O 55: Poster Session III - MA 141/144 (Methods: Atomic and Electronic Structure; Particles and Clusters; Heterogeneous Catalysis; Semiconductor Substrates: Epitaxy and Growth+Adsorption+Clean Surfaces+Solid-Liquid Interfaces; Oxides and Insulators: Solid-Liquid Interfaces+Epitaxy and Growth; Phase Transitions; Metal Substrates: Adsorption of Inorganic Molecules+Epitaxy and Growth; Surface Chemical Reactions; Bimetallic Nanosystems: Tuning Physical and Chemical Properties; Oxides and insulators: Adsorption; Organic, polymeric, biomolecular films; etc.)

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

O 55.1 Wed 18:30 Poster F

Lagrange Functions for Electronic Structure Calculations — •Christine Broelemann, Peter Krüger, and Johannes Pollmann — Institut für Festkörpertheorie, WWU Münster

We have examined the efficiency of Lagrange functions, as compared to plane waves, for calculating electronic properties of atoms, molecules, solids and surfaces within density functional theory. Real space Lagrange functions provide – like plane waves – an orthonormal and complete basis set. Our results show that the efficiency of both methods is the same for bulk calculations. In contrast to the plane wave method, however, it is possible within the Lagrange function method to conveniently adapt the real space grid for a given system. Taking advantage of this fact, the number of grid points can be reduced in vacuum regions, in particular. Lagrange functions can be used for periodic as well as for finite systems alike. It turns out that they are particularly useful for electronic structure calculations of charged systems. Problems occuring within the plane wave method due to long-range Coulomb interactions can be avoided that way.

O 55.2 Wed 18:30 Poster F

Combined direct and inverse photoemission experiment: A thorough characterization of energy, angle and spin resolution — •Michael Budke, Tobias Allmers, and Markus Donath — Physikalisches Institut, WWU Münster, Wilhelm-Klemm-Str. 10, 48149 Münster

We present an experimental setup that combines spin- and angle-resolved direct (PE) and inverse photoemission (IPE) in one UHV chamber [1], allowing measurements of the spin-resolved electronic structure below and above the Fermi level of the same sample preparation. The system for PE operates with a gas discharge lamp and an electron analyzer combined with a SPLEED detector. Our spectrometer for IPE [2] is home-made and comprises a spin-polarized electron source and energy-selective Geiger-Müller counters for photon detection. The achievable energy resolutions are better than 50 meV for PE and better than 200 meV for IPE. The latter value states an improvement of a factor of two compared to other state-of-the-art IPE spectrometers. The high energy resolution makes the setup especially suitable for studies in the close vincinity of the Fermi level.

In this contribution, the two spectrometers are characterized concerning energy and angle resolution by means of the Fermi-level crossing of the L-gap surface state on Cu(111). Spin-resolved measurements of Co/Cu(100) will be presented combined with a characterization of the spin polarization of the electron beam and the Sherman function of the SPLEED detector. [1] M. Budke *et al.*, RSI **78**, (in press).

[2] M. Budke *et al.*, RSI **78**, 083903 (2007).

O 55.3 Wed 18:30 Poster F

Two-photon Photoemission spectroscopy of the clean and alkali-doped 1T-TiSe$_2$ transition-metal dichalcogenide — •Martin Wiesenmayer, Jens Buck, Timm Rohwer, Kai Rossnagel, Lutz Kipp, and Michael Bauer — Institut für Experimentelle und Angewandte Physik, Universität Kiel, 24098 Kiel, Germany

The transition-metal dichalcogenide 1T-TiSe$_2$ has attracted considerable attention in the recent past due to a structural phase transition at $T \approx 200$ K accompanied by the formation of a charge density wave (CDW) state. In a two-photon photoemission (2PPE) study we investigated the electron excitation spectra of these two phases in the vicinity of the Γ point of the Brillouin zone and their modification due to the adsorption and intercalation of different alkali species. We are able to identify a characteristic excitation band as well as phase- and intercalation specific modifications in the vicinity of the Fermi edge. Our experiments are furthermore supported by time-resolved 2PPE measurements addressing the ultrafast decay dynamics of the electron excitations. Our results will be discussed under consideration of corresponding results from past photoemission and inverse photoemission studies.

O 55.4 Wed 18:30 Poster F

Atomically Resolved Kelvin Probe Force Microscopy Measurements Analysed by a nc-AFM simulator — •Thilo Glatzel[1] and Laurent Nony[2] — [1]Department of Physics, University of Basel, Klingelbergstr. 82, 4056 Basel, Switzerland — [2]L2MP, UMR CNRS 6137, Univ. d'Aix-Marseille III, 13397 Marseille Cedex 20, France

Amplitude-Modulation Kelvin probe force microscopy (AM-KPFM) experiments have shown frequently atomically resolved contact potential difference (CPD) images. In this work, we report numerical investigations performed with a modified scheme of our nc-AFM simulator [1], with the goal to address the origin of such a contrast.

For that purpose, the core of our simulator has been modified to mimic the AM-KPFM setup. In AM-KPFM, the bias voltage that is applied between the tip and the surface is modulated at a frequency that matches the one of the second eigenmode of the cantilever. The long-range, short-range and electrostatic forces used to describe the system are derived from analytical expressions. The coupling between the first and the second eigenmodes of the cantilever will also be discussed.

Our results reproduce the experimental observations, thus showing that atomic variations of the CPD that are observed experimentally very likely reveal the atomic variations of the electrostatic potential at the surface of the ionic crystal.

[1] L. Nony et al., Phys Rev B 74, 235439 (2006).

O 55.5 Wed 18:30 Poster F

Photoelectron Spectroscopy at FLASH: Limits and Perspectives — •Martin Marczynski-Bühlow, Matthias Kalläne, Stefan Hellmann, Sabrina Lang, Claas Thede, Tim Riedel, Sönke Harm, Kai Rossnagel, and Lutz Kipp — Institut für Experimentelle und Angewandte Physik, Universität Kiel, D-24098

The Free Electron Laser in Hamburg (FLASH) produces very brilliant, ultrashort, and coherent photon pulses in the VUV regime.

Employing high-intensity monochromatic VUV–pulses ($h\nu$ = 115.5 eV, FEL 3^{rd} harmonic) delivered by the PG2 beamline of FLASH we performed angle resolved as well as core–level photoelectron spectroscopy (PES) on the transition metal dichalcogenide 1T–TaS$_2$ in the Mott insulating phase (T = 140 K). For high photon intensities strong space charge (SCE) effects have been observed. To determine the limit where PES is still feasible, the measurements are compared with simulations of SCEs based on the Barnes & Hut Treecode Algorithm originally developed for simulating planetary movements. Furthermore, the perspectives of PES with FEL light in terms of time-resolved pump-probe experiments, spatially and angularly resolved PES with photon sieves [1], and the influence of high photon intensities on the momentum resolved electronic structure as well as on the photoemission process itself will be illustrated.

This work is supported by the Innovationsfond des Landes Schleswig-Holstein.

[1] L. Kipp, M. Skibowski, R. L. Johnson, R. Berndt, R. Adelung, S. Harm and R. Seemann, Nature 414, 184 (2001).

O 55.6 Wed 18:30 Poster F

Electronic structure of the non-polar GaN($1\bar{1}00$) surface — •Marco Bertelli[1], Peter Löptien[1], Jörg Malindretos[1], Martin Wenderoth[1], Rainer G. Ulbrich[1], Angela Rizzi[1], Maria Clelia Righi[2], and Alessandra Catellani[2,3] — [1]IV. Physikalisches Institut and Virtual Institute of Spin Electronics (VISel), Georg-August Universität Göttingen, D-37077 Göttingen, Germany — [2]CNR-INFM

National Center on nanoStructures and bioSystems at Surfaces (S^3) and Dipartimento di Fisica, Università di Modena e Reggio Emilia, I-41100 Modena, Italy — [3]CNR-IMEM, Parco Area delle Scienze, 37A, I-43010 Parma, and (S^3), Italy

Cross-section scanning tunneling microscopy (STM) and scanning tunneling spectroscopy (STS) have been performed on the non-polar $GaN(1\bar{1}00)$ surface (m-plane).
The unintentionally n-doped GaN(0001) samples were thinned down to $\sim 100\ \mu m$, cleaved along the m-plane in ultra high vacuum and measured in-situ by STM at room temperature. The experimental empty state topographies collected with sample bias from +2.9 V to +4.0 V show an unreconstructed surface.
First principle DFT-LDA calculations of the surface electronic properties were performed. In agreement with experiment, the calculations predict a relaxed surface but no reconstruction. Two surface bands appear inside the semiconductor band gap at the borders of the surface Brillouin zone, one empty band localized on the Ga-atoms and one filled band on the N-atoms. Up to now this theoretical prediction has not been confirmed by the STS experiment.

O 55.7 Wed 18:30 Poster F

Electronic structure of transition metal dichalcogenide misfit compounds — •Matthias Kalläne, Kai Rossnagel, and Lutz Kipp — Institute for Experimental and Applied Physics, University of Kiel, D-24098 Kiel, Germany

The incommensurate layered transition metal dichalcogenide (TMDC) misfit compounds are composed of alternatingly stacked slabs of hexagonally ordered TMDCs and cubic monochalcogenides, leading to a lattice mismatch in one direction parallel to the surface. In spite of the incommensurability, however, the slabs are in a very high stacking order perpendicular to the layers and the crystals show a high stability. In order to investigate the bonding perpendicular to the layers and the influence of the incommensurability on the electronic structure we have employed angle–resolved photoelectron spectroscopy on different TMDC misfit compounds. By studying the electronic structure at the Fermi surface, we could directly observe a charge transfer to the TMDC layers, while the electronic band dispersion perpendicular to the layers was found to be negligible. Therefore, the interlayer bonding seems to be dominated by ionic contributions, similar to intercalated TMDC compounds. To reveal possible incommensurability effects we have analyzed the band dispersion in different crystal directions and have found signatures of both subsystems in the electronic structure.

The photoemission experiments were carried out at the ALS in Berkeley. Work at the University of Kiel is supported by DFG Forschergruppe FOR 353.

O 55.8 Wed 18:30 Poster F

Plasma Electrochemistry in Ionic Liquids: Deposition of Copper-Nanoparticles — •Mareike Brettholle[1], Oliver Höfft[1], Sebastian Mathes[2], Sherif Zein El Abedin[1], and Frank Endres[1] — [1]Institut für Metallurgie, TU Clausthal, 38678 Clausthal-Zellerfeld, Germany — [2]Institut für Physik und Physikalische Technologien, TU Clausthal, 38678 Clausthal-Zellerfeld, Germany

Ionic liquids 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 their low vapour pressure low pressure plasmas can easily be applied. The idea is to use the free electrons of the plasma to reduce the dissolved metal atoms in the liquid and generate this way the metal particles. In ionic liquids this principle was utilized recently by Meiss et al. [2]. Here we present our results using an argon plasma as electrode for the electrochemical deposition of copper nanoparticles (5-100 nm) from a Cu solution in 1-butyl-1-methylpyrrolidinium bis(trifluoromethylsulfonyl)amide [BMP]Tf2N and 1-ethyl-3-methylimidazolium bis(trifluoromethylsulfonyl)amide [EMIm]Tf2N. XPS, REM, EDX and Dynamic light scattering (DLS) were used to characterise the particles. [1] F. Endres, S. Zein El Abedin , Phys. Chem. Chem. Phys., 8 (2006) 2101; [2] S. A. Meiss, M. Rohnke, L. Kienle, S. Zein El Abedin, F. Endres and Jürgen Janek, Chem. Phys. Chem., 8 (2007) 50

O 55.9 Wed 18:30 Poster F

Fluorescence in the presence of metallic nanoparticles — •Philipp Reichenbach, Thomas Härtling, and Lukas M. Eng — Institut für Angewandte Photophysik, Technische Universität Dresden, 01062 Dresden, Germany

When fluorescent molecules (being excited by incident light) are placed in the neighbourhood of metallic nanoparticles, big changes of the observed fluorescence rate can occur. On the one hand, the excitation of the molecule can be strongly enhanced as a result of the scattering of the exciting light at the nanoparticle. On the other hand, part of the fluorescent radiation will be absorbed by the nanoparticle. The dependence of these two factors from the system parameters like excitation wavelength, relative position of molecule and particle as well as surrounding medium was investigated. As a result, we are able to clearly identify set-ups for which enhanced fluorescence microscopy/spectroscopy becomes feasible.

O 55.10 Wed 18:30 Poster F

***Ab initio* study on electronic and optical properties of silicon nanocrystals embedded in SiO_2 matrices** — •Kaori Seino[1], Friedhelm Bechstedt[1], and Peter Kroll[2] — [1]Institut für Festkörpertheorie und -optik, Friedrich-Schiller-Universität, Jena, Germany — [2]Department of Chemistry and Biochemistry, University of Texas at Arlington, Arlington, TX, USA

Although a high control of size and arrangement of Si nanocrystals (NCs) embedded in a SiO_2 can be obtained experimentally, theoretical works for Si NCs embedded in SiO_2 are limited. We study electronic and optical properties for Si NCs embedded in an amorphous SiO_2 matrix by means of first-principles calculations. Many theoretical results are available for hydrogenated Si NCs. We investigate the dependence on the diameter of the Si NCs, varying in the range from 0.8 to 1.6 nm. The calculations for optical properties have been widely performed within the independent-particle approximation. The results for Si NCs embedded in SiO_2 are compared with the corresponding results for hydrogenated Si NCs of the same size. The electronic confinement effects are much reduced with respect to crystallites without host. The optical absorption spectra show a pronounced peak somewhat blueshifted to the bulk E_2 peak similarly to measured spectra. We extract dielectric functions of the NC material from the calculated spectra using different effective-medium theories.

O 55.11 Wed 18:30 Poster F

W_nS_m-Clusters: Possible Building Blocks for New Nano-Materials? — Wilko Westhäuser[1], •Tobias Mangler[1], Tim Fischer[1], Sibylle Gemming[2], Gotthard Seifert[2], and Gerd Ganteför[1] — [1]University of Konstanz, Germany — [2]University of Dresden, Germany

Since bulk WS_2 forms layered structures similar to bulk graphite, this material might also built up stable cage-like fullerene structures. Large graphite-like structures (multiwall fullerenes, nanotubes) have been found in TEM experiments, but so far no anorganic fullerenes have been detected in the size regime of C_{60}. Thus, we started a search for WS_2 fullerenes by combining gas phase and deposition experiments. In the gas phase, we identified a variety of different structures (nanowires, nanoplatelets) in the size regime up to 30 metal atoms [1-3].

To investigate the suitability as building blocks, in a first attempt small size-selected W_nS_m-clusters were soft-landed on Ag- and Si-substrates at ultrahigh vacuum conditions. These samples were analysed via HREELS and XPS. The HREELS spectra are different for the different cluster sizes indicating that these clusters survived the soft-landing on the substrate and do not coalesce to bulk-like structures.
[1] S. Gemming, J. Tamuliene, G. Seifert, N. Bertram, Y.D. Kim and G. Ganteför, Appl. Phys. 82, 161 (2006)
[2] N. Bertram, Y.D. Kim, G. Ganteför, Q. Sun, P. Jena, J. Tamuliene and G. Seifert, Chem. Phys. Lett. 396, 341 (2004)
[3] N. Bertram, J. Cordes, Y.D. Kim, G. Ganteför, S. Gemming and G. Seifert, Chem. Phys. Lett. 418, 36 (2006)

O 55.12 Wed 18:30 Poster F

Crystal structure of transition metal oxide nano particles synthesized form ferritin — •Michael Krispin, Florian Sedlmeir, Aladin Ullrich, and Siegfried Horn — Lehrstuhl für Experimentalphysik II, Universität Augsburg, D-86135 Augsburg

We have investigated the local crystal structure of nanosized transition metal oxides by extended x-ray absorption fine structure (EXAFS). Iron and cobalt oxide nanoparticles of different diameters were produced by thermal treatment of horse spleen ferritin molecules and remineralized apo-ferritin molecules, respectively. The structure of these particles was compared to various iron oxide and ferrihydrite references as well as cobalt oxide references. The Fourier transformed (FT) EXAFS spectra of the iron oxide nanoparticles differ significantly from hematite and maghemite reference spectra and change systematically as a function of particle diameter, signalling a corresponding evolution of the structure. A possible explanation therefore is the mixture of hematite and maghemite phases in a core-shell model, in which the fraction of a γ-Fe_2O_3 like particle shell increases while the hematite core decreases with decreasing particle size. In the case of cobalt oxide nanoparticles we find good agreement of the FT EXAFS spectra to the Co_3O_4 reference.

O 55.13 Wed 18:30 Poster F

Interaction of slow highly charged ions with surfaces — •Christian Haake, Thorsten Peters, Andreas Wucher, and Marika Schleberger — Universität Duisburg-Essen, Lotharstraße 1, 47048 Duisburg, Germany

A new ion beam installation has been built to investigate the mechanisms of energy dissipation in a substrate after the impact of highly charged ions. First experiments at the TU Wien made successful use of metal-insulator-metal (MIM) junctions to measure electronic excitations in the irradiated metal [1]. These MIM-junctions offer the unique possibility to detect excitations below the work function which limits the external emission of electrons. In order to separate effects induced by either the kinetic or the potential energy of the projectile, both contributions need to be controlled independently. In the Vienna experiment the ions had medium charge states of q=1 up to to q=8 and kinetic energies of 400 eV to 12 keV. The new set-up offers higher charge states and is designed for kinetic energies of less than 100 eV/q. This will enable us to produce extremely slow highly charged ions. In addition, external electron emission as well as secondary and neutral mass spectrometry (SIMS/SNMS) will be used to follow the external pathways of energy dissipation.

[1] T. Peters, C. Haake, D. Diesing, D. Kovacs, A. Golczewski, G. Kowarik, F. Aumayr, A. Wucher and M. Schleberger, Hot electrons created by (rather) cold ions, submitted to Phys. Rev. Lett.

O 55.14 Wed 18:30 Poster F

Swift Heavy Ion (SHI) modification of Ag/Au-TiO_2 nanocomposite thin films prepared by co-sputtering. — Venkata Sai Kiran Chakravadhanula[1], Venkata Girish Kotnur[1], Amit Kulkarni[1], Yogendra Kumar Mishra[2], Devesh Kumar Avasthi[2], Dietmar Fink[3], Thomas Strunskus[1], •Vladimir Zaporojtchenko[1], and Franz Faupel[1] — [1]Chair for Multicomponent Materials, Institute for Materials Science, Christian-Albrechts University at Kiel, Kaiserstr. 2, Kiel, Germany, 24143. — [2]Inter University Accelerator Centre, New Delhi, India, 110067. — [3]Hahn Meitner Institut, Glienicker Str. 100, Berlin, Germany, 14109.

Ag-TiO_2 and Au-TiO_2 nanocomposites with different volume fractions of metal nanoparticles were prepared by co-sputtering. The morphology of these nanocomposites was investigated by transmission electron microscopy (TEM). Metal volume fractions were determined by SEM-EDX. Optical characterization of these nanocomposites was carried out using UV/Vis/NIR spectroscopy. The nanocomposites were then irradiated by Swift Heavy Ions (SHI) with 100 MeV (Ag^{8+} ions) at different fluences ranging from 1 X 10^{12} to 1 X 10^{13} ions/cm^2. The extinction spectra of the pristine samples show plasmon resonances at wavelengths which depend on the volume fraction of metal, particle size and morphology of the composites. The influence of the SHI fluences, on the microstructure and the extinction spectra were observed. The changes in the properties of these nanocomposites are discussed in terms of ion-material interactions.

O 55.15 Wed 18:30 Poster F

X-Ray Absorption (XAS) and Magnetic Circular Dichroism (XMCD) Measurements of Mn_6Cr Single-Molecule-Magnets Adsorbed on Various Surfaces — •Fabian Merschjohann[1], Aaron Gryzia[1], Armin Brechling[1], Marc D. Sacher[1], Ulrich Heinzmann[1], Maik Heidemeier[2], Thorsten Glaser[2], Sönke Voss[3], Mikhail Fonin[3], Michael Burgert[3], Ulrich Rüdiger[3], and Eberhard Goering[4] — [1]Dep. of Physics, Bielefeld University — [2]Dep. of Chemistry, Bielefeld University — [3]Dep. of Physics, Konstanz University — [4]MPI für Metallforschung, Stuttgart

We report on the electronic configuration of Mn_6Cr-Single-Molecule Magnets (SMM) adsorbed on various surfaces. We investigated the substrate/molecule interaction, in particular the exchange of the electrons with the substrate. The manganese atoms of the Mn_6Cr-SMM are trivalent. X-Ray absorption measurements at the Mn-L_2- and L_3-edge indicated a certain amount of divalent Mn-atoms. This suggests a reduction of the Mn_6Cr molecules due to an electron transfer to the substrate. This transfer depends on the electronic configuration of the substrate material. Thus we investigated Mn_6Cr-SMM adsorbed on insulating (SiO_2), metallic (Au) and semiconducting (Highly Ordered Pyrolytic Graphite HOPG) materials. To determine the fraction of Mn^{II}- and Mn^{III}-ions we calculated the measured spectral shape by using di- and trivalent reference spectra. We will also show XMCD measurements of the adsorbed SMM performed at BESSY in Berlin which reflect the expected magnetic configuration of Mn and Cr.

O 55.16 Wed 18:30 Poster F

STM-Study of clean ZnO surfaces and Cu growth on ZnO — •Kroll Martin, Kuschel Thomas, Löber Thomas, and Köhler Ulrich — Ruhr Universität Bochum, Experimentalphysik IV - AG Oberflächen, Bochum, Germany

STM was used to study the polar, zinc terminated ZnO(0001)-Zn surface, the polar, oxygen terminated ZnO($000\bar{1}$)-O surface and the non-polar, mixed terminated ZnO($10\bar{1}0$) surface. The influence of atomic hydrogen and water present during different annealing procedures on the large scale morphology of flat and miscut surfaces was investigated. The morphology of the clean ZnO(0001)-Zn surface with characteristic triangular islands changes dramatically when water is present during annealing and on vicinal ZnO($10\bar{1}0$) surfaces the regularity of the step train is crucially dependent on the preparation conditions.

Additionally the deposition of Cu using MBE and CVD on the zinc terminated surface were studied. The formation of (111)-orientated Cu-clusters at room-temperature is followed by in-situ applied STM. Kink-sites at step edges and especially the apexes of triangular ZnO-substrate terraces act as preferred nucleation sites. At room temperature the decay of small Cu-islands takes place on a time scale of minutes. Larger Cu-coverages lead to an ensemble of interconnected 3D-islands of uniform height separated by trenches down to the substrate. Further annealing up to 400 °C points to a partial entrenching of the islands into the oxide support and (or) an alloy formation.
Lit: Kroll, M.; Köhler, U.; Surf. Sci. 601 (2007) 2182

O 55.17 Wed 18:30 Poster F

Trends in Reactivity: Gold Catalysis — •Guido Walther[1], Søren Jensen[2], and Sebastian Horch[1] — [1]CAMD, Department of Physics, DTU, 2800 Lyngby, Denmark — [2]MIC, Department of Micro and Nanotechnology, DTU, 2800 Lyngby, Denmark

Gold, as the noblest of all the metals, becomes catalytically active for several chemical reactions, when its particle size is less than 5 nm. Beside the particle size, there are many other effects, which maybe contribute to the surprisingly high activity of gold nano-particles, like support and/or electronic effects. But it is still not understood in detail yet, what accounts for these unique properties of nano-sized gold.

In a new microreactor setup, CO and H_2 oxidation were studied on TiO_2 supported Au catalysts of various well defined particle sizes. The particle size was confirmed using TEM. To analyze the reaction products, the microreactor was interfaced to a gas chromatograph.

We show a trend in reactivity in catalysis by gold for these reactions. By switching the oxidation agent from O_2 to N_2O, an investigation whether the rate-limiting step is associated with O_2 or CO, was feasible. This gives an experimental indication that CO oxidation follows an alternative pathway via a CO–O_2 intermediate.

O 55.18 Wed 18:30 Poster F

Homogeneous and front-induced surface transformations during catalytic oxidation of ammonia over Pt(1 0 0) — •Florian Lovis[1], Matias Rafti[2], Yingfeng Zeng[1], and Ronald Imbihl[1] — [1]Institut für Physikalische Chemie und Elektrochemie, Leibniz-Universitat Hannover, Callinstr. 3-3a, D-30167 Hannover, Germany — [2]INIFTA, Dto. de Química, Fac. de Cs. Exactas, Universidad Nacional de La Plata, Diag. 113 y 64, CC 16 suc. 4, (1900) B1871DCR La Plata, Argentina

The ammonia + oxygen reaction over Pt(1 0 0) single-crystal surface was studied under UHV conditions using photoemission electron microscopy (PEEM) as spatially resolving method and work function measurements via a Kelvin probe and temperature programmed reaction (TPR) experiments as integral methods. A broad hysteresis in the reaction rates occurs and one finds reaction fronts as well as spatially homogeneous transitions in the adsorbate layer.

O 55.19 Wed 18:30 Poster F

Mass selected Ag cluster based catalysis: size and shape effects — •Kristian Sell[1], Ingo Barke[1], Viola von Oeynhausen[1], Karl-Heinz Meiwes-Broer[1], Stefan Vajda[2], Sungsik Lee[2], Yu Lei[2,3], Byongdu Lee[2], Jeffrey W. Elam[2], Michael J. Pellin[2], Sönke Seifert[2], Randall E. Winans[2], Randall J. Meyer[2], and Arantxa Fraile-Rodríguez[4] — [1]Universität Rostock, Institut für Physik, Rostock, Deutschland — [2]Argonne National Laboratory, Argonne, USA — [3]University of Illinois at Chicago, USA — [4]Swiss Light Source, Paul Scherrer Institut, Villigen, Switzerland

The exceptional performance of nanocatalysts has motivated intense research as highly dispersed nanocatalysts are widely used in commercial applications. Here we study size-selected silver particles under realistic conditions in a reaction of industrial relevance.

Supported size selected Ag clusters of sub-nm to several nm size are produced by laser evaporation and an arc charge ion source (ACIS) and deposited on Al2O3 supports. These are prepared by atomic layer deposition of thin Al2O3 films on the native silicon oxide surface of Si wafers. The catalytic properties of the supported clusters are studied under atmospheric pressure reaction conditions. We use a unique approach which allows for in situ, real-time monitoring of changes in size and shape of the nanocatalysts by grazing-incidence small-angle x-ray scattering (GISAXS) with simultaneous detection of the reaction products. The relationship between cluster size/shape and its function in catalytic activity and selectivity in direct epoxidation of propylene on Ag clusters will be discussed.

O 55.20 Wed 18:30 Poster F

Inverse Au/TiO$_2$ model catalysts studied with in-situ high-pressure XPS — •Dumbuya Karifala, Lucasczyk Thomas, Schirmer Michael, Marbach Hubertus, Gottfried Michael, and Steinrück Hans-Peter — Lehrstuhl für Physikalische Chemie II, Universität Erlangen-Nürnberg

We have prepared and investigated planar inverse TiO$_2$/Au model catalysts using XPS and SEM. In addition, we have studied the surface composition and the electronic structure in the presence of CO and O$_2$ at pressures of up to 1 mbar using high-pressure XPS. The model systems have been prepared and characterized on a polycrystalline Au foil and on an Au(111) surface. Initially, we used a recipe reported by Biener et al.[1] and prepared the TiO$_2$ clusters by vapor deposition of Ti on the Au surfaces at 300 K, followed by oxidation with O$_2$ at 300 K and annealing at 600-900 K in vacuum. We found that part of the deposited Ti forms an Au-Ti alloy during this procedure. To prevent alloying, we have developed a modified procedure in which the TiO$_2$ clusters are annealed in an O$_2$ atmosphere. SEM images of the nanoparticles on Au foil show a particle size distribution in the 10 nm range for an initial Ti coverage of 0.25 ML. At high coverages, exposure to CO and O$_2$ did not reveal significant changes in the oxidation states of either Au or Ti, probably because of a buried TiO$_2$/Au interface. In contrast, at lower TiO$_2$ coverages (initial Ti coverage 0.25 ML) and CO pressures above 0.1 mbar, the in-situ XP spectra show changes that are attributed to the interaction between CO and Ti. 1. Biener et al.

O 55.21 Wed 18:30 Poster F

The chemical state of iron during N$_2$O decomposition over iron modified zeolites ZSM-5: A high-pressure XPS study — •Karifala Dumbuya[1], Saiprasath Gopalakrishnan[2], Wilhelm Schwieger[2], J. Michael Gottfried[1], and Hans-Peter Steinrück[1] — [1]Universität Erlangen-Nürnberg, Lehrstuhl für Physikalische Chemie II — [2]Universität Erlangen-Nürnberg, Lehrstuhl für Chemische Reaktionstechnik

Iron containing ZSM-5 zeolites are employed as catalysts for the abatement of N$_2$O in waste gases and in partial oxidation reactions with N$_2$O as the oxidant. The chemical state of the active Fe centers during reaction is unknown; however, it has been speculated that an α-Fe(II) species is the active site.[1] NaOH-treatment increases the activity, which has been attributed to the alteration of the Fe centers.[2] We have studied commercial ZSM-5 (as-supplied and NaOH-treated) using XPS and in-situ XPS during N$_2$O exposure (pressure $\leq$ 1 mbar). No Fe was found in the surface region of the commercial ZSM-5 before or after ion-exchange with NaOH, contrary to ICP-AES results. As expected, significant amounts of Fe (mainly in the +2 and +3 oxidation states) were detectable with XPS, following Fe doping of both catalysts. The Fe content in the surface region of the NaOH-modified ZSM-5 did not change with temperature (300-650 K), while the as-supplied sample showed Fe segregation in this temperature range. Details about the electronic state of Fe in the Fe doped, NaOH-modified catalyst in the presence of N$_2$O ($5*10^{-8}$ - 1 mbar) will be discussed. [1] Dubkov et al., J. Catal. 207 (2002) 341. [2] Groen et al., J. Catal. 243 (2006) 212.

O 55.22 Wed 18:30 Poster F

Silver, oxygen and hydrogen deposited on the Bi terminated prestructured Si/Ge surface — •Vasily Cherepanov and Bert Voigtländer — Institute of Bio- and Nanosystems (IBN 3), and cni – Center of Nanoelectronic Systems for Information Technology, Research Centre Jülich, 52425 Jülich, Germany

Si-Ge based nanostructures like wires or dots are attractive objects since they are compatible with an existing silicon technology. The similar nature of Si and Ge allows to grow epitaxial Si/Ge nanostructures using a surfactant like Bi to suppress Si-Ge intermixing. A well ordered array of 2-3 nm wide and atomic layer in heigh Ge nanowires can be formed in a controlled way at Si(111) substrate. However to utilize the electrical properties of those structures one would need to increase the difference in the electrical properties of the wires and the substrate. The Si/Ge structures thus can be used as templates for a next step of selforganized growth of different material which selectively bonds to Si or Ge. The challenge is to find a material which at some condition would stick or interact selectively to Si or Ge. We made an attempt to explore a possible chemical selectivity for Si and Ge surface. The Bi covered surface contained Si and Ge areas was exposed to flux of silver, oxygen and atomic hydrogen at various conditions. The resulting surface structure was examined by scaning tunneling microscopy.

O 55.23 Wed 18:30 Poster F

Surface Characterisation of MOCVD Single Source Precursor Grown GaSb-films — •Andreas Seemayer[1], Alexander Hommes[1], Sascha Hümann[1], Ralf Hunger[2], Stephan Schulz[3], and Klaus Wandelt[1] — [1]University of Bonn, Institute for Physical Chemistry, Wegelerstr. 12, 53115 Bonn — [2]Hahn-Meitner-Institute Berlin GmbH c/o BESSY, Albert-Einstein-Str. 15, 12489 Berlin — [3]University of Paderborn, Department Chemie, Warburger Str. 100, 33098 Paderborn

III-V semiconductor films used for opto- and microelectronic devices have traditionally been grown by (MO)MBE and LPE processes. An alternative metal-organic CVD-process, which has been established in the last two decades for high-throughput and low-cost fabrication works for nitrides, phosphides and arsenides, but is problematic for antimonides. In particular, for GaSb films an alternative route is a CVD-process using the heterocyclic single source precursor $[tBu_2GaSbEt_2]_2$.

Subject of the present work is the investigation of the surface physical properties of the produced films as well as the gas phase behaviour of the used precursor. Therefore films were produced on a Si(100) substrate in a HV-MOCVD reactor and investigated using AES, S-XPS and AFM. In addition, growth experiments under UHV conditions were performed. The results are discussed in terms of a correlation of the electronic properties with the composition and structure of the films.

O 55.24 Wed 18:30 Poster F

Growth of large laser deposited Cu-pyramides on Si at raised temperatures — •Susanne Seyffarth and Hans-Ulrich Krebs — Institut für Materialphysik, Universität Göttingen, Friedrich-Hund-Platz 1, 37077 Göttingen

Thin Cu films were prepared on Si(111) and Si(100) substrates using pulsed laser deposition (PLD) in ultra high vacuum. Especially the effect of elevated substrate temperatures on the growth of Cu on Si was investigated. While for low substrate temperatures closed films with small grains are observed, for temperatures above 200 °C epitaxial growth of three dimensional pyramides with edge lengths of a few micrometers is observed using scanning electron microscopy (SEM) and atomic force microscopy (AFM). Depending on the orientation of the substrate the base area of the islands is a triangle for Si(111) and a square for Si(100). In both cases the height of the pyramides is up to 500 nm. The epitaxial relationships with the Si substrates, the dependences of the pyramidal sizes on the number of laser pulses, the stability of the structures and possibilities for an ordering of the islands are discussed.

O 55.25 Wed 18:30 Poster F

Magnetic and structural investigations of thin iron layers on GaAs(001) and GaAs(110) surfaces with and without an MgO intermediate layer — •Carsten Godde[1], Sani Noor[1], Christian Urban[1], Igor Barsukov[2], Jürgen Lindner[2], and Ulrich Köhler[1] — [1]Institut für Experimentalphysik IV/ AG Oberflächen, Ruhr-Universität Bochum, Germany — [2]Institut für Experimentalphysik / Festkörperphysik, Universität Duisburg / Essen, Germany

The structure and the magnetic behaviour of Fe-layers on GaAs(001) and GaAs(110) were studied in a UHV system that offers the means for structural analysis by STM and LEED and magnetic characterization by MOKE during deposition. The preparation of the GaAs(001) and GaAs(110) polished wafer surfaces consisted of cycles of sputtering and annealing, in the case of the cleaved GaAs(110) surface no in situ preparation was necessary. On all samples the structure of the Fe-layer when grown at 20°C is strongly influenced by the substrate morphology. At elevated growth temperature a disrupted Fe-layer develops. Using MgO as an intermediate layer the structural quality is substantially reduced. The uniaxial anisotropy of Fe on GaAs(110) surfaces is profoundly influenced by the MgO intermediate layer. The effect of annealing up to 500°C on the structure and the magnetic behaviour were studied. Although smooth layers with large islands develop, STM shows that Ga and As from the substrate diffuse to the Fe-island top. On GaAs(001) the substrate reconstruction changes from an initially present (2x6) to a As-rich (2x4).

O 55.26 Wed 18:30 Poster F

Magnetic in situ characterization by MOKE and Kerr microscopy — •Sani Noor, Carsten Godde, Christian Urban, and Ulrich Köhler — Institut für Experimentalphysik IV, AG Oberflächen, Ruhr-Universität Bochum, Germany

A UHV system is being introduced that offers both the structural analysis by LEED and STM and the magnetic analysis by MOKE and Kerr microscopy of thin films. These can be grown by sets of MBE sources that are pointing at the sample in the STM, MOKE and Kerr microscopy positions allowing in situ measurements respectively. Our focus here shall be the magnetic characterization. The combination of a longitudinal MOKE setup and polar Kerr microscopy, which is based on a long distance microscope, enables the recording of magnetization loops for in and out of plane magnetization. The former provides angular dependent measurements by azimuthal rotation of the sample, the latter can be obtained by spatial integration of the acquired Kerr images. Test measurements have been performed including the study of the anisotropic behaviour of Fe on InAs(001)(4x2) and the Kerr microscopy of FeGd ((0.5 nm Fe/0.5 nm Gd) x 70) multilayers which feature a strong out of plane anisotropy at room temperature as confirmed by SQUID measurements.

O 55.27 Wed 18:30 Poster F

STM and STS study of atomic and electronic structure of epitaxial graphene on SiC(0001) — Peter Lauffer[1], Konstantin V. Emtsev[1], Sergey Reshanov[2], Ralf Graupner[1], •Thomas Seyller[1], Gerhard Pensl[2], Heiko B. Weber[2], and Lothar Ley[1] — [1]Lehrstuhl für Technische Physik, Universität Erlangen-Nürnberg, Germany — [2]Lehrstuhl für Angewandte Physik, Universität Erlangen-Nürnberg, Germany

Epitaxial growth of graphene on SiC surfaces by solid state graphitization is a promising route for future development of graphene based electronics. In the present work we have studied the morphology, atomic scale structure, and electronic structure of thin films of few-layer graphene on SiC(0001) by scanning tunneling microscopy (STM) and spectroscopy (STS). We discuss the determination of layer thickness based on atomically resolved images and show that such identification can be supported by evaluation of the roughness induced by the interface. We also present and interpret thickness dependent tunneling spectra, which can serve as an additional fingerprint for the determination of the layer thickness.

O 55.28 Wed 18:30 Poster F

Morphology of epitaxial graphene films on SiC(0001) determined by LEEM — Taisuke Ohta[1,2], Farid El Gabaly[3], Aaron Bostwick[1], Jessica L. McChesney[1], Konstantin V. Emtsev[4], Andreas K. Schmid[3], •Thomas Seyller[4], Karsten Horn[3], and Eli Rotenberg[1] — [1]Advanced Light Source, Lawrence Berkeley National Laboratory, Berkeley, California, USA — [2]Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, Germany — [3]National Center for Electron Microscopy, Lawrence Berkeley National Laboratory, Berkeley, California, USA — [4]Lehrstuhl für Technische Physik, Universität Erlangen-Nürnberg, Germany

Epitaxial films of graphene on SiC surfaces are interesting from a basic physics as well as applications-oriented point of view. In the present work we use low-energy electron microscopy (LEEM) and angle-resolved photoemission (ARPES) to study the morphology of epitaxial graphene films grown on SiC(0001) by solid state graphitization in ultrahigh vacuum (UHV). Different layer thicknesses were witnessed by characteristic electron reflectivity spectra. After relating these to the thickness dependent π-band structure determined by ARPES it is possible to unambiguously assign regions in the LEEM images to the interfacial layer and single-layer as well as bilayer graphene. This information will aid the improvement of the morphology of large scale epitaxial graphene films through optimization of preparation conditions.

O 55.29 Wed 18:30 Poster F

Interface investigations for III-V solar cells — •Ulf Seidel, Henning Döscher, and Thomas Hannappel — Hahn-Meitner-Institut, Glienicker Str. 100, 14109 Berlin, Germany

III-V multi-junction solar cells currently represent the most efficient photovoltaic devices. The device structures of the tandem solar cells, which were prepared in this work via MOVPE, contain many different layers of III-V semiconductors. For the best performance of the solar cells a sharp hetero-interface preparation via MOVPE was necessary. Here, the investigation of two interfaces is presented in detail: (1) InGaAs/GaAsSb that is needed in the tunnel junction of our low band gap multi-junction solar cell and (2) Si/GaP that is needed for the epitaxy of our III-V solar cells on silicon(100) substrates instead of InP(100). Both interfaces were characterized in-situ during the MOVPE-growth with reflectance difference spectroscopy (RDS) and after a contamination free transfer in ultra high vacuum with X-ray photoelectron spectroscopy (XPS) and low energy electron diffraction (LEED). Additionally AFM micrographs were recorded.

O 55.30 Wed 18:30 Poster F

Resistance of a single atom: scattering of electrons by single adatoms and small islands during homoepitaxial growth of Bi(111) films — •Hichem Hattab, Giriraj Jnawali, Boris Krenzer, and Michael Horn-von Hoegen — Fachbereich Physik, Universität Duisburg-Essen, Lotharstr. 1, 47048 Duisburg, Germany

Atomically smooth Bi(111) films on Si(001) were prepared following a recipe of G. Jnawali et al. (PRB 74 , 195340 (2006)) and were used as template to study the resistivity change during additional growth of Bi at 80 K by using a 4-probe technique and SPA-LEED. At very low Bi coverage of less than 0.01 bilayer (BL) a linear increase of the film resistivity was observed which suddenly changes to a square root dependence up to 0.5 BL. This behaviour is explained by a combination of Venables nucleation theory and Fuchs-Sondheimer behaviour. At very low coverage each deposited Bi adatom acts as single scatterer, which ultimately scatters the conduction electrons diffusively. The linear increase of the resistivity is proportional to the density of adatoms. With increasing Bi adatom density suddenly stable 2-dim. islands nucleate, the adatom density drops, and the islands grow in size at constant island density. Now the electrons are scattered at the step edges which density increase as square root of the coverage. At higher coverage the resistivity shows a bilayer oscillation indicating the oscillation in roughness which is followed by a 1/d behavior described by Fuchs-Sondheimer. From the slopes of the two initial regimes the effective cross-section for diffuse scattering of a single Bi adatom and of a bilayer step edge is calculated.

O 55.31 Wed 18:30 Poster F

Laser Treatment of Stainless Steel — •Christian Holzheu, Matthias Laske, and Othmar Marti — Institute of Experimental Physics, University of Ulm, 89069 Ulm, Germany

Laser treatment of stainless steel and the resulting material changes are studied. By irradiating the steel surface with short laser pulses the adhesion of polymers and especially fluorinated polymers is improved. The experiments were designed to evaluate the influence of different laser parameters on adhesion, surface morphology and composition and on surface tension. Corrosion behaviour and the durability of the material after laser treatment in comparison to untreated samples are studied in long time tests. Salt fog and mechanical pulses are used to simulate nearly realistic conditions.

O 55.32 Wed 18:30 Poster F

STM studies of surface plasmon mediated laser annealing of gold films — •Markus Schmotz, Armin Fubel, and Paul Leiderer — Universität Konstanz, Konstanz, Germany

Using a Kretschmann configuration we illuminate thin polycrystalline gold films under the surface plasmon resonance angle. Thus, a frequency doubled Nd:YAG laser locally heats the films at different intensities. The investigation of structural changes of the gold surfaces is done in situ by a homebuilt STM. To gain quantitative information we study FFT-data (fast Fourier transformation) like PSD-spectra (power-spectrum-density) and autocorrelation functions beneath typical roughness parameters like RMS (root-mean-square) and MPP-values (mean-peak-to-peak). The influence of single and multi-shot treatment is also determined at higher and lower intensities, respectively.

Preliminary results show broadening and flattening of the typical gold mounds at low intensities and thus increasing correlation lengths and grain sizes. Reproducibility checks and analysis of detailed annealing mechanisms will be reported.

O 55.33 Wed 18:30 Poster F

Interfacial layering of room temperature ionic liquids based on the tris(pentafluoroethyl)trifluorophosphate anion at the sapphire interfaces — •Markus Mezger[1], Heiko Schröder[1], Sebastian Schramm[1], Harald Reichert[1], Sebastian Schöder[1], John Okasinski[1], Moshe Deutsch[2], Benjamin Ocko[3], Emerson De Souza[1], John Ralston[4], and Helmut Dosch[1] — [1]Max-Planck-Institut für Metallforschung, Stuttgart — [2]Bar-Ilan University, Ramat-Gan, Israel — [3]Brookhaven National Laboratory, Upton, NY, USA — [4]Ian Wark Research Institute, Adelaide, Australia

A new group of room temperature ionic liquids (RTIL) based on the tris(pentafluoroethyl)trifluorophosphate (FAP) anion reveals intriguing features in comparison to conventional molten salts. Especially the improved chemical and thermal stability make them interesting candidates for a variety of technological processes. Using high energy x-ray reflectivity we get access to deeply buried solid-liquid interfaces and gain real space information with Å-resolution. In this study, we discuss reflection patterns of FAP based ionic liquids, recorded at different temperatures ranging from the highly supercooled metastable liquid state to 120 °C. By parameter refinement of a two-component distorted-crystal model we disclose pronounced layering of the anions and cations close to the solid wall. With increasing temperature, the decay length of the interfacial ordering decreases.

O 55.34 Wed 18:30 Poster F

High energy x-ray reflectivity study of the room temperature ionic liquids $[bmim]^+$ $[PF_6]^-$ and $[bmim]^+$ $[BF_4]^-$ at solid interfaces — •Sebastian Schramm[1], Markus Mezger[1], Heiko Schröder[1], Harald Reichert[1], John Okasinski[1], Moshe Deutsch[2], Benjamin Ocko[3], Emerson De Souza[1], and Helmut Dosch[1] — [1]Max-Planck-Institut für Metallforschung, Stuttgart — [2]Bar-Ilan University, Ramat-Gan, Israel — [3]Brookhaven National Laboratory, Upton, NY, USA

Room temperature ionic liquids (RTILs), being composed solely of ions, are very promising new materials. Their physical properties make them suitable for many technological processes, e.g. as solvents in catalytic reactions and electrolysis. In particular for the understanding of reactions at an interface, knowledge on the spatial arrangement of the ions at hard walls is essential. In our study, we used high energy (~ 70 keV) x-ray reflectivity to probe the structure of these liquids at the sapphire interface. The results give evidence for interfacial layering in 1-butyl-3-methylimidazolium hexafluorophosphate ($[bmim]^+$ $[PF_6]^-$), in contrast to 1-butyl-3-methylimidazolium tetrafluoroborate ($[bmim]^+$ $[BF_4]^-$) where no layering was found. In combination with the analysis of the bulk liquid structure factor, the recorded reflection patterns give both the molecular layer spacing, as well as the decay length of the spatial ordering. We compare the x-ray scattering results with optically obtained surface and interfacial tension data to gain detailed information about the nature of the chemical interaction between the sapphire substrate and the ions of the RTIL.

O 55.35 Wed 18:30 Poster F

Post annealing investigations of thin praseodymia films on Si(111) — Sebastian Gevers, •Daniel Bruns, Thomas Weisemöller, Carsten Deiter, and Joachim Wollschläger — Fachbereich Physik, Universität Osnabrück, Barbarastr. 7, 49076 Osnabrück, Germany

Due to its large oxygen capacity and oxygen mobility praseodymia is interesting for applications in modern heterogenous catalysis. For instance the selectivity of praseodymia for carbon compounds is advantageous in olefiant gas synthesis. The investigation of annealing processes leads to a better understanding of the oxygen transport in the praseodymia films. In this context thin PrO2 films were annealed at temperatures from 300°C up to 600°C under UHV conditions before they were analysed with Spot Analysis Profile Low Electron Energy Diffraction (SPALEED). The diffraction pattern indicates a phase transition to Pr2o3 at the surface. Furthermore X-Ray Diffraction experiments (XRD) show a partial subsurface phase transition from PrO2 into various oxidation states including Pr2O3.

O 55.36 Wed 18:30 Poster F

Adsorption of benzene on the Si(001)-(2×1) and the SiC(001)-(3×2) surfaces – a comparative theoretical study — •Jürgen Wieferink, Peter Krüger, and Johannes Pollmann — Institut für Festkörpertheorie, Universität Münster

We have investigated the adsorption of benzene (C_6H_6) on (001) surfaces of Si and SiC employing the generalized-gradient approximation of density functional theory together with norm-conserving pseudopotentials. Using the quadratic string method [1] we have explored reaction pathways to possible final adsorption states.

At Si(001)-(2×1), we find C_6H_6 to initially adsorb via electrophilic addition in a butterfly configuration by binding two opposite (1,4) carbon atoms to the silicon atoms of one surface dimer. The energetically most favorable tight-bridge structure can then be reached by the formation of two additional bonds between the (2,3) carbon atoms and an adjacent silicon dimer [2].

At SiC(001)-(3×2), the silicon dimers are further apart from each other. As a result, this surface cannot feature bridging geometries and is thus expected to generate an ordered monolayer of butterfly benzene, where each molecule exhibits two π-bonds that are available for further reactions. An energetically more favorable dissociated adsorption structure is also discussed and shown to be kinetically unreachable. Finally, the electronic structure of the optimized geometries is examined and discussed.

[1] S. K. Burger, W. Yang, J. Chem. Phys. **124**, 054109 (2006)
[2] J.-Y. Lee, J.-H. Cho, Phys. Rev. B **72**, 235317 (2005)

O 55.37 Wed 18:30 Poster F

Insulating Ground State of Sn/Si(111)-($\sqrt{(3)} \times \sqrt{(3)}$)R30° — •Silvio Modesti[1,2,3], Luca Petaccia[1,4], Gustavo Ceballos[1,5], Ivana Vobornik[1], Giancarlo Panaccione[1], Giorgio Rossi[1], Luca Ottaviano[6], Silvano Lizzit[4], and Andrea Goldoni[4] — [1]Laboratorio Nazionale TASC-INFM, S.S. 14 Km 163.5, 34012 Trieste, Italy — [2]Dipartimento di Fisica, Universita' di Trieste, v. Valerio 2 I-34127, Trieste, Italy — [3]Institut für Angewandte Physik, Universität Hamburg, Jungiusstr. 11, D-20355 Hamburg — [4]Sincrotrone Trieste S.C.p.A., S.S. 14 Km 163.5, 34012 Trieste, Italy — [5]ICN, UAB Campus, E-08193 Bellaterra (Barcelona), Spain — [6]Universita' dell'Aquila, via Vetoio 10, 67010 Coppito-L'Aquila, Italy

The Sn/Si(111)-($\sqrt{(3)} \times \sqrt{(3)}$)R30° surface, having an odd number of electrons per surface unit cell, was so far believed to be metallic according to the electron counting argument. One third of a monolayer of tin adatoms in the T4 site forms a narrow surface state band that is half filled, and therefore prone to structural and electronic instabilities. We show, by using tunneling spectroscopy, scanning tunneling microscopy, photoemission, and photoelectron diffraction, that below 70 K this surface has a very low density of states at the Fermi level and is not appreciably distorted [1]. The experimental results are compatible with the magnetic insulating Mott-Hubbard ground state predicted by LSDA + U calculations [2]

[1] S. Modesti, et al., Phys. Rev. Lett. 98, 126401 (2007) [2] G. Profeta and E. Tosatti, Phys. Rev. Lett. 98, 086401 (2007).

O 55.38 Wed 18:30 Poster F

First-Principles Investigation of an Epitaxial Silicon Oxynitride Layer on a 6H-SiC(0001) Surface — •Peter Krüger, Björn Baumeier, and Johannes Pollmann — Institut für Festkörpertheorie, Universität Münster

Recently, Shirasawa et al. [1] have experimentally shown that incorporation of nitrogen at the interface of a silicate adlayer on 6H-SiC(0001) leads to the formation of a well ordered, highly stable epitaxial silicon oxynitride (SiON) layer without dangling bond states. Scanning tunneling spectroscopy data for this system show an amazingly large band gap of about 9 eV.

We have investigated the structural and electronic properties of this novel system by employing density functional theory with self-interaction-corrected pseudopotentials. Our results support the structural model inferred from low-energy electron data [1]. In addition, our calculated filled- and empty-state scanning tunneling microscopy images are in excellent agreement with the experimental data clearly revealing that the O and Si surface states, respectively, of the silicate double-layer on top of the system give rise to the observed images.

The calculated surface band structure exhibits a surface band gap of 9 eV whose physical origin is clarifed. Further investigations show that SiON overlayers on 6H-SiC(0001) and 6H-SiC(000$\bar{1}$) have qualitatively different electronic structures. While the former is free from gap states, the latter possesses two N-derived states in the fundamental band gap.

[1] Shirasawa et al., Phys. Rev. Lett. **98**, 136105 (2007)

O 55.39 Wed 18:30 Poster F

Energy barriers for dissociative adsorption of H_2 molecules on Si, SiC, and diamond (001) surfaces: A comparison — •Xiangyang Peng[1], Peter Krüger[2], and Johannes Pollmann[2] — [1]Department of Physics, Uppsala University, SE-75121 Uppsala, Sweden — [2]Institut für Festkörpertheorie, Wilhelm-Klemm-Str. 10, 48149 Münster

We report first-principles investigations of the reaction of molecular hydrogen with the Si(001)-(2×1) and C(001)-(2×1) surfaces and discuss the results in light of our previous studies of H_2 reaction with two different SiC(001) surfaces, one of which is highly reactive to H_2 uptake. The calculations reveal that the reaction of H_2 with all above surfaces depends crucially on intricate combined effects of the substrate lattice constant, the arrangement of the surface dimers as well as the orientation and spatial extent of their dangling bond orbitals. In agreement with experiment, our results confirm that Si(001) and C(001) are inert to H_2 adsorption at room temperature because all adsorption pathways considered exhibit substantial energy barriers. They are in satisfying agreement with previous density functional and quantum Monte Carlo calculations which have been carried out for two specific reaction pathways only. Guided by our earlier studies on H_2 reaction with SiC(001) surfaces, we have considered a third reaction pathway which actually turns out to have the lowest energy barrier on C(001). A comparison of the energy barriers and reaction energies for the different surfaces addressed turns out to be particularly revealing.

O 55.40 Wed 18:30 Poster F

Laser Activated Vapour Phase Processes for Silicon Substrate Cleaning — •Ulrich Abelein, Andreas Assmuth, Torsten Sulima, and Ignaz Eisele — Universität der Bundeswehr München, Institut für Physik, Werner-Heisenberg-Weg 39, 85577 Neubiberg, Germany

One of the most important issues in today's nanoelectronics fabrication is the in situ cleaning of silicon substrates, i. e. the removal of organic impurities and SiO_2, before epitaxial growth.

The currently used vapour phase methods, like the hydrogen bake, require high process temperatures above 800 °C to activate the chemical reaction which leads to the desired effect. To avoid the diffusion of dopands or the formation of SiC clusters during the cleaning process a reduction of the necessary temperature below 700 °C is desirable.

Possible solutions to achieve this aim are the activation of the gas molecules by a plasma source or by laser light. As plasma processes cause damages to insulating layers and roughen the surface the use of a laser to provide the energy is more suitable.

We have integrated a process chamber, equipped with a 193 nm ArF Excimer Laser and up to four gases, in an UHV cluster tool. The laser beam is guided parallel to the substrate to ensure that only the gas molecules are affected and not the silicon. An RTP lamp heater can be used to adjust the substrate temperature independent from the laser energy. The efficiency of this approach will by demonstrated by the results achieved with a cleaning process using laser activated GeH_4 to remove carbon and SiO_2.

O 55.41 Wed 18:30 Poster F

The interface between diamond and aqueous electrolyte — •Markus Dankerl, Moritz Hauf, Ulrich Stützel, Andreas Reitinger, Jose Garrido, and Martin Stutzmann — Walter Schottky Institut, Technische Universität Müunchen, Am Coulombwall 3, 85748 Garching

Diamond, which is terminated with hydrogen at the surface, shows the intriguing property of being p-type surface conductive with a two-dimensional hole gas forming beneath the surface. If brought into electrolyte solutions, this surface conductivity shows a dependence on the diamond electrode potential. This allows for the fabrication of in-plane FETs with the electrolyte functioning as gate, therefore called EGFETs. We report on the characterization of the surface conductivity of single crystalline hydrogen terminated diamond in contact with electrolyte. The focus is put on the effect coulombic screening of charge at the interface by salts with different valency has on the surface conductivity. Experimental results are compared to simulations based on the screening effect. In this context the mechanism of the pH sensitivity is discussed, where the effect of ionic strength on pH sensitivity suggests, that pH-dependent surface charges have an equivalent effect on the surface conductivity as a change of the electrode potential.

O 55.42 Wed 18:30 Poster F

Scanning tunneling microscope study of Fe, Co, and Cu- Phthalocyanine growth on metal surfaces — •Shih-Hsin Chang[1], Alessandro Scarfato[1,2], Germar Hoffmann[1], and Roland Wiesendanger[1] — [1]Institut für Angewandte Physik, Universität Hamburg, Germany — [2]Dipartimento di Fisica, University of Salerno, Italy

The growth behaviour of Fe-, Co-, and Cu- Phthalocyanine (Pc) molecules on Cu(111) surfaces has been studied by a variable-temperature scanning tunneling microscope. For all three kinds of Pcs, we find perfect alignment of one molecular axis relative to one of the equivalent crystallographic axis of Cu(111) at submonolayer coverage. At about 1 ML short-range ordered domains appear and molecular configurations are found to have a mismatch angle from the crystallographic axis of Cu(111) due to molecule-molecule interaction. Above 1 ML, well-ordered domains of second layer molecules are formed. Based on STM images molecules were found to be tilted out-of-plane. Still, a substantial variation of the growth behaviour for the different Pc is observable. We will discuss these variations in terms of molecule-molecule and molecule-substrate interactions.

O 55.43 Wed 18:30 Poster F

Design and construction of a 300 mKelvin / 17 Tesla ultra-high vacuum scanning tunneling microscope for molecular studies — •Jörg Schwöbel, Matthias Nohme, Robert Ravlić, Jan Wienhausen, Germar Hoffmann, and Roland Wiesendanger — Institut für Angewandte Physik, Universität Hamburg, Germany

The detailed investigation of molecular excitations and molecular magnetism is a prerequisite to establish molecules as building blocks for tailor made materials. Here, we present the design of a new ultra-high vacuum system for the local study of molecular magnetism with scanning tunneling microscopy (STM) and spectroscopy (STS).

To resolve magnetic molecular levels this system operates at ultra-low temperatures (300 mK), thereby increasing energy resolution, and is equipped with a 17 Tesla magnetic field to achieve splitting of magnetic states. Organic magnetic molecules will be prepared on metal substrates as well as on substrates covered by insulating layers for electronic decoupling. For the preparation of heterogeneous layers from different materials and of single molecules we developed new vacuum components for a flexible growth at temperatures between 1 and 500 K. Metal and molecule evaporators are mounted on individual sample holders. Therefore, evaporators can be easily exchanged and operated in the preparation chamber as well as within the 300 mK cryostat.

We will discuss the design concept of the STM system and the vacuum components we developed on portable evaporators, as well as for the preparation of crystals with high melting temperatures. First results on the in-situ preparation of molecular systems will be presented.

O 55.44 Wed 18:30 Poster F

STM / STS investigation of porphyrin and corrole molecules on surfaces — •Germar Hoffmann, Stefan Kuck, Jens Brede, and Roland Wiesendanger — Institute of Applied Physics, University of Hamburg

Porphyrins and corroles are metallo-organic compounds with a single metal ion in their central positions. Previous studies of porphyrin systems revealed unique electronic and magnetic features[1] making this class an interesting material for future spintronic devices. These spectroscopic features are influenced by the structural adsorption of the molecule on the surface. We employ scanning tunneling microscopy to compare the adsorption of tetra-phenyl-porphyrin and tri-phenyl-corrole revealing a saddle deformation of the molecule's aromatic core. The influence of the deformed molecular macrocycle on the molecular states near the Fermi energy is studied in detail by means of scanning tunnelling spectroscopy (STS). To investigate the metal-molecule interaction, molecules with different ligands and thin isolating layers of NaCl are employed to electronically decouple the molecules from the metallic substrate.

[1] H.Wende et al., Nature Materials, 6:516-519 (2007).

O 55.45 Wed 18:30 Poster F

Water adsorption on stepped and flat Pt(111) surfaces – combined TDS and STM measurements — •Alexander Picolin[1], Alex Redinger[1], Carsten Busse[1], Markus Morgenstern[2], and Thomas Michely[1] — [1]II. Physikalisches Institut, Universität zu Köln, Germany — [2]II. Physikalisches Institut B, RWTH Aachen, Germany

An extensive insight into the water-metal-bonds and a deeper understanding of corrosion and catalytic reactions require knowledge about the behaviour of water molecules on metallic surfaces. Therefore, adsorption mechanism, resulting phases, and preferred bonds of the ice double layer on Pt(111) are investigated with thermal desorption spectroscopy (TDS) and scanning tunneling microscopy (STM).

After adsorption of water at 120 K on a flat Pt(111) surface, TDS measurements only show the well-known multilayer (at 150-160 K) and monolayer desorption peaks (∼168 K). When the sample is prepared by 5 keV Ar$^+$ ions (fluence 10^{17} ions/cm^2) under grazing incidence (83° against surface normal) a rippled morphology with a high step density (∼5% of adsorption sites) results. Subsequent TDS on this surface shows a shift in temperature of the monolayer peak as well as two further desorption peaks at 180 K and 195 K. These two additional peaks are absent, if a small amount of CO is adsorbed at 400 K prior to H_2O adsorption. As CO binds preferentially to steps, the two additional H_2O desorption peaks from the clean surface are attributed to molecules bound to {100} and {111}-microfacetted steps. Binding energies and the order of desorption for step edges are determined. The preference of step edge occupation is also observed in STM images.

O 55.46 Wed 18:30 Poster F

STM observation of antiphase boundaries in Fe$_3$O$_4$(001)/MgO thin epitaxial films — •David Serrate[1], Julia M. Orna[2], Luis Morellón[2], Andre Kubetzka[1], Kirsten von Bergman[1], and Roland Wiesendanger[1] — [1]Institute of Applied Physics, University of Hamburg, Hamburg, Germany — [2]Instituto de Nanociencia de Aragón, University of Zaragoza, Zaragoza, Spain

Due to its high Curie temperature and half-metallic nature, Fe$_3$O$_4$ thin films are archetypal candidates as electrodes for spin-valve type devices. However, the spin filtering effects achieved at room temperature up to date are modest[1]. The reason is that the properties of the Fe$_3$O$_4$ surface play a mayor role on the TMR of magnetic tunnel junctions, and therefore a better understanding of the surface termination is mandatory. Several STM experiments have been published on the (001) surface of bulk single crystals, but the surface of artificial thin films remains unexplored. The most likely defects occurring in Fe$_3$O$_4$ epitaxial films are the so-called antiphase boundaries (APB)[2], which arise from the coalescence of two crystallographic domains. We report the direct observation of APB in thin epitaxial Fe$_3$O$_4$ (40 nm) by means of STM topography showing atomic resolution. Fe3O4(001) was grown on MgO(001) by pulsed laser deposition. Surface preparation for STM measurements consisted of cycles of Ar$^+$ etching and O$_2$ annealing at 5×10^{-7} mbar. The results provide a structural model for the APB and confirm the origin of the in-plane MR characteristic of ultrathin Fe$_3$O$_4$ films[2]. [1] H. Matsuda et al., Jpn. J. Appl. Phys. 41, L387 (2002) [2] W. Eerestein et al., Phys. Rev. Lett. 88, 247204 (2002)

O 55.47 Wed 18:30 Poster F

Metal coatings prepared by organometallic chemical vapour deposition (OMCVD) — •Jörn Wochnowski[1], Thimo Göllnitz[1,2], Germar Hoffmann[2], Roland Wiesendanger[2], and Jürgen Heck[1] — [1]Institute of Inorganic and Applied Chemistry — [2]Institute of Applied Physics; University of Hamburg

In microtechnology, the coating of temperature-sensitive substrates with high melting-point materials is challenging. The use of volatile organometallic compounds can be an answer to solve this ambitious task. We developed an experimental set-up for the deposition of elements, oxides, and functional composites in glass hollowware by means of OMCVD. With the first experimental set-up [1], the thermally induced decomposition of numerous elementorganic and metallorganic precursors has been tested for the deposition of catalytic or optic materials.

Here, we will present experimental data of the thermal deposition of different metals as tungsten [2] on a glass surface. We used Atomic Force Microscopy as one standard analytical surface method to obtain structural and morphological information of the deposited metal layers. We will discuss the preparation and the analytics of the prepared surfaces. With the objective to bring the deposition temperature of W(CO)$_6$ further down to room temperature, we developed a new photolytic OMCVD set-up. We will demonstrate and discuss the realization of our experimental setup.

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[2] J.Wochnowski, doctoral thesis Hamburg 2007.

O 55.48 Wed 18:30 Poster F

Study of formation and thermal stability of Fe layers on ZnO surfaces — Alexander Demund, Daniel Wett, Sylvia Reiche, Rüdiger Szargan, and •Reinhard Denecke — Wilhelm-Ostwald-Institut für Physikalische und Theoretische Chemie, Universität Leipzig, Linnéstr. 2, 04103 Leipzig

Formation and thermal stability of Fe layers on ZnO surfaces have been studied by means of X-ray Photoelectron Spectroscopy and Low Energy Electron Diffraction. Experiments were performed on the polar surfaces ZnO(0001) and ZnO(000-1) and on the non-polar (1120) surface. The results indicated a pseudo 2D growth mode for iron on ZnO at room temperature, which was less pronounced on the Zn-terminated (0001) surface. Under ultra high vacuum conditions low coverages of deposited Fe^0 on all ZnO single crystal surfaces were partially oxidized by a small fraction of residual -OH-groups and ZnO to FeO. A strong temperature dependence of the interface reactivity was found upon annealing. Starting from 200 - 300°C iron was first oxidized to bivalent iron oxide. After complete oxidation of Fe^0 to Fe^{2+} at around 400°C, Fe^{2+} reacted to Fe^{3+}. Above temperatures of 500°C the deposited metallic iron was completely oxidized to trivalent iron. Differences observed for the different surface orientations will be discussed.
Work has been supported by DFG (FG 404 Sz58/15).

O 55.49 Wed 18:30 Poster F

Investigation of MgO thin films on Mo(100) by scanning tunneling microscopy and spectroscopy — •Mike Pezzotta, Dinesh Subramaniam, Marco Pratzer, and Markus Morgenstern — II. Physikalisches Institut B, Otto-Blumenthal-Straße, RWTH Aachen and JARA-FIT, 52074 Aachen

Oxide thin films on metallic substrates offer the possibility of investigating the electronic structure of metallic or ferromagnetic atoms at low electronic coupling to the substrate. Magnesium oxide films on a molybdenum substrate are favored because of their flat and nearly defect-free epitaxial growth [1].

We studied the growth of MgO islands on Mo(100) by scanning tunneling microscopy and spectroscopy on the clean Mo surface as well as on the Mo-carbide reconstruction. MgO thin films were prepared by molecular beam epitaxy of magnesium in oxygen athmosphere ($p=1*10^{-7}$ mbar). The oxidation process has been controlled by Auger spectroscopy. Annealing temperatures in the range of 900 K to 1100 K result in MgO island sizes up to 50 nm in width and up to 1 nm in height. First spectroscopic dI/dU and dz/dU measurements are presented.

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O 55.50 Wed 18:30 Poster F

Direct metalation of phthalocyanine and tetraphenylporphyrin on Ag(111) with co-adsorbed iron atoms — •Yun Bai, Florian Buchner, Matthew Wendahl, Robert Staehle, Ina Kellner, Andreas Bayer, Hubertus Marbach, Jörg Michael Gottfried, and Hans-Peter Steinrück — Universität Erlangen-Nürnberg, Lehrstuhl für Physikalische Chemie II, Egerlandstr. 3, 91058 Erlangen, Germany

Metalloporphyrins and metallophthalocyanines are promising candidates for the functionalization of surfaces on the nanoscale because they combine a reactive metal ion with a planar organic ligand, which serves as a structure-forming element. Potential applications of such functionalized surfaces include heterogeneous catalysts with well-defined active sites and sensor systems. In this contribution, we report the in-situ preparation of related model systems, in particular Fe(II)-phthalocyanine and Fe(II)-tetraphenylporphyrin monolayers on Ag(111). Both complexes are sensitive toward oxidation and react readily with molecular oxygen, which makes the preparation of the adsorbates by ex-situ metalation of the ligands in solution and subsequent deposition difficult. Instead, we deposited monolayers of the less reactive metal-free ligands and metalated them with the stoichiometric amounts of vapour-deposited Fe atoms in an ultra-high vacuum environment. This surface-mediated redox reaction was studied with XPS and STM and was found to proceed with high yield (up to 95%). Supported by the DFG through SFB 583.

O 55.51 Wed 18:30 Poster F

Enhancement of photodesorption by vibrational excitation — •Tijo Vazhappilly[1], Stephanie Beyvers[1], Tillmann Klamroth[1], Rigoberto Hernandez[2], and Peter Saalfrank[1] — [1]Institut

für Chemie, Universität Potsdam, D-14476 Potsdam, Germany — [2]School of Chemistry and Biochemistry, Georgia Institute of Technology,Atlanta, GA 30332-0400

The effect of selective excitation of adsorbate vibrations by tailored IR laser pulses, on the photodesorption of H_2 and D_2 from a Ru(0001) surface has been investigated theoretically. A two-dimensional model is used for the Desorption Induced by Electronic Transitions (DIET) limit. A jumping wavepacket algorithm is employed with different initial states, starting from ground vibrational state to vibrationally excited states and vibrational wavepackets[1]. This model is extended to Desorption Induced by Multiple Electronic Transitions (DIMET) by incorporating electronic temperatures from femtosecond UV/vis laser excitation of metal electrons. In this regime, the IR+UV/vis strategy to control the photodesorption is realized by the Monte Carlo Wave Packet (MCWP) method [2], and Molecular Dynamics (MD) with electronic friction. Vibrational preexcitation appears to be successful in both DIET and DIMET.

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O 55.52 Wed 18:30 Poster F

Adsorption, Dissociation and Desorption of Acetylene on Steel

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One way to improve the hardness and wear resistance of crude steel is low-pressure carburisation. In this process, the surface near region of steel is enriched with carbon, produced in-situ by dissociative adsorption of hydrocarbons followed by diffusion of carbon atoms into the bulk. In order to gain a detailed understanding of this process, adsorption, dissociation and desorption of acetylene (C_2H_2) on steel at temperatures between 500 and 1200 K were studied by mass spectrometry and Auger electron spectroscopy utilising molecular beam techniques. At low temperatures ($T<700$ K), the sticking probability for C_2H_2, measured by the technique of King and Wells, is very small. Nevertheless, an increase in surface carbon coverage can be seen at 500 K, indicating a slow diffusion rate at this temperature. Upon raising temperature, the sticking coefficient reaches a maximum of 0.3 at 1000-1050 K. For even higher temperatures, the sticking probability decreases again due to nitrogen, segregating to the surface and blocking the adsorption of C_2H_2. Increasing the kinetic energy of C_2H_2 molecules by seeding with helium leads to smaller sticking coefficients at all temperatures, proposing a non-activated adsorption process.

This work was supported by BMBF (03X2506C).

O 55.53 Wed 18:30 Poster F

Chemical reactivity of the polar O-ZnO(000-1) surface investigated by vibrational spectroscopy

— •Hengshan Qiu, Yuemin Wang, and Christof Wöll — Lehrstuhl für Physikalische Chemie I, Ruhr-Universität Bochum, 44780 Bochum, Germany

Zinc oxide is an important material with a wide range of technological applications in catalysis, solar cells, as gas sensor and in semiconductor devices [1]. In catalysis, the heterogeneous catalyst system Cu/ZnO has been widely applied for the industrial methanol synthesis. Recently, the oxygen terminated polar (000-1) surface has been demonstrated to be the most active surface for methanol synthesis from syngas ($CO/CO_2/H_2$) on ZnO powders [2]. It is found that the clean, H-free O-ZnO(000-1) surface is (1x3) reconstructed and exposes 0.33 ML O vacancies. In this contribution, the interaction of different molecules (CO, CO_2 CH_2O and HCOOH) with the clean O-ZnO(000-1) surface was studied by high-resolution electron energy loss spectroscopy (HREELS), thermal desorption spectroscopy (TDS) and low-energy electron diffraction (LEED). The present results provide detailed information about the chemical reactivity of defect sites (in particular O vacancies) towards different adsorbates. The corresponding reactions can be monitored by vibrational spectroscopy.

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O 55.54 Wed 18:30 Poster F

SPA-LEED investigations on the growth of NiO films on MgO passivated Ag(001)

— •Lars Boewer[1], Bernd Zimmermann[2], and Joachim Wollschlaeger[2] — [1]Fakultät Physik / DELTA, Technische Universität Dortmund, D-44221 Dortmund — [2]Fachbereich Physik, Universität Osnabrück, D-49076 Osnabrück

Thin oxide films are important for nanoelectronic devices. For instance, they serve as tunneling barriers for tunneling magneto resistors (TMR). NiO is used for TMR devices due to its antiferromagnetic properties.

In this work we studied the growth of NiO on Ag(001) as model for lattice matched oxide films on metals. In addition, we deposited MgO films, which are also lattice matched, prior to the deposition of NiO to passivate the Ag substrate and to avoid alloying of Ni and Ag.

Oxide films were prepared by MBE of metals (Ni or Mg) in oxygen atmosphere at room temperature. The stoichiometry was investigated by AES. SPA-LEED was used to study the morphology of the oxide films at different growth stages. The NiO film initially nucleates with islands of two monolayer height. After completion of 2ML the growth continues in the layer-by-layer growth mode. Finally, we observe the formation of mosaics due to misfit dislocations.

O 55.55 Wed 18:30 Poster F

Properties of ultrathin In layers on the Ni(111) face

— •Wojciech Linhart, Tomasz Tokarz, Agnieszka Gorzelska, Zbigniew Jankowski, and Aleksander Krupski — Institute of Experimental Physics, University of Wroclaw, pl. Maxa Borna 9, 50-204 Wroclaw, Poland

The atomic structure and morphology of ultrathin In layers on the Ni(111) face deposited in ultrahigh vacuum at the substrate temperature ranging from 150 K to 700 K were investigated with the use of Auger electron spectroscopy (AES), low-energy electron diffraction (LEED) including I-V LEED and directional elastic peak electron spectroscopy (DEPES).

O 55.56 Wed 18:30 Poster F

Phases with long-range order observed in the interaction of silver with the Re($10\bar{1}0$) surface.

— •Viktor Scherf[1], Christian Pauls[1], Lyria Messahel[1,2], and Klaus Christmann[1] — [1]Institut für Chemie und Biochemie der FU Berlin, D-14195 Berlin — [2]University of Sciences and Technology H. Boumediène, U.S.T.H.B., Faculty of Chemistry, B.P.32, El-Alia 16111, Bab Ezzouar, Algiers, Algeria.

We have studied the interaction of silver with the Re($10\bar{1}0$) surface in UHV in the temperature range between 300 and 800 K by means of low-energy and medium-energy electron diffraction (LEED and MEED) as well as with temperature-programmed thermal desorption (TPD). Deposition of Ag from submonolayer to multilayer coverages was accomplished in small coverage increments; the monolayer concentration was calibrated using MEED and examined using LEED-(I,V) calculations. Short annealing at 800 K ensured thermodynamic equilibrium of the Ag phases formed, since it is not until 950 K that Ag desorbs in noticeable amounts. Within the submonolayer coverage regime the following ordered LEED phases could be observed with increasing Ag coverage: c(2x2); p(1x4); p(1x5), and (1x1), whereby all phases turn out to be uniquely correlated with temperature and surface coverage. We develop structure models of the Ag phases and discuss and compare our data with recent studies of Au on Re($10\bar{1}0$) and Ag on Ru($10\bar{1}0$) surfaces.

O 55.57 Wed 18:30 Poster F

A Monte Carlo study of surface diffusion driven growth of a single droplet

— •Robert Heimburger — Institute for Crystal Growth, Berlin, Germany

The Vapour-Liquid-Solid-Mechanism (VLS) is proven to be a promising way to grow spatially arranged seed crystals for the growth of polycrystalline silicon layers on amourphous substrates. The study of coalescence and growth of liquid metal droplets on partially wetted surfaces is of great interest as the process is an important partial step of the Vapour-Liquid-Solid-Mechanism.

We present a detailed study of the diffusion driven evolution of droplet size in dependence of growth temperature, surface roughness and deposition rate neglecting coalescences of droplets using the Monte Carlo method. Additionally spatial concentration profiles of the growing matter are discussed. The estimates will be compared with experimental results of droplet formation on a molybdenum surface by evaporation of indium.

O 55.58 Wed 18:30 Poster F

Vibrational features of copper adatoms on Cu(111)

— •Diana

Vogel, Olaf Skibbe, and Annemarie Pucci — Kirchhoff-Institut für Physik, Universität Heidelberg, Im Neuenheimer Feld 227, D-69120 Heidelberg

It is known that some stepped copper surfaces show vibrational features that are introduced by the steps [1]. The energies of some of these vibrations are higher than those of the bulk phonons. We found with high-resolution electron energy loss spectroscopy (HREELS) similar features by looking at the Cu(111) surface on which we evaporated copper at liquid nitrogen temperature. The behavior of these vibrational features will be shown as a function of the amount of added copper and the annealing temperature, respectively.

The aim of this study is to characterize the roughened surface which can serve as a nano-structured template for the adsorption of molecules. The interaction of adsorbates with the surface is known to be influenced strongly by the presence of defect sites [2].

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[2] O. Skibbe, M. Binder, A. Otto, and A. Pucci, in preparation.

O 55.59 Wed 18:30 Poster F

The growth and structure of titania films on a rhenium(0001) surface — •Susanne Schubert and Klaus Christmann — Institut für Chemie und Biochemie der FU Berlin, Germany

In view of the significance of titanium dioxide as a catalyst support for low-temperature CO oxidation we have studied the epitaxy and chemical properties of titanium dioxide films grown on a clean and oxygen-covered Re(0001) surface. Titania films were prepared by co-deposition of Ti vapor in an oxygen atmosphere at elevated temperatures ($T \geq 830$K). The structure and chemical (surface) composition of these films were analyzed by means of low-energy electron diffraction (LEED), low-energy ion scattering (LEIS) and X-ray photoelectron spectroscopy (XPS) as a function of deposition rate and film thickness starting from the monolayer regime up to concentrations of 10 to 40 monolayers. While the overall film stoichiometry is close to TiO_2 (rutile) independent of film thickness we find a moiré LEED pattern at low surface concentrations, faceting with hexagonal phases in three domains of rutile(110) rotated by 120° against each other in the medium coverage regime, and well-ordered unfaceted rutile films for thicknesses beyond ≈ 40 monolayers. The respective growth behavior can be described by a Stranski-Krastanov mechanism.

O 55.60 Wed 18:30 Poster F

The Pt_xRu_{1-x}/Ru(0001) surface alloy formation process studied by STM — •Andreas Bergbreiter, Harry E. Hoster, and R. Jürgen Behm — Institute of Surface Chemistry and Catalysis, Ulm University, D-89069 Ulm, Germany

Pt_xRu_{1-x}/Ru(0001) surface alloys were prepared by vapor deposition of Pt on a Ru(0001) single crystal, followed by annealing to 1350 K. According to high resolution STM analyses with chemical contrast, the composition of the Pt_xRu_{1-x}/Ru(0001) surface is homogeneous on both nanometer and micrometer length scale. For $x<0.8$, the amount of Pt exactly matches the initial coverage by pseudomorphic Pt islands. Even after alloy formation we find islands on the surface. These islands are more compact in shape and larger in size than the initial Pt islands, but have the same Pt:Ru ratio as the surrounding terraces. Together with the homogeneous composition, the conserved amount of Pt surface atoms means, that virtually no Pt is buried below these alloy islands. Pt deposition at high temperatures and Ru overgrowth of Pt islands show that the absence of Pt in the subsurface layer (below the islands) can be rationalized by a preference of both Pt and Ru to occupy Ru 3-fold sites. High exchange rates between Pt (Ru) adatoms and atoms in the underlying layer allow equilibration of the topmost layers. The site preferences fit well to effective pair interaction energies derived from lateral atomic distribution within the Pt_xRu_{1-x}/Ru(0001) surface alloys.

O 55.61 Wed 18:30 Poster F

Temperature effects in the growth of Ru on Pt(111) — András Berkó[1,2], •Andreas Bergbreiter[1], Petra M. Erne[1], Harry E. Hoster[1], and R. Jürgen Behm[1] — [1]Institute of Surface Chemistry and Catalysis, Ulm University, D-89069 Ulm, Germany — [2]Permanent Adress: Institute of Surface Chemistry and Catalysis, University of Szeged, H-6701 Szeged, Dóm tér 7, Hungary

The growth of Ru on Pt(111) at substrate temperatures in the range of 50-500°C was studied by high resolution STM and Auger electron spectroscopy (AES). Ru deposition at temperatures up to 250°C leads to the formation of triangular bilayer islands [1]. The lateral dimensions of these bilayer islands become more uniform with increasing substrate temperature, but show little dependence on evaporation rate and Ru coverage. At deposition temperatures of 300°C or higher, in contrast the islands are only of monoatomic height. Based on STM-imaging with chemical contrast and AES analyses, this is associated with the onset of surface alloy formation. The influence of the different strengths of Pt-Pt, Pt-Ru, and Ru-Ru interactions as well as the role of lattice mismatch effects are discussed.

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O 55.62 Wed 18:30 Poster F

Atomic-scale self-organization of Fe nanostripes on stepped Cu(111) surfaces — •Nikolay N. Negulyaev[1], Valeri S. Stepanyuk[2], Wolfram Hergert[1], Patrick Bruno[2], and Jurgen Kirschner[2] — [1]Physics Department, Martin-Luther-University, Halle-Wittenberg, 06099 Halle, Germany — [2]Max Planck Institute of Microstructure Physics, 06120 Halle, Germany

Growth of Fe nanostripes on a vicinal Cu(111) surface is investigated on the atomic scale performing molecular dynamics and kinetic Monte Carlo simulations [1]. We involve in our study the kinetic mechanisms of incorporation of Fe atoms into the stepped Cu(111) surface. The atomic processes responsible for the interlayer mass transport and the self-assembly of 1 ML high Fe stripes are identified. The role of temperature is revealed. We demonstrate that strain relaxations at steps have a strong impact on the self-assembly of one-dimensional Fe atomic structures on vicinal Cu(111).

1. N.N. Negulyaev et al., Phys. Rev. B, submitted.

O 55.63 Wed 18:30 Poster F

Influence of sputtering effects during homoepitaxial growth of Cu(100) using electron-beam evaporation — •Henning Prüser, Martin Wenderoth, Alexander Weismann, and Rainer G. Ulbrich — IV. Physikalisches Institut der Georg-August-Universität Göttingen

It is well known that ion assisted deposition influences the growth processes in thin film formation. Electron beam evaporators which apply high voltage to the crucible produces a significant fraction of ionized atoms that are accelerated to the sample. We have investigated the impact of this effect on the homoepitaxial growth of copper films using Scanning Tunneling Microscopy. During growth different electrical fields were applied to suppress ion bombardment at varied substrate temperatures. At room temperature without ion suppression a nanostructured surface is found. Rectangular shaped vacancy islands are created quite similar to those obtained by [1]. If an electric field is applied, a multilayer growth mode can be observed. Ion-free deposition at higher substrate temperatures results in a layer by layer growth. This work was supported by DFG SFB 602 TPA3.

[1] M. Ritter et al, Surface Science **348** (1996) 243-252

O 55.64 Wed 18:30 Poster F

The growth of Co on Fe/W(110)investigated by STM and STS — •Torsten Methfessel and Hans-Joachim Elmers — Johannes Gutenberg-Universität Mainz, Institut für Physik, Staudingerweg 7, D-55099 Mainz

Highly spinpolarised metals are of great interest e.g. for the application in spin-valves. Recently observed large tunneling magnetoresistance (TMR) effect values of 410 % at room temperature for Co/Fe(100) electrodes indicate a high spin-polarisation at the Fermi energy of bcc Co [1]. Instead of a (100) oriented substrate, we grow bcc Co on Fe(110), where the symmetry change from hcp to bcc becomes obvious in the (110) surface plane, in contrast to the (100) orientation. In order to prepare a Fe(110) substrate, we deposited a 8 ML Fe film on W(110) that was annealed to 500 K. The annealing results in large separated islands with an ideal Fe(110) surface, that serves as a substrate for the deposition of Co. Using scanning tunneling microscopy and spectroscopy (STM and STS) we investigated the local structural and electronic properties of the bcc Co films. The first monolayers of Co grow as pseudomorphic bcc layers, which shows periodic lattice distortions similar to the growth of Co on Cr(110) [2]. Single point spectroscopy reveals a peak of the LDOS at +1 eV in contrast to the peak at +0.6 eV observed for the second monolayer bcc Co/Cr(110), which might be explained by the differences in the lattice constants of Fe and Cr.

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O 55.65 Wed 18:30 Poster F

Adsorption of CO, O$_2$ and ethene on Pt$_x$Ce/Pt(111) surface alloys. A HREELS-, TPD-study. — Jan Markus Essen, •Conrad Becker, and Klaus Wandelt — Institut für Physikalische und Theoretische Chemie, Universität Bonn, Wegelerstrasse 12, 53115 Bonn, Germany

It is well known that alloying can change the adsorption and reaction properties of surfaces significantly. In this study we investigated the Pt-Ce system. Evaporating Ce onto Pt(111) followed by annealing to 1000 K forms ordered alloys. Depending on the cerium fraction a (2x2) and a (1,96x1,96)+(1,96x1,96)R30° LEED pattern is observed. Our TPD and HREELS study of CO, O$_2$ and ethene adsorption shows a very low reactivity of these surface alloys. Concerning CO adsorption we find a significantly decreased desorption temperature of about 280 K compared to 400 K for a CO saturation coverage on pure Pt(111). Likewise oxygen adsorbed at 90 K, followed by annealing, cannot oxidize these surface alloys. In comparison with Pt(111) neither is molecularly bonded oxygen observed at 90 K nor can desorption of oxygen caused by recombination of atomic oxygen at 750 K be detected as on Pt(111). Our results support the model for the Pt$_x$Ce/Pt(111) surface alloy consisting of a Pt Kagomé net as the top layer. Because of the low reactivity we conclude that the top layer of the surface alloy contains no Cerium-atoms.

O 55.66 Wed 18:30 Poster F

Preparation and investigation of galvinoxyl on potassium bromide — •Miriam Klusmann and Marika Schleberger — Universität Duisburg-Essen, Fachbereich Physik, Lotharstraße 1, D-47048 Duisburg, Germany

Molecular magnets are supposed to offer storage densities up to some tera bits per square inch. But before any technical application can be realized a suitable preparative method to produce well-ordered structures of such molecular assemblies is required. Most of the molecular magnets cannot be deposited on surfaces by conventional techniques like organic molecular beam epitaxy (OMBE) due to thermal decomposition of the molecules below the operating temperature of the evaporator. To avoid this problem we use a pulsed valve to spray a solution that contains molecular magnets onto the bare substrat. Preparation takes place under ultra-high vacuum (UHV) conditions. The idea is that the solvent evaporates while the molecules adsorb (ideally intact) onto the surface. We report on results obtained with the stable radical galvinoxyl (C$_{29}$H$_{41}$O$_2$) dissolved in ethanol p. a. and injected onto a freshly cleaved (100)-surface of the insulator potassium bromide (KBr). Investigation of the surface before and after injection is done by atomic force microscopy in the nondestructive dynamic mode (FM-AFM) under ultra-high vacuum conditions.

O 55.67 Wed 18:30 Poster F

Contact charging between insulators by organic molecule adsorption — •Wei Chen, Christoph Tegenkamp, and Herbert Pfnuer — Leibniz-Universität Hannover, Institut für Festkörperphysik, Appelstr. 2, 30167 Hannover, Germany

It has been shown that adsorption of simple organic acids on wide band gap insulators can introduce unoccupied electronic states in the band gap. These unoccupied states of adsorbates can lower electron excitation energy significantly, which makes it possible for charge exchanges between insulators. The adsorbates are thus decisive for contact charging problems as the electronic states of the surfaces are well defined by the them.

In this paper, the electronic states of benzoic acids attached to various functional groups are investigated by density functional theory calculations. The results show that salicylic acid (SA) and anthranilic acid (AA) are ideal for contact charging between insulators because of their higher binding energy of the uppermost π_z orbital of the COOH group. The corresponding anti-bonding state (i.e. the LUMO) is thus located closer to the VB edge of the insulators, resulting a smaller effective band gap. Moreover, the HOMO-LUMO separation of AA is 0.12 eV smaller compared to SA. Further, we represent first results of atomic force microscopy measurements which are performed on organic molecule adsorbed NaCl surface using KCl coated cantilevers in order to study contact charging between the alkali chlorides.

O 55.68 Wed 18:30 Poster F

The structure of the first layer of acetylene adsorbed on NaCl(100) — Aldo Cartagena, •Jochen Vogt, and Helmut Weiss — Chemisches Institut der Universität Magdeburg, Universitätsplatz 2, 39106 Magdeburg

Acetylene adsorbed on NaCl(100) is considered as a model system of physisorption under the conditions of a moderate lattice mismatch and, moreover, the formation of hydrogen bonds between neighboring molecules. Hydrogen bonds are known to cause red-shifts of the IR-active C–H stretch modes of the molecules. In low-energy electron diffraction experiments, a $(3\sqrt{2}\times\sqrt{2})$R45° symmetry of the first layer of acetylene is observed at 75 K, in agreement with a previous study [1]. Under the same conditions, polarization infrared spectroscopy reveals a splitting of the asymmetric stretch mode in three absorptions at 3227.3, 3230.5, and 3248.7 cm^{-1}, respectively, also in agreement with a previous study [2]. We use potential calculations to determine the structure of the adlayer and vibrational exciton theory guided by ab initio calculations to give a new assignment of the observed IR transitions to molecules on inequivalent sites, the latter being interlinked by different numbers of hydrogen bonds.

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O 55.69 Wed 18:30 Poster F

Oxygen incorporation from CO2 and H2O in Fe-doped SrTiO3 single crystals — •Florian Voigts[1], Dominik Schwendt[1], Sebastian Dahle[1], Pradyot Datta[2], Jana Grosse-Brauckmann[2], Lars Dörrer[2], Christos Argirusis[2], and Wolfgang Maus-Friedrichs[1] — [1]Institut für Physik und Physikalische Technologien, TU Clausthal, Leibnizstrasse 4, 38678 Clausthal-Zellerfeld, Germany — [2]Institut für Metallurgie, TU Clausthal, Robert-Koch-Strasse 42, 38678 Clausthal-Zellerfeld, Germany

Strontium titanate is a promising candidate for the development of a new generation of resistive high temperature oxygen sensors. The analysis of automobile exhaust is regarded as a possible main application. An interpretation of the sensors signal in such an environment will only be possible with an understanding of the cross-sensitivity of the strontium titanate for other present gases like water or carbon dioxide.

Our results for the interaction of donor-doped strontium titanate single crystals with these species are presented in this poster. Metastable Induced Electron Spectroscopy and Ultraviolet Photoelectron Spectroscopy are used to study adsorption and dissociation processes under ultra high vacuum conditions. Oxygen tracer diffusion experiments performed under realistic conditions using Secondary Ion Mass Spectroscopy as well as investigations with X-ray Photoelectron Spectroscopy and Temperature Programmed Desorption give evidence to the oxygen incorporation into the strontium titanate. Furthermore, diffusion processes can be investigated. We try to correlate the results to develop a model for the occurring interaction processes.

O 55.70 Wed 18:30 Poster F

Interaction of SrTiO$_3$ nanoparticles with reactive gases — •Dominik Schwendt[1], Florian Voigts[2], Wolfgang Maus-Friedrichs[2], Christos Argirusis[3], and Jana Grosse-Brauckmann[3] — [1]Institut für Materialien und Bauelemente der Elektronik, Leibniz Universität Hannover, Appelstr. 11A, 30167 Hannover, Germany — [2]Institut für Physik und Physikalische Technologien, TU Clausthal, Leibnizstr. 4, 38678 Clausthal-Zellerfeld, Germany — [3]Institut für Metallurgie, TU Clausthal, Robert-Koch-Straße 42, 38678 Clausthal-Zellerfeld, Germany

SrTiO$_3$ is known for its capability as high temperature oxygen sensor. The most interesting application of this sensor would be the analysis of automobile exhaust, allowing the optimisation of fuel injection and catalytic oxidation of toxic exhaust.

Metastable Impact Electron Spectroscopy as wells as Ultraviolet Photoelectron Spectroscopy are used to analyse the valence band structure of SrTiO$_3$ and its adsorbates, while we use X-ray Photoelectron Spectroscopy to check the stoichiometry of the samples. In this poster we present the results of the interaction of SrTiO$_3$, produced via a sol-gel-route, with different reactive gases, such as H$_2$O, CO$_2$, CO, and NO. The results are being compared to the interaction of these gases with SrTiO$_3$(100) single crystalls.

O 55.71 Wed 18:30 Poster F

Growth Study of Salene Molecules on NaCl(001) — •Knud Lämmle, Alexander Schwarz, and Roland Wiesendanger — Institut für Angewandte Physik, Jungiusstrasse 11a, 20355 Hamburg

Combining magnetism with the properties of organic molecules opens new options to develop unique materials. An example would be a transparent magnet. For our investigation we choose Salenes which exhibit a metallic centre and a planar structure. By exchanging the centre atoms, it is possible to tune the magnetic properties. Moreover, several molecules can be attached to each other to study the intramolecular magnetic coupling between the metallic centres via chemical bonds in such molecules. As a first step we study the growth of Co-Salene molecules using atomic force microscopy. To investigate these molecules without hybridisation effects we use the large bandgap insulator NaCl(001) as substrate. The molecules were evaporated with a homebuilt Knudsen cell at temperatures around 220 °C, while the evaporation rate was monitored by a quartz crystal microbalance. At low coverages the molecules decorate step edges only. At increased coverages the molecules form wires which also grow across large terraces. Increasing the amount of evaporated material further leads to network formation. We observed that the wires grow primarily oblique to the crystallographic axes.

O 55.72 Wed 18:30 Poster F

Spin-dependent Electron Transmission through Organized Organic thin Films — •Benjamin Göhler[1], Arne Rosenfeldt[1], Volker Hamelbeck[1], Georg F. Hanne[1], Helmut Zacharias[1], and Ron Naaman[2] — [1]Physikalisches Institut, Universität Münster — [2]Department of Chemical Physics, The Weizmann Institute, Rehovot, Israel

Electron dichroism has been reported for vapours of chiral molecules [1]. The interaction of longitudinally spin-polarized electrons with chiral molecules can be different for two enantiomers or stated the other way around for one enantiomer and electrons of opposite helicities. The attenuation of polarized electron beams shows a dependence upon the spin of the electrons.

Here photoelectrons are detected that are emitted from a gold surface covered by an organized organic thin film (OOTF). Photoelectrons excited from gold by circularly polarized light have a longitudinal spin polarization of up to 15% [2]. The photoelectron yield of gold covered with OOTF also varies with the circular polarization of the incident laser light [3]. When the photon energy applied (5.9 eV) is not sufficient to ionize the adsorbed molecules but emit electrons from the gold substrate, those results suggest that the electron transmission through the organic layer is spin dependent. To analyze this spin filter effect a new set-up is built with a small-size conventional electron polarimeter (Mini Mott) to determine the spin polarization of the transmitted electrons through the OOTF. [1] PRL 74, 4803, 1995. [2] PRL 47, 374, 1981. [3] Science 283, 814, 1999.

O 55.73 Wed 18:30 Poster F

Self-assembled monolayers on gold containing azobenzene ligands — •F. Vogel[1], M. Borg[1], F. Bretthauer[2], U. Siemeling[2], and F. Träger[1] — [1]Institut für Physik and Center for Interdisciplinary Nanostructure Science and Technology - CINSaT, Universität Kassel, Kassel — [2]Institut für Chemie and Center for Interdisciplinary Nanostructure Science and Technology - CINSaT, Universität Kassel, Kassel

Two azobenzene-derivatized 1,2-dithiolanes were synthesized and used for the preparation of self-assembled monolayers (SAM) on gold. Azobenzene derivatives can be switched between their "cis" and "trans" isomers by irradiation with light and represent the most widely studied system for photoresponsive SAMs. However, in SAMs based on thiols and symmetric disulfids on gold, the chromophores are densly packed and show little free volume to allow photoisomerisation. The binding unit of the investigated molecules with their two attachment points and increasing size should lead to considerable void spaces between the individual photoresponsive azo units. Photoswitching was confirmed by ellisometric measurements. The kinetics of film formation of the two molecules have been compared by in situ optical second harmonic generation (SHG). It has been shown that the absorption of the molecules on the gold substrate is best described by second order Langmuir kinetics for the investigated concentration of 100 μmol/l.

O 55.74 Wed 18:30 Poster F

Vapour phase deposition of biphenylthiol self-assembled monolayers — •Laxman Kankate, Andrey Turchanin, and Armin Gölzhäuser — Department of Physics, Physics of Supramolecular Systems, University of Bielefeld, D-33615 Bielefeld

Self-assembled monolayers (SAMs) with aromatic moieties caused recently a particular interest due to their applications in molecular electronics, nanolithography and biotechnology. To achieve high reproducibility of the SAM-based devices and nanostructures the utilization of high quality, well defined monolayers is necessary. The traditional *wet chemistry* preparation of SAMs suffers from solvent, ambient and substrate contaminations resulting often in poor quality of the molecular assemblies. On the contrary, the preparation of SAMs in UHV provides a high degree of control over the experimental parameters. We have studied the formation of 1,1*-biphenyl-4-thiol (BPT) and 4*-nitro-1,1*-biphenyl-4-thiol (NBPT) SAMs on Au surfaces by vapour deposition in UHV. The deposition parameters and the quality of monolayers were optimized and characterized by mass spectrometry and X-ray photoelectron spectroscopy (XPS). The formation of both SAMs was tuned from the sub-monolayer to the monolayer regimes.

O 55.75 Wed 18:30 Poster F

Vapour phase deposition of biphenylthiol self-assembled monolayers — •Laxman Kantake, Andrey Turchanin, and Armin Gölzhäuser — Department of Physics, Physics of Supramolecular Systems, University of Bielefeld, D-33615 Bielefeld

Self-assembled monolayers (SAMs) with aromatic moieties caused recently a particular interest due to their applications in molecular electronics, nanolithography and biotechnology. To achieve high reproducibility of the SAM-based devices and nanostructures the utilization of high quality, well defined monolayers is necessary. The traditional *wet chemistry* preparation of SAMs suffers from solvent, ambient and substrate contaminations resulting often in poor quality of the molecular assemblies. On the contrary, the preparation of SAMs in UHV provides a high degree of control over the experimental parameters. We have studied the formation of 1,1*-biphenyl-4-thiol (BPT) and 4*-nitro-1,1*-biphenyl-4-thiol (NBPT) SAMs on Au surfaces by vapour deposition in UHV. The deposition parameters and the quality of monolayers were optimized and characterized by mass spectrometry and X-ray photoelectron spectroscopy (XPS). The formation of both SAMs was tuned from the sub-monolayer to the monolayer regimes.

O 55.76 Wed 18:30 Poster F

Valence band spectroscopy on functionalized cellulose surfaces — •Lothar Klarhöfer[1], Kai Volgmann[1], Wolfgang Maus-Friedrichs[1], Volker Kempter[1], and Wolfgang Viöl[2] — [1]TU-Clausthal, Institut für Physik und Physikalische Technologien, Leibnizstraße 4, D-38678 Clausthal-Zellerfeld — [2]HAWK FH Hildesheim/Holzminden/Göttingen, Fakultät Naturwissenschaften und Technik, Von-Ossietzky-Straße 99, 37085 Göttingen

XPS (X–Ray Photo–Electron Spectroscopy) has become a popular technique in pulp and paper science. Nevertheless, neither XPS valence band spectra nor UPS spectra (Ultra Violet Photo Electron Spectroscopy) were reported so far, although valence band spectra is well–known to provide detailed information of the chemical state at the surfaces enabling the analysis of different treatments.

We use XPS core level and valence band spectra in combination with UPS (HeI/HeII) and MIES (Metastable Impact Electron Spectroscopy). In order to understand the recorded spectra of cellulose several spectra of so–called "fingerprint" molecules were prepared and compared with the origin cellulose spectra.

Both the Cellulose and the model surfaces, were plasma treated by a dielectric barrier discharge in order to enhance the wetting behavior of the surface. Untreated and synthetic–air–plasma treated model surfaces were compared with respect to the surface composition of functional groups. Functionalities containing oxygen were significantly increased on plasma–treated samples, shown both with core level XPS and UPS and MIES.

O 55.77 Wed 18:30 Poster F

Surface investigations of wood constituents and wood-based compounds — •Thomas Haensel[1], Andreas Comouth[1], Nicolas Zydziak[2], Pierre Lorenz[1], Syed Imad-Uddin Ahmed[1], Stefan Krischok[1], Axel Kauffmann[2], and Juergen A. Schaefer[1] — [1]Institut für Physik and Institut für Mikro- und Nanotechnologien, TU Ilmenau, P.O. Box 100565,Germany — [2]Fraunhofer Institut für Chemische Technologie (ICT), Joseph-von-Fraunhofer-Straße 7, 76327 Pfinztal, Germany

Graphite is a common bipolar plate material in direct methanol fuel cells. However, the graphite used is synthetically manufactured in an energy intensive and costly process. Efforts are underway to replace synthetic graphite with pyrolyzed compounds that consist largely of natural wood-based components. In this study, the surface characteristics of unpyrolyzed and pyrolyzed cellulose and lignin were investigated using contact angle measurements and X-ray photoelectron spectroscopy. Since an important consideration for any replacement material is its reactivity to methanol, the adsorption process on these surfaces was also examined by offering methanol. All results were compared with highly oriented pyrolytic graphite. The results indicate that methanol does not react in any significant manner with the pyrolyzed surfaces. The charging and X-ray degradation problems associated with the study of native compounds are also discussed.