30 P4

Second Harmonic Generation and Two Photon Photoemission from Cs on Cu(111) — •Mariusz Pazgan, Cheng-Tien Chiang, Aimo Winkelmann, and Jürgen Kirschner — Max-Planck-Institut für Mikrostrukturphysik, Weinberg 2, D-06120 Halle (Saale), Germany

We report on a combined study of nonlinear-optical Second Harmonic Generation (SHG) and Two-Photon Photoemission (2PPE) from the system of Cs on Cu(111). The SHG and photoemission signals were simultaneously measured during real time deposition of Cs atoms on Cu(111) surface. Clear resonances in 2PPE and SHG were observed in measurements at 140K and 300K. We interpreted our results by optical transitions between the occupied Cu(111) Shockley surface state band and the unoccupied Cs anti-bonding state at the photon energy of 3.07eV used in the experiment.

O 60.94 Wed 17:30 P4

Investigation of spin-polarized electron transmission through Co/C/Co tunnel junctions — •Felix Huerkamp, Bernd Stärk, Peter Krüger, and Johannes Pollmann — Institut für Festkörpertheorie, Universität Münster, Germany

We investigate transmission properties of electrons at the interfaces of Co/C/Co metal-semiconductor hybrid systems within an ab-initio approach. The considered open system is a tunnel junction consisting of three parts: the left and right semi-infinite cobalt leads, as well as the scattering region built by N layers of carbon atoms. We employ spin-polarized density-functional theory within the generalized gradient approximation to calculate the spin-polarized transmission. To this end, we use a Greens function technique which is based on the representation of the wave functions by Gaussian orbitals. This enables us to treat the scattering problem as a localized perturbation of a Co crystal. In a first step, we calculate self-consistently the potential in the region of the C layers and the neighboring Co layers. Then we construct the exact self-energies from the potential of bulk Co. Finally, we evaluate the transmission coefficient T(E) calculating the Greens function in the subspace of the perturbation. We have investigated junctions of hexagonal Co with C layers grown in (111) direction, as well as junctions of fcc Co with C layers oriented in (001) direction. The results for the transmission are discussed as a function of the number of C layers in the scattering region.

O 60.95 Wed 17:30 P4

Electronic States of Polar and Non-polar Surfaces within the Quasiparticle Approach — •Abderrezak Belabbes and Friedhelm Bechstedt — Institut für Festköpertheorie und -optik, Friedrich-Schiller-Universität, Max-Wien-Platz 1, 07743 Jena, Germany

DFT provides an incorrect description of the band gap and excited states of InN. The correction of this error is of considerable importance in understanding the surface physics and semiconducting properties of InN. The purpose of this work is to reevaluate the quasiparticle band structure using the novel LDA-1/2 method for the surfaces states of InN. We restrict ourselves to a discussion of the electronic structure of the clean polar and non-polar surfaces. Our calculations allow us to explain the n-type conductivity of polar InN surfaces and the pinning of the Fermi level. The electronic structure of non-polar InN surfaces is found to be very different from that of the polar surface. It shows a semiconduting behavior, but with surfaces states that energetically overlap with bulk states. Therefore, these findings suggest an absence of electron accumulation on the non-polar InN surfaces. Our results agree with the previous calculations by C. G. Van de Walle and experimental observations by Wu et al, who provided evidence for an unpinned Fermi level at non-polar surfaces. The results have been obtained with low computational effort, similarly to standard LDA calculations, much in contrast to the GW quasiparticle approach.

O 60.96 Wed 17:30 P4

Defects in amorphous silica : from density functional to many-body perturbation theory — •David Waroquiers[1,2], Matteo Giantomassi[1,2], Martin Stankovski[1,2], Gian-Marco Rignanese[1,2], and Xavier Gonze[1,2] — [1]Université Catholique de Louvain IMCN-NAPS, Louvain-la-Neuve, Belgique — [2]European Theoretical Spectroscopy Facility (ETSF)

Amorphous silica is of particular technology interest for its electronic and optical properties. It is commonly used in a lot of devices such as optical fibers, lenses, filters, gate dielectrics in MOS transistors, . . . In the present work, we investigate the effect of hydrogen on the properties of amorphous silica.

Accurate electronic structure is obtained using many-body perturbation theories such as GW approximation. Till recently, this method could only be applied to small systems because of its large computational cost. New theoretical and algorithmic developments in the version 6 of ABINIT [1] (extrapolar method, band parallelism and projector-augmented wave formalism) now enable us to perform GW calculations in large supercells with a reasonable cost in CPU time.

We report results obtained for several hydrogen-containing silica cells of 72 atoms. The electronic structure has been computed using many-body perturbation theory in its GW approximation. Formation energies are calculated at the DFT and GW level [2]. Some preliminary results on the optical properties are also presented.

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O 60.97 Wed 17:30 P4

H-Adsorption and surface resonances on Pd and Pt — •Alexander Menzel[1], Peter Amann[1], Michael Cordin[1], Erminald Bertel[1], Josef Redinger[2], Sebastian Stolwijk[3], Karen Zumbrägel[3], and Markus Donath[3] — [1]Inst. f. Phys. Chemie, Univ. Innsbruck, Austria. — [2]Dep. of Appl. Physics, Techn. Univ. Wien, Austria. — [3]Physikal. Institut, Univ. Münster, Germany

In this contribution, the influence of Hydrogen adsorption on the isoelectronic surfaces Pt(110) and Pd(110) is observed with ARPES (in some cases spin resolved) and compared with DFT-calculations. A strong surface resonance at $\overline{S}$ can be identified experimentally in ARPES by backfolding due to adsorbate-induced changes of surface-symmetry. Whereas Hydrogen adsorption induces no energetic shift of the surface resonance at $\overline{S}$ in Pt(110), a downward shift on Pd(110) is observed. This difference is related to the different adsorption sites for hydrogen on both surfaces and compares favourably with DFT calculations [2]. Interestingly, upon hydrogen adsorption a pairing-row reconstruction on Pd(110) develops together with a satellite peak of the $\overline{S}$ resonance. The band dispersion of this satellite is parallel to the dispersion of the main resonance, but is shifted to lower energies by roughly 400meV. The spectra resemble Ni(110), however, a spin polarization could not be detected. Possible origins of the satellite peak are discussed.

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O 60.98 Wed 17:30 P4

Field Emission Resonances on the Quasi One-Dimensional Si(111)5x2-Au Reconstruction — •Stefan Polei, Ingo Barke, Kristian Sell, Viola von Oeynhausen, and Karl-Heinz Meiwes-Broer — Institut für Physik, Universität Rostock, D-18051, Rostock, Germany

Scanning tunnelling spectroscopy measurements of field emission resonances (FER) have shown to be a suitable tool to investigate local work function variations particularly on metal surfaces [1]. About FER on semiconductors or nanostructured surfaces less literature can be found. In this contribution we compare FER on different regions of a Si(111)7x7 substrate which is partially covered by the quasi one-dimensional Si(111)5x2-Au structure. Across a transition between Si(111)7x7 and Si(111)5x2-Au a shift of the FER peak positions is found which can be attributed to changes of the local work function. At increased spatial resolution dI/dV maps reveal a periodic shift of the higher order FER in the direction perpendicular to the chains of Si(111)5x2-Au. This effect appears on a length scale of less than one nanometer and is caused by surface-potential variations. Model calculations are shown to quantify their amplitude.

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O 60.99 Wed 17:30 P4

Energy-filtered PEEM at ferroelectric nanostructures: Fingerprints of the ferroelectric polarization in the electronic structure of $PbZr_{0.52}Ti_{0.48}O_3$ — •Ingo P. Krug[1], Nick Barrett[2], Astrid Besmehn[4], Alessio Morelli[3], Ayan Roy Chaudhuri[3], Ionela Vrejoiu[3], Marten Patt[1], Olivier Renault[5], Fausto Sirotti[6], and Claus M. Schneider[1] — [1]IFF-9, Forschungszentrum Jülich GmbH, Jülich, GERMANY — [2]DSM/IRAMIS/SPCSI, C.E.A. Saclay, Gif-sur-Yvette, FRANCE — [3]MPI für Mikrostrukturphysik, Halle, GERMANY — [4]ZCH, Forschungszentrum Jülich GmbH, Jülich, GERMANY — [5]LETI group, MINATEC, C.E.A. Grenoble, Grenoble, FRANCE — [6]TEMPO beamline, Synchrotron SOLEIL, Gif-sur-Yvette, FRANCE

Ferroelectrics are promising materials for nanoelectronic devices. Their versatility offers a widespread range of applications, for example, non-volatile memory-cells, controllable surface catalysts, or energy harvesting devices. The key to improved functionality is to understand the interrelations between electronic structure and ferroelectricity. Many ferroelectrics are thought to exhibit a combined structural and electronic reconstruction upon ferroelectric ordering. While the structural aspects can easily be investigated by diffraction, determining the electronic structure by photoemission is often challenging due to the insulating nature of this material class. Nevertheless, as we show for the case of $PbZr_{0.52}Ti_{0.48}O_3$ (PZT), spectromicroscopic studies in these materials are rewarding: Energy-filtered PEEM by a NanoESCA microscope reveals polarization effects in core-levels and the valence-band.

O 60.100 Wed 17:30 P4

Development of an impurity-embedding code based on the Korringa-Kohn-Rostoker (KKR) Green function method — •David Bauer, Phivos Mavropoulos, Rudolf Zeller, and Stefan Blügel — Peter Grünberg Institut & Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, 52425 Jülich, Germany

We present a new implementation of the KKR Green function method for performing electronic structure calculations based on the density functional theory of impurity atoms embedded in a periodic host.

Our code is able to treat impurity atoms positioned unrelated to the host sites. This became possible by a two step approach: For large deviations of the impurity from the host position a virtual atom method is used where the host Green function is expanded around the new impurity position. Then, small displacements are treated as described in [1].

In addition, we include in our code a recently developed accurate method to directly solve the coupled Lippmann-Schwinger equations for non-spherical potentials via systems of linear equations obtained by Chebyshev expansions for radial variables. This is especially important for the irregular solutions when spin-orbit coupling is included in the presence of a magnetic field, since then, the effective potential close to the origin is not necessarily spherical. Further, the code has been parallelized in energies, which enables us to use typically 100 processors with an almost linear speedup.

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O 60.101 Wed 17:30 P4

Angle-resolved photoelectron spectroscopy of strained $SrRuO_3$ thin films — •Arndt Quer[1], Erik Kröger[1], Matthias Kalläne[1], Adrian Petraru[2], Rohit Soni[2], Hermann Kohlstedt[2], Lutz Kipp[1], and Kai Rossnagel[1] — [1]Institute of Experimental and Applied Physics, University of Kiel, 24098 Kiel, Germany — [2]Department of Nanoelectronics, Technical Faculty, University of Kiel, 24143 Kiel, Germany

The magnetoelectric effect in composites based on oxides and in particular the coupling mechanism between the electric and magnetic order parameters have recently attracted much attention in basic research. By combining different piezoelectric and magnetostrictive substances it is possible to optimize the magnetoelectric properties of the composite, for example, with regard to technological applications such as ultra-sensitive magnetic sensors. Due to its adequate electrical conductivity in combination with lattice-strain induced changes of the magnetic moment, ferromagnetic $SrRuO_3$ is a good test candidate for the magnetostrictive component of the magnetoelectric composite. Our goal here was to study the magnetostrictive behavior by analyzing the electronic structure of $SrRuO_3$ thin films in different strain-states. To this end, we prepared pulsed-laser-deposition grown $SrRuO_3$ films on different oxide substrates. The samples were annealed by O_2 under various conditions, resulting in atomically clean and mostly defect-free surfaces. The samples were studied by low-energy electron diffraction and angle-resolved photoelectron spectroscopy. This work was supported by the DFG through SFB 855.

O 60.102 Wed 17:30 P4

Theoretical approach to adatom structures on semiconductor surfaces: Ab-initio studies and explicit many-body extensions. — •Sergej Schuwalow and Frank Lechermann — I. Institut für Theoretische Physik, Universität Hamburg, D-20355 Hamburg, Deutschland

Single adatoms, dimers and general quasi-twodimensional adsorbate arrays on semiconductor surfaces exhibit a great variety of interesting effects, while having the advantage of being directly accessible via surface-sensitive experimental probe techniques. The reduced dimensionality and the coupling to the substrate can produce, e.g., peculiar magnetic effects and also correlation effects may become important due to strong electron localization at the adatom sites.

Within this work, we investigate the electronic structure of submonolayer surface systems, namely the Sn/Si(111) and the Sn/Ge(111) alpha surfaces [1], as well as single magnetic adatoms (Fe,Co,Ni) on the InSb(110) substrate [2] by density-functional theory (DFT) and, where appropriate, its combination with explicit many-body methods. Our main focus lies on determining the structural, bonding and magnetic properties, and in case of the Sn submonolayer systems, the influence of a finite Hubbard U on the surface states.

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O 60.103 Wed 17:30 P4

The plasma treatment of Titanium in Oxygen, Nitrogen, Argon and air studied with MIES, UPS and XPS — •René Gustus[1], Sebastian Dahle[1], and Wolfgang Maus-Friedrichs[1,2] — [1]Institut für Physik und Physikalische Technologien, TU Clausthal, Leibnizstr. 4, 38678 Clausthal-Zellerfeld, Germany — [2]Clausthaler Zentrum für Materialtechnik, TU Clausthal, Leibnizstr. 4, 38678 Clausthal-Zellerfeld, Germany

The treatment of Titanium with different kinds of plasma is commonly used for etching, oxidation, carbonization or nitriding. During some of these techniques, a lot of heat is carried into the material, whereas

others operate at room temperature. All of the processes reported so far have in common that cover gas is needed. The gas is choosen in terms of application, thus Nitrogen-rich or Carbon-rich gases are utilized for hardening and pure Argon as inert gas. It is also reported that an Oxygen plasma can be used for the removal of a TiN film.
We investigated the reaction and etching rates of an Oxygen and a Nitrogen dielectric barrier discharge (DBD) plasma and opposed both in an air plasma. The etching depth and surface purgation in an air plasma is then compared to an Argon plasma, to determine the use of an air plasma for technical applications. For our studies, we employed Metastable Induced Electron Spectroscopy (MIES), Ultraviolet Photoelectron Spectroscopy (UPS), and X-ray Photoelectron Spectroscopy (XPS).

O 60.104 Wed 17:30 P4

An Overview of Methanol Reactions on Ru based Catalyst Surfaces under UHV Conditions — •Pawel Gazdzicki and Peter Jakob — Fachbereich Physik, Philipps-Universität Marburg, Deutschland

The conversion of methanol to CO_2 is of substantial importance referring to the direct methanol fuel cell where CO from methanol dehydrogenation is responsible for the poisoning of the electrodes. In this comprehensive study thermally induced reaction pathways ($T = 20 - 600$ K) of methanol on various Ru based catalysts (Ru(0001), (sub)monolayer Cu/Ru(0001), Cu(111)/Ru(0001), pseudomorphic Pt/Ru(0001) and Pt_xRu_{1-x}/Ru(0001) surface alloys) have been investigated in detail using Fourier transform infrared spectroscopy, temperature programmed desorption and photoelectron spectroscopy. Particular interest is devoted to the influence of preadsorbed oxygen on the formation and stability of the various reaction intermediates. Among the various stable surface species hydroxyl, formaldehyde, formate, methoxy and carbon monoxide have been identified. A reaction scheme is presented to illustrate trends.

O 60.105 Wed 17:30 P4

In-situ alkylation reaction of two ionic liquids studied by X-ray photoelectron spectroscopy (XPS) — •Inga Niedermaier[1], Claudia Kolbeck[1], Florian Maier[1], Nicola Taccardi[2], Peter Wasserscheid[2], and Hans-Peter Steinrück[1] — [1]Lehrstuhl für Physikalische Chemie II, Egerlandstr. 3, 91058 Erlangen — [2]Lehrstuhl für Chemische Reaktionstechnik, Egerlandstr. 3, 91058 Erlangen

Ionic liquids (ILs) - salts with a melting temperature below 100 °C - have highly attracted attention due to their great potential in many fields, e.g. in catalysis or electrochemistry, and as a new class of tailored solvents. Due to their extremely low vapour pressure, ILs can be investigated with X-ray photoelectron spectroscopy (XPS) under ultra-high vacuum conditions allowing for in-situ studies of reactions in the near-surface region.

For the first time, an in-situ alkylation could be directly monitored by XPS in a 1:1 mixture of the two ILs $[C_8C_1Im][Cl(CH_2)_3SO_3]$ (IL 1) and $[(Me_2N(CH_2)_3)C_1Im][Tf_2N]$ (IL 2). In this thermally activated reaction, the amine group of the $[(Me_2N(CH_2)_3)C_1Im]^+$ cation (2) reacts quantitatively with the $[Cl(CH_2)_3SO_3]^-$ anion (1), producing an ammonium group in a new cation and a free chloride anion. Cl 2p spectra directly reflect the transformation of the covalently bound chlorine of (1) into the chloride anion. Additionally, angle resolved XPS (ARXPS) provides information on surface enrichment and orientation effects of the pure ILs and in the binary mixture before and after alkylation. - This work was supported by the DFG through SPP 1191 and the Cluster of Excellence 'Engineering of Advanced Materials'.

O 60.106 Wed 17:30 P4

Investigations of different techniques for oxygen termination of ultrananocrystalline diamond films — •Alexandra Voss, Hermann Koch, Cyril Popov, and Johann Peter Reithmaier — Universität Kassel, Institut für Nanotechnologie und Analytik, Heinrich-Plett-Straße 40, 34132 Kassel, Germany

Due to the high electrochemical potential window and high chemical stability, combined with a number of superior physical properties, all types of diamond films are ideal candidates for platforms for biosensors and DNA-chips. In almost all cases, after growth the surfaces of these films are hydrogen terminated and require photo-, plasma-, electro- or thermochemical processes to change the termination or to attach desired surface functionalities. In the current work we present the results for the surface modification of ultrananocrystalline diamond/amorphous carbon (UNCD/a-C) composite films by two different methods for oxygen termination, a O_2-plasma process and a UV/ozone treatment. The surfaces emerging from both modification ways were characterized by contact angle (CA) measurements, SEM, XPS, ToF-SIMS and STM, and their longtime stability with respect to different storage conditions was observed. In addition, the rate of the modification was determined with time dependent experiments to achieve highly hydrophilic surfaces (CA below 10°). The modification of the UNCD/a-C films increases their versatility for tailoring the surface properties for applications in biosensors, which requires a variety of functionalities in order to immobilize biomolecules.

O 60.107 Wed 17:30 P4

Conductivity of nano-porous Titania (TiO_2) during UV-illumination — •Thomas Kriesche[1] and Thomas Bürgi[2] — [1]Phys.-Chem.-Institut, Im Neuenheimer Feld 253, 69120 Uni Heidelberg — [2]Faculté des Sciences, Séction de Chimie, Département de Chimie Physique, Quai Ernest-Ansermet 30, CH-1211 Genève 4

The photocatalytic property of TiO_2 is used in many applications as solar cells for the production of hydrogen and electric energy, degradation of harmful substances, corrosion-protective coating. It is also investigated for energy storage (solar-to-fuel). Absorbed UV-light creates electrons and holes in the semiconductor, which recombine or can do reduction respectively oxidation on surface adsorbed molecules. The change of the conductivity during UV-irradiation reveals fundamental information about processes in nano-porous TiO_2 layers. Time resolved measurements offer the possibility to combine information from other methods like infrared spectroscopy, especially ATR-FTIR in MIR range. Data from scanning-electron-microscopy is used to show the porous structures. The conductivity is measured on top of a TiO_2 pill via a four point method in an Argon or Nitrogen atmosphere. It is possible to change the temperature and the humidity. For UV irradiation a Xenon lamp or 350nm diodes are in use with $\sim 0,5-1mW/cm^2$. The received data should be a step to describe the electron behavior of nano-porous TiO_2 under UV-irradiation.

O 60.108 Wed 17:30 P4

Spectroscopic Identification of initial decomposition mechanism of Prenal on a Platinum Model Catalyst — •Jan Haubrich[1], David Loffreda[2], Francoise Delbecq[2], Philippe Sautet[2], Yvette Jugnet[3], Conrad Becker[4], and Klaus Wandelt[1] — [1]Inst. für Phys. und Theo. Chemie, Uni. Bonn — [2]Lab. de Chimie, Ecole Normale Supérieure de Lyon — [3]Inst. de Rech. sur la Catalyse, Villeurbanne — [4]CINAM, Aix-Marseille Uni.

The prediction of reaction mechanisms consisting of complex networks of elementary steps and the identification of corresponding intermediates are major challenges in multifunctional catalysis and surface chemistry. We demonstrate that this difficulty can be overcome by tracking the temperature dependent formation of the intermediates and identifying the decomposition pathways in the case prenal, an α,β-unsaturated aldehyde, on the Pt(111) model catalyst surface by combining vibrational spectroscopy, temperature-programmed reaction spectroscopy and DFT analysis. Desorption states of H_2 (280 K, 410 K and 473 K) and CO (414 K) suggest that the loss of H and the CO functions are among the first elementary steps. HREELS performed after annealing to specific temperatures results in spectra which can be assigned to several subsequently formed surface intermediates with the help of complementary theoretical vibrational analysis. The most likely reaction pathway obtained from DFT for intial decomposition occurs from the strongly bonded prenal adsorption structures via an dehydro-η^3-triσ(CCC)-H1 intermediate to the η^1-isobutylidyne species at high temperatures.

O 60.109 Wed 17:30 P4

Monitoring and adjusting the temperature of ultra-thin metal catalysts *in situ* — •Ievgen Nedrygailov, Kevin Stella, Cordelia Soostmeyer, Eckart Hasselbrink, and Detlef Diesing — Fakultät für Chemie, Universität Duisburg-Essen, D-45117 Essen, Germany

Despite the widespread usage of metal thin films in surface science experiments, the *in situ* measurement of the thin film temperature using traditional methods remains challenging. To address this problem the technique of adjusting and measuring the temperature of metal thin films by passing an electric current through them is proposed. The current flowing directly through the thin film serves for both: Joule heating of the thin film and monitoring the temperature using the temperature dependence of the thin film resistance. Direct heating is used to clean the platinum thin films (15-20 nm) on top of the silicon based electronic devices under ultra high vacuum conditions. Temperature programmed desorption of water and CO molecules from the polycrystalline platinum surface of the devices is studied to characterize the chemical state of the device surface.

O 60.110 Wed 17:30 P4

Photoinduced CO oxidation by association with defect-bound atomic oxygen on thin MgO films — •Philipp Giese, Harald Kirsch, Christian Frischkorn, and Martin Wolf — Fritz-Haber-Institut, Abt. Physikalische Chemie, Faradayweg 4-6, 14195 Berlin

As a prototype system for chemistry of defect-bound atomic oxygen on MgO, the CO oxidation has been studied. Atomic oxygen species were generated by photoinduced N_2O dissociation on thin MgO films grown on Ag(100). CO oxidation was studied as a function of photon exposure and initial CO coverage. The reaction products were studied by temperature programmed desorption spectroscopy (TPD). Carbon monoxide was co-adsorbed on films with atomic oxygen (10^{13} atoms/cm^2) at 20 K. If the coadsorbate is irradiated with UV light (5 eV), a CO_2 desorption peak at about 300 K appears, accompanied by a depletion of the atomic oxygen. The amount of CO oxidation increases with photon exposure and stops when the atomic oxygen is completely depleted. However, this process does not happen by irradiation of CO without previous atomic oxygen preparation, thus a direct reaction between the adsorbed CO molecules can be excluded. In addition, without UV excitation of the coadsorbate no reaction occurs either, revealing that the activation barrier for the CO oxidation on MgO surfaces is too high for a thermally activated reaction.

O 60.111 Wed 17:30 P4

Selforganization in ultrathin, K-promoted V-oxide layers on Rh(111) during the O2+H2 reaction. — •Martin Hesse, Fernando Sotoca Usina, and Ronald Imbihl — Institut für Physikalische Chemie und Elektrochemie, Leibniz-Universität Hannover, Callinstr. 3 - 3a, D-30167 Hannover, Germany

Alkali metals (AM's) promoted V-oxides play an important role as catalysts in a number of industrial partial oxidation reactions. As catalytic model system we studied the behaviour of K-promoted ultrathin V-oxide films (0.25 ML of V) on Rh(111) in the O2+H2 reaction using photoemission electron microscopy (PEEM) as spatially resolving method. With LEED, ordered phases of the ternary system V+K-O were detected. Similar to the unpromoted system stationary patterns develop under reaction conditions formed by stripes of V+O+K surrounded by bare Rh(111) surface. In addition, we observe also dynamic chemical wave patterns leading to K redistribution and enrichment of K at interfaces. The main effect of the addition of the AM is that it makes the VOx system very dynamic as evidenced by violent chemical turbulence. Tentatively, the stationary patterns were explained as being a consequence of reactive phase separation.

O 60.112 Wed 17:30 P4

Chemical trends in the metal-substrate interaction for adsorbed Pt atoms — •Chong Gao and Axel Gross — Institut für Theoretische Chemie, Universität Ulm, D-89069 Ulm, Germany

Catalysts typically consist of small metal particles deposited on a oxide substrate. The interaction of the support with the metal particles can play quite a significant role for the catalytic activity of the particles. Using density functional theory, we have addressed the catalytic activity of small supported Pt clusters with up to 6 atoms. As the support, we considered Au, Ru, Si and TiO_2 substrates in order to derive chemical trends from metals to semiconductors and oxides. The electronic structure of the adsorbed Pt atoms and calculated CO adsorption energies on these metal-support systems are used as a probe of the chemical reactivity. The results are compared to recent results of the local reactivity of surface alloy systems [1,2]. In general, we find a strong anti-correlation between the binding energies of the Pt clusters on the substrates and the CO adsorption energies on the metal clusters.

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O 60.113 Wed 17:30 P4

Cluster chemistry in the gas phase: a new approach for laser spectroscopy — •Kathrin Lange, Bradley Robert Visser, Martin Tschurl, Ulrich Kaspar Heiz, and Ulrich Boesl-von Grafenstein — Lichtenbergstr. 4, 85748 Garching

The characterization and determination of organic molecules which exist as enantiomers or diastereomers are today of crucial importance especially for the pharmaceutical industry. It has been shown that chiral metal clusters are able to catalyse one form of the enantiomer or diastereomer [1].

The aim of the present work is to build a new setup to produce chiral metal clusters and to implement the idea of separating enantiomers by laser spectroscopy.

The chiral metal clusters will be produced by a laser vaporisation cluster source [2] and reacted with target organic species in the gas phase.

In this work we will describe the setup of our apparatus and a number of laser spectroscopy techniques (REMPI, CD Spectroscopy) in detail. These techniques will be used to induce photochemical processes in the metal cluster and molecule complexes to achieve enantiomeric or diastereomeric sensitive separation and detection [3].

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O 60.114 Wed 17:30 P4

Experimental setup of a time-of-flight mass spectrometer for reaction product detection in heterogeneous catalysis — •Andreas Winbauer, Martin Tschurl, Josef Kiermaier, and Ulrich Kaspar Heiz — Lichtenbergstraße 4, 85748 Garching

Mass spectrometry is a very powerful analytical tool for the study of heterogeneous catalysis. It's often used to study reaction processes by analyzing the reaction products, both in a qualitative and in a quantitative way.

Often mass spectrometers work by using electron impact ionization, where a discrimination between isomers is difficult to achieve. Their fragmentation patterns must differ to a large extent.

A powerful and soft method for selective ionization is REMPI (Resonant Enhanced Multiphoton Ionization). In this technique a laser of specific wavelength is employed to ionize only one isomer through resonant intermediate states. Other isomers cannot be ionized as they are non resonant at the energy used.

For the study of catalytic reactions on metal clusters supported on single crystal surfaces under UHV conditions a new experimental setup was built. For the spectroscopic studies custom ion optics were designed to incorporate the crystal support and enable future desorption-ionization studies.

In this work we will present our experimental setup, in which we combine time of flight mass spectrometry with resonance enhanced multiphoton ionization. Furthermore we will show first experimental results and possible applications for our setup.

O 60.115 Wed 17:30 P4

First-Principles Calculations of Hydrogen Generation Due to Water Splitting on Polar GaN Surface — •Po-Tuan Chen — Physics Department, Osnabrueck, Germany

We present the chemical reactions leading to hydrogen gas generation via water splitting on polar GaN surfaces, which can be a significant source of renewable energy. To build an understanding at the atomic level of the activations afforded by the GaN (0001) and (000-1) surfaces, we determine the reaction mechanism of hydrogen generation on the polar faces using density functional theory calculations. The calculation results show that the first H splitting from water can occur with ground-state electronic structures; the barriers of H2O splitting are 0.10 and 0.34 eV on the Ga-face and the N-face, respectively. However, the second H splitting requires huge energies of 1.42 and 1.73 eV, respectively, on the Ga-face and the N-face. Although the polar GaN surface can catalyze the first hydrogen splitting from water, we suggest that photoexcitation should be necessary for the second splitting.

O 60.116 Wed 17:30 P4

In-situ spectroscopic investigation of adsorption and reaction of pyridine molecules on Pt surfaces — •Claudia Wöckel[1], Kristina Fischer[1], Andre Dorsch[1], Sandra Wickert[1], Regine Streber[2], Hans-Peter Steinrück[2], and Reinhard Denecke[1] — [1]Wilhelm-Ostwald-Institut, Universität Leipzig, Linnestr. 2, 04103 Leipzig, Germany — [2]Physikalische Chemie II, Department Chemie, Friedrich-Alexander-Universität Erlangen-Nürnberg, Germany

Using high-resolution and time-dependent XPS adsorption and reaction processes can be followed in-situ. We are applying this method to pyridine molecules adsorbed on Pt. Using a regularly stepped Pt(355) and a Pt(111) surface, C 1s and N 1s core level data are recorded during adsorption at various temperatures. As additional parameter, the free Pt terrace width is varied by deposition of Ag atoms on the surface, forming rows along the step edges at 300 K. Temperature-programmed XPS allows to follow the thermal reaction of the adsorbed species. The experiments have been performed at BESSY II in Berlin.

In line with literature reports about a temperature- and coverage-dependent reorientation from flat to upright[1], we observe changes in the core level binding energies and intensities during the uptake. Upon heating the strong N 1s feature observed at 200K is transformed into a contribution at higher binding energy. This is accompanied by respective changes in the C 1s data, suggesting again temperature- and coverage-dependent changes, here towards α -pyridyl. Supported by BMBF (05 ES3XBA/5).
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O 60.117 Wed 17:30 P4

Solar2Fuel: XPS and TPD characterization of functionalized TiO_2 surfaces for photocatalytic reduction of CO_2 — •Florian Staier, Michael Grunze, and Michael Zharnikov — Angewandte Physikalische Chemie, Universität Heidelberg, INF 253, 69120 Heidelberg

The handling of CO_2 produced by industrial installations and power plants has become a very important environmental issue nowadays because of it's generally accepted impact on the green house effect. In this context, a storage of CO_2 or its conversation to fuel or useful chemicals are highly desirable. Along these lines, the solar2fuel project, funded by BMBF, aims on photocatalytic conversion of CO_2 to methanol with a sufficient quantum efficiency which can justify and make rentable an industrial realization of the process. As the primary catalytic system TiO_2 nanoparticle powder coatings are used. These particles are doped with metals to enhance their catalytic activity and functionalized with specially designed dyes which promote photocatalytic reaction and move the absorption spectrum from UV (characteristic of TiO_2) to the visible range. We present first results on characterization of these catalytic systems by several complimentary techniques as well as on temperature-programmed-desorption of CO_2 and methanol from these functionalized surfaces.

O 60.118 Wed 17:30 P4

Gold-containing model catalysts studied with in-situ XPS — •Martina Pistor, Karifala Dumbuya, Ole Lytken, Lorenz Ringel, Jörg Michael Gottfried, and Hans-Peter Steinrück — Universität Erlangen-Nürnberg, Lehrstuhl für Physikalische Chemie II

The noble metal gold, if supported as nanoparticles on oxides such as TiO_2, is a promising catalyst for many oxidation reactions. Up to now, it is still debated why gold, which is not active as a bulk material, becomes active in the dispersed state (with optimum particle sizes 2-5 nm). Explanations include quantum size effects, low-coordinated gold atoms, the substrate/gold perimeter interface and anionic as well as cationic gold species. Using in-situ X-ray photoelectron spectroscopy (XPS), we have studied various gold-based powder catalysts and model catalysts, both in the presence of CO, O_2 and propene and under ultrahigh vacuum conditions. The studied systems include gold nanoparticles supported on $TiO_2(110)$ and titania nanoparticles supported on Au(111) as well as reference powder catalysts. Depending on the experimental conditions, especially the oxygen partial pressure, the intrinsic catalytic activity of the system is superimposed by X-ray-induced effects such as the formation of gold oxide. On the basis of these beam damage effects, we will discuss possible limitations of in-situ XPS. This work is supported by the DFG through grant GO 1812/1 and by the Cluster of Excellence "Engineering of Advanced Materials" granted to the Universität Erlangen-Nürnberg.

O 60.119 Wed 17:30 P4

Investigation of new Catalysts for PEM Fuel Cells — •Roy Mbua[1], Ulricke Kramm[2], Klaus Mueller[1], Matthias Richter[1], Karsten Henkel[1], Ioanna Paloumpa[1], and Dieter Schmeisser[1] — [1]Brandenburgische Technische Universitaet Cottbus, Angewandte Physik/Sensorik, K. - Wachsmann-Allee 1, 03046 Cottbus — [2]Helmholtz-Zentrum für Materialien und Energie, Berlin

Increasing green house emissions amplify global warming concerns worldwide. Fuel cells, based on polymer electrolyte membranes (PEM) are part of the solution to this issue. We aim at developing and testing new catalysts for fuel cells. Platinum catalysts perform best in PEM fuel cells to date but they are very expensive. For fuel cells to be perfectly applicable and economically affordable, an alternative catalyst with similar or even greater efficiency should be developed.

Metal phthalocyanines are known to be good oxygen reduction catalysts and are associated with high electron transfer properties. We investigated Cobalt Phthalocyanine in its pure state mixed with Carbon Black (CoPc:Carbon Black=1:9) untreated and also after a treatment in N2 at several temperatures, up to 1000°C for 30 minutes.

Results of XPS and EDX analyses reveal that the treatment at higher temperatures causes a rearrangement in the chemical states of Co, N and C atoms. Furthermore, results of cycling voltammetry (CV) analysis reveal that CoPc treated in N2 at 800°C exhibited a higher current density, in conclusion, a higher catalytic activity than the untreated CoPc.

O 60.120 Wed 17:30 P4

Methanol synthesis over binary Cu/ZnO surfaces: exploration of energy surfaces for determining adsorption sites for CO_2 — •luis martínez suárez[1], johannes frenzel[1], bernd meyer[2], and dominik marx[1] — [1]Ruhr University Bochum, Theoretical Chemistry, Bochum, Germany — [2]Interdisziplinäres Centrum für Molekulare Materialien (ICMM) and ComputerChemieCentrum (CCC), Department Chemie und Pharmazie, Friedrich-Alexander-Universität Erlangen-Nürnberg, Erlangen, Germany

Methanol is synthesized from syngas over Cu/ZnO in a heterogeneous catalytic process with CO_2 as carbon source. Atomistic insight into the strong metal substrate interaction (SMSI) effect in Cu/ZnO catalysts has been obtained in a static picture. Calculations of surface phase diagrams by *ab initio*-thermodynamics determined realistic structures of a small Cu_8 cluster on $ZnO(000\bar{1})$ in a hydrogen atmosphere with temperature and pressure conditions as required in the industrial process. These structures are stabilized by the interplay of structural changes as a result of redox properties of the syngas with realistic saturation of the catalyst surface by hydrogen interacting with defect sites. Herein the global energy landscape of the CO_2 reactant over several thermodynamically relevant catalyst surface structures is explored with spatial resolution employing density functional theory. After having identified all possible adsorption sites on the complex Cu/ZnO surfaces the adsorption modes of the complexes are refined investigating their individual structures.

O 60.121 Wed 17:30 P4

Ceria promoted CO oxidation on Pt(111): Oxygen-spillover and active border concept — Stefan Becker[1], •Kathleen Müller[1], Rafal Wróbel[1,2], and Helmut Weiss[1] — [1]Otto-von-Guericke-University Magdeburg, Institute of Chemistry, Universitätsplatz 2, D-39106 Magdeburg, Germany — [2]West Pomeranian University of Technology, Institute of Chemical and Environmental Engineering, Pulaskiego 10, 70-322 Szczecin, Poland

The influence of CeO_x nanoformations on the heterogeneously catalysed CO oxidation above the bistable region was investigated. A well-defined CeO_x/Pt(111) model catalytic system with homogeneous 2D islands has been produced by evaporating Ce on Pt(111) in oxygen ($5\cdot10^{-8}$ mbar). The clean Pt(111) surface was characterised by XPS, LEED and STM and the inverted model catalysts CeO_x/Pt(111) by XPS, STM and CO titration. The temperature and pressure dependency of the reaction rate was analysed via mass spectrometry. An enhanced reactivity was observed for a surface covered with CeO_x islands as compared to clean Pt(111). The CeO_x leads to a change in the adsorption characteristics for oxygen as well as for carbon monoxide (promotional effects). An active border concept for oxygen and carbon monoxide and a spillover mechanism for oxygen are suggested.

O 60.122 Wed 17:30 P4

Hydrogen adsorption on $RuO_2(110)$ — •Bianca Eifert[1], Christian Heiliger[1], Jan Philipp Hofmann[2], Herbert Over[2], and Ari Paavo Seitsonen[3] — [1]Physikalisches Institut, Justus Liebig University Giessen, D-35392, Germany — [2]Physikalisch-Chemisches Institut, Justus Liebig University Giessen, D-35392, Germany — [3]Physikalisch-Chemisches Institut, University of Zurich, CH-8057, Switzerland

Complementary to experimental work, density functional theory calculations are utilized to gain a deeper insight into the adsorption and insertion behavior of hydrogen and water species on the $RuO_2(110)$ surface at an atomic level. This is important for an improved understanding of RuO_2 as a model and real catalyst system in reactions spanning from oxide-catalyzed dehydrogenation to a wide range of electrochemical reactions.

[1] M. Knapp, D. Crihan, A. P. Seitsonen, E. Lundgren, A. Resta, J. N. Andersen and H. Over, J. Phys. Chem. C 111, 5363 (2007)

O 60.123 Wed 17:30 P4

Spectroscopic and microscopic characterization of potential catalysts for the hydrogenation of CO2 — •David Hoffmannbeck, Matthias Richter, Matthias Städter, Ioanna Paloumpa, Karsten Henkel, and Dieter Schmeisser — BTU-Cottbus, LS Angewandte Physik II - Sensorik K.-Wachsmann-Allee 1, D-03046 Cottbus

The reduction of CO2 emissions is a general demand of the society in order to avoid irreversible climate changes. We are investigating potential catalysts for the hydrogenation of CO2 in particular for its application in the so called oxyfuel combustion process.

In order to understand the catalytic behavior of the investigated materials we use the techniques X-Ray Photoemission (XPS) and -absorption (XAS) Spectroscopy as well as X-Ray Diffraction (XRD) and Scanning Electron Microscopy (SEM). The prospective of our work is to figure out the electronic and structural properties of the material and to optimize proper catalysts or design new ones for best catalytic activity. Beside the spectro-microscopic investigations the catalysts are tested under Sabatier reaction conditions in terms of activity, stability and sensitivity against poisoning. In our preliminary work we constructed a Sabatier reactor system with analytical parts based on infrared absorption and mass spectroscopy modules. First spectroscopic and catalytic results achieved on a commercially available Ru/Al2O3 catalyst will be presented.

O 60.124 Wed 17:30 P4

Reduction of Thin NiO Films by Carbon Monoxide — •Oliver Höfert[1], Wei Zhao[1], Karin Gotterbarm[1], Andreas Bayer[1], Junfa Zhu[2], Christian Papp[1], and Hans-Peter Steinrück[1] — [1]Lehrstuhl für Physikalische Chemie II, Universität Erlangen-Nürnberg, Egerlandstr. 3, 91058 Erlangen — [2]National Synchrotron Radiation Laboratory, University of Science and Technology of China, Hefei 230029, People's Republic of China

NiO is an important material in heterogeneous photocatalysis for degradation of azodyes [1] or water splitting [2]. We studied the reactivity of different thin NiO films on Pd(100) towards CO by in situ XPS applying synchrotron radiation at BESSY II. Our data shows that closed and well ordered NiO films with less than 2 ML are indeed reduced to metallic Ni by exposure to CO above 400 K. The reduction of NiO by CO is chemically reversible as was shown by subsequent reoxidation of the metallic Ni by O_2. The influence of Pd to the reaction could be excluded. Our kinetic investigations revealed a coupling of diffusion and reaction in the reduction process. For both mechanisms we determined the activation energy. Additionally, the reoxidized films showed a different behaviour and could not be fully reduced due to structural changes.

This work was supported by BMBF (05 ES3XBA/5) and the DFG through the Cluster of Excellence "Engineering of Advanced Materials".

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[2] Kato, H. et al (2001),J. Phys. Chem. B, 105 (19)

O 60.125 Wed 17:30 P4

Nucleation, growth and thermal behaviour of Au and Cu-clusters on ZnO — •Dietmar Rother, Martin Kroll, and Ulrich Köhler — Institut für Experimentalphysik IV / AG Oberflächenphysik, Ruhr-Universität Bochum

The growth of Au and Cu on $ZnO(10\bar{1}0)$ single crystal surfaces was studied as a first step to understand complex catalytically active systems, often consisting of small metal clusters on metal oxide surfaces. Thermal evolution of Au and Cu clusters on $ZnO(10\bar{1}0)$ was studied in-situ with STM at elevated temperature. Au and Cu were deposited using MBE sources at room temperature. On the mixed terminated $ZnO(10\bar{1}0)$ surface separated Cu clusters are formed at room temperature. A partial entrenching of Cu into the ZnO substrate at elevated temperature of $T > 670K$ was found and points to a reaction of the Cu-clusters with the ZnO support. Au on ZnO shows a different behaviour: Annealing RT-deposited Au-clusters to comparable temperatures shows no reaction of Au-Clusters with the ZnO-substrate. After the initial coarsening, Au on ZnO shows no changes while scanning in-situ at elevated temperature up to 770K on a time scale of hours. The minimum cluster density is already reached at 420K. The behaviour on $ZnO(10\bar{1}0)$ is compared to other ZnO surfaces and to $TiO_2(110)$.

O 60.126 Wed 17:30 P4

CO oxidation reaction on thin mesoporous Au/TiO_2 layers — •Matthias Roos[1], Dominique Böcking[2], Kwabena Offeh Gyimah[1], Gabriela Kucerova[1], Joachim Bansmann[1], Nicola Hüsing[2,3], and R. Jürgen Behm[1] — [1]Institute of Surface Chemistry and Catalysis, Ulm University, D-89069, Germany — [2]Institut für Anorganische Chemie II, Ulm University, D-89069, Germany — [3]Abteilung Materialchemie, Universität Salzburg, A-5020, Austria

The catalytic properties of thin homogeneous layers of mesoporous Au/TiO_2 [1] deposited onto silicon substrates to study the CO oxidation reaction was investigated. The mesoporous TiO_2 layers are fabricated using a sol-gel process followed by the precipitation-deposition of Au nanoparticles. The measurements on the catalytic activity were performed in a vacuum system using a quadrupole mass spectrometer which allows to collect the reaction gases very close to a specific region on the surface [2]. Using this setup, the activation energy and the reaction orders of CO and O_2 were measured and compared to respective measurements on planar Au/TiO_2(110) model catalysts and standard Au/TiO2 powder catalysts. Furthermore, the catalytic stability and the deactivation behaviour of the mesoporous Au/TiO_2 films was studied. To test the accessibility by reaction gases of deeper lying regions within the catalytically active films, the thickness of the TiO_2 layers was varied for different measurements.

[1] Y. Denkwitz et al., Appl. Cat. B 91 (2009) 470

[2] M. Roos et al., J. Chem. Phys. 133 (2010) 094504

O 60.127 Wed 17:30 P4

HR-EELS studies on zinc oxide powders samples — •Sebastian Frey, Martin Kroll, Dietmar Rother, and Ulrich Köhler — Ruhr-Universität Bochum, Deutschland

Zinc oxide powders are an important catalyst for a number of organic reactions, e.g. the synthesis of methanol. Corresponding surface science studies, on the other hand, mainly deal with single crystalline surfaces. Since this situation is quite different from a real catalyst, this work concentrates on the vibrational spectroscopy analysis of ZnO powder samples using high resolution electron energy loss spectroscopy (HR-EELS) to deliver supplementary information to the existing single crystal studies. At first we present different approaches to fix the ZnO powder on a gold substrate for vacuum treatment including XRD and SEM-analysis. Finally, the results of our HR-EELS measurements of the ZnO powder samples exposed to different organic molecules like methanol and formic acid are displayed in comparison to the (0001), (000-1) and (10-10) single crystal surfaces.