O 35: Poster Session II (Polymeric biomolecular films; Nanostructures; Electronic structure; Spin-orbit interaction; Phase transitions; Surface chemical reactions; Heterogeneous catalysis; Particles and clusters; Surface magnetism; Electron and spin dynamics; Surface dynamics; Methods; Electronic structure theory; Functional molecules)

Time: Tuesday 18:15–21:45 Location: Poster B

O 35.1 Tue 18:15 Poster B

Interfacial behaviour of thin films of ionic liquids on mica — •Alexey Deyko, Florian Rietzler, Hans-Peter Steinrück, and Florian Maier — Lehrstuhl für Physikalische Chemie II, Egerlandstr. 3, Erlangen, 91058, Germany

We present a comprehensive study of ultrathin films of ionic liquids (ILs) deposited on mica surface. The ILs used are [C1C1Im][Tf2N] (1,3-dimethylimidazolium bis(trifuoromethyl)imide), and [C4C1Im][Tf2N] (1-butyl-3-octylimidazolium bis(trifuoromethyl)imide). These ILs can be successfully employed in a variety of electrochemical applications, for instance in solar cells. However, little information is available on the interfacial structure of ILs at charged surfaces. Due to its atomically flat surface and relatively simple preparation, mica is an ideal candidate for our studies. Ultra thin films of ILs in the sub-monolayer regime up to several nm thicknesses were prepared using a physical vapour deposition method under ultra high vacuum conditions. Employing angle resolved x-ray photoelectron spectroscopy (ARXPS), top and interface layers were probed with respect to adsorption behaviour, molecular orientation, and growth mode. It was found that the investigated ILs grow in a three-dimensional fashion and form islands on mica surface, even at coverages below one monolayer. That result is noticeably different to a case, when ILs are deposited on a metal surface, such as Au(111), where films grow in a layer-by-layer fashion wetting the Au surface. Supported by the DFG through SPP 1191 and by the Cluster of Excellence Engineering of Advanced Materials.

O 35.2 Tue 18:15 Poster B

Photonic Crystal Fibres Coated with Ionic Liquids in a Surface Science Approach — •Florian Rietzler[1], Till Cremer[1], Alexey Deyko[1], Florian Maier[1], Mathias Schmidt[2], Bastian Etzold[2], Peter Wasserscheid[2], and Hans-Peter Steinrück[1] — [1]Lehrstuhl für Physikalische Chemie II, Egerlandstr. 3, 91058 Erlangen — [2]Lehrstuhl für Chemische Reaktionstechnik, Egerlandstr. 3, 91058 Erlangen

Ionic liquids (ILs), organic salts with melting points below 100 °C, are often denoted as "green" solvents because of their extremely low vapour pressure. In catalysis one major problem of ILs is related to their high viscosity-induced mass transfer limitations. In the so-called Supported Ionic Liquid Phase concept this problem can be overcome by immobilizing a thin layer of IL on a solid support. Transferring this concept to Photonic Crystal Fibres (PCFs), i.e. coating the inner surface of light transmitting PCFs with a thin IL film, potentially allows in-situ monitoring of chemical reactions. Until now, the morphology of the IL film and the IL-glass interface is not well understood. In a surface science approach ultrathin films of the IL 1,3-dimethylimidazolium bis(trifluoromethylsulfonyl)imide were evaporated onto flat silica glass (as a model for the PCF surface) and investigated by ARXPS. In order to overcome the observed island formation of the IL on pristine Suprasil, two types of surface modifications were performed, both leading to a better wetting. This work was supported by DFG-SPP1191 and the Cluster of Excellence "Engineering of Advanced Materials".

O 35.3 Tue 18:15 Poster B

Silver nanosctructure formation in cinnamyl alcohol — •Sebastian Dahle[1,2], Lienhard Wegewitz[1,3], and Wolfgang Maus-Friedrichs[1,3] — [1]Institut für Physik und Physikalische Technologien, Technische Universität Clausthal, Leibnizstrasse 4, 38678 Clausthal-Zellerfeld, Germany — [2]Hochschule für Angewandte Wissenschaft und Kunst, Fakultät für Naturwissenschaften und Technik, Von-Ossietzky-Straße 99, 37085 Göttingen, Germany — [3]Clausthaler Zentrum für Materialtechnik, Technische Universität Clausthal, Leibnizstrasse 4, 38678 Clausthal-Zellerfeld, Germany

Metastable Induced Electron Spectroscopy, Ultraviolet Photoelectron Spectroscopy, X-ray Photoelectron Spectroscopy, and Atomic Force Microscopy have been employed to study the adsorption of silver and cinnamyl alcohol on Au(111) and Si(100) substrates. Initially, these investigations were carried out preceding the investigation of the adsorbtion behavior of silver on wood surfaces, where cinnamyl alcohol is used as precursor for lignin. Even though cinnamyl alcohol has only one technical application by now, some interesting properties of nanostructure formation and catalytic decomposition have been found.

O 35.4 Tue 18:15 Poster B

Inelastic tunnelling spectroscopy of protein monolayers — •Robert Lovrincic[1], Lior Sepunaru[1], Israel Pecht[2], and David Cahen[1] — [1]Department of Materials and Interfaces, Weizmann Institute of Science, Rehovot, Israel — [2]Department of Immunology, Weizmann Institute of Science, Rehovot, Israel

Electron transfer (ET) through proteins has been studied intensively in aqueous solutions. Based on our previous work on temperature-dependent current-voltage measurements across proteins in a solid-state configuration[1], we tried to gain deeper insight to the ET mechanism through macroscopic solid-state protein junctions, using inelastic tunnelling spectroscopy (IETS). IETS is a is an all-electronic spectroscopy that measures the vibronic structure of non-equilibrium molecular transport, where even Raman- and IR-forbidden transitions may be observed as strong bands. By assigning the observed peaks to known vibrations of the protein, we prove that at least some of the electrons actually pass through the proteins, a finding that presents a first step towards tracing the electron transport pathways through complex biomolecules.

1 L. Sepunaru, I. Pecht, M. Sheves, and D. Cahen, Journal of the American Chemical Society 133, 2421-2423 (2011).

O 35.5 Tue 18:15 Poster B

Covalently bonded mixed chains of Br-NDI and Br-TTP molecules — •Finn Lorbeer[1], Isabel Fernandez Torrente[1], Martina Corso[1], Lena Kaufmann[2], Max Kerbs[2], Arno Wiehe[2], Christoph A. Schalley[2], Andrew DiLullo[3], Saw-Wai Hla[3], José Ignacio Pascual[1], and Katharina J. Franke[1] — [1]Institut für Experimentalphysik, Freie Universität Berlin, Arnimallee 14, 14195 Berlin, Germany — [2]Insitut für Chemie und Biochemie, Freie Universität Berlin, Takustraß e 3, 14195 Berlin, Germany — [3]Dept. of Physics and Astronomy, Clippinger Lab 251B, Athens, OH 45701, USA

A promising route for the synthesis of a junction composed of a molecular charge donor and an acceptor on a surface resembling a diode, is the controlled formation of a covalent bond between individual organic donor and acceptor species. Here we use low temperature scanning tunneling microscopy (STM) and scanning tunneling spectroscopy (STS) to investigate the brominated naphthalenediimide (Br-NDI) and tetra(4-bromophenyl)porphyrin (Br-TPP) bond formation on Au(111).

For preparation temperatures of 300 K the Br-NDI and Br-TPP form H-bonded networks. Above 650 K annealing temperature we debrominate the two species and covalently bonded chains are formed. The electronic properties of the TPP remain unaffected after the bond formation. In contrast the flexible NDI molecule is geometrically distorted in the chains and the energy level alignment depends on this deformation as well as on the neighbors in the chain. We can change the geometric configuration of the NDI by vertical manipulation and hence shift the energy levels without affecting the covalent chains.

O 35.6 Tue 18:15 Poster B

Formation of Dysprosium clusters on Si(111)7x7 and Si(001)2x1 surfaces — •Martin Franz, Stephan Appelfeller, Michael Theurer, Monir Rychetsky, and Mario Dähne — Institut für Festkörperphysik, Technische Universität Berlin, Hardenbergstr. 36, D-10623 Berlin, Deutschland

Clusters on surfaces are of high interest because of their fascinating quantum properties and their possible application in future nanodevices or catalysis. Here, dysprosium induced clusters on the Si(111)7x7 and on the Si(001)2x1 surface were studied using scanning tunneling microscopy. The clusters were grown by molecular beam epitaxy using submonolayer metal coverages and moderate annealing temperatures. It was found that the 7x7 reconstructed Si(111) surface acts as a template for cluster formation, where the clusters grow self-organized preferentially on the faulted halves of the 7x7 unit cells. Here different cluster types could be observed, depending on the growth conditions. For post-growth annealing off-center clusters which are located at an edge of the 7x7 half unit cells form, while at deposition directly on the heated substrate the preferential growth of centered clusters is observed. On the Si(001) surface no such template effect exists. Here, clusters are observed that show a one-dimensional ordering resulting in the presence of cluster-chains on the surface. This project was supported by the DFG through FOR 1282 project D.

O 35.7 Tue 18:15 Poster B

Fabrication of nanostructures for detecting single nanoparticles using the meniscus-force-method — •Daniela Schön, Kathrin Kroth, Sabrina Darmawi, and Peter J. Klar — I. Physikalisches Institut, Justus-Liebig-Universität, Heinrich-Buff-Ring 16, DE-35392 Gießen, Germany

We present an array of holes that can be used for separating and arranging nanoparticles. The structure is created on a glass substrate via electron beam lithography (EBL), using PMMA as resist. In order to remove electrostatic charges during the EBL, a conductive polymer is applied on top of the PMMA. By creating a cavity array with lateral and vertical dimensions in the sub-micrometer range, particles with diameters smaller than 100 nm can be separated. A drop of a solution containing nanoparticles, such as TiO_2, CaO or ZnO, can be applied on top of the structure. During the evaporation of the drop the particles are drawn into the cavities by the meniscus-force. The structure containing the separated nanoparticles can be investigated by SEM and Raman imaging.

O 35.8 Tue 18:15 Poster B

Combined experimental STM and atomistic KMC modelling study of Ru cluster growth on graphene/Ru(0001) — •Albert K. Engstfeld[1], Christoph U. Lorenz[1], Harry E. Hoster[2], Yong Han[3], Jim W. Evans[3], and R. Jürgen Behm[1] — [1]Ulm University, Institute of Surface Chemistry and Catalysis, D-89069 Ulm, Germany — [2]Technische Universität München, Centre for Electromobility, 50 Nanyang Drive, Singapore 637553 — [3]Iowa State University, IPRT and Department of Physics & Astronomy, Ames, IA 50011 USA

The inhomogeneous potential energy surface (PES) for Ru on graphene/Ru(0001) leads to the formation of Ru clusters on specific trap sites within the moiré unit cells. We determine the fraction of populated moiré cells (versus coverage, deposition flux, and temperature), as well as the spatial distribution of clusters quantified by a SRO analysis. Behaviour is elucidated by KMC simulations of an atomistic model for cluster formation on a suitable non-uniform PES. The simulated evolution of the cluster density versus coverage, and the spatial cluster distribution, agree with experiments. An unusually weak dependence on deposition flux seen in experiment is not yet recovered by the current simulation parameters. Simulation also provides the cluster size distribution, not readily accessible with STM. Varying diffusion barriers for Ru used in the simulation are compatible with DFT results for Ru on flat graphene.

O 35.9 Tue 18:15 Poster B

Self-organized controlled positioning of nanoparticles based on the meniscus-force method — •Kathrin Kroth, Sabrina Darmawi, Torsten Henning, and Peter J. Klar — I. Physikalisches Institut, Justus-Liebig-Universität, Heinrich-Buff-Ring 16, DE-35392 Gießen, Germany

With the help of a periodic array of cavities, nanoparticles in solution can be separated and arranged. Arrays of cavities in the micrometer range were created in a thin layer of PMMA on a silicon substrate via EBL. A drop of solution containing nanoparticles, such as polystyrene-latex, Au and SiO_2 in the range of (300 ... 500) nm were deposited onto the array. During the evaporation of the drop the nanoparticles are shoved into the cavities by the meniscus-force. Since the meniscus-force is dependent on the contact angle, different surfactants were added to the solution. The approach of evaporating a thin film of metal on top of the structure was also used to manipulate the contact angle. A characterization of the particles inside the cavities was carried out via SEM and Raman mapping.

O 35.10 Tue 18:15 Poster B

Spin polarized surface states on stepped magnetic surfaces : ab-initio approach. — •Oleg Stepanyuk[1], Oleg Polyakov[1], and Valeri Stepanyuk[2] — [1]Faculty of Physics, Moscow State University, 119899 Moscow, Russia — [2]Max-Planck-Institut für Mikrostrukturphysik, Weinberg 2, D-06120 Halle, Germany

It was shown that surface states electrons become spin polarized above magnetic layers and nanoislands[1]. In the present work we perform the state of the art ab-initio studies of surface state electrons at steps of magnetic metals. We focus on steps of 3d metals on Cu(111) surface. We have revealed a spin-dependent charge transfer at step ages which is explained by Smoluchowski effect. Strongly inhomogeneous spin polarization of surface statates[1] at steps is revealed. Our results indicate that tunneling magnetoresistance at steps can exhibit very strong changes at the atomic scale. [1]* L. Diekhoner et. al. Phys. Rev. Lett. 90, 236801

O 35.11 Tue 18:15 Poster B

Characterization of Pt and Au nanoparticles on Fe3O4/Pt(111) thin film — •Alessandro Sala, Francesca Genuzio, Hagen Klemm, Thomas Schmidt, and Hans-Joachim Freund — Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, Germany

Pt and Au nanoparticles are catalytically active systems which show a peculiar strong metal-support interaction [1]. The formation of such nanoparticles over a iron oxide thin film has been observed in-situ and in real-time with SMART; this Low Energy and PhotoEmitted Electron Microscope can combine microscopy, spectroscopy and diffraction with high resolution and transmission to collect information about the morphology, the chemical distribution and the structural and electronic properties of complex systems. Particularly, XPEEM images reveal under particular conditions the formation by dewetting of FeO domains and the different nucleation of Au nanoparticles on this domains respect to the Fe3O4 area. LEEM, LEED, XPEEM and XPS permits to characterize the growth, the morphology and the electronic properties of Pt nanoparticles and their encapsulation by FeO, under different deposition conditions. [1] Z.-H. Qin, M. Lewandowski, Y.-N. Sun, S. Shaikhutdinov, and H.-J. Freund, J. Phys. Chem. C 2008, 112, 10209-10213

O 35.12 Tue 18:15 Poster B

Three-dimensional TiO2 nanotube arrays for photo-device application — •Ahmed al-Haddad[1,2], Yaoguo Fang[1], Huaping Zhao[1], and Yong Lei[1] — [1]Fachgebiet 3D-Nanostrukturierung, Institut für Physik & Zentrum für Mikro- und Nanotechnologien (ZIK MacroNano), Technische Universität Ilmenau, 98693 Ilmenau, Germany. — [2]Department of Physics, College of Science, University of Al-Mustansiryah, Baghdad, Iraq

Thin films of high purity titanium were deposited on p-Si surface by physical vapour deposition (electron beam deposition) and followed by anodization of the deposited titanium thin film in an ethylene glycol solution at room temperature. TiO2 nanotubes are well aligned and organized into high-order uniform arrays. The morphology and crystallization of the resulting three-dimensional TiO2 nanotubes were investigated by scanning electron microscopy and X-ray diffraction. Current-voltage and capacitance-voltage characteristics and photo responsivity was measured for these arrays.

O 35.13 Tue 18:15 Poster B

Surface morphology of Silicon nanowires in dependence of different doping concentrations — •Stefan Weidemann, Ulrike Heiden, Jürgen Sölle, and Saskia Fischer — Neue Materialien, Institut für Physik, Humboldt-Universität zu Berlin, 12489 Berlin

Silicon nanowires (SiNWs) with rough surfaces have strongly decreased thermal conductivities and, hence, are promising candidates for thermoelectric devices [1]. However, the mechanism of formation of rough surfaces is still unclear and remains to be investigated. Here, we concentrate on producing NWs of defined length and study their structural and surface properties.

We fabricate SiNW arrays on wafer scale with tuneable lengths between 10-50 μm, and diameter in the range between 50-300 nm by the method of metal-assisted chemical etching [2]. We investigate the preparation of solid, rough and porous NW surfaces of different Boron-doped Si-substrates with resistivities of 5 mΩcm, 20Ωcm and $>$10kΩcm.

[1] A. I. Hochbaum et al., Nature 451, 163 (2008)

[2] M.-L. Zhang et al., J. Phys. Chem. C, 112 2008

O 35.14 Tue 18:15 Poster B

Manipulating and contacting single InAs Nanowires at GaAs edges — •Kilian Flöhr[1], Yusuf Günel[2], Kamil

Sladek[2], Robert Frielinghaus[2], Hilde Hardtdegen[2], Carola Meyer[2], Marcus Liebmann[1], Thomas Schäpers[1,2], and Markus Morgenstern[1] — [1]II. Physikalisches Institut, RWTH Aachen and JARA Jülich Aachen Research Alliance, 52074 Aachen, Germany — [2]Peter Grünberg Institut, Forschungszentrum Jülich and JARA Jülich Aachen Research Alliance, 52425 Jülich, Germany

We investigated methods to spatially control InAs nanowires on a substrate using micromanipulators attached to an optical microscope with the goal of producing InAs tips for scanning tunneling microscopy. The wires, which were grown by metalorganic vapor phase epitaxy (MOVPE) on a GaAs wafer without catalysts, could be picked up individually using a sharp indium tip exploiting adhesion forces. Later, the wires were placed with submicrometer precision onto the desired position somewhere at the edge of a cleaved GaAs wafer or on other substrates, e.g. a perforated Si_3N_4 membrane [1]. We established a new method to realize ohmic contacts for partly suspended nanowires at the wafer edge with standard electron beam lithography.

[1] K. Flöhr, M. Liebmann, K. Sladek, H.Y. Günel, R. Frielinghaus, F. Haas, C. Meyer, H. Hardtdegen, Th. Schäpers, D. Grützmacher, M. Morgenstern, Rev. Sci. Instrum. 82, 113705 (2011)

O 35.15 Tue 18:15 Poster B

***p*- and *n*-type Silicon Nanowires from Metal-Assisted Chemical Etching** — •U. Heiden[1], J. Sölle[1], S. Weidemann[1], R. Heimburger[2], T Teubner[2], T. Boeck[2], R. Fornari[2], and S.F. Fischer[1] — [1]Neue Materialien, Institut für Physik, Humboldt-University zu Berlin, D-10099 Berlin — [2]Leibniz-Institut für Kristallzüchtung, Max-Born-Str. 2, D-12489 Berlin

Metal-assisted chemical etching (MACE) is a top-down procedure to form silicon nanowires (SiNWs) [1]. A precise control of etching parameters and the understanding of their influence on the nanowire morphology are topical research issues. They are extremely important to achieve process reproducibility.

Vertical and single crystalline SiNWs were produced with a two-step MACE procedure. Silver nanoparticles are used as catalyst. The etchant includes hydrofluoric acid (HF) and hydrogen peroxide (H_2O_2). We investigate the difference between highly doped p and n SiNWs regarding to the length, porosity and their density on the wafer.

p-type SiNWs are longer and show a higher density on the wafer compared to n-type NWs. Longer etching times lead to longer NW lengths. Increasing the concentration of H_2O_2 in the etchant, accelerates the etching reaction and decreases the NW density. A higher growth rate causes the NWs to stick together at the top and form sheaves which is in accordance with the previous report in [1].

[1] M. Zhang et al., J. Phys. Chem. C 112, 4444-4450 (2008).

O 35.16 Tue 18:15 Poster B

Stability of In/Si(111)-(4x1) nanowires — •Martin Babilon, Stefan Wippermann, Uwe Gerstmann, and Wolf Gero Schmidt — Universität Paderborn, Germany

Quasi one-dimensional structures, such as artificial atomic-scale wires, have attracted considerable attention recently [1]. They do not only show fascinating physical properties, but also have a large technological potential, e.g., as atomic-scale interconnects. Highly anisotropic surface superstructures are suitable model systems to explore atomic-scale wires both experimentally and computationally. The In/Si(111)-(4x1) surface [2, 3] is probably the most intensively investigated system in this context.

In this work, we present first-principles calculations on the influence of relativistic effects affecting the stability of (4x1) and (8x2) surface. A reversible phase transition from the metallic Si(111)-(4x1)-In zigzag chain structure to an insulating (8x2) reconstruction below 125 K is observed [4]. Here, our goal is to investigate the influence of relativistic effects and the treatment of the In core electrons on the phase transition temperature.

[1] N. Nilius, T. M. Wallis and W. Ho, Science 297, 1853 (2002).

[2] O. Bunk et al., Phys. Rev. B 59, 12228 (1999).

[3] S. Wippermann, N. Koch, W. G. Schmidt, Phys. Rev. Lett. 100, 106802 (2008).

[4] A. A. Stekolnikov, K. Seino, F. Bechstedt, S. Wippermann, W. G. Schmidt, Phys. Rev. Lett. 98, 026105 (2007).

O 35.17 Tue 18:15 Poster B

Tomonaga-Luttinger Liquid Behavior in Au/Ge(001) Nanowires — •Sebastian Mietke[1], Christian Blumenstein[2], Jörg Schäfer[2], Sebastian Meyer[2], Michael Lochner[1], René Matzdorf[1], and Ralph Claessen[2] — [1]Fachbereich Naturwissenschaften, Experimentalphysik II, Universität Kassel, 34132 Kassel, Germany — [2]Physikalisches Institut, Universität Würzburg, 97074 Würzburg, Germany

Atomic nanowires formed by self-organization of metal adatoms on semiconductor surfaces offer a vast playground for physics in low dimensions. Recently, Au-induced chains on Ge(001) have been found to exhibit Tomonaga-Luttinger liquid behavior (TLL) [1], which has not been found in a surface system before. Here we scrutinize the electronic properties of these Au chains by scanning tunneling spectroscopy (STS) and angle-resolved photoemission (ARPES) over a wide temperature range. Density of states maps reveal a 1D conduction path in real space, thereby clearly identifying conducting filaments in chain direction over a wide energy range. A power-law behavior upon energy is found in the density of states, characteristic of a TLL. The corresponding exponent α is found independently by both STS and ARPES. Furthermore, *universal scaling behavior* is observed as a hallmark of TLL physics. This renders the Au/Ge(001) chains the first TLL system at a surface, opening new possibilities to probe modified interactions from specific atomic configurations. [1] Nature Physics, Vol. 7, 776-780 (Oct. 2011).

O 35.18 Tue 18:15 Poster B

Sensitive gas sensor device obtained from the combination of 3D surface nano-patterns technique with atomic layer deposition — Zhibing Zhan[1,2], Yan Mi[1,2], Hui Sun[1,2], Fabian Grote[1,2], Huaping Zhao[1,2], and •Yong Lei[1,2] — [1]Fachgebiet 3D-Nanostrukturierung, Institut für Physik & Zentrum für Mikro- und Nanotechnologien (ZIK MacroNano), Technische Universität Ilmenau, 98693 Ilmenau, Germany — [2]Institut für MaterialPhysik, Westfälische Wilhelms-Universität Münster, 48149 Münster, Germany

Combined atomic layer deposition (ALD) with an innovative three-dimensional (3D) surface nano-structuring technique, ultrathin alumina membranes (UTAMs), we obtained a gas sensor device with sensitivity reaching PPB level to NO2. To our knowledge, this value has not been reported before for commercial gas sensors. Due to the characteristic of high regularity and controllability from ALD and our 3D nano-patterns technique, it is feasible to investigate the surface chemistry and physics, and hence to optimize the parameters of the gas sensor device. Our method used to prepare this gas sensor device is compatible to semiconductor device industry, which exhibit tremendous application potentials in the fields of environmental protection and atmospheric quality monitoring.

O 35.19 Tue 18:15 Poster B

Confined metallic thin films obtained by epitaxy on Si nanorods — •Lisa Kühnemund, Christoph Tegenkamp, and Herbert Pfnür — Institut für Festkörperphysik, Leibniz Universität Hannover

Understanding the properties of structures on the nanoscale is the key to realize miniaturization in electronic systems. Transport and local spectroscopy of thin but spatially extended Ag layers performed so far have revealed that indeed the morphology in metallic films is essential for (mesoscopic) transport [1,2]. We are interested in the effect of confining these films to structures on the nanoscale. This enables us to control also the current paths and monitor the effective defect structures.

To obtain these structures we used Si nanorods as masks for growing constricted nano-sized Ag films. The Si nanorods of 1μm in length and 100 nm in diameter [3] were transferred, after an HF-dip, onto Si substrates. The deposition of Ag at low temperatures reveals metallic and contiguous films of a few atomic layer thickness. First results of this technique as well as local transport measurements obtained by means of a 4 point probe STM-SEM system will be presented.

[1] M. Henzler et al., Phys. Rev. B **58**, 10046 (1998).

[2] J. Schmeidel et al., Phys. Rev. B **80**, 115304 (2009).

[3] The Si rods were grown by phase shift lithography and plasma etching at the IMTEK, Freiburg.

O 35.20 Tue 18:15 Poster B

Large area Zirconium carbide surface nanopatterns towards smart sunlight-heat conversion — Zhenyang Wang[1,2], Hui Sun[1,2], Yan Mi[1,2], Fabian Grote[1,2], Huaping Zhao[1,2], and •Yong Lei[1,2] — [1]Fachgebiet 3D-Nanostrukturierung, Institut für Physik & Zentrum für Mikro- und Nanotechnologien (ZIK MacroNano), Technische Universität Ilmenau, 98693 Ilmenau, Germany. — [2]Institut für MaterialPhysik, Westfälische Wilhelms-Universität Münster, 48149 Münster, Germany

Manipulation and/or conversion of sunlight energy are eternal research topics, since the inexhaustible solar energy is one of the most ideal candidates to conquer the increasingly terrible energy sources crisis. In this work, highly regular ZrC nanopatterns were assembled, by combination of an atomic layer deposition (ALD) and ultra-thin alumina membranes (UTAMs). The as-grown ZrC nanopatterns are in large area up to several square centimeters, and can be self-supported. Assisted with the sacrificed zinc oxide, size and spacing of the nanopatterns can be manipulated in even larger scale. Solar thermal property investigation shows that this kind of carbide of the transition metal can efficiently convert the sunlight into heat. This kind of nanopatterns has great potential in both solar-thermo usage and solar-thermo enhanced thermo-chromic smart windows.

O 35.21 Tue 18:15 Poster B

Single one-dimensional nanolines and atom chains on the semiconductiong Si(001) surface — •Sigrun A. Köster[1], François Bianco[1], James G. H. Owen[1], David R. Bowler[2], and Christoph Renner[1] — [1]University of Geneva, Switzerland — [2]University College London/London Centre of Nanotechnology, UK

Single-atom chains on a wide gap substrate are a very attractive embodiment of a truly one-dimensional system to explore the remarkable physical properties emerging in such low dimensions. We present examples of self-assembled one-dimensional systems on the Si(001) surface, that is, Bi nanolines [1], Haiku stripes [2,3] and single atom Mn chains. All lines grow perpendicular to the Si(001) dimer rows, at densities which can be adjusted by means of the growth parameter. Therefore we can establish chains isolated on a semiconducting background or produce a dense array of possibly interacting chains. High resolution scanning tunneling microscopy (STM) micrographs are in perfect agreement with density functional theory (DFT), providing detailed insight into the chain structures. We further discuss low temperature STM spectroscopy suggesting that our chains are indeed suitable candidates to investigate the electronic properties in one dimension.

[1] J. H. G. Owen, K. Miki, D. R. Bowler, J. Mater. Sci. **41** (2006) 4568

[2] F. Bianco, J. H. G. Owen, S. A. Köster, D. Mazur, Ch. Renner and D.R. Bowler, Phys. Rev. B **84**, 035328 (2011)

[3] J. H. G. Owen, F. Bianco, S. A. Köster, D. Mazur, D. R. Bowler and Ch. Renner, Appl. Phys. Lett. **97** (2010) 093102

O 35.22 Tue 18:15 Poster B

Fabrication and the characterization of the electrical, optical and field emission properties of regular ZnO and PbSe nanowires arrays — •Yaoguo Fang[1,2], Kin Mun Wong[1,2], André Devaux[3], Liaoyong Wen[1,2], Luisa De Cola[3], and Yong Lei[1,2] — [1]Fachgebiet 3D-Nanostrukturierung, Institut für Physik & Zentrum für Mikro- und Nanotechnologien (ZIK MacroNano), Technische Universität Ilmenau, 98693 Ilmenau, Germany. — [2]Institut für Materialphysik, Westfälische Wilhelms-Universität Münster, 48149 Münster, Germany. — [3]Physikalisches Institut, Westfälische Wilhelms-Universität, 48149 Münster, Germany.

ZnO nanowires (NWs) and nanostructures of different length and shape were fabricated on silicon substrates by different methods such as chemical vapour deposition (CVD), hydrothermal or by chemical etching of the NWs grown by the CVD process. Well aligned ZnO NWs arrays of different length and size could be obtained by the CVD method and the shape of the NWs could be modified by chemical etching which produces needlelike ZnO NWs arrays. Conversely, doping the ZnO NWs with indium produces leaf-like ZnO nanostructures. With the use of the dry contact printing method, the regular and long ZnO NWs arrays could be used for the realizations of the NWs in Schottky device applications. In addition, the electrical, optical, stoichiometric, doping concentrations, field emission as well as the defect properties of the different morphologies of the ZnO nanostructures were obtained by a number of different spectroscopic techniques. On the other hand, p-PbSe nanowire arrays have also been fabricated and characterized.

O 35.23 Tue 18:15 Poster B

Fabrication and Characterization of Self-Assembled and Self-Aligned Single-Walled Carbon Nanotubes — •Harald Budde, Nicolai Hartmann, Nina Rauhut, and Achim Hartschuh — Department Chemie und CeNS, LMU, München, Germany

We report on the fabrication of horizontally aligned single-walled carbon nanotube arrays and their electro-optical properties. The arrays were obtained via a simple solution-based evaporation method on different substrates and were characterized by atomic force and optical microscopy [1, 2]. The nanotube alignment was determined by polarization-sensitive photoluminescence (PL) measurements. Electrically contacted arrays exhibit ohmic transport characteristics. Upon applying a bias voltage, electroluminescence (EL) from semiconducting nanotubes could be detected [3]. We investigate the bias dependence of the electroluminescence and compare PL and EL spectra for the same sample position. Arrays of aligned nanotubes are rather robust and bright sources of broad range emission as compared to single nanotubes and could be useful for optoelectronic applications.

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[2] M. Engel, J. Small, M. Steiner, M. Freitag, A. Green, M. Hersam, P. Avouris, ACS Nano 2 (12), 2445-2452, 2008.

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O 35.24 Tue 18:15 Poster B

Embedding Nanowires by means of Spin Coating — •Jan Schmidtbauer, Franziska Schuette, Roman Bansen, Thomas Teubner, and Torsten Boeck — Leibniz-Institute for Crystal Growth

Nanowires are promising structures for future optoelectronic devices as well as for thermoelectric applications, gas sensors and Li-ion batteries. Typically, nanowires are removed from the substrate for electric characterization. However, contacting nanowires turns out to be challenging without removing them from the substrate. For this purpose, embedding nanowires in an insulating matrix which is protruded by the nanowire tips can provide a promising way to contact the wire using an AFM. We propose an embedding process by means of spin coating hydrogen silsesquioxane (HSQ) and curing the layer subsequently. The curing process is conducted at temperatures up to 700°C. Thus, the HSQ layer transforms from a Si-O-Si cage-like structure into a Si-O-Si network (SiO_2). Different approaches are compared to uncover the nanowire tips.

O 35.25 Tue 18:15 Poster B

Directional photochemical growth in gold nanoparticle arrays — •Susan Derenko[1], Andrew Sarangan[2], and Thomas Härtling[1] — [1]Fraunhofer Institute for Nondestructive Testing, Dresden Branch, Maria-Reiche-Str. 2, 01109 Dresden, Germany — [2]Electro-Optics Program, University of Dayton, 300 College Park, Dayton, Ohio, USA

Plasmonic nanoparticle arrays are interesting building blocks for optical sensors. For their integration into devices one may wish to modify their geometry locally within an array to tune the surface plasmon resonance in certain array sections. We present a method to induce local particle growth by exposure of lithographically fabricated Au-nanoparticle arrays to a HAuCl4 solution. Illumination of the system activates the gold ions in solution, whereas the nanoparticles act as seeds and induce particle growth. We monitor the modification via the shift of the plasmon resonance wavelength. For discoidal particles a growth preferentially perpendicular to the array plane is obtained resulting in a blue-shifted resonance. These findings are supported by AFM and SEM measurements and simulations.

O 35.26 Tue 18:15 Poster B

Coupling of plasmons to molecular excitons — •Hongdan Yan[1], Peter Lemmens[1], Johannes Ahrens[2], Martin Bröring[2], Sven Burger[3], Gerhard Lilienkamp[4], Winfried Daum[4], Ulrich Krieg[5], Herbert Pfnür[5], Fatih Kalkan[5], Karina Morgenstern[5], Aidin Lak[6], and Meinhard Schilling[6] — [1]IPKM, TU-BS, Braunschweig, Germany — [2]IAAC, TU-BS, Braunschweig, Germany — [3]ZIB, Berlin, Germany — [4]IEPT, TU Clausthal, Germany — [5]FKP, LU Hannover, Germany — [6]EMG, TU-BS, Braunschweig

We investigate plasmon/molecule interaction using Au nanowire arrays that have strongly polarized plasmonic modes. The energy of the longitudinal mode is tuned by varying the aspect ratio of the nanowires. A coupling to molecular excitons is evident from an analysis of the lineshape of the optical absorption. Theoretical modelling of the plasmonic spectrum confirms our experimental findings. Work supported by B-IGSM and NTH School for Contacts in Nanosystems.

O 35.27 Tue 18:15 Poster B

Instability types at ion-assisted alloy deposition: from surface to bulk nanopatterning — Gintas Abrasonis[1] and •Klaus Morawetz[2,3] — [1]Institute of Ion Beam Physics and Materials Research, Helmholtz-Zentrum Dresden Rossendorf, PF 51 01 19, 01314

Dresden, Germany — [2]Münster University of Applied Sciences, Stegerwaldstrasse 39, 48565 Steinfurt, Germany — [3]International Institute of Physics (IIP) Av. Odilon Gomes de Lima 1722, 59078-400 Natal, Brazil

Ion irradiation assistance of the film growth has a strong impact on structural properties. Here, we demonstrate that ion irradiation of growing binary alloys leads to the formation of composition-modulated surface patterns. Be means of linear stability analysis we show that the ion-to-atom arrival ratio is the pattern control parameter. Close to the instability threshold we identify different regimes of instabilities driven by ion-induced surface roughness processes or roughness-composition feedback interactions. In particular, the synergistic effects of the curvature-dependent displacement coupling to the preferential sputtering or to the diffusivity are found to induce instabilities and pattern formation. Depending on the film growth and ion-irradiation conditions the instabilities show stationary or oscillating behavior. This presents opportunities to grow 3D laterally or vertically ordered nanostructures.

O 35.28 Tue 18:15 Poster B

Diamond-Like Carbon Coatings on Industrial Polyethylene Surfaces — •Magdalena Rohrbeck[1], Christian B. Fischer[1], Stefan Wehner[1], Matthias Richter[2], and Dieter Schmeisser[2] — [1]Universität Koblenz-Landau, IfIN - Physik, 56070 Koblenz, Germany — [2]BTU Cottbus, Angewandte Physik II / Sensorik, 03046 Cottbus, Germany

Synthetic materials are used in a wide variety of fields. Depending on the intended application the plastic material must meet specific requirements. Since the material always interacts with its environment, particular attention is required regarding the surface. Possible damage of the plastic material and further risks could be caused by the adhesion of bacteria, biofilm formation and encrustations. Therefore, bacteria-repellent coatings and surface-modified materials that allow for an effective removal of adhered bacteria are of extremely high interest for many applications. In this study Polyethylene (PE) is chosen as simplest model for relevant plastic materials. Surface modification of PE samples is accomplished by plasma-deposited diamond-like carbon (DLC) coatings to achieve increased abrasion strength and bacterial resistance. Two types of nanometer-scaled DLC films with different layer thicknesses are compared by multiscale microscopic analysis. Further spectroscopic measurements with synchrotron radiation are performed. These results will provide an enhanced understanding of layer formation at the interface between the basic plastic material and the DLC coating and will possibly lead to optimal parameters for the surface coating to achieve improved product characteristics.

O 35.29 Tue 18:15 Poster B

Replication of nanometer size structures by laser embossing in thin metal foils — •Martin Ehrhardt, Pierre Lorenz, and Klaus Zimmer — Leibniz Institut für Oberflächenmodifizierung, Permoserstr. 15, 04318 Leipzig

Laser embossing is a micromanufacturing technology which enables the direct fabrication of three dimensional structures in metal foils. In the present study a novel arrangement of pulsed laser microembossing is introduced which allows a more flexible fabrication process with laser microembossing. To demonstrate the capability of the manufacturing process micro and nanostructures were successfully transferred from moulds into silver and copper foils by using UV Excimer laser pulses. The replicated patterns had high accuracy regarding the shape and the spatial resolution. An almost linear correlation between the used laser fluence and the height of the embossed microstructures was observed for both investigated materials. The achieved surface qualities were analysed with scanning electron microscopy (SEM), Atomic Force Microscopy (AFM) and reflection measurements.

O 35.30 Tue 18:15 Poster B

Complex quantum well states/resonances in magnetic thin films — •Christoph Seibel[1], Andreas Nuber[1], and Friedrich Reinert[1,2] — [1]Physikalisches Institut, Experimentelle Physik VII und Wilhelm Conrad Röntgen Research Center for Complex Material Systems (RCCM), Universität Würzburg, D-97074 Würzburg — [2]Gemeinschaftslabor für Nanoanalytik, Karlsruher Institut für Technologie KIT, D-76021 Karlsruhe

Low dimension effects are attracting more interest as they are becoming more relevant for future applications. In particular ultra thin Ni or Fe films are suitable model systems for nanostructured magnetic devices.

Using angle-resolved photoelectron spectroscopy (ARPES) we measured quantum well states/resonances in the close vicinity to the Fermi energy along high symmetry directions and the Fermi surface of the Fe/W(110) and Ni/W(110) films. In Fe/W(110) we find minority quantum well states, which are highly anisotropic in their dispersion due to the rather weak structural anisotropy of the bcc (110) crystal surface. Due to hybridisation effects of the measured quantum well states in Ni/W(110), the origin of the apparent splitting remains to be discussed.

O 35.31 Tue 18:15 Poster B

Two-site Kondo effect in atomic chains — Nicolas Néel[1], Richard Berndt[1], •Jörg Kröger[2], Tim Wehling[3], Alexander Lichtenstein[3], and Mikhail Katsnelson[4] — [1]University of Kiel, Germany — [2]Technical University of Ilmenau, Germany — [3]University of Hamburg, Germany — [4]University of Nijmegen, The Netherlands

Linear $CoCu_nCo$ clusters on Cu(111) are fabricated by means of atomic manipulation. They represent a two-site Kondo system with tunable interaction. Scanning tunnelling spectroscopy reveals oscillations of the Kondo temperature T_K with the number n of Cu atoms for $n \geq 3$. Density functional calculations show that the Ruderman-Kittel-Kasuya-Yosida interaction mediated by the Cu chains causes the oscillations. Calculations find ferromagnetic and antiferromagnetic interaction for $n = 1$ and 2, respectively. Both interactions lead to a decrease of T_K as experimentally observed. Financial support through SFB 668 is acknowledged.

O 35.32 Tue 18:15 Poster B

X-ray spectroscopic investigation of YVO_3 — •Olga Schuckmann[1], Stefan Bartkowski[1], Anna Buling[1], Christine Derks[1], Karsten Küpper[2], Stephen Blundell[3], Ewa Talik[4], and Manfred Neumann[1] — [1]Fachbereich Physik, Universität Osnabrück, Germany — [2]Abteilung Festkörperphysik, Universität Ulm, Germany — [3]Clarendon Laboratory, University of Oxford, United Kingdom — [4]University of Silesia, Institute of Physics, Katowice, Poland

Orthovanadate YVO_3 is a particularly interesting material, due to multiple orbital-, spin ordering and structural phase transitions as a function of temperature. The dynamic of such phase transition plays a key role in optical rewritable data storages, due to the limitation of the switching rate by the phasechange rate.

Moreover YVO_3 is a strongly correlated electron system, thus the interplay between the kinetic energy and Coulomb interaction manipulates the electronic and magnetic properties of matter. Due to the strong correlation between d electrons a variety of physical properties, such as Mott transition and so insulating phases, can occur.

By means of X-ray spectroscopic techniques XPS, XES and XAS, the electronic structure and microscopic formation of physical properties of YVO_3, as the origin of the band gap, satellites and the valence states are investigated. As a first result we identified YVO_3 as a real Mott-insulator with a nominal band gap of minimum 1.1 eV.

O 35.33 Tue 18:15 Poster B

Formation of an ideal Schottky barrier by Au/n-type β-Ga_2O_3 — •Mansour Mohamed[1], Christoph Janowitz[1], Klaus Irmscher[2], and Recardo Manzke[1] — [1]Institute of Physics, Humboldt University of Berlin, Newtonstr. 15, D-12489 Berlin, Germany — [2]Leibniz Institute for Crystal Growth, Max-Born-Str. 2, D - 12489 Berlin, Germany

High resolution angular-resolved photoelectron spectroscopy (ARPES) was applied to study the formation of a Schottky barrier on cleaved β-Ga_2O_3 single crystals with a carrier concentration of 6x10^{16} cm^{-3}, which were grown by the Czochralski method. A coverage-dependent surface photovoltage effect induced by the synchrotron radiation was observed. The shift of the valence band- and semicore- states at low Au- coverage and the work functions of Au and β-Ga_2O_3 were determined in situ by ARPES. From these experimental data the Schottky barrier height was found to be 1.01 eV in nearly perfect agreement to the value of 1.07 eV obtained from the current-voltage characteristics. The system Au/n-type β-Ga_2O_3 matches nearly ideally the characteristics of a pure Schottky barrier.

O 35.34 Tue 18:15 Poster B

Spin-orbit splitting in the valence bands of ZrS_xSe_{2-x} — •Mohamed Moustafa, Ali Ghafari, Christoph Janowitz, and

Recardo Manzke — Institut für Physik, Humboldt Universität zu Berlin, Newtonstr. 15, D-12489 Berlin, Germany

Angle-resolved photoemission spectroscopy using synchrotron radiation was performed for ternary layered transition metal dichalcogenides ZrS_xSe_{2-x}, where x varies from 0 to 2. A characteristic splitting of the chalcogen p-derived valence bands along high symmetry directions was observed. The splitting size at the A point of the Brillouin zone is found to increase from 0.06 eV to 0.31 eV with increasing atomic number of the chalcogenide as progressing from ZrS_2 towards $ZrSe_2$, respectively. An almost linear behaviour of the splitting size upon the composition parameter x is observed. Our electronic structure calculations based on the density functional theory prove that this splitting is due to spin-orbit (SO) coupling. When considering spin-orbit coupling, the degeneracy of the valance bands is lifted.

O 35.35 Tue 18:15 Poster B

Two dimensional Rare-Earth ordered alloys — •Lucia Vitali[1,2] and Enrique Ortega[1,3] — [1]Material Physics Center- University of Basque Country, San Sebastian (Spain) — [2]Ikerbasque Foundation, Bilbao (Spain) — [3]Fisica Aplicada, University of Basque Country (spain)

The reported fast magnetization/demagnetization, key features for spintronics and data storage, has raised the scientific and technological interest for thin ferromagnetic layers supported on non-magnetic metal-substrates. The physical principle behind these observations is the interaction between quasi-particles and the role of the interface. Recent work has reported on the formation of a new ordered stoichiometric alloy of GdAu2 formed by deposition of Gd atoms on Au(111) surface at high temperatures [1]. The observed layer by layer growth shows different structural, electronic and magnetic properties with respect to bulk GdAu2 structure although the stoichiometric structure is preserved. Indeed, contrary to the antiferromagnetic behaviour of this alloy as bulk material, the first two layers of GdAu2 grown on Au(111) show a ferromagnetic character [1]. Here, we report that, similarly to GdAu2, also GdAg2 and GdCu2 surface alloys can be obtained. Topographic and spectroscopic characterization of the local density of state of the three epitaxially grown surface alloys of Gd have been performed with a commercial 1K-STM. Here, the similarity and peculiarity of these surface alloys will be explained in terms of the influence of the s, p and d orbitals of the supporting substrates. [1] M.Corso, et al. PRL 105, 016101 (2010)

O 35.36 Tue 18:15 Poster B

Two-dimensional fitting data analysis in Angle-resolved photoemission spectroscopy — •Lucas Barreto, Richard Hatch, Marco Bianchi, and Philip Hofmann — Department of Physics and Astronomy, Interdisciplinary Nanoscience Center, Aarhus University, 8000 Aarhus C, Denmark

Angle-resolved photoemission spectroscopy (ARPES) is a well-established technique used to investigate the electronic properties of materials. ARPES data is frequently analyzed by considering scans taken at fixed emission-angle (EDC) or binding energy (MDC). In a number of cases, however, this approach does not permit one to extract all the useful information and may even lead to a misinterpretation of results [1]. Furthermore, recent ARPES developments have heightened the importance of analyzing the entire two-dimensional data set. Assuming an initial dispersion and a self-energy, the spectral function is calculated and then, using a search procedure, the parameters are optimized in order to obtain a good agreement between the measured and calculated spectra. The customary way to perform this search is to minimize χ^2. In this work, we propose an alternative way of comparing the calculated and the measured spectra that gives more weight to the regions with higher intensities by using derivatives. We will present results of both methodologies for ARPES measurements on Bi_2Se_3 exposed to CO [2] and compare the two methods in order to verify the applicability of the suggested approach.

[1] I. A. Nechaev et al. PRB, **80**,113402 (2009).

[2] M. Bianchi et al. PRL,**107**,086802 (2011).

O 35.37 Tue 18:15 Poster B

Nitridation of diamond - a possible way to *n*-type surface-conductivity? — •Nora Jenny Vollmers, Uwe Gerstmann, and Wolf Gero Schmidt — Theoretische Physik, Universität Paderborn

Diamond has a lot of outstanding qualities but the lack of a suitable *n*-type donor has hindered this material to gain broad technological application. Nevertheless, nitrogen doping was already successfully used to improve the emission behavior of field emission devices based on *a*-C:H diamond thin films [1, 2, 3]. In this theoretical work we want to propose a possible way to *n*-type surface conductivity at the clean diamond (001) (2×1) reconstructed surface which consists of flat dimer rows. Using density functional theory together with the Quantum ESPRESSO PWscf package [4], we compare the electronic and magnetic properties for different N incorporation depths. Built-in directly at the surface, N gives rise to localized surface states similar to intrinsic carbon dangling bond-like states. Otherwise N is able to introduce surface conductivity as demonstrated by ab initio calculated effective mass tensors. In addition, the extreme anisotropy of the effective mass tensor comparable with those of metallic indium-chains on silicon substrates indicates the possibility to achieve *n*-type 1D surface-conductivity along the dimer-chains.

[1] R.S. Balmer et al., J. Phys.: Cond. Matt. 21, 364221 (2009).

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[3] M. Kaukkonen et al., Phys. Rev. Lett. 83, 5346 (1999).

[4] Ch.J. Pickard, F. Mauri, Phys. Rev. Lett. 88, 086403 (2002).

O 35.38 Tue 18:15 Poster B

Electronic spectrum of pure and doped Si(111)-(2x1) surfaces — •M. Pötter[1], M. Rohlfing[1], K. Löser[2], M. Wenderoth[2], T.K.A. Spaeth[2], J.K. Garleff[2], and R.G. Ulbrich[2] — [1]Fachbereich Physik, Universität Osnabrück — [2]IV. Physikalisches Institut, Universität Göttingen

We discuss the electronic structure of the Pandey-chain terminated Si(111)-(2x1) surface, as resulting from density-functional theory and from the GW approximation of many-body perturbation theory. Our theoretical investigations are complemented by experimental scanning-tunneling microscopy and spectroscopy studies. We focus on two issues:

(i) The Pandey chain can be buckled in two possible configurations (positive and negative buckling). The corresponding electronic spectra show distinctively different fundamental gaps, that can be used to identify the buckling.

(ii) When Pandey-chain Si atoms are substituted by phosphorus (e.g. from n-type doping), the geometry and potential are modified, and the additional electron further changes the electronic structure of the system. We discuss the spatial and spectral signatures of this modification.

O 35.39 Tue 18:15 Poster B

Photo-induced tunneling current microscope setup for UHV applications — •Uwe Schmitt, Andreas Englisch, and Uwe Hartmann — Institute of Experimental Physics, Universität des Saarlandes, P.O. Box 15 11 50, D-66041 Saarbrücken

In order to measure photo-induced tunneling currents on clean metal and semiconductor surfaces an UHV-STM-system was completed with suitable optical components which allows a simultaneous illumination of the sample with two wavelengths. The wavelengths can be modulated in the intensity with different modulation frequencies in order to detect the influence of both wavelengths with a lock-in-amplifier. The modulation deep can be chosen in a way that the DC-part of the light intensity determines the time independent photo conductivity and consequently the tunnel gap which is controlled by the feed-back-loop. In the original UHV-system (Omicron VT-STM) the Scala-electronic was replaced by a low cost controller from Soft dB.

O 35.40 Tue 18:15 Poster B

Cluster Models for Surface Reactions on Copper Oxide — •Martin Schmeisser[1], Jörg Schuster[2], Stefan E. Schulz[1,2], Ulrich Biedermann[3], and Alexander Auer[1,3] — [1]Chemnitz University of Technology, Gemany — [2]Fraunhofer ENAS, Chemnitz, Germany — [3]Max-Planck Institute for Iron Research, Düsseldorf, Germany

Copper is the most widely used material in semiconductor interconnect technology. Atomic Layer Deposition has recently been proposed as a means to deposit copper oxide on nanostructured surfaces with high aspect ratio for possible integration in the metalization step of device fabrication. A reduction step is required to convert the deposited copper oxide film into metallic copper. Several reduction agents have been used but little experimental data is available on the reduction reaction pathways.

Thus, a theoretical investigation has been started to model reduction reactions on a copper oxide surface. As a starting point different cluster model systems of a Cu2O surface have been proposed and tested for consistency with system size and against similar slab models. Adsorption mechanisms of formic acid were investigated and stable adsorbed structures are reported. A few reactions of an adsorbed formic acid molecule were modeled within a synchronous transit scheme at the b-p/TZVP level of theory.

O 35.41 Tue 18:15 Poster B

Topographic deconvolution of molecular photoemission spectra — •Serguei Soubatch[1], Peter Puschnig[2,3], Eva Reinisch[3], Thomas Ules[3], Georg Koller[3], Markus Ostler[4], Lorenz Romaner[2], Claudia Ambrosch-Draxl[2], Stefan Tautz[1], and Michael Ramsey[3] — [1]Peter Grünberg Institut, Forschungszentrum Jülich — [2]Chair of Atomistic Modeling and Design of Materials, Montanuniversität Leoben — [3]Institut für Physik, Karl-Franzens Universität Graz — [4]Lehrstuhl für Tech- nische Physik, Universität Erlangen-Nürnberg

We propose a method of photoemission spectra interpretation based on tomographic deconvolution of spectral features into individual orbitals suitable for cases when two or even several molecular orbitals overlap in the same energy interval. Suggested approach utilizes the earlier finding that the ARPES intensity distribution from a single molecular state is related to the Fourier transform of respective molecular orbital. Deconvoluting the entire experimental datacube of photoemission current recorded with toroidal electron analyzer into momentum dependent and energy dependent components and approximating the momentum dependent part by the Fourier transform of a chosen molecular orbital, one achieves the energy distribution of corresponding orbital. In the photoemission experiments on PTCDA/Ag(110), using tomographic deconvolution, four orbitals situated within an energy range of only 0.4 eV were successfully differentiated demonstrating applicability of the method even for strongly interacting molecule/metal interfaces.

O 35.42 Tue 18:15 Poster B

Spin-resolved photoemission experiments of Rashba-split quantum-well electron states — •Sebastian Jakobs[1,2], Andreas Ruffing[1], Sabine Steil[1], Indranil Sarkar[1], Stefan Mathias[1], Mirko Cinchetti[1], and Martin Aeschlimann[1] — [1]Department of Physics and Research Center OPTIMAS, University of Kaiserslautern, 67663 Kaiserslautern, Germany — [2]Graduate School Materials Science in Mainz, University of Kaiserslautern, D-67663 Kaiserslautern, Germany

The Rashba-Bychkov effect in a two-dimensional electron gas originates from spin-orbit interaction and an asymmetric confinement of the electron gas. It can produce spin-split energy bands in nonmagnetic materials without the need of applying any external magnetic field. This effect has been shown on various surfaces, and the resulting spin-split surface-state bands show a high spin polarization directed in the surface plane, perpendicularly to the k-vector of the photoelectrons [1]. Recently, we reported on the observation of a giant Rashba spin-orbit splitting of quantum-well state bands in the unoccupied electronic structure of a Bi monolayer on Cu(111) [2]. In this poster we will present first spin-resolved photoemission experiments of both commensurate and incommensurate structure of the quantum-well system Bi/Cu(111), which confirm the Rashba-character of the splitting.

[1] J.H. Dil, J. Phys.: Condens. Matter 21, 403001 (2009)
[2] S. Mathias et al., Phys. Rev. Lett. 104, 066802 (2010)

O 35.43 Tue 18:15 Poster B

Spin Splitting Mechanism in Surface Alloys investigated by Circular Dichroism in the Angular Distribution of Photoelectrons — •Carola Strasser, Isabella Gierz, Hadj-Mohamed Benia, Klaus Kern, and Christian R. Ast — MPI für Festkörperforschung, Stuttgart

Circular dichroism in the angular distribution (CDAD) of photoelectrons refers to the difference of the measured photocurrent for right and left circularly polarized light. The CDAD signal contains information about the photoemission process and is determined by the experimental geometry, the orbital composition of the initial state and also the relative phase between different final state partial waves.

We used an ARPES (angular resolved photoemission spectroscopy) setup with different light polarizations and applied this technique to the band structure of two surface alloys on the Ag(111) surface with different spin splitting. Both systems show a clear CDAD signal but variant features. To get more information about the spin splitting mechanism we combined tight binding calculations with general theoretical descriptions of CDAD to explain the characteristic patterns in the experimental data.

O 35.44 Tue 18:15 Poster B

Angular resolved photoemission study of a two-dimensional electron system induced by Cs adsorption on InSb(110). — •Alexander Georgi[1], Carola Strasser[2], Isabella Gierz[3], Stefan Becker[1], Marcus Liebmann[1], Christian Ast[2], and Markus Morgenstern[1] — [1]II. Physikalisches Institut B and JARA-FIT, RWTH Aachen University, Aachen, Germany — [2]Max-Planck-Institut für Festkörperforschung, Stuttgart, Germany — [3]Max Planck Research Department for Structural Dynamics, University of Hamburg, Centre for Free Electron Laser Science, Hamburg, Germany

Using angular resolved photoemission (ARPES) at 70 K, we investigated the band structure of a two-dimensional electron system (2DES) created by Cs adsorption on p-type InSb(110). Cs induces a large band bending on the surface of p-type InSb(110) and creates a 2DES in the inversion layer. ARPES measurements reveal the parabola of the first 2DES subband exhibiting an effective mass of only $m^* = 0.022\,m_0$ in accordance with theory.

The large electric field within the 2DES leads to a large Rashba parameter estimated to be about $\alpha = 7\times10^{-11}$eVm. Scanning tunneling spectroscopy studies [1] indeed show a beating pattern in the Landau levels of the system which can be attributed to this Rashba spin splitting. Experiments to probe this spin splitting by ARPES are under way.

[1] S. Becker, Phys. Rev B 81, 155308 (2010)

O 35.45 Tue 18:15 Poster B

Phase behavior of chain molecules on surface: Monte Carlo simulation — •Pritam Kumar Jana and Andreas Heuer — Institute of Physical Chemistry, University of Muenster, Corrensstr. 28/30, Muenster, Germany

Self assembled monolayers of organic molecules on solid substrate build well defined surfaces, which can be structured efficiently on a nanometer scale. Self assembled monolayers are formed by organic molecules which spontaneously chemisorb on solid substrate [1,2], e.g. alkanethiolates attaching to gold surfaces with their sulfur head groups. We have studied an idealized model of chain molecules adsorbed on a flat substrate by means of extensive Monte Carlo Simulations. Our study focuses on phase transitions within a monolayer rather than on self aggregation. We model the molecules as rigid chains of Lennard-Jones spheres with one head group. As chain molecules are considered as rigid rod, all intra molecular degrees of freedom have been neglected. The Monte Carlo dynamics involves translational move in 3D space and rotational moves in 2D space. In the course of the simulation the concentration of chain molecules is increased with a fixed flux. We determine the phase diagram in dependence of the different energetic and structural parameters (e.g. chain length) of the model.

[1] A. Ulman, Chem.Rev., 96, 1533, 1996. [2] G. E. Poirier, Chem. Rev., 97, 117, 1997.

O 35.46 Tue 18:15 Poster B

Atomistic Simulations of Pressure-Induced Structural Transformations in Ice Nanocrystals — •Konstantin Weber[1,2] and Carla Molteni[1] — [1]King's College, Physics Department, London, UK — [2]ICMM/CCC, University of Erlangen-Nürnberg, Germany

Ice has a very complex and widely studied phase diagram, which includes many crystalline phases (stable as, e.g., ice Ih, ice II, and ice III, and metastable ones as ice Ic) as well as amorphous phases. Pressure can be used to induce structural transitions between these phases, allowing the study of transition mechanisms and of phase dependent properties. Ice nanocrystals of variable size add an extra dimension to the phase diagram, and it is interesting to understand how size affects the phase transformations. We present the results of a series of simulations where we have modeled pressure-induced structural transformations in ice Ih nanocrystals using the classical TIP4P force field, a constant pressure molecular dynamics method for finite systems, and the metadynamics technique for accelerating rare events. Metadynamics allows us to study the phase transformations at realistic pressure conditions, without the need to overpressurize the systems as in conventional molecular dynamics because of time scale limitations.

O 35.47 Tue 18:15 Poster B

Depth profiling X-ray photoemission investigation and its impact into the field of Fusion Energy Materials — •Stephanie Rädel[1,2,3], Martin Köppen[3], Martin Oberkofler[3], Johann Riesch[3], Heike Löchel[1], Max Bauer[1], Antje Vollmer[1], and

Christian Linsmeier[3] — [1]Helmholtz Zentrum Berlin für Materialien und Energie GmbH, Berlin, Germany — [2]TU Berlin, Berlin Germany — [3]Max-Planck-Institut für Plasmaphysik, Garching, Germany

The next step of the roadmap in fusion energy research is the construction of the experimental fusion reactor ITER. Due to particle collision and energy deposition in the reactor vessel, requirements for first wall materials are extremely high. Therefore it is crucial to gain knowledge on the interaction of the plasma and the surface of ITER. During operation, diffusion, erosion and re-deposition occur. For a successful operational scenario, these reactions need to be predicted. In this study we investigate selected surface processes by XPS measurements. By using synchrotron radiation, it is possible to tune photon energies (kinetic energy of photo-electrons) achieving different information depths. Following diffusion processes and chemical reactions by depth profing becomes feasible. Here we present the ternary system Be/W/C and its chemical and physical behaviour upon annealing. This understanding is a step towards predictions of the behaviour of the elements at the ITER first wall under different reaction conditions during operation.

O 35.48 Tue 18:15 Poster B

Patterning of the surface termination of ultrananocrystalline diamond films — •Mahsa Mozafari, Alexandra Voss, Cyril Popov, and Johann Peter Reithmaier — Universität Kassel, Institut für Nanostrukturtechnologie und Analytik, Heinrich-Plett-Straße 40, 34132 Kassel, Germany

Diamond and diamond films attract an ever increasing interest for different biotechnological applications due to their extraordinary properties, like excellent biocompatibility, high chemical stability, wide electrochemical window, high wear resistance and optical transparence, etc. Further advantage of the diamond surface is the possibility to tailor the surface termination and respectively the surface properties, including the wettability and conductivity. These properties are decisive for the interactions with any bioentity (cells, proteins, RNA, DNA). In the current work we present the results for the surface modification of ultrananocrystalline diamond/amorphous carbon (UNCD/a-C) composite films and its patterning. The surface of these films is H-terminated after growth, which determines the hydrophobic character and the p-type surface conductivity. Applying O_2-plasma, NH_3/N_2-plasma or UV/O_3 modifications it can be rendered hydrophilic and insulating due to the change of the surface termination. The modified surfaces were investigated by contact angle measurements, SEM, AFM, XPS and electrical measurements. Further, the possibility to pattern the surface termination by electron, ion and laser beams was also studied.

O 35.49 Tue 18:15 Poster B

Molecular beam studies of methane dissociation on Ru(0001) — •Harald Kirsch, Zefeng Ren, R. Kramer Campen, and Martin Wolf — Fritz-Haber-Institut , Abt. Physikalische Chemie, Faradayweg 4-6, 14195 Berlin

Understanding the dissociation of methane on transition metal surfaces is a challenge in heterogeneous catalysis. We have investigated the dissociation products of CH_4 and CD_4 on a Ru(0001) surface with vibrational sum-frequency spectroscopy (SFG) and temperature-programmed desorption(TPD). To overcome the dissociation barrier under UHV conditions, a supersonic molecular beam of CH_4/CD_4 seeded in He or H_2 has been used to generate adsorbed methyl radicals. The system was studied as function of surface temperature (300K - 500K) and coverage. Coverage was determined after each measurement by oxygen coadsorption and recombinative C + O desorption. High resolution (<5 cm^{-1}) vibrational sum-frequency generation spectroscopy has allowed the observation of new features in the C-H stretching region. For adsorption at surface temperatures below 350K just one resonance could be observed at 3000 cm^{-1}, which is identified as the CH stretching mode. At temperatures higher than 350K, two additional red shifted peaks appear. These observation could help to identify intermediates of the methane dehydrogenation and complement previously discovered decomposition pathways.

O 35.50 Tue 18:15 Poster B

Catalytic activity of free and graphene-supported transition metal clusters — •Sanjubala Sahoo, Markus E. Gruner, and Peter Entel — Faculty of Physics and Center for Nanointegration CeNIDE, University of Duisburg-Essen, Lother Str. 1, 47048 Duisburg

We have studied the CO oxidation reaction for CO adsorbed on a Pt_{13} cluster and for CO adsorbed on a graphene sheet. The reaction pathway is identified and the activation barrier is calculated. Our results show that the activation barrier in case of the Pt_{13} cluster is similar in magnitude to that of the Pt(111) surface. On the other hand, we find that the activation barrier for CO oxidation on graphene alone is lower compared to that of a free Pt cluster. In future, we also explore the reaction for Pt13 cluster is deposited on graphene. The studies are done with the nudged elastic band method [1] by employing the total energy calculations from density functional theory within generalized gradient approximation as implemented in Vienna ab-initio simulation package (VASP) [2].

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[2] G. Kresse et al., Comput. Mater. Sci. **6**, 15 (1996).

O 35.51 Tue 18:15 Poster B

Flame-Synthesis of Tailored Metal-Oxide Nanoparticle Surfaces for Highly Selective and Reactive Gas Sensors — •Antonio Tricoli — Particle Technology Laboratory, Department of Mechanical and Process Engineering, ETH Zurich, 8092 Zurich, Switzerland

Metal-oxide nanoparticles such as SnO_2 and TiO_2 are state-of-the-art materials for the assembly of solid-state chemical gas sensors. The remarkable chemical and temperature stability of these wide band-gap semiconductors allows operation in very harsh environments as for exhaust oxygen sensors in modern fuel control feedback loop. The high reactivity of their surface with simple and complex gaseous compounds allows detection of important analytes down to particle per billion concentrations (ppb). However, this is usually achieved by exploitation of spill-over effects on noble-metal clusters post-deposited (e.g. by impregnation) on their surface. This drastically limits the stability of their sensing performance at the elevated operation temperatures ($250 - 600\,^\circ$C) of these metal-oxides and considerably increases the cost for their production. Additionally, such gas sensing metal-oxides suffer of very poor selectivity confining their application to relatively simple gas mixtures. This is a main limitation to their utilization as gas sensors in novel applications such as non-invasive medical diagnostics by breath analysis. Development of noble-metal-free metal-oxide nanoparticles with high selectivity to trace concentrations (ppb) of the target analyte is a key-step toward the fabrication of portable and wearable gas sensing technology with numerous applications. Here, the one-step flame-synthesis of tailored multi-oxide nanoparticles is presented as a tool for the production of very selective and sensitive gas sensors. In particular, the synthesis of highly reactive $SnO_2 - SiO_2$ nanocomposites with limit of detection (LOD) in the ppb range is demonstrated as a valid alternative to the utilization of noble-metals leading to considerably higher sensitivity and stability. In particular, the thermal stabilization of very fine SnO_2 nanocrystals with size below twice their Debye length up to very high temperatures ($900\,^\circ$C) is shown as a reliable method for the synthesis of wide band-gap semiconductors with surface states-controlled conductivity and thus very high sensitivity. Additionally, the flame-synthesis of $SnO_2 - TiO_2$ solid solutions with rutile crystal structure is presented as a powerful approach to control the selectivity of such metal-oxide surfaces against disturbing agents such as water vapor, an omnipresent and varying component in gas sensing.

O 35.52 Tue 18:15 Poster B

Solar2Fuel: Spectroscopic and electrochemical characterization of functionalized semiconductor surfaces for photocatalytic reduction of CO_2 — •Florian Staier, Michael Grunze, and Michael Zharnikov — Angewandte Physikalische Chemie, Universität Heidelberg, Im Neuenheimer Feld 253, 69120 Heidelberg

The handling of CO_2 produced by industrial installations and power plants has become a very important environmental issue nowadays because of it's generally accepted impact on the green house effect. In this context, storage of CO_2 or its conversation to fuel or useful chemicals are highly desirable. Along these lines, the Solar2Fuel project, funded by German BMBF (13N11793), aims on photocatalytic conversion of CO_2 to methanol with a sufficient quantum efficiency to make an industrial realization of the process profitable. As the basic catalytic system, semiconductor nanoparticle powder coatings are used. These particles are functionalized with dye molecules to promote the photocatalytic reaction and to move the absorption spectrum from UV to the visible range. Here we present first results on the adsorption kinetics, absorption character, and photoactivity for a variety of the relevant systems. These properties were primary addressed by X-ray photoelectron spectroscopy and electrochemical methods.

O 35.53 Tue 18:15 Poster B

Solar2Fuel: ATR-IR-Spectroscopic characterization of functionalized semiconductor surfaces for photocatalytic reduction of CO_2 — •Leo Pöttinger[1] and Thomas Bürgi[2] — [1]Physikalisch-Chemisches Institut, Universität Heidelberg, Im Neuenheimer Feld 253, 69120 Heidelberg — [2]Département de Chimie Physique Université de Genève, 30 Quai Ernest-Ansermet CH-1211 Genève 4

The handling of CO_2 produced by industrial installations and power plants has become a very important environmental issue nowadays because of it's generally accepted impact on the green house effect. In this context, storage of CO_2 or its conversation to fuel or useful chemicals are highly desirable. Along these lines, the Solar2Fuel project, funded by German BMBF (13N11793), aims on photocatalytic conversion of CO_2 to methanol with a sufficient quantum efficiency to make an industrial realization of the process profitable. As the basic catalytic system, semiconductor nanoparticle powder coatings are used. These particles are functionalized with dye molecules to promote the photocatalytic reaction and to move the absorption spectrum from UV to the visible range. ATR-IR-Spectroscopy during adsorption of different dyes and CO_2 on the nanoparticles is performed, as well as the reaction upon visible light irradiation.

O 35.54 Tue 18:15 Poster B

Oxidation behavior of orientated brass surfaces investigated with STM, XPS and LEED — •Andreas Zychma, Renate Wansing, and Alexander Birkner — Lehrstuhl für Physikalische Chemie I, Ruhr-Universität Bochum

In heterogeneous catalysis, especially in methanol synthesis, the system Cu/ZnO plays an important role. Particularly the metal-substrate interaction of copper and zinc oxide is of great interest. While many groups therefore study the system copper on zinc oxide, we investigate the behavior of zinc oxide on copper, the so called 'inverse system'. For that we use brass single crystals with an amount of 15 percent zinc. After oxygen exposure in ultra high vacuum at different substrate temperatures the stepwise formation of zinc oxide and copper oxide can be observed with x-ray photoelectron spectroscopy (XPS). Additionally low energy electron diffraction (LEED) and scanning tunneling microscopy (STM) as well as spectroscopic measurements with the STM are performed to investigate the formation process of zinc oxide and copper oxide on brass surfaces with different crystal orientation.

O 35.55 Tue 18:15 Poster B

Reactivity of Acetylene on thin NiO films and on Pd(100) — •Oliver Höfert, Wei Zhao, Karin Gotterbarm, Andreas Bayer, Christian Papp, and Hans-Peter Steinrück — Lehrstuhl für Physikalische Chemie II, Universität Erlangen-Nürnberg, Egerlandstr. 3, 91058 Erlangen

NiO is an important material in heterogeneous photocatalysis for degradation of azodyes [1] or water splitting [2]. We studied different thin NiO films on Pd(100) and Pd (100) towards their reactivity with C_2H_2 by in situ XPS, applying synchrotron radiation at BESSY II. Our data shows that acetylene adsorbs molecularly on the substrate; the thermal evolution studies point to a reaction at 300 K leading to an intermediate that was shown to be CCH [3]. At higher reaction temperatures further decomposition and reaction is found. On thin, highly stressed NiO films acetylene adsorbs on many different adsorption sites leading to a broad peak in the C 1s photoelectron spectrum. Thermal treatment of C_2H_2 leads to an intermediate similar to the one on the clean substrate. At higher temperatures carbon is produced which reacts with the NiO to CO and desorbs.

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

[1] Hu, X. et al, J. Chem. Tec. & Biotec., 85 (2010) 11

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

[3] Camplin, J. P. et al, Phys. Chem. Chem. Phys. 2 (2000) 4433

O 35.56 Tue 18:15 Poster B

Methanol synthesis on ZnO(000$\bar{1}$): CO reduction at oxygen vacancies. — •Johannes Frenzel, Nora Graf, and Dominik Marx — Lehrstuhl für Theoretische Chemie, Ruhr-Universität Bochum, 44780 Bochum, Germany

In the heterogeneous catalytic synthesis of methanol on the ZnO(000$\bar{1}$) surface with oxygen vacancies [1] gives rise to a complex free energy landscape[2] for the reduction of CO on this catalyst at high temperature and pressure conditions as required in the industrial process. Using *ab initio* metadynamics for computational heterogeneous catalysis the underlying complex reaction network from CO to methanol has been generated in the first place by exploring the global free energy, that allowed a subsequent refinement of individual reaction pathways.[2]

In the present study, the complex reduction process from CO to methanol is studied by exploring the electronic structure of reaction intermediates with density functional theory. After comparing the electronic bands and molecular orbitals involved we find the reduction state of surface and O vacancy bound adsorbates to be controlled by the charge states of the F–center, which is defined by the gas phase conditions.[1] Monitoring the reduction process of reaction paths obtained by metadynamics sampling of the free energy surface at the electronic structure level on snapshots reaction allows further mechanistic insight into the catalytic process.

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O 35.57 Tue 18:15 Poster B

The dynamic redox properties of MoV oxide catalysts for the selective oxidation of alkanes studied by in-situ microwave cavity perturbation — •Christian Heine, Maik Eichelbaum, Annette Trunschke, and Robert Schlögl — Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, Germany

The semiconducting M1 phase MoVNbTeOx is a selective catalyst for the direct oxidation of propane yielding about 50% acrylic acid. During the redox reaction a charge transfer between the catalyst and the chemisorbed reactants takes place. To study the interaction between the gas phase and the catalyst surface, we developed a method based on the microwave cavity perturbation technique enabling the investigation of (di)electric properties of powder catalysts under operation in a contact-free manner, thus completely avoiding contact resistance and electrode-related problems (Eichelbaum et al., PCCP, DOI 10.1039/C1CP23462E). This method offers the possibility to probe the electronic structure of the catalyst under reaction conditions. It is known from in-situ photoelectron spectroscopy studies that the surface of the M1 phase behaves dynamically and changes its electronic and geometric structure during the catalytic reaction, which is associated with a modification of the surface density of states. As a consequence, the equilibrium between surface and bulk states is shifted modifying the surface states-induced band bending. The impact of the surface electronic structure on the electrical conductivity of the catalyst will be discussed.

O 35.58 Tue 18:15 Poster B

Micro-flow tube reactor for investigations on the catalytic activity of model catalysts — Kwabena Offeh Gyimah, Matthias Roos, •Joachim Bansmann, and R. Jürgen Behm — Institute of Surface Chemistry and Catalysis, Ulm University, D-89069 Ulm

Here, we report on a newly developed glass reactor for investigating the catalytic activity of model catalysts which usually exhibit very small surface areas and, as a consequence, very low reactions rates. The design of the reactor is based on a reactor developed by Wong et al. [1], it is fabricated from glass, allows temperatures up to 400°C, and is connected to a quadrupole mass spectrometer. Due to its small reaction volume, it is only suitable for small samples (e.g., 3mm x 3mm). The reactor has been tested for the CO oxidation reaction on thin film based Au/TiO_2 catalysts [2] in the pressure regime of several mbars (CO and O_2). Due to its design, it allows fast measurements on the activation energy of catalysts. The properties of this reactor will be compared to other reactors, e.g. [1,3].

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O 35.59 Tue 18:15 Poster B

Low cost low noise amplifier for charged nanoparticle beam detection — •Sebastian Schleicher, Wolfgang Rosellen, and Mathias Getzlaff — Institute of Applied Physics,University Duesseldorf

For our investigations we generate nanoparticles in the gas phase by a UHV compatible Arc Ion Cluster Source (ACIS)[1]. Nearly 50% of the beam consists of charged nanoparticles with sizes between 5 nm and 15 nm. For beam positioning and controlling, the nanoparticles are detected by a very low noise current amplifier in an embedded system. The charged nanoparticle beam has an electrical current of a couple of pico-Ampere. By amplifying this signal by a magnitude of 10^{15}, it can be quantified. The main problem to overcome when amplifying a signal is to minimize the noise. There are four known noise sources, which need to be considered ($1/f$ noise, $1/f^2$ noise, Johnson-Nyquist Noise and Shot noise). We use a transimpedance amplifier. For this purpose the construction elements, like the power supply and the transimpedance amplifying circuit, were made by low-cost components. Each construction element was chosen by their highest possible noise suppression according to signal enhancement. The final signal will be converted by a 24-bit delta-sigma analog-to-digital converter. The system will be designed as an embedded microcontroller system.

[1] R.-P. Methling, V. Senz, E.-D. Klinkenberg, Th. Diederich, J. Tiggesbäumker, G. Holzhüter, J. Bansmann, K.-H. Meiwes-Broer, European Physical Journal D **16**, 173 (2001)

O 35.60 Tue 18:15 Poster B

Ag clusters on SiO_2 and in matrices: effects of cluster-structure and surroundings — •Sabrina Hoffmann[1], Stefanie Duffe[1], Kamil Latussek[1], David Engemann[1], Christoph J. Sahle[1], Christian Sternemann[1], Heinz Hövel[1], Ralph Wagner[2], and Pieter Glatzel[3] — [1]TU Dortmund, Experimentelle Physik I/DELTA, Dortmund, Germany — [2]BU Wuppertal, Fachgruppe Physik-Materialwissenschaften, Wuppertal, Germany — [3]ESRF, Grenoble, France

Embedding Ag clusters produced in a supersonic expansion using THECLA, a THErmal CLuster Apparatus [1,2] into a polydimethylsiloxane (PDMS) / SiO_2 aerogel matrix enables the investigation of a much higher amount of separated clusters [3] which on a SiO_2 substrate is limited by coalescence and electromagnetic coupling [2]. The plasmon resonances of Ag clusters on SiO_2 and in PDMS / SiO_2 aerogel before and after exposure to air were investigated by optical spectroscopy [4]. XANES measurements at the Ag $L_{1,2,3}$ absorption edges [5] carried out at the synchrotron radiation sources DELTA and ESRF were compared to ab initio multiple scattering calculations (FEFF) for different cluster sizes and structures.

[1] O. F. Hagena, Z. Phys. D 20, 425 (1991). [2] H. Hövel et al., Phys. Rev. B 48, 18178 (1993). [3] L. Ravagnan et al., J. Phys. D 42, 082005 (2009). [4] U. Kreibig et al., In: Advances in Metal and Semiconductor Clusters Vol. 4, (ed. M.A. Duncan), JAI press Inc., 345 (1998). [5] P. Behrens et al., Z. anorg. allg. Chem. 625, 111 (1999).

O 35.61 Tue 18:15 Poster B

Cluster aus fokussierten Ionenstrahlen - Massenspektroskopische Untersuchung von Flüssigmetall-Ionenquellen — •Martin Wortmann, Dirk Reuter und Andreas D. Wieck — Ruhr-Universität Bochum, Universitätsstr. 150, 44780 Bochum

Bei der Untersuchung der Cluster-Emission aus Flüssigmetall-Ionenquellen (LMIS) war man bisher durch die Auflösung der in herkömmlichen FIB-Systemen (focused ion beam) verwendeten $E \times B$ – Massenfilter limitiert. Die Auflösung nimmt mit zunehmender Masse der untersuchten Cluster rapide ab. Will man auch im Bereich größerer Cluster ($n > 10$) eine hinreichende Massenseparation erreichen, werden also hochauflösende Massenspektrometer benötigt.

Die durch die Verwendung von LMIS erreichbaren Clusterströme eröffnen außerdem die Möglichkeit, derartige Quellen zur Erzeugung monodisperser Cluster zu verwenden. Durch ein geeignetes elektrisches Potential können die Cluster abgebremst und auf Substraten deponiert werden.

In diesem Beitrag werden die Designüberlegungen für den in Bochum im Aufbau befindlichen hochauflösenden Massenfilter diskutiert. Die Massentrennung kann sowohl durch einen $E \times B$ – Filter als auch durch Time-of-Flight-Spektroskopie erreicht werden. Präsentiert werden Details des experimentellen Aufbaus, sowie Ergebnisse der ionenoptischen Berechnungen, die für die Planung einer solchen Anlage zwingend notwendig sind. Außerdem werden die Ergebnisse der bereits durchgeführten Messungen diskutiert.

O 35.62 Tue 18:15 Poster B

Mass selected copper clusters on graphite (HOPG): Photoelectron spectroscopy with ultraviolet light — •Christoph Schröder[1], David Engemann[1], Niklas Grönhagen[1], Natalie Miroslawski[1], Bernd von Issendroff[2], and Heinz Hövel[1] — [1]Technische Universität Dortmund, Experimentale Physik I, Germany — [2]Albert-Ludwigs-Universität Freiburg, Physikalisches Institut, Germany

We investigated mass selected copper clusters between 34 and 92 atoms deposited at 125 K on graphite (HOPG) using ultraviolet photoelectron spectroscopy (UPS). The clusters were softlanded with less then 0.1 eV per atom kinetic energy. Cluster were deposited with different coverage for each cluster size and measured at 125 K. For a better interpretation we subtracted normalized HOPG spectra from the measured cluster spectra to extract the d-band structure of the clusters. Afterwards we annealed the sample for 1 hour at RT and observed changes in the UPS spectra depending on the cluster coverage. For these investigations the source of exciting radiation was a He-gas discharge lamp (hν=21,2 eV). In order to get more information about the clusters we will use Ar (hν=11,6 eV) instead of He in our discharge lamp for future experiments. For this reason we have installed a heatable LiF-window.

O 35.63 Tue 18:15 Poster B

Catalytic activity of supported Pt clusters compared to Pt(111) — •Andrew S. Crampton, Claron. J. Ridge, Florian F. Schweinberger, and Ulrich Heiz — Technische Universität München, Catalysis Research Center, Chair of Physical Chemistry, Lichtenbergstr. 4, 85748 Garching, Germany.

Softlanding size-selected metal clusters, generated with a laser ablation source and mass selected with a QMS, onto a metal oxide support enables independent size and coverage control. These model systems then provide a direct path for the experimental chemist to probe electronic and geometric effects by changing the particle size by one single atom. The reactivity of these systems is investigated using a variety of surface science methods such as TPD/TPR, pMBRS, IRRAS, UPS and MIES. Recent studies on adsorbates have proven the potential of MIES to study adsorbate systems with a superior sensitivity compared to UPS. With these methods the kinetics and thermodynamics of reactions on clusters can be examined, as well as the electronic structure and vibrational properties of the adsorbates. Of particular interest are common model systems and demanding reactions, such as hydrogenation of olefins, on Pt clusters in the range from a single atom to nano crystallites (1-80 atoms). Comparing the results of measurements on the clusters with Pt(111) within the same experimental setup allows for a precise and comprehensive understanding of the effects on catalytic activity imparted by particle masses in the non-scalable size regime. The information obtained from these experiments contributes to deciphering fundamental catalytic mechanisms on the nanoscale.

O 35.64 Tue 18:15 Poster B

Linear and nonlinear spectroscopy of size selected metal clusters on surfaces — •Philipp Heister, Tobias Lünskens, Martin Tschurl und Uli Heiz — Technische Universität München, Lehrstuhl für physikalische Chemie

The catalytic activity of small metal clusters has been shown to vary by orders of magnitude upon addition of a single metal atom. A better understanding of the interplay between the electronic and geometrical structure and the catalytic activity of the clusters may be gained through a precise knowledge of the electronic structure and geometry from spectroscopic studies. Therefore we use different spectroscopic methods to investigate size selected and unselected metal clusters on surfaces under UHV conditions. We use highly sensitive techniques such as surface Cavity Ring-Down spectroscopy (s-CRD) and surface Second-Harmonic-Generation spectroscopy (s-SHG) for observing the obtical properties of these clusters. The interest mainly focuses on the size and shape dependent electronic structures and plasmon-like transitions of small deposited clusters. With these plasmon oscillations we are able to gain further information about oxidation and reduction of the supported size selected clusters. We also observe interesting cluster-plasmon size effects, for example a sudden increase in plasmon resonances (parallel to the surface normal) for increasing cluster size. It seems that these clusters need to be at least three atomic layers thick in order to show plasmon oscillations, whereas thinner clusters (one or two atomic layer) do not show any plasmon oscillations.

O 35.65 Tue 18:15 Poster B

Setup and characterisation of CRD and SHG spectrometer for measuring optical response of supported metal clusters and evaporated molecules under UHV conditions — •Tobias Lünskens, Philipp Heister, Martin Tschurl und Uli Heiz — Technische Universität München, Lehrstuhl für physikalische Chemie

Supported metal clusters have attracted considerable interest due to their special catalytic properties. Optical and catalytic properties of these metal clusters are determined by their electronic structure which can be studied by optical absorption spectroscopy as well as surface second harmonic generation (s-SHG) spectroscopy under UHV conditions. The interest mainly focuses on the size and shape dependent electronic structure of deposited cluster. Due to their low absorption cross-section and the low surface coverage that is necessary to avoid agglomeration of the clusters highly sensitive techniques such as surface cavity ring-down (s-CRD) spectroscopy and s-SHG-spectroscopy are needed. By s-CRD-spectroscopy we also investigate evaporated molecules and their interaction with different substrates und size selected metal clusters. We present the experimental setup which is composed of two main parts: A cluster deposition unit including laser vaporization cluster source, ion optics, and mass selection device and three different spectroscopic methods, including s-CRD spectroscopy in the UV-Vis- (from 400 nm to 900 nm) and in the IR-region (from 2500 nm to 3500 nm), and s-SHG-spectroscopy for measurements down to 200 nm. A transfer chamber allows fast change of support materials without breaking UHV.

O 35.66 Tue 18:15 Poster B

STM of size selected silver and copper clusters deposited on $Au(111)$ and $C_{60}/Au(111)$ — •David Engemann[1], Niklas Grönhagen[1], Natalie Miroslawski[1], Bernd von Issendorff[2], Tommi T. Järvi[3], Michael Moseler[2,3,4], and Heinz Hövel[1] — [1]Technische Universität Dortmund, Experimentelle Physik I — [2]Albert-Ludwigs-Universität Freiburg, Physikalisches Institut — [3]Fraunhofer-Institut fuer Werkstoffmechanik IWM, Freiburg — [4]Freiburger Materialforschungszentrum

Size selected silver and copper clusters with sizes in between 34 atoms to 147 atoms were soft landed on clean $Au(111)$ and $Au(111)$ covered with 1 and 2 ML C_{60} and measured with scanning tunneling microscopy (STM) at $77K$. We observed a deformation of the cluster shape due to the strong metallic interaction between the clusters and $Au(111)$. The silver clusters became epitaxial and developed a structure composed of several monolayers. The number of these monolayers depends on the number of atoms in the clusters and the deposition energy. The larger the cluster mass the more monolayers the clusters develops on $Au(111)$ and the larger the deposition energy the fewer monolayers occur. These results are compared with molecular dynamic simulations and other atomistic calculations. The clusters were annealed up to room temperature and afterwards measured with STM at $77K$. On 1 ML C_{60} all cluster heights became smaller after annealing. We compare these results for copper and silver clusters. Resulting differences may be explained with the fact that for the same number of atoms copper clusters are smaller than silver clusters.

O 35.67 Tue 18:15 Poster B

Photocatalysis with supported size-selected metal clusters — •Martin Tschurl[1], Josef Kiermaier[1], Andreas Winbauer[1], Friedrich Esch[1], Claude Henry[2], and Ulrich Heiz[1] — [1]TU München, Catalysis Research Center, Lichtenbergstr. 4, 85748 Garching, Germany — [2]CINaM-CNRS, Campus de Luminy, Case 913, 13288 Marseille Cedex 09, France

In this work we present a setup for the study of the photochemical properties of size-selected clusters softlanded on various support materials. The apparatus consists of a laser ablation cluster source with ion optics for guiding the cluster beam and a quadrupole for mass selection. The size-selected clusters are softlanded on a special temperature-adjustable sample holder and can then be further characterized.

To determine the photocatalytic activity of the clusters, reaction products will be monitored. For this purpose our setup is equipped with a standard quadrupole mass selector with electron ionization. In addition, we have developed a new type of time-of-flight mass spectrometer, which is used in combination with REMPI (Resonant Enhanced Multiphoton Ionization). This spectrometer is specially designed to study the formation of different isomers. In this case, discrimination can be achieved by selecting a wavelength, which is in resonance with the electronic states of just one of the reaction products. This resonant process will greatly enhance the ionization yield of this particular species, which can then be detected in the time-of-flight spectrometer with very high sensitivity.

O 35.68 Tue 18:15 Poster B

d^0 ferromagnetic interface between non-magnetic perovskites — •Riku Oja and Risto M. Nieminen — Aalto University, Helsinki, Finland

In perovskite oxides, oxygen p bands are narrow and have a high density of states just below the band gap. Also, oxygen p electrons have a strong exchange coupling. Hence, Stoner criterion for itinerant ferromagnetism is fulfilled in hole-doped d^0 perovskites, if the hole density is high enough. Obtaining high hole densities, moving the Fermi level to the oxygen p band, is easily done by so-called intrinsic doping by a charge-imbalanced interface between two d^0 perovskites. This introduces holes (for p type interface) or electrons (for n type interface) confined in the interface region.

We have performed DFT and DFT+U calculations with both LSDA and GGA for both types of $\mathrm{KTaO_3/SrTiO_3}$ interfaces. The atomically sharp p type interface has been observed in experiments. The hole on oxygen $2p$ orbitals is localized on $\mathrm{SrTiO_3}$ side of the interface and is spin-polarized. Very small values of on-site Hubbard interaction U on oxygen p orbitals cause complete spin-polarization and half-metallic, ferromagnetic holes. The antiferromagnetic solution has higher energy. For the n type interface, on the other hand, electrons on Ti d orbitals do not magnetize completely.

As the density of states at the top of the O p band is higher than at the bottom of the Ti d band, we conclude that p type interfaces between d^0 perovskites are good materials for interfacial ferromagnetism below ferroelectric thin films.

O 35.69 Tue 18:15 Poster B

A new mode of operation of electron energy loss spectrometers: Application to surface magnon and surface vibration spectra — •Rajeswari Jayaraman, Harald Ibach, and Claus Michael Schneider — Peter Grünberg Institut, Forschungszentrum Jülich, 52425 Jülich, Germany

Using advanced simulations of the electron optics we have found a new mode of operation for the lens system in electron energy loss spectrometers (EELS) in which the cardinal planes of the lenses are closer to the sample. The product of transmission and solid angle angle accepted by the analyzer thereby increases by a factor of 3-5, yielding a corresponding gain in the intensity. The effect is demonstrated for a recently developed high-intensity spectrometer [1] with spectra of surface spin waves on fcc cobalt. Using this new mode we have been able to obtain spin wave spectra with 7meV resolution. Commercially available EEL-spectrometers can likewise be operated in the new mode. We demonstrate this with vibration spectra of water on Ag(115). The electron optical calculations furthermore allow an absolute calibration of the cross section for inelastic electron scattering. [1] H. Ibach, J. Rajeswari, C. M. Schneider, to be published.

O 35.70 Tue 18:15 Poster B

Investigation of ultrathin Fe films on Ag(001) using linear and nonlinear photoemission — •Thiago Peixoto[1], Mariusz Pazgan[1], Francesco Bisio[1,2], Aimo Winkelmann[1], Maciej Dabrowski[1], Marek Przybylski[1], and Jürgen Kirschner[1] — [1]MPI of Microstructure Physics, Halle-Saale, Germany — [2]CNR-SPIN, Genova, Italy

Investigations of iron films grown on silver surfaces have shown an intriguing thickness-dependent oscillatory magnetic anisotropy [1,2]. This behaviour was explained by the appearance of quantum well states (QWS) in the Fe film. In order to access the relevant electronic states, we investigated ultrathin Fe/Ag(001) films by angle- and spin-resolved one-photon (1PPE, $h\nu = 6\,eV$) and multi-photon photoemission (2PPE, 3PPE, $h\nu = 3\,eV$) at 150 K. Consistent with the observation of 5.6 ML oscillations of QWS in Fe/Ag(001) [2], we report periodic thickness- and energy-dependent intensity variations of electronic transitions in 1PPE and 2PPE spectra. Using different incident light polarizations, we identify the presence of specific unoccupied states in 2PPE. The Fe films show an average spin-polarization of about 30% near E_F in 2PPE and 10% in 1PPE. This difference is attributed to the influence of unoccupied states. By means of angle-dependent 3PPE, the $n = 1$ image-potential state of Fe/Ag(001) is identified, with an estimated electron effective mass of $m_{eff} = 0.75 m_e$ and a binding energy of $E_B = 0.77$ eV with respect to the vacuum level.

[1] U. Bauer and M. Przybylski, Phys. Rev. B 81, 134428 (2010).

[2] J. Li *et al.*, IEEE Trans. Magn. 47, 1603 (2011).

O 35.71 Tue 18:15 Poster B

Twin-Photoemission Electron Microscopy System (Twin-PEEM) — •Alexander Krasyuk[1], Christian Tusche[1], Gerd Schönhense[2], and Jurgen Kirschner[1] — [1]Max-Planck-Institut für Mikrostrukturphysik, Weinberg 2, D-06120 Halle, Germany —

[2]Johannes Gutenberg Universität Mainz, Staudinger Weg 7, D-55128 Mainz, Germany

We will present an innovative twin photoemission electron microscopy system (Twin-PEEM), which consists of two fully functionally crossed PEEMs. The Twin-PEEM was calculated with commercial software to design charged particle optics devices and constructed using professional 3D CAD software. The new design allows to place a single crystalline target directly after the cathode lens of the microscope in such a way that the low energy electrons diffracted on the single crystal can be imaged in a 90° mirror-like geometry. As was recently shown [1,2] such electron mirror can be used as a highly efficient spin-filter for 2D PEEM images. We characterize a few micro-structured samples obtained with Twin-PEEM using unpolarised deep ultraviolet light (discharge lamp) with the aim to demonstrate the potential of the novel electron microscope. We will discuss also the possibility of using the Twin-PEEM as tool for spin-resolved photoemission experiment.

[1] C. Tusche, M. Ellguth, A. A. Ünal, C.-T. Chiang, A. Winkelmann, A. Krasyuk, M. Hahn, G. Schönhense, and J. Kirschner, APL 99, 032505 (2011)

[2] M. Kolbe, P. Lushchyk, B. Petereit, H.J. Elmers, G. Schönhense, A. Oelsner, C. Tusche, and J. Kirschner. PRL 107, 207601 (2011)

O 35.72 Tue 18:15 Poster B

Time-resolved ARPES studies with high-oder harmonic radiation — •Björn Frietsch[1,2], Robert Carley[1,2], Martin Teichmann[1,2], Kristian Döbrich[1], Cornelius Gahl[2], and Martin Weinelt[2] — [1]Max-Born-Institut, Max-Born-Straße 2A, 12489 Berlin, Germany — [2]Freie Universität Berlin, Fachbereich Physik, Arnimallee 14,14195 Berlin, Germany

We present results from a high-order harmonics XUV source and beamline. The setup produces XUV photons between 20-65 eV, at an energy resolution of 150 meV and a pulse duration of 100 fs for time-resolved photoelectron spectroscopic studies of laser-driven dynamics in correlated systems. To create harmonics, 40-fs pulses from a commercial amplified Ti:Sapphire laser system running at 10 kHz repetition rate are focused into an argon-filled gas cell. The XUV wavelength and energy resolution are selected using a toroidal grating monochromator. We have used the instrument to study ultrafast magnetization of the lanthanide metals Gadolinium and Terbium, and to perform preliminary experiments on laser-driven phase transitions in VO2.

O 35.73 Tue 18:15 Poster B

$[\mathrm{Mn}_6^{\mathrm{III}}\mathrm{Cr}^{\mathrm{III}}]^{3+}$-SMMs and its counterions on HOPG analyzed by Means of FM-KPFM — •Aaron Gryzia[1], Natalie Frese[1], Armin Brechling[1], Ulrich Heinzmann[1], Veronika Hoeke[2], and Thorsten Glaser[2] — [1]Molecular and Surface Physics, Bielefeld University — [2]Anorganic Chemistry I, Bielefeld University

$[\mathrm{Mn}_6^{\mathrm{III}}\mathrm{Cr}^{\mathrm{III}}]^{3+}$ is a single-molecule-magnet (SMM) consisting of two bowl-shaped fragments, each containing three Mn-atoms, which are bridged by a central Cr-complex. For charge neutrality, counterions have to be coupled to the SMM. The SMM creates different kinds of structures on HOPG such as flat islands consisting of one or two layers of **$[\mathrm{Mn}_6^{\mathrm{III}}\mathrm{Cr}^{\mathrm{III}}]^{3+}$** or agglomerations at step edges. Data is acquired by means of nc-AFM. The position of the counterions is not yet known exactly, neither can they, if visible, be discriminated from the SMM by AFM. We expect the counterions to have a big influence on how the SMM adsorbs onto the substrate. The SMM is triply positive charged and each counterion carries a negative charge therefore differences in the contact potentials occur. If these differences are strong enough we are able to observe them and identify the SMM and its counterions by means of FM-KPFM (Frequency Modulated - Kelvin Probe Force Microscopy). Most recent results of our KPFM-Data will be shown and discussed with respect to the counterions.

O 35.74 Tue 18:15 Poster B

Using a two-dimensional electron mirror for efficient spin-resolved bandstructure mapping — •Christian Tusche, Martin Ellguth, Aimo Winkelmann, Alexander Krasyuk, and Jürgen Kirschner — Max-Planck-Institut für Mikrostrukturphysik, 06120 Halle, Germany

We measure the spin-polarization of photoelectrons emitted from several atomic layers thick Co films grown on Cu(100) using a momentum microscope. This instrument, consisting of a photoemission electron microscope (PEEM) and an aberration corrected electrostatic energy analyzer directly records the parallel momentum component, $k_{||}$, of photoelectrons emitted from the sample. Spin-filtering is based on the diffraction of low energy electrons in the (00)-LEED spot of a W(100) crystal, installed at the exit of the energy filter. In the spatial imaging mode, PEEM images of the magnetic domain structure of the Co films showed that 3800 image points can be recorded simultaneously [1].

A series of constant-energy cuts through the Brillouin zone gives direct access to the valence band electronic structure of the ultra-thin Co-film. By inserting the W(100) electron mirror into the electron optical path, the spin-resolved distribution of photoelectrons as a function of $k_{||}$(x,y) is recorded simultaneously with unprecedented efficiency. By exploiting the energy dependent spin-sensitivity of the low energy diffraction process, the absolute value of the spin-polarization can be obtained without magnetization reversal of the sample.

[1] Tusche, Ellguth, Ünal, Chiang, Winkelmann, Krasyuk, Hahn, Schönhense and Kirschner, Appl. Phys. Lett. **99**, 032505 (2011)

O 35.75 Tue 18:15 Poster B

(001) and (011) Surfaces of MnO and NiO — •Mihail Granovskij[1,2], Andreas Schrön[1,2], and Friedhelm Bechstedt[1,2] — [1]Institut für Festkörpertheorie und -optik, Friedrich-Schiller-Universität Jena, Max-Wien-Platz 1, 07743 Jena, Germany — [2]ETSF

In the paramagnetic state the ground-state crystal structure of the $3d$ transition metal oxides (TMOs) MnO and NiO is given by an ideal rock-salt (rs) structure. Below their respective Néel temperature, however, they are characterized by the formation of an antiferromagentic ordering AFM2 which is acompanied by a rhombohedral distortion along the [111] direction. The intersection of the thermally swichable magnetic ordering AFM2 with the crystal surfaces makes TMO surfaces ideal benchmark-materials for the investigation of recent magnetic surface probing techinques such as spin-polarized scanning tunneling microscopy (SP-STM) and magnetic exchange force microscopy (MExFM).

We present a density functional theory (DFT) study of the (001) and (011) surfaces of MnO and NiO. Exchange and correlation are treated within the generalized-gradient approximation (GGA) to DFT within the parametrization of Perdew, Burke, and Ernzerhof (PBE). For a proper treatment of the on-site Coulomb interaction, we correct with an effective interaction U according to Dudarev's approximation (GGA+U).

O 35.76 Tue 18:15 Poster B

Metal- Porphyrins on metallic and superconducting surfaces — •Nino R. Hatter, Benjamin W. Heinrich, Lukas Z. Braun, Tobias R. Umbach, Jose I. Pascual, and Katharina J. Franke — Institut für Experimentalphysik, Freie Universität Berlin, Germany

While magnetic properties of single magnetic molecules on metal surfaces have been vividly studied in the last years, only little research has been done on magnetic impurities on superconducting substrates. On metal surfaces spin-excitations or Kondo screening can be observed. On a superconductor exchange coupling to Cooper pairs adds another complex many-body interaction, which is competing with Kondo screening[1,2,3]. Here we present a comparative study of metal-porphyrins on Au(111) and on the type-I superconductor Pb(111) using Scanning Tunneling Microscopy/Spectroscopy (STM/STS).

[1] K.J. Franke, G. Schulze, J.I. Pascual, Science 332, 940 (2011), [2] A. Yazdani et al., Science 275, 1767 (1997), [3] H. Shiba, Prog. Theor. Phys. 40, 435 (1968)

O 35.77 Tue 18:15 Poster B

Magnetic and structural investigations of thin ferromagnetic CrSb layers on GaAs(110)/GaAs(001) — •Carsten Godde and Ulrich Köhler — Institut für Experimentalphysik IV, AG Oberfläche, Ruhr-Universität Bochum, Germany

Thin CrSb layers grow in the metastable zinc blende structure on III-V semiconductors and are predicted to be halfmetallic with a spin polarization of 100% at the Fermi-level. Thus, these systems are of great interest because of their possible use as spin aligning layers for spintronic devices. In this contribution we present structural and magnetic measurements of thin CrSb layers on the GaAs(110) and GaAs(001) surfaces for different coverages and annealing temperatures by STM and SQUID magnetometry. STM reveals for both surfaces a Volmer-Weber growth mode of the CrSb layers and atomic resolution show an ordering alongside the lattice structure of the substrate. Particularly with regard to the existence of different phases at the GaAs(001) surface, we investigate the influence of a Ga- and an As-terminated surface of the substrate for the film deposition. SQUID magnetometry measurements show ferromagnetic characteristics of the thin CrSb layers up to 4 ML thickness with a magnetic moment per Cr-atom of up to 5 μ_B.

O 35.78 Tue 18:15 Poster B

Susceptibility measurements of Ni clusters embedded in organic matrices — •Mariella Denk, Robert Mittermair, Daniel Queteschiner, Richard Denk, Michael Hohage, Lidong Sun, and Peter Zeppenfeld — Institut für Experimentalphysik, Johannes Kepler Universität Linz, A-4040 Linz, Austria

Reflectance Difference-Magneto Optic Kerr spectroscopy (RD-MOKE) and Atomic Force Microscopy (AFM) was used to study the morphologic and magnetic properties of organic magnetic molecules, namely, cobalt tetramethoxyphenylporphyrin (CoTMPP) on Cu(110)-(2x1)O. The magneto optic Kerr signal of the organic molecules strongly depends on the photon energy [1]. Thick layers ($\approx$ 100 nm) of organic molecules were used as host material for subsequent Ni cluster growth. The size, shape and distribution of the Ni particles strongly influences their optical and magnetic properties. By using an embedding organic matrix, we try to tune the interparticle interactions as well as the coupling between the organic molecules and the metal clusters, which, for instance, will affect the superparamagnetic limit of the nanoparticles. In order to address superparamagnetic effects the experimental setup was upgraded to measure the magnetic susceptibility, directly, and over the whole spectral range from 1.5 to 5 eV.

[1] M. Fronk, B. Bräuer, J. Kortus, O. G. Schmidt, D. R. T. Zahn and G. Salvan, Phys. Rev. B 79, 235305 (2009)

O 35.79 Tue 18:15 Poster B

Electronic states on Si(111)-(5×2)-Au — •Kerstin Biedermann and Thomas Fauster — Lehrstuhl für Festkörperphysik, Universität Erlangen-Nürnberg, Staudtstr. 7, D-91058 Erlangen, Germany

Submonolayers of gold on vicinal Si(111) surfaces form a variety of atomic chain structures and hence serve as a model system for one-dimensional electronic systems. We concentrate here on the Si(111)-(5×2)-Au surface, which exhibits three gold chains per unit cell.

Angle- and time-resolved two-photon photoemission experiments were carried out using infrared (IR, E_{IR}=1.55 eV) and ultraviolet (UV, E_{UV}=4.65 eV) femtosecond laser pulses. For photoemission (UPS) experiments the fourth harmonic (IR+UV) provided a source of 6.2 eV photons. The polarization of all beams could be chosen independently. Using optical dipole-selection rules, at normal emission, we evaluated the parity of the electronic states, which is either even or odd with respect to the $(1\bar{1}0)$ mirror plane orthogonal to the gold chains.

Apart from bulk transitions we observed an even, short-lived ($\tau <$ 20 fs) $n = 1$ image-potential resonance and a long lived feature ($\tau >$ 600 fs) within the bulk band gap of silicon. States related to the gold chains were detected at high emission angles. We present here an analysis of our time-, angle- and energy-resolved measurements and compare our findings to the Si(557)-Au and Si(553)-Au surfaces.

O 35.80 Tue 18:15 Poster B

Photoemission study of occupied and unoccupied states on Si(553)-Au — •Stefan Regensburger[1], Kerstin Biedermann[1], Thomas Fauster[1], Franz J. Himpsel[2], and Steven C. Erwin[3] — [1]Lehrstuhl für Festkörperphysik, Universität Erlangen-Nürnberg, Staudtstraße 7, 91058 Erlangen, Germany — [2]Department of Physics, University of Wisconsin-Madison, 1150 University Avenue, Madison, WI 53706, USA — [3]Center for Computational Materials Science, Naval Research Laboratory, Washington, DC 20375, USA

Atomic gold chains on vicinal Si(111) surfaces serve as model system for one-dimensional electronic states. For the characterization of the electronic states near the $\bar{\Gamma}$-point we used angle- and time-resolved two-photon photoemission with photon energies of 1.55 eV and 4.65 eV, as well as photoemission with 6.2 eV photon energy. Information about the symmetry of the electronic states was obtained from the polarization dependence of the spectra.

In addition to bulk transitions, the Rasha-split gold bands [1] and the $n = 1$ image-potential resonance we find two states related to the step-edge atoms. We observe an unoccupied state with even symmetry in the bulk band gap of silicon with a lifetime of $\tau = 125$ fs. It is assigned to the spin-polarized step-edge atoms predicted by theory [2]. An occupied state located 0.42 eV below the Fermi level corresponds to non-magnetic step-edge atoms coupled in pairs.

[1] Crain, J. N. et al., Phys. Rev. B **69**, 125401 (2004)

[2] Erwin, S. C. and Himpsel, F. J., Nat. Commun. **1**, 58 (2010)

O 35.81 Tue 18:15 Poster B

Two-photon photoemission from Si(111) 7×7 — •Jens Güdde, Andreas Damm, Marcel Reutzel, Alexander Lerch, and Ulrich Höfer — Fachbereich Physik und Zentrum für Materialwissenschaften, Philipps-Universität, D-35032 Marburg

The dynamics of photoexcited electrons in unoccupied states of the Si(111) 7×7 surface has been investigated by time- and angle-resolved two-photon photoemission (2PPE) for different sample temperatures. Aside from non-resonant 2PPE from the occupied S_2 surface band and the valence band maximum we observe the population dynamics in the initially filled (S_1) and and empty (U_1) surface bands as well as in the X valley of Si close to the surface. The population in the conduction band (CB) shows a temperature-dependent delayed rise on the same time scale of several hundred femtoseconds as the electron thermalization in the U_1 band. The photoemission from the S_1/U_1 as well as from the CB is completely quenched by hydrogen adsorption. Together with the delayed population rise, this suggests that the CB is populated by electrons which were initially excited in the U_1 band. The investigation of the population dynamics for different parallel momenta along the $\overline{\Gamma}$-$\overline{\mathrm{K}}$-direction reveals that the intraband relaxation within the CB proceeds on a time scale of few picoseconds while the population at the conduction band minimum decays with a time constant of several tens of picoseconds.

O 35.82 Tue 18:15 Poster B

Photoemission studies of graphene on Pt(111) — •David Nobis, Daniel Niesner, and Thomas Fauster — Lehrstuhl für Festkörperphysik, Universität Erlangen-Nürnberg, Staudtstr. 7, D-91058 Erlangen, Germany

Graphene can be grown on a variety of metal surfaces with different quality. On the Pt(111) surface graphene was prepared by decomposition of hydrocarbons. Ultraviolet photoelectron spectroscopy (UPS, 6.22 eV) and two-photon photoemission (2PPE, pump pulse 4.66 eV, probe pulse 1.55 eV) experiments were carried out on the graphene-covered surface.

The UPS experiments show a downward-dispersing state 260 meV below the Fermi level. This state fits well to a Shockley surface state from the bare Pt(111) surface calculated by the phase accumulation model. The graphene layer increases its binding energy.

By 2PPE the first two image-potential states with binding energies of 820 meV and 210 meV were observed. Lifetimes were determined to 13 fs and 79 fs and effective masses are close to the free-electron mass. Compared to the clean Pt(111) surface [1] the graphene layer enlarges the binding energy (mostly of n=1 image-potential state) and the lifetime of the image-potential states. This can be understood by the screening of the charge being dominated by the graphene. Angle-resolved spectra show maximum intensity around $\mathbf{k}_{\parallel} = 0.1$ Å^{-1} which is attributed to a resonance with the Shockley surface state.

[1]Link, S. *et al.*, Phys. Rev. B **63** (2001) 115420

O 35.83 Tue 18:15 Poster B

Towards time- and angle-resolved photoemission at a free-electron laser with an angle-resolving ToF spectrometer — •Christian Sohrt[1], Michael Bauer[1], Wilfried Wurth[2], Lutz Kipp[1], and Kai Rossnagel[1] — [1]Institut f\"ur Experimentelle und Angewandte Physik, Kiel, Germany — [2]Institut f\"ur Experimentalphysik and Center for Free-Electron Laser Science, Hamburg, Germany

The Free-Electron Laser (FEL) in Hamburg (FLASH) generates highly brilliant, ultrashort pulsed radiation with pulse durations down to 50 fs and photon energies up to 1000 eV. This enables unique experiments, as for example time-resolved core-level photoelectron spectroscopy. However, to establish photoelectron spectroscopy as a completely viable technique at an FEL, one has to develop a detection scheme with maximum efficiency, because the pulse repetition rates of FELs are notoriously low and the available beam time is extremely scarce. Our proposed solution is a photoelectron spectroscopy experiment based on a novel angle-resolved time-of-flight spectrometer. Compared to traditional detection schemes the instrument is expected to enhance the detection efficiency by a factor of about 200–due to the larger acceptance angle–and the temporal resolution by a factor of seven to about 100 fs–due to single-pulse detection. Thus, it will become possible to correlate core-level dynamics which is sensitive to changes in the charge distribution around specific atomic sites, with the dynamics of electrons at the Fermi surface in a single experiment. Here we present the progress of this project. This work is supported by the BMBF (FSP 301 FLASH).

O 35.84 Tue 18:15 Poster B

Thickness dependence of ion induced eletron emission —

•Kevin Kusmierek[1], Christian Haake[1], Andreas Wucher[1], Marika Schleberger[1], and Detlef Diesing[2] — [1]Universität Duisburg-Essen, Fakultät für Physik, 47057 Duisburg, Germany — [2]Universität Duisburg-Essen, Fakultät für Chemie, 45117 Essen, Germany

Ion bombardment of thin metal films leads to electronic excitations causing the well known secondary electron emission. When the film thickness is in the range of the excited carrier's mean free path, reflection of carriers at the back side of the film and subsequent passage through the front side to the vacuum may increase the secondary electron emission yield. This increase of the yield is influenced by the relaxation of the ion induced electronic excitation. Thus, we present a study on the thickness dependence of the secondary electron emission yield. Our metal films are evaporated on glass and AFM studies show a mean roughness of 3 nm. The films have thicknesses between 10 and 100 nm and are bombarded with keV Ar ions.

O 35.85 Tue 18:15 Poster B

Surface and Image-Potential States of Ni(111) Investigated with Spin- and Time-Resolved 2PPE — Thomas Odebrecht[1,2], •Beatrice Andres[1,2], Marko Wietstruk[1,2], Anke B. Schmidt[3], Markus Donath[3], and Martin Weinelt[1,2] — [1]Max-Born-Institut, 12489 Berlin — [2]Fachbereich Physik, Freie Universität Berlin, 14195 Berlin — [3]Physikalisches Institut, Westfälische Wilhelms-Universität Münster, 48149 Münster

The surface electronic structure of Ni(111) does not only exhibit occupied *sp*- and *d*-derived bulk states and surface resonances [1], but also a partially occupied Shockley-like surface state (SSS) as well as a Rydberg-series of image-potential states (IPS) close to the vacuum enegy. In two-photon photoemission experiments (2PPE) using the fundamental ($1h\nu = 1.6$ eV) and the third harmonic ($3h\nu = 4.8$ eV) of our Ti:Sa laser, we gain information on exchange splitting, spin polarization and spin-dependent lifetimes of these states.

We can either populate the unoccupied minority component of the SSS with a $1h\nu$ pulse and probe with $3h\nu$ or use a $3h\nu$-pump and $1h\nu$-probe pulse to reach the energetic region of the IPS. Populating the IPS out of the occupied components of the surface and bulk states we create a spin-polarized population in these unoccupied states which allows us to study their spin-dependent properties.

[1] Okuda *et. al.*, *Phys. Rev. B* **80**, 180404 (2009).

O 35.86 Tue 18:15 Poster B

Thermal desorption spectroscopy of interstellar relevant molecules on Forsterit and Olivine — •Robert Frigge, Tushar Suhasaria, Nadine Heming, Björn Siemer, and Helmut Zacharias — Physikalisches Institut, Universität Münster, Germany

Chemical surface reactions on dust grains are a possible way of molecule formation in the Interstellar Medium (ISM). These grains typically consists of carbonaceous and silicate particles embedded in icy mantles which are formed by molecules like CO, CO_2, H_2O or CH_4. Temperature programmed desorption (TPD) is used to investigate the binding energy and reaction order of several interstellar relevant molecules like D_2, CO, CO_2, CH_4, and D_2O on different interstellar silicate analogues like Forsterite (Mg_2SiO_4) and Olivine ($Mg_xFe_{1-x}SiO_4$). The experimental set-up consists of a quadrupole mass spectrometer, a dosing chamber and a liquid helium cooled sample holder. Due to this set-up it is possible to investigate the behavior of these molecules at very low temperatures ($\approx 5\,K$) comparable to the ISM. Further due to the dosing chamber it is possible to prepare a sample with a precise and low coverage. We present desorption spectra, binding energies and their coverage dependence on both Olivine and single crystal Forsterite.

O 35.87 Tue 18:15 Poster B

On the relation between fluctuations in STM currents and diffusion coefficients of molecules on surfaces — •Susanne Hahne[1], Julian Ikonomov[2], Moritz Sokolowski[2], and Philipp Maass[1] — [1]Department of Physics, University of Osnabrück, Barbarastr. 7, 49076 Osnabrück, Germany — [2]Institute of Physical and Theoretical Chemistry, University of Bonn, Wegelerstr. 12, 53115 Bonn, Germany

A widely used method to measure surface diffusion coefficients is by tracking particles via STM, FEM or FIM. To obtain reliable data one needs a good statistic, which is generally quite extensive. Also these methods are limited to sufficiently small mobilities. An alternative experimental approach is the recording of the signal fluctuations in time from a locally fixed microscope [e.g. tunneling current in case of STM; frequency/height in case of AFM]. This procedure on the other hand needs a good theoretical description in order to obtain reliable results. Three different methods can be applied to analyze this signal fluctuations: (i) Determination of the autocorrelation-function or extraction of the peaks in the fluctuation, where either (ii) the distribution of peak widths is studied or (iii) the distribution of peak to peak distances. We critically discuss and extend analytical theories underlying these methods and evaluate their power by comparison to recent experiments [1].

[1] J. Ikonomov, P. Bach, R. Merkel, and M. Sokolowski, Phys. Rev. B 81, 161412(R) (2010).

O 35.88 Tue 18:15 Poster B

Surface and bulk states at Ge(100) - Binding energies, lifetimes and dispersions — •Jens Kopprasch[1,2], Kristof Zielke[1,2], Cornelius Gahl[1,2], Christian Eickhoff[1,2], Jörg Schäfer[3], and Martin Weinelt[1,2] — [1]Max-Born-Institut, Max-Born-Straße 2a, 12489 Berlin, Germany — [2]Freie Universität Berlin, Fachbereich Physik, Arnimallee 14, 14195 Berlin, Germany — [3]Universitat Würzburg, Fakultät für Physik und Astronomie, Am Hubland, 97074 Würzburg, Germany

Germanium (Ge) is a material of growing interest in semiconductor industry. Increased industrial engineering has opened a broad field of applications for Ge, e.g. solar cells, high-power transistors, infrared optics and X-ray detectors.

We observed band bending at n-doped samples and flat-band conditions on p-doped samples. In this way we determine the Ge(100) ionisation potential. A series of two-photon-photoemission measurements with variing photon energies allows us to identify the dangling-bond states D_{up}, D_{down} and the first image-potential state n=1. We determined the binding energies, lifetimes and dispersions of these states. Furthermore we observed bulk-band transitions at 90K which lead to carrier dynamics on a picosecond timescale. In addition we observe ultrafast interband scattering between the conduction band and Γ-valley.

O 35.89 Tue 18:15 Poster B

Electronic energy dissipation - obtain mechanisms and models from TDDFT — •Michael Grotemeyer and Eckhard Pehlke — Institut für Theoretische Physik und Astrophysik, Universität Kiel, Germany

Molecular dynamics simulations based on time-dependent density-functional theory to describe the electron dynamics and Ehrenfest dynamics for the motion of the nuclei have provided detailed information about the electronic energy dissipation of vibrationally highly excited HCl molecules in front of a metal surface. Inspection of the time development of the electronic excitation spectra reveals the energy transfer mechanism and helps to identify the diabatic states responsible for the dissipation. The striking asymmetry between the excitation spectra of the holes and the electrons pinpoints the importance of the energetical position of the molecular resonances in the energy range of the unoccupied states. This leaves us with the question how to produce simple tight-binding like models and whether there is a unifying description of the energy dissipation process that holds the potential to be generalized to arbitrary molecular trajectories. Already a one-dimensional tight-binding model including only the LUMO is capable of describing the energy transfer process and illustrates many effects of the *ab initio* TDDFT-MD simulations. By adding an additional unoccupied molecular orbital into the model we obtain an improved description of the excitation spectra at the maximum of the dissipation. We suggest the resonance width of the LUMO plays a decisive role for the nonaddiabatic effects.

O 35.90 Tue 18:15 Poster B

Dynamic space charge effects in time-resolved photoelectron spectroscopy — •Lars Oloff, Stefan Hellmann, Christian Sohrt, Ankatrin Stange, Timm Rohwer, Michael Bauer, Lutz Kipp, and Kai Rossnagel — Institut für Experimentelle und Angewandte Physik, Universität Kiel, 24118 Kiel, Germany

The development of fs-pulsed lightsources, e.g. Free-Electron Lasers or High Harmonic Generation sources (HHG), opened up a new field of photoelectron spectroscopy (PES) in terms of time-resolved pump-probe-experiments. The high intensity of these sources leads to the effect that the interaction beween the photoelectrons emitted in such an ultrashort time frame can not be neglected anymore. This phenomenon known as space charge effect results in general in non-negligible impact on kinetic energy and detected angle of the emittted electrons. Specifically in time-resolved pump-probe-PES in the high pump-power regime a further intensity-caused effect can be recognized: Via multiphoton-processes the low energy pump-pulse may lead to unwanted emission of electrons from the material. This pump electron cloud interacts via Coulomb forces with the electron cloud emitted through the probe pulse resulting in shifted and broadened photoelectron spectra. We investigated these dynamic space charge effects at a HHG source (42.66 eV, 27th Harmonic) on $TiSe_2$ and $Pt(111)$ demonstrating their dependency on material, intensity and chosen delay between the two pulses. The results can be interpreted via molecular dynamic simulations.

O 35.91 Tue 18:15 Poster B

Preparation and spectroscopic studies of benzo[ghi]perylene dye on SiC — •Nils Fabian Kleimeier[1], Deb Kumar Bhowmick[1], Nabi Aghdassi[1], Steffen Linden[1], André Devaux[1,2], Luisa De Cola[1,2], and Helmut Zacharias[1,2] — [1]Physikalisches Institut, Westfälische Wilhelms-Universität, Wilhelm-Klemm-Str. 10, 48149 Münster, Germany — [2]CeNTech GmbH, Center for Nanotechnology, Heisenbergstr. 11, 48149 Münster, Germany

Organic-inorganic hybrid systems have gained increasing interest due to their versatile applications, e.g., as organic solar cells, biosensors, light emitting devices, or molecular electronics. Our research focuses on polyaromatic hydrocarbons (PAHs) due to their characteristically high fluorescence yield and the possibility to tune their photophysical and electrochemical properties. SiC substrates are functionalized with aminopropyl triethoxysilane (APTES) molecules by a siloxane bond. The benzo[ghi]perylene-1,2-dicarboxylic anhydride is then bound covalently to the APTES via imide bonds. Covalent attachment of the dye to the surface is verified by X-ray photoemission spectroscopy and FT-IR spectroscopy. UV absorption and time-resolved fluorescence and two-photon photoemission spectroscopy (TR-2PPE) measurements have been performed, yielding lifetimes between τ_1=1.4 to 1.8 ns and τ_2=4.3 to 4.7 ns for the fluorescence and τ=84 fs for the TR-2PPE measurement.

O 35.92 Tue 18:15 Poster B

Real-time observation of electron propagation in condensed matter — •Stefan Neppl[1], Elisabeth M. Bothschafter[1,2], Ralph Ernstorfer[3], Adrian L. Cavalieri[4], Johannes V. Barth[1], Dietrich Menzel[1], Reinhard Kienberger[2], and Peter Feulner[1] — [1]TU München — [2]Max-Planck-Institut für Quantenoptik — [3]Fritz-Haber-Institut — [4]CFEL

Photo-ionization with isolated attosecond (1 asec = 10^{-18} s) XUV pulses simultaneously dressed by a precisely timed NIR electric field is envisaged as a tool for probing the ultrafast dynamics of electrons in condensed matter [1]. Here we demonstrate the ability of this streaking technique for real-time probing the motion of photo-excited electrons in thin metal films as they traverse single atomic layers. By growing epitaxial layers of magnesium on a W(110) substrate, we are able to follow the time evolution of the XUV-induced photoelectron wave packets originating from the W4f and Mg2p core states and the joint conduction band with a time resolution of only a few attoseconds. Depending on the initial state character of the released electrons, we measure relative time delays in their emission ranging from 10 to 200 asecs, with different dependencies on the thickness of the overlayer. The results will be compared to corresponding streaking experiments performed on magnesium and tungsten single crystals

[1] Cavalieri et al. Nature 449, 1029 (2007)

O 35.93 Tue 18:15 Poster B

Nonequilibrium phonon gas in laser-excited solids — •Isabel Klett[1], Orkhan Osmani[1,2], and Bärbel Rethfeld[1] — [1]TU Kaiserslautern, 67663 Kaiserslautern, Germany — [2]Universität Duisburg-Essen, 47048 Duisburg, Germany

Irradiation of metals with a femtosecond laser pulse leads to a hot electron gas, while the lattice stays nearly cold. Due to the excitation, the electronic system is out of thermal equilibrium, so after laser irradiation, two main processes occur: The first is the electron thermalization, the second is the energy transfer from the electrons to the lattice due to the electron-phonon-coupling. Both processes have been described by assuming a thermalized distribution function for the phononic system. However, due to the fact that only longitudinal phonon modes can absorb the energy of the electrons, this assumption does not hold. Besides, with THz-Lasers [1], different phonon modes can be excited directly, leading to a thermal nonequilibrium within the phononic system. Furthermore, in thin films phonon confinement effects have been observed [2], which is also an indication for a nonequilibrium distribution of the phonons. We describe the phonon-phonon interaction and phonon thermalization with a Boltzmann collision integral. Our aim is to model nonequilibrium phonon distributions and the resulting observable effects after ultrashort laser-matter interaction.

[1] S. Kumar et al., Appl. Phys. Lett. 84, 2494*2496 (2004)

[2] B. Krenzer et al., Phys. Rev B 80, 024307 (2009)

O 35.94 Tue 18:15 Poster B

Time-resolved femtosecond Se 3d core level spectroscopy in the Mott insulator TiSe2 — •Hatem Dachraoui[1], Tobias Milde[1], Michael Porer[2], Norbert Müller[1], Recardo Manzke[3], Walter Pfeiffer[1], Rupert Huber[2], and Ulrich Heinzmann[1] — [1]Molecular and Surface Physics, Faculty of Physics, Bielefeld University, Germany — [2]Ultrafast Quantum Electronics and Photonics, Faculty of Physics, Regensburg University, Germany — [3]Elektronische Eigenschaften und Supraleitung, Faculty of Physics, Humboldt-University Berlin, Germany

Strongly correlated materials exhibit interesting dynamics and phase transitions for which the underlying mechanisms are still under debate. Fs-laser induced dynamics provide information about the phase transition mechanism. The recent progress in the creation of femtosecond EUV pulse generation (by means of high harmonic Generation HHG) offers the feasibility of time-resolved core level photoelectron spectroscopy which is capable of probing ultra-fast light driven processes at surfaces. Here we use 20 fs EUV-pulses to directly study the ultrafast dynamics of the charge density wave in TiSe2 after near-infrared excitation (1.5 eV). Structural transitions, evidenced by a dynamic shift of Se 3d core-levels, occurs before electrons lattice thermalization is established.

O 35.95 Tue 18:15 Poster B

2PPE-measurement on Cu(1 1 11) with an angle-resolving time-of-flight spectrometer — •Thomas Kunze[1,2], Jens Kopprasch[1,3], Martin Teichmann[1,3], Thorsten U. Kampen[2], and Martin Weinelt[1,3] — [1]Max Born Institut, Max-Born-Straße 2a, 12489 Berlin, Germany — [2]SPECS GmbH, Voltastr. 5, 13355 Berlin, Germany — [3]Freie Universitat Berlin, Fachbereich Physik, Arnimallee 14, 14195 Berlin, Germany

We aim at the implementation of an advanced concept for photoemission spectroscopy into a robust and reliable experiment for time- and energy-resolved photoemission with ultrahigh transmission. The basic idea is to combine a parallel imaging technique comprising ultimate $\vec{k}$-resolution with time-of-flight energy dispersion. Therefore we developed, in cooperation with SPECS GmbH, the angular-resolving Time-of-Flight spectrometer THEMIS. This instrument allows us to measure energy E over parallel momentum $k_{x\|}$ and $k_{y\|}$ without rotating the sample.

We present two-photon photoemission measurements on Cu(1 1 11), a vicinal copper surface with (001)-terraces. The dispersion of the image-potential states reveals back-folding and mini-gap opening with the periodicity of the step superlattice. The lifetimes of the image-potential states at Cu(1 1 11) depend on the parallel momentum of the photoemitted electrons.

O 35.96 Tue 18:15 Poster B

Charge-transfer collisions of H^+ with He using Time-Dependent Density Functional Theory — •Guillermo Avendano-Franco, Xavier Gonze, and Bernard Piraux — Université Catholique de Louvain, Louvain-la-Neuve, Belgium

We present a theoretical study of the Charge-transfer collisions of H^+ with He using Time-Dependent Density Functional Theory. The energies of the projectile were between 70 keV to 1.2MeV. We found some charge being transferred to the proton and we considered those results in relation to current theoretical descriptions of the collision processes.

O 35.97 Tue 18:15 Poster B

Investigations of the Patch Effect with a Scanning Kelvin Probe — •Gertrud Konrad[1,2], Stefan Baessler[3], Iain Baikie[4], Henry Bonner[3], Werner Heil[2], Rachel Hodges[3], Thorsten Lauer[2], Sean McGovern[3], and Xuying Tong[3] — [1]Atominstitut, TU Wien, Austria — [2]Universität Mainz, Germany — [3]University of Virginia, Charlottesville, USA — [4]KP Technology Ltd., Wick, UK

Precision measurements of observables in neutron beta decay address important open questions of particle physics and cosmology, and are generally complementary to direct searches for new physics beyond the Standard Model in high-energy physics.

The analysis of the decay protons is based on a precise energy measurement, by means of an electrostatic filter or by TOF measurement. Then the electric potential between the decay and filter regions has to be known with an accuracy of better than 10 mV. Possible inhomogeneities of the work function (WF) at the electrode surface vary the electric field distribution. On the inside of a cylindrical electrode, a spatial variation of order of 100 meV over a distance of several cm was found. A scanning Kelvin probe (SKP) has been used to map the WF, with a spatial resolution of 2 mm and a WF resolution of $1-3$ meV. To minimize the WF variations, different surface materials, treatments, and coatings are being investigated. A platinized surface yielded a RMS WF value of better than 10 meV. Coating adhesion and surface roughness have a significant influence on the measured WF values.

The physics motivation, the SKP technique as well as the status of the investigation will be presented in this talk.

O 35.98 Tue 18:15 Poster B

Dynamische Rasterreibungskraftmikroskopie: Bildkontrast bei höheren Moden auf HOPG — •Felix Mertens, Karsten Krischker, Thomas Göddenhenrich und André Schirmeisen — Institut für Angewandte Physik, Justus-Liebig-Universität Gießen, D-35392 Gießen

Es wird ein Modulations-Reibungsmikroskop präsentiert, das für Topographie- und Reibungsmessungen unter UHV Bedingungen geeignet ist [1]. Eine modifizierte Lock-In Technik regt die Probe zu Schwingungen entlang der Hebelarmlängsachse an [2]. Durch den Spitze-Probe Kontakt werden dem Hebelarm Oszillationen aufgeprägt, die durch ein Glasfaserinterferometer detektiert werden. Entspricht die Anregungsfrequenz der modulierten Probenschwingung einem ganzzahligen Bruchteil der Hebelarmbiegeresonanz, so setzt sich die Hebelarmoszillation sowohl aus niederfrequenten als auch aus hochfrequenten Schwingungsanteilen zusammen. Die niederfrequenten Schwingungsanteile korrespondieren mit der Topographie, die Anregung der hochfrequenten Schwingungsanteile wird durch den Reibungskontakt verursacht. Die Anwendung dieser Technik auf hochorientiertem Pyrographit ermöglicht Reibungsaufnahme, bei denen die Orientierung der Kornstruktur einen wesentlichen Kontrastmechanismus der Aufnahme darstellt. [1] T. Göddenhenrich, S. Müller, and C.Heiden, Rev. Sci. Instrum. 65, 2870 (1994) [2] A. Spychalski-Merle, K. Krischker, T. Göddenhenrich, and C. Heiden, Appl. Phys. Lett. 77, 501 (2000)

O 35.99 Tue 18:15 Poster B

Nanoparticle Manipulation With Combined AFM/SEM — •Michael Feldmann[1], Antoni Tekiel[2], Jessica Topple[2], Dirk Dietzel[1], Peter Grutter[2], and André Schirmeisen[1] — [1]Institut für Angewandte Physik, JLU Giessen, Germany — [2]Department of Physics, McGill University, Montréal, Canada

To understand friction on a fundamental level the investigation of friction with nanoparticles has presented itself as a very promising approach[1][2]: a nanoparticle is pushed by an AFM tip to measure the friction between the particle and a substrate. These experiments allow to study friction of extended single asperity nanocontacts. If this kind of experiment is executed with just a single AFM tip as a probing channel, the tip can either move the particle or image it, but not both at the same time. To gain a better understanding of the involved processes and to increase control over the manipulation, we performed nanoparticle manipulations with a combined AFM / SEM system. This setup enabled us to move the particles with the AFM, while simultaneously observing the particle translations with scanning electron microscopy. We observed that the AFM tip is not only able to push the particles, but also to pull the particles over the substrate due to the adhesion between tip and particle. On the other hand complete detachment of the particles from the substrate did never occur, consistent with the assumption of having very flat interfaces and thus high adhesion between particle and substrate.

[1] D. Dietzel et. al., Phys. Rev. Lett. 101, 125505 (2008)

[2] D. Dietzel et. al., Phys. Rev. B 82, 035401 (2010)

O 35.100 Tue 18:15 Poster B

Charge transport mesasurements performed with an ultra compact multi-tip STM — •Marcus Blab, Vasily Cherepanov, Peter Coenen, and Bert Voigtländer — Peter Grünberg Institut (PGI-3), Forschungszentrum Jülich, 52425 Jülich, Germany, and JARA-Fundamentals of Future Information Technology

An ultra compact 4-tip STM was constructed in order to investigate the charge transport through nanostructures. Examples for systems which can be studied with such a microscope include nanowires, graphene and nanoscale semiconductor devices. The instrument diameter of 50 mm leads to high mechanical stability and low thermal drift. The heart of this multi tip STM is the ultra compact Koala Drive nanopositioner. We will show the characteristics of this new machine like drift and noise. Furthermore first measurements at test samples and lithographic structured samples of nanowires will be presented.

O 35.101 Tue 18:15 Poster B

Radio frequency optimized STM for the use with pulsed tunneling voltages — •Christian Saunus, Marco Pratzer, and Markus Morgenstern — II. Physikalisches Institut, RWTH Aachen University, Aachen Germany

The measurement of fast surface dynamics with an STM suffers from the low readout bandwidth given by the high gain preamplifier. To overcome this limit, Sebastian Loth introduced an all electrical pump-probe measurement which enabeled him to measure electron spin relaxation at the order of 100 ns by a commercial standard STM [1]. To increase this time resolution even more we designed a very compact STM with an insitu tip exchange mechanism operating with high frequency voltage pulses. We have shown that a time resolution of 710 ps is achieved by using the non-linearity of the I(V) curve on HOPG. The microscope is designed to work in a 4 K UHV system with 7 T rotatable magnetic field.

[1] S. Loth, Science 329, 1628 (2010)

O 35.102 Tue 18:15 Poster B

Ion conduction in glass ceramics: Influence of nanoscopic boundary surfaces in experiment and simulation — •Marvin Stiefermann[1], Dirk Dietzel[2], André Schirmeisen[2], Harald Fuchs[1], and Bernhard Roling[3] — [1]Physikalisches Institut, University of Münster and CeNTech, Center for Nanotechnology, Münster — [2]Institut für Angwandte Physik, University of Gießen — [3]Department Chemie, Universität Marburg

The ongoing progress in miniaturization leads to a constantly increasing number of mobile electronic devices. The largest factor limiting the usability of the devices is the battery endurance. Hence further research is needed for a better understanding leading to higher battery performance. We analysed a solid electrolyte as found in modern batteries using a N2 cooled variable temperature atomic force microscope. Electrostatic force spectroscopy in the time domain (TDEFS) was employed to study the relaxation times of ions within nanoscopic subvolumes of a phase separated glass ceramic, consisting of a well conducting glassy phase and poorly conducting crystalline phase. An effect observed earlier in ion conduction studies was the decrease of relaxation time when increasing the fraction of weakly conducting crystalline phase[1]. To understand this phenomenon we compared the experimental TDEFS spectra with simulations based on a Comsol Multiphysics finite element simulation. The model built consists of 2500 elements allocated to well and poor conducting phases randomly. By varying the fraction of both phases, the trend of nanoscopic ion conduction can be reproduced and related to the amount of surface boundaries.

O 35.103 Tue 18:15 Poster B

Contact size effects for the β-relaxation of PMMA using friction force microscopy — •Johannes Sondhauss[1], Bernd Gotsmann[2], Mark A. Lantz[2], and André Schirmeisen[3] — [1]Institute of Physics, University of Münster, Germany — [2]IBM Zurich Research Laboratory, Rüschlikon, Switzerland — [3]Institute of Applied Physics, University of Giessen, Germany

The importance of polymer films for different technical applications brought increased attention to polymer surface studies. In addition polymers are an ideal model system for tribology due to their distinct modes of dissipation. The friction force microscope (FFM) has been recently proved useful to study surface processes in polymers. In this work we performed friction experiments using different Si-tips sliding on a PMMA film. We varied the applied load, the scan velocity and the sample temperature. In addition we used three different cantilevers with tip radii between 18 nm and 2.65 μm. Latter were produced by attaching a spherical Si-particle to the modified tip apex of a cantilever. Within the chosen parameter range we observed the β-relaxation as well as the onset of the α-relaxation and we were able to determine the activation energy of the β-relaxation for each of the data sets measured with the different tips. The observed activation energy increases for increasing tip radii.This trend seems to follow the Eyring model which describes the influence of the shear stress on the activation energy. Furthermore, a conversion of the scan velocity to frequency [1] allowed us to combine the individual data sets to one curve.

[1] Tocha et al., Soft Matter 5, 1489 – 1495 (2009)

O 35.104 Tue 18:15 Poster B

Nano-Raman Microscope with Novel Probe Design for High-Resolution Surface Investigations — •Christoph Zeh[1], Daria Kovalenko[1], Martin Küttner[1], Bernd Köhler[1], Jörg Opitz[1], and Lukas M. Eng[2] — [1]Fraunhofer Institut für Zerstörungsfreie Prüfverfahren, Institutsteil Dresden, Maria-Reiche-Str. 2, 01109 Dresden — [2]Institut für Angewandte Photophysik, TU Dresden, 01069 Dresen

Optical Raman signals contain a wealth of information about the physical and chemical properties of many different substances. In this work, we demonstrate our home-built Nano-Raman microscope (NRM) and special optical fiber probes. The NRM comprises a standard microscope as optical detection system and a scanning near-field optical (SNOM) head. It is intended for investigations of nano-structured materials for novel industrial applications. The probe acts as a nanoscale light source and locally illuminates the sample. In each examined point of the sample, light scattered from the surface is collected through the microscopes objective lens and sent to an optical detector, e.g. spectrometer. The smaller the light source is, the higher is the resolution. To achieve a small spot size and high light intensities at the same time, we use sharp optical fiber tips prepared from a special optical fiber. The fiber has a refractive index profile allowing better polarization control, especially for circular light distributions. These modes of the optical field allow for a higher efficiency of the fiber probe. We will present recent results on the fabrication of suitable fiber tips.

O 35.105 Tue 18:15 Poster B

Implementing a setup to detect ballistic and inelastic transport channels in an LT-STM experiment — •Maren C. Cottin, Johannes Schaffert, Rolf Möller, and Christian A. Bobisch — Faculty of Physics, Center for Nanointegration Duisburg-Essen, University of Duisburg-Essen, 47048 Duisburg, Germany

As low cost and easy to process alternatives to conventional inorganic semiconductors, organic molecules are already applied in a variety of electronic devices. For an improvement in speed, energy consumption and lifetime of these devices the understanding of the electronic transport through the molecules is essential. Electrons injected into a molecule by the tip of a scanning tunneling microscope (STM) may lead to an electronic excitation. The relaxation may follow different pathways, one of which is a radiative decay, i.e. the emission of photons [1]. The spectral analysis of these photons combined with the ultimate lateral resolution of the STM has been demonstrated to allow a mapping of dissipative channels within a single molecule [2]. Here, we present the implementation of a detection unit for light emission which is integrated into an existing home built low temperature STM experiment. As a complementary technique, ballistic electron emission microscopy (BEEM) can be used to identify ballistic transport channels [3]. The combination of both techniques will give further access to study transport phenomena on an atomic scale.

[1] R. Berndt et al., Science 262, 1425 (1993). [2] C. Chen et al., Phys. Rev,. Lett. 105, 217402 (2010). [3] A. Bannani et al., Science 315, 1824 (2007).

O 35.106 Tue 18:15 Poster B

STM characterization of self-assembled organic compounds on metallic surfaces — •Oscar Diaz Arado[1,3], Lars Jansen[1], Hendrik Wagner[2], Amido Studer[2], and Harald Fuchs[1] — [1]Physikalisches Institut and Center for Nanotechnology, Muenster — [2]Organisch-Chemisches Institut, Westfaelische Wilhelms-Universitaet, Muenster — [3]Centro de Estudios Avanzados de Cuba, CEAC, La Habana, Cuba.

Chemical reactions on surfaces (2D reactions) through the self-assembly of organic compounds have been an uprising field of research in the last years, being a promising alternative to construct covalent-linked organized structures, something thought to be impossible up to now [1]. Therefore, we investigate the possibility to initiate a chemical reaction between two organic compounds, 2,5-Dihexylterephthalaldehyde and Octanehydrazide, on Au (111), a simple geometry to study their possible 2D reactions [2]. These compounds were initially studied with a scanning tunneling microscope (STM) under a liquid environment, where no self-assembly process was observed. Organic molecular beam epitaxy is a method suitable to perform a controlled layer-by-layer deposition of organic compounds in the ultra high vacuum (UHV) regime. We present our preliminary results of the combination of the OMBE deposition technique with a room temperature STM under UHV conditions. The successful deposition and self-assembled structure formation of each compound is presented here. [1] D. F. Perepichka, F. Rosei, Science 2009, 323, 216 [2] T. R. Linderoth et. al., Angew. Chem. 2007, 119, 9387

O 35.107 Tue 18:15 Poster B

Thermal Scanning Probe Lithography: Progress and Applications — •Felix Holzner[1,2], Philip Paul[1], Cyrill Kuemin[1,2], Ute Drechsler[1], James L. Hedrick[3], Heiko Wolf[1], Nicholas Spencer[2], Urs Duerig[1], and Armin Knoll[1] — [1]IBM Research, Rueschlikon, Switzerland — [2]Laboratory of Surface Science and Technology, ETH Zurich, Switzerland — [3]BM Research, Almaden, USA

The presented poster summarizes our recent advances in Thermal Scanning Probe Lithography with polyphthalaldehyde (PPA) as resist material. The polymer responds to the presence of a hot tip by depolymerization and local desorption. Thereby arbitrarily shaped patterns in the form of topographic reliefs can be written.

Patterning speeds with up to 500000 pixels/s and a positioning error of less than 10 nm at 10 mm/s scan speed were achieved. The written reliefs were imaged with the same cantilever with similar scan speeds leading to short fabrication turn-around times. In addition, we show that it is possible to use the surface roughness of the polymer films as fingerprints for the alignment of subsequently written patterns. The method achieves a stitching accuracy of <5 nm.

First applications shown on the poster include "Ultra long-term data preservation" and "Removable templates for directed placement of gold nanorods".

[1] Holzner et al., Nano Letters, 2011, 11, 3957-3962 [2] Paul et al., Nanotechnology, 2011, 22, 275-306 [3] Knoll et al., Advanced Materials, 2010, 22, 3361-3365 [4] Holzner et al., Appl. Phys. Lett., 2011, 99, 023110 [5] Pires et al., Science, 2010, 328, 732

O 35.108 Tue 18:15 Poster B

Electron induced dynamics of hepthathioether β-cyclodextrin molecules — •Avijit Kumar[1], René Heimbuch[1], Kim S. Wimbush[2], Hasan Atesci[1], Adil Acun[1], David N. Reinhoudt[2], Aldrik H. Velders[2,3], and Harold J W Zandvliet[1] — [1]Physics of Interfaces and Nanomaterials, MESA+ Institute for Nanotechnology — [2]Supramolecular Chemistry and Technology, MESA+ Institute for Nanotechnology — [3]Biomolecular Chemistry, MIRA Institute for Biomedical Technology and Technical Medicine, University of Twente, the Netherlands

Macroscopic junctions using Self Assembled Monolayers (SAMs) are prevalent in charge transport studies in molecular electronics. However, the macroscopic nature of metal-molecules contacts lead to an ensemble averaging of the transport events that occur across array of contacted molecules. Here, we have performed variable temperature scanning tunneling microscopy (STM) and spectroscopy (STS) measurements on hepthathioether β-cyclodextrin (β-CD) SAMs on Au to investigate dynamical behavior, which is not apparent in ensemble averaged studies. The dynamics is reflected in the tunneling current-time (I-t) traces, which were recorded with the STM feedback disabled. The dynamics is temperature independent, but increases with increasing tunneling current and sample bias, indicating that the conformational changes of the β-CD molecules are induced by electrons that tunnel inelastically. Even for sample biases as low as 10 mV we observe well-defined levels in the I-t traces. We attribute these jumps to the excitations of the molecular vibration of the macrocyclic β-CD molecule.

O 35.109 Tue 18:15 Poster B

Chromium Bulk Tips for Spin-Polarized Scanning Tunneling Microscopy — •Christian Hanneken, André Kubetzka, Kirsten von Bergmann, and Roland Wiesendanger — Institute of Applied Physics and Microstructure Research Center, University of Hamburg, Jungiusstrasse 11, D-20355 Hamburg, Germany

For the investigation of magnetic nanostructures using spin-polarized scanning tunneling microscopy (SP-STM), one would like to avoid uncontrolled magnetic interactions between tip and sample and the tip and an external magnetic field. Antiferromagnetic material features these properties, therefore being desirable as a tip material. In this work, a new method is presented for the production of antiferromagnetic chromium bulk tips. The electrochemically etched tips were characterized *ex situ* using scanning electron microscopy. In order to demonstrate the magnetic sensitivity of the produced tips, one tip was characterized *in situ* using SP-STM. The polar angle of the tip magnetization and its variation after different tip changes is determined and is found not to change significantly. In addition, it is shown that an external magnetic field has no effect on the tip magnetization up to B = ±2 T. To conclude, this Chromium bulk tip is found to be similar to Cr coated W tips with the advantage of a nearly infinite amount of magnetic material.

O 35.110 Tue 18:15 Poster B

Conductive AFM for CNTs characterisation — •Marius Toader[1], Holger Fiedler[2], Stefan E. Schulz[2,3], and Michael Hietschold[1] — [1]Chemnitz University of Technology, Institute of Physics, Solid Surfaces Analysis Group, D-09107 Chemnitz, Germany — [2]Chemnitz University of Technology, Center for Microtechnologies, D-09126 Chemnitz, Germany — [3]Fraunhofer Research Institute for Electronic Nano Systems, D-09126 Chemnitz, Germany

Within a continuous downscaling tendency, the remarkable mechanical and electrical properties of Carbon NanoTubes (CNTs) recommend them as suitable candidates for nanoscale electronics and interconnects. A versatile technique able to address simultaneously morphological and electrical measurements within such nanosystems is Conductive Atomic Force Microscopy (C-AFM). In this work, MWCNTs networks were vertically grown by chemical vapour deposition on a conductive bottom contact line as described in [1]. Using C-AFM, topographic information as well as current mapping of CNTs networks within distinct trenches were obtained. Current-voltage (I-V) characteristics were recorded down to single CNTs bundles. The corresponding reproducibility was checked over multiple measurements sets and distinct locations. Moreover, the sample bias used during the spectroscopy measurements was found to have no influence on the I-V response. The outcome I-V spectra were found to be highly reproducible and consistent with the voltage dependent current mapping of the CNTs networks. [1] Fiedler et al. online via DOI: 10.1109/IITC.2011.5940346

O 35.111 Tue 18:15 Poster B

Experiments on molecular heat transport — •Nils Könne, Ludwig Worbes, David Hellmann, Konstantin Kloppstech, Hanna Fedderwitz, and Achim Kittel — EHF, Fak. V, Physik, Carl von Ossietzky Universität Oldenburg

The aim of our research is the heat transfer through a single molecule a topic which has attracted a lot of interest in recent years [1]. We have developed a near field scanning thermal microscope (NSThM) to investigate heat transfer under ultra high vacuum conditions across distances ranging from fractions of a nanometer to a few nanometers. The microscope has a lateral resolution in the range of a few nanometers. In the present project we are using this instrument to investigate the molecular heat transfer. To address this we are using self assembled mono layers as a model system. For this purpose different thiols are arranged on a gold covered substrate to which the thiol group of the molecule is bound covalently. Firstly, we characterize the degree of coverage of the film by means of atomic force microscopy. The heat transfer is investigated under ultra high vacuum conditions by cooling (about 120K) or heating the sample (350K) and keeping the NSThM tip at room temperature. First result will be presented. [1] Yonatan Dubi and Massimiliano Di Ventra, Rev. Mod. Phys. 83, 131 (2011).

O 35.112 Tue 18:15 Poster B

A combined LT-STM/FIM for tip specific tunnelling experiments — •Ben Wortmann and Rolf Möller — Faculty of Physics, Center for Nanointegration Duisburg-Essen, University of Duisburg-Essen, 47048 Duisburg, Germany

We present details on a homebuilt, compact, low temperature scanning tunnelling microscope that allows in situ field ion microscopy of a cooled tunnelling tip inside the STM. Therefore a characterization of the tip is possible without transfer to a different position in the UHV system. This guarantees that the tip characterized by FIM is identical to the one used for the STM experiment. The geometry of the microscope resembles a cylinder with a height of only 13 cm and a diameter of 4 cm. Shutters at the bottom of the microscope can be opened to expose the tip to a channel plate or closed to assure even lower temperatures and minimal thermal drift while tunnelling. A combination of two piezo-electric accentuators is used to move a magnetically attached unit (*slider*) by a slip-stick motion. The tip is spot welded to the slider which can be easily exchanged in vacuum. The STM is screwed directly onto a commercially available continuous flow cryostat which allows cooling to about 5-7 K. Insulation from vibration is provided by a combination of springs and eddy current damping. An almost identical system already shows the performance of the STM setup[1]. The very compact design minimises helium consumption to about 1 litre/hour. [1] (H. Karacuban, M. Lange, J. Schaffert, O. Weingart, Th. Wagner and R. Möller, Surf. Sci. Lett., 603, Issue 5, L39 (2009).

O 35.113 Tue 18:15 Poster B

On the characterization of thermal properties of Near-field scanning thermal microscope (NSThM) thermocouple-sensors by means of 3-ω technique — •Konstantin Kloppstech, David Hellmann, Ludwig Worbes, Nils Könne, Hanna Fedderwitz, and Achim Kittel — EHF, Fak. V, Physik, Carl von Ossietzky Universität Oldenburg

The experimental analysis of near-field heat transfer from defined surfaces by a NSThM is founded on accurate knowledge of thermal properties of the thermocouple sensor, particularly the thermal resistance κ. The fact that the sensor consists of a multi-material system complicates common analysis methods. The 3ω method provides an alternative for determining κ and in addition to this the effective heat capacity c_p and the Seebeck-coefficient S. The method bases on a very small AC heating current at angular frequency ω which is sent through a wire, resulting in a temperature and thus in a resistance fluctuation at 2ω. This periodic change in resistance leads to an alternating voltage at 3ω angular frequency, from which κ, c_p, and S can be determined. In our approach we use a 5 μ thin glass fiber coated with 2 nm Pt and 80 nm Au whose thermal properties are determined with the 3-ω method in a first step. Held in UHV the glass fiber is approached with a NSThM sensor adding a second channel for heat drain, resulting in a measurable change in κ that gives access to κ of the sensor. As the 3-ω method relies on established theoretical formulation it gives access to a value of thermal resistance and an exact error estimation. In summary we show that this method is first class in characterizing NSThM-sensors.

O 35.114 Tue 18:15 Poster B

Scanning near-field optical microscopy with single color centers — •Thomas Oeckinghaus, Julia Tisler, Rainer Stöhr, Roman Kolesov, Rolf Reuter, Friedemann Reinhard, and Jörg Wrachtrup — Universität Stuttgart, 3. physikalisches Institut

We are using single color centers as a light source for apertureless scanning near-field optical microscopy. Specifically, we use a nanodiamond of a size below 10nm, containing only a single nitrogen-vacancy color center, which we attach to the tip of an AFM. Close to a sample, the fluorescence of the color center is modulated by fluorescence resonance energy transfer (FRET), a short ranged dipole-dipole interaction. This interaction quenches the fluorescence of the donor (color center), whenever it is approached to an acceptor (sample). Because of the short range of FRET, high resolution scanning images can be obtained in this way. We successfully acquired SNOM images of a graphene monolayer with a resolution of 20 nm.

Furthermore, we present a technical development, stroboscopic detection of an oscillating tapping-mode AFM tip. This allows to scan at a specific height above the sample or to reduce stress on the sample by avoiding contact mode scanning.

O 35.115 Tue 18:15 Poster B

A next-generation room-temperature AFM setup with optical access for NV-magnetometry — •Dominik Schmid-Lorch, Tobias Staudacher, Friedemann Reinhard, and Jörg Wrachtrup — 3. Physikalisches Institut und Forschungszentrum SCoPE, Universität Stuttgart, Germany

The nitrogen-vacancy (NV) color center in diamond can be used as a magnetic field sensor with sub-nanometer special resolution. This is due to the fact that its spin sublevels are sensitive to magnetic fields and that they can be monitored using optically detected magnetic resonance (ODMR). Using this center as a scanning probe in an AFM [1] the sensing and imaging of single spins under ambient conditions might be feasible.

We present a novel integrated design for such a scanning probe diamond nano-magnetometer as well as our planed experiments, such as single spin MRI and single molecule SNOM.

[1] G. Balasubramanian et al., Nature Vol 455 (2008)

O 35.116 Tue 18:15 Poster B

Recent progress on the open source software package GXSM — •Thorsten Wagner^1 and Percy Zahl^2 — ^{1}Johannes Kepler University Linz, Institute of Experimental Physics, Linz, Austria — ^{2}Brookhaven National Laboratory, Upton, USA

Since 1998 the open source software package GXSM has an increasing community of users and developers all over the world. [1] The linux based software packages provides in combination with a digital signal processor (DSP) a very flexible tools for acquiring and processing data of all kinds of scanning probe microscopes. [2] With the implementation of the vector probe engine [3], GXSM developed to a full spectroscopic system. Besides traditional point spectroscopy (STS) it acquires spectroscopic data on grids and does atom tracking and manipulation. Just recently new algorithm for the automatic drift correction and tip crash prevention (for force spectroscopy) were implemented. With intelligent over sampling it goes beyond the 16bit limit of the hardware. Up to four input channels, like tunnel current and oscillation frequency, can be used simultaneously and mixed for the Z feedback control. The new hardware platform "SR-MK3Pro" will also allow an internal PLL feedback to drive tuning fork and needle sensors.

[1] http://gxsm.sf.net and http://sranger.sf.net

[2] P. Zahl, M. Bierkandt, S. Schröder, and A. Klust, Rev. Sci. Instr. 74 (2003) 1222

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O 35.117 Tue 18:15 Poster B

Investigations by intermittent contact AFM on free-standing static and mechanically vibrating nanowires — •Moid Bhatti, Ivo Knittel, and Uwe Hartmann — Institut für Experimentalphysik, Uni Saarland

The scanning speed of the atomic force microscope (AFM) is mainly limited by the resonant frequency of the (conventionally micron-sized) cantilever (fc) and the feedback control loop for height control with piezo resonant frequency fz. A reduction of the cantilever size leads to a higher fc for instance a nano-sized cantilever has fc typically in MHz range. Scanning at such high speeds will require a correspondingly fast feedback control loop (high fz). Besides, an understanding of the interaction between a sample surface and a static or oscillating nanowire (NW) or "nanocantilever (NC)" is required.

We have been studying the contact mechanics of the cantilever-sample system in the context of dynamic mode AFM using NCs of various types: (1)Nanowires grown on a substrate. (2)Carbon nanotubes attached to an AFM cantilever. (3)Focused-Ion-Beam (FIB)-structured AFM cantilevers. (4)FIB-structured NC at the tip of an optical fiber whereby the light transmission capability of the fiber can be utilized for the integrated detection of the NC oscillating at its tip.

We will present distance-dependent resonance curves and show various oscillatory states of an AFM cantilever interacting with a static NW and of NCs tapping on a sample surface. NWs were excited piezoelectrically and electrostatically up to 100 MHz. The detection of such vibrations is discussed.

O 35.118 Tue 18:15 Poster B

Low noise, wide band current to voltage amplifier for low temperature scanning tunneling microscope operation — •Hanna Fedderwitz, David Hellmann, Ludwig Worbes, Konstantin Kloppstech, Nils Könne, and Achim Kittel — EHF, Fak.V Physik, Carl von Ossietzky Universität Oldenburg

We are interested in the heat transfer across a nanoscale vacuum gap between two surfaces mediated by evanescent electromagnetic fields [1]. The characteristic length scale depends on the temperature of the two opposing surfaces and increases drastically at low temperatures. To investigate this effect we are setting up a low temperature scanning tunneling microscope (LT-STM) which can be equipped with a coaxial thermocouple tip [2]. Therefore it is necessary to apply the tunnel voltage to the sample instead of the STM-tip as in most STM setups. We achieve this by choosing a two stage setup. The first stage features low-noise transimpedance amplification by using a commercial high performance FET operational amplifier together with a high-ohm feedback resistor. Giving access to the current which is drained into the tip at tunnel voltage level the amplifier has to be powered by a floating supply voltage. A second stage is employed to reference the output signal to ground needed by the feedback electronics. This stage makes use of a commercial instrumentation amplifier. The two-stage system shows a low inherent total current noise of 4pA and a stable frequency response up to 10kHz cutoff frequency. [1] Achim Kittel et al., Appl. Phys. Lett. 93, 193109 (2008). [2] Uli F. Wischnath et al., Rev. Sci. Instrum. 79, 073708 (2008).

O 35.119 Tue 18:15 Poster B

Investigations by intermittent contact AFM on free-standing static and mechanically vibrating nanowires — •Moid Bhatti, Ivo Knittel, and Uwe Hartmann — Institut für Experimentalphysik, Uni Saarland

The scanning speed of the atomic force microscope (AFM) is mainly limited by the resonant frequency of the (conventionally micron-sized))cantilever (fc) and the feedback control loop for height control with piezo resonant frequency fz. A reduction of the cantilever size leads to a higher fc for instance a nano-sized cantilever has fc typically in MHz range. Scanning at such high speeds will require a correspondingly fast feedback control loop (high fz). Besides, an understanding of the interaction between a sample surface and a static or oscillating nanowire (NW) or "nanocantilever (NC)" is required.

We have been studying the contact mechanics of the cantilever-sample system in the context of dynamic mode AFM using NCs of various types: (1)NWs grown on a substrate. (2)Carbon nanotubes attached to an AFM cantilever. (3)Focused-Ion-Beam(FIB) structured AFM cantilevers. (4)A FIB structured NC at the tip of an optical fiber whereby the light transmission capability of the fiber can be utilized for the integrated detection of the NC oscillating at its tip.

We will present distance-dependent resonance curves and show various oscillatory states of an AFM cantilever interacting with a static NW and of a NC tapping on a sample surface. Free-standing NWs were excited piezoelectrically by using LiNbO3 single crystal and electrostatically in an electron microscope using a microwave line.

O 35.120 Tue 18:15 Poster B

A low-temperature facility for spin-polarized scanning tunneling microscopy — •Lihui Zhou, Peter Löptien, Focko Meier, Jens Wiebe, and Roland Wiesendanger — Institute of Applied Physics, University of Hamburg, Germany

Spin-polarized scanning tunneling microscopy (SP-STM) is a well-established technique to give insights into magnetic properties [1]. To investigate atomic-scale magnetism of atomic-size nanostructures where the typical energy scale is on the order of sub-meV [2] a facility being able to conduct measurements at a temperature in the range of one Kelvin is a prerequisite. We have planned and constructed a low-temperature facility capable of SP-STM measurements. The commercial main chamber (SPECS, Berlin) contains a scanning tunneling microscope cooled by a Joule-Thomson cryostat resulting in a base temperature of 1.2 K using ^{4}He. The microscope integrates a lateral positioning stage enabling to perform cross-sectional STM investigations. This chamber also includes evaporators directing to the microscope's sample receptacle enabling to deposit single atoms onto cold surfaces. There are two additional home-built vacuum chambers for *in situ* magnetic sample and spin-polarized tip preparation. These chambers contain evaporators, a sample heating manipulator, an e-beam heater, and a sputter gun. We will present measurements demonstrating both the spatial and the energy resolutions, and SP-STM measurements of the Fe double layer on W(110).

[1] R. Wiesendanger, Rev. Mod. Phys. **81**, 1495 (2009)

[2] J. Wiebe et al., J. Phys. D: Appl. Phys. **44**, 464009 (2011)

O 35.121 Tue 18:15 Poster B

A scanning tunneling microscope control system based on a field programmable gate array — •Peter-Jan Peters, Thomas Jürgens, and Richard Berndt — Institut für Experimentelle und Angewandte Physik, Christian-Albrechts-Universität zu Kiel, 24098 Kiel, Germany

A new scanning tunneling microscope control device based on a field programmable gate array (FGPA) and a real time computer is presented. Industry standard PXI data acquisition cards and custom design digital to analog converter circuits are used. The custom converters show a noise density of 950 nV/$\sqrt{Hz}$ in the relevant frequency range. New modes of measurement can be implemented in a flexible manner owing to the programmability of the FPGA. A layered software design is used to hide the detail of the FPGA programming from most users. Test measurements on Au(111) surfaces performed at ambient temperatures resolving the surface reconstruction show that state of the art performance is achieved.

O 35.122 Tue 18:15 Poster B

Setup and characterization of a new-built 300 mK ul-

tra high vacuum scanning tunneling microscope — •Danny Baumann[1], Torben Hanke[1], Christian Hess[1], Marko Kaiser[2], Ralf Voigtländer[2], Dirk Lindackers[2], and Bernd Büchner[1] — [1]Institut für Festkörperforschung, IFW Dresden — [2]Bereich Forschungstechnik, IFW Dresden

We present the setup and characterization measurements of a newly built ultra high vacuum (UHV) 300 mK scanning tunneling microscope (STM). The used cryostat is a bottom loading ^{3}He single shot system equipped with a 9T superconducting magnet and connected to a three-chamber UHV system. The UHV system gives the possibility to prepare, store and analyze tips and samples and mount them in the STM without breaking the UHV conditions.

Furthermore, we show the very high spatial resolution as well as the very high long-term stability of the STM system with measurements on standard samples and investigations on the iron pnictide superconductor LiFeAs.

Additionally, we have performed scanning tunneling spectroscopic measurements with a superconducting Niobium tip to show that the energy resolution of the STM at base temperature is close to the thermal limit.

O 35.123 Tue 18:15 Poster B

Investigations on nanowire-cantilever interactions — •Moid Bhatti, Ivo Knittel, and Uwe Hartmann — Institut für Experimentalphysik, Universität des Saarland

High speed (video rate and beyond) atomic force microscopy (AFM) requires a height feedback with a bandwidth of 100 kHz and more, for which solutions are emerging. On the other hand, cantilevers with resonant frequencies (f) in the MHz range are required. Nano-sized cantilevers with f in the MHz range can fulfill this requirement. However, an understanding of the interaction between a sample and a static or oscillating nanowire (NW) or nanocantilever (NC) is needed.

We have been studying the contact mechanics of the cantilever-sample system in the context of dynamic mode AFM using NCs of various types: (1)NWs grown on a substrate (whose dynamic behavior is equivalent to a cantilever with a NW attached to it). (2)Carbon nanotubes attached to an AFM cantilever. (3)Focused-Ion-Beam-(FIB)-structured AFM cantilevers. (4)A FIB-structured NC at the tip of an optical fiber, whereby the light transmission capability of the fiber can be utilized for the integrated detection of the NC oscillating at its tip.

We will present distance-dependent resonance curves and show various oscillatory states of an AFM cantilever interacting with a static NW and of a NC tapping on a sample. A dedicated piezoelectric element was excited to vibrations of up to 100 MHz. The detection of such vibrations is discussed besides a technique for the electrostatic excitation of mechanical vibrations of free-standing NWs in MHz range.

O 35.124 Tue 18:15 Poster B

Development of a cryogenic scanning tunneling microscope with integrated optical lenses — •Jeannette Kemmer, Jens Kügel, Pin-Jui Hsu, Paolo Sessi, and Matthias Bode — Institute of Experimental Physics II, University Würzburg, Am Hubland, 97074 Würzburg

We present the current status of a home-built low-temperature Scanning Tunneling Microscope (STM) with integrated lenses for in-situ optical excitation studies. The STM design includes an x-y-stage for sample positioning as well as lenses for back- and front-side focused laser illumination. It is integrated into a two-chamber UHV system equipped with a commercial LHe cryostat with a projected hold time of t >100 h. Test measurements performed under ambient conditions (HOPG), UHV and at low-temperatures will be presented.

O 35.125 Tue 18:15 Poster B

An oxygen annealing chamber for the preparation of clean hard metal substrates — •Johannes Friedlein, Andreas Sonntag, Benjamin Ehlers, Stefan Krause, and Roland Wiesendanger — University of Hamburg, Institute of Applied Physics, Jungiusstr. 11A, 20355 Hamburg, Germany

Reproducible measurements on the atomic scale require surfaces of high purity. The preparation of hard metal substrates like W and Mo crystals for scanning tunneling microscopy experiments involves creating a surface impurity depletion zone by annealing in oxygen atmosphere ($p \leq 1 \times 10^{-6}$ mbar) at high temperature ($T \leq 2000$ °C) [1-2].

We present the design and construction of a dedicated preparation chamber for clean W and Mo surfaces. It has a separate pumping system, consisting of turbo, ion getter and titanium sublimation pump. An ion gauge and a mass spectrometer allow for the control and analysis of vacuum conditions. The preparation process is conducted via remotely controlled O_2 leak valve and electron beam heating. During the annealing process the surroundings heat up leading to an increase of their degasing rates. To avoid this we implement a water cooling system for the chamber wall as well as for the heating stage.

[1] M. Bode, S. Krause, L. Berbil-Bautista, S. Heinze, R. Wiesendanger, Surface Science **601**, 3308 (2007).
[2] Kh. Zakeria, T.R.F. Peixotoa, Y. Zhanga, J. Prokopa, J. Kirschner, Surface Science **604**, L1 (2010).

O 35.126 Tue 18:15 Poster B

Advanced pulse-shaper design for simultaneous phase, amplitude, and polarization control of femtosecond laser pulses — •Christoph Schwarz, Ole Hueter, Fabian Ebert, and Tobias Brixner — Institut für Physikalische und Theoretische Chemie, Universität Würzburg, Am Hubland, 97074 Würzburg

The technique of femtosecond pulse shaping is an essential tool for recent advances in the area of optical near-field control and spectroscopy. So far the commonly used pulse-shaper setups are restricted in terms of their degrees of freedom. Either the amplitude and phase of a single polarization state or the phases of two perpendicular polarizations can be modulated. In the latter case, shaping is limited to certain polarization states. To achieve shaping of the full vector field we introduce an improved pulse-shaper design. In contrast to other approaches a single dual-layer liquid-crystal spatial light modulator (LC-SLM) is employed in order to shape independently phase and amplitude of two mutually perpendicular polarization components. To maximize the number of usable pixels of the LC-SLM for both polarizations, it is important to achieve almost equal frequency distributions in the Fourier plane of the zero-dispersion compressor. Numerical calculations and ray-tracing simulations are employed to optimize these distributions. To realize the calculated parameters experimentally we use a tailor-made thin-film polarizer for generation of two perpendicularly polarized pulses and a volume phase holographic grating for the zero-dispersion compressor. By recombining the two polarizations in a common-path setup we achieve control over the complete vector field of the resulting pulse.

O 35.127 Tue 18:15 Poster B

Development of a System measuring Adhesion Forces in Powder Collectives — •Stefanie Wanka[1], Michael Kappl[1], Markus Wolkenhauer[2], and Hans-Jürgen Butt[1] — [1]Max Planck Institute for Polymer Research, Mainz, Germany — [2]Boehringer Ingelheim Pharma GmbH & Co. KG, Ingelheim, Germany

Fine powders commonly have poor flow ability and dispersibility due to interparticle adhesion that leads to formation of agglomerates. Knowing about adhesion in particle collectives is indispensable to gain a deeper fundamental understanding of particle behavior in powders. Especially in pharmaceutical industry a control of adhesion forces in powders is mandatory to improve the performance of inhalation products. Typically the size of inhalable particles is in the range of 1-5 μm. To measure adhesion forces in fine powder collectives a new method was developed which is based on particle detachment from a surface caused by its inertia. To achieve detachment of particles in the relevant size range, accelerations in the order of 500 000g are necessary. Existing techniques for measurement of particle adhesion forces are experimentally demanding and time consuming. Therefore we aim to develop a system that will allow routine measurements of adhesion in particle collectives. The acceleration required for particle detachment is provided by a shock excitation system based on the Hopkinson bar principle (SPEKTRA GmbH Dresden) and measured via laser vibrometry. Particle detachment events are detected by optical video microscopy. First test measurements showed successful detachment of particles < 10 μm and thus a proof of concept.

O 35.128 Tue 18:15 Poster B

Soft Landing of Macromolecules using Electrospray Ionization — •Richard Steinacher, Seung Cheol Oh, Julian Lloyd, Hartmut Schlichting, and Johannes V. Barth — Physik Department, E20, TU München, Germany

Recent developments in research towards positioning macromolecules on surfaces, relevant for organic electronics or materials, made it desirable to deposit and investigate species that can not be sublimated by thermal evaporation techniques. We present a set-up with several stages, where an ion beam of macromolecules is produced by an electrospray ionization source, focused by electrodynamic funnels, and guided by electrostatic lenses. Furthermore, a quadrupole is used, to mass-selectively seperate the constituents of the ion beam. The apparatus allows to bring the molecules into a clean UHV environment and deposit them on a substrate, for the production of films with high purity. Beyond the generation and the guidance techniques of the ion current, the set-up is compact and thus very versatile. This will enable the usage of one instrument with multiple devices, such as scanning probe microscopes or for the production of hybrid organic-semiconductor components.

O 35.129 Tue 18:15 Poster B

Preparation and application of highly polarized Xe with variable ^{129}Xe content — •Alexander Potzuweit, Richard Kastelik, Hagen Allmrodt, Lars Kraft, Anuschka Schaffner, and Heinz Jänsch — Fachbereich Physik, Philipps-Universität Marburg, D-35032 Marburg

We employ NMR of hyperpolarized ^{129}Xe to investigate surface phenomena and diffusion. To increase the sensitivity towards structurally caused, local inhomogeneities a small line width is favorable. In solid Xe the line width is dominated by dipolar interaction with neighboring nuclear spins. This can be substantially reduced by diluting the NMR-active isotope ^{129}Xe in the NMR-inactive isotope ^{132}Xe. Thus we are able to investigate ordering effects like annealing. Dynamic processes at the bulk surfaces can be monitored by exchange spectroscopy (EXSY) of the bulk and surface atoms ($\Delta\nu \approx 100$ ppm). Here we present the technical development of the apparatus and discuss first results.

O 35.130 Tue 18:15 Poster B

High-Resolution Double-Photoelectron Spectroscopy from superconducting Surfaces — •Tobias Bauer, Robert Wallauer, Stefan Voss, and Reinhard Dörner — Institut für Kernphysik, Goethe Universität, 60486 Frankfurt am Main, Germany

It is theoretically predicted that the breakup of Cooperpairs by a single XUV photon leads to the emission of two electrons which formed the pair. First experiments which have been performed with a custom-build Time-of-Flight spectrometer, failed to show evidence for this process due to the low energy resolution.

With a new developed experimental setup which includes a new spectrometer (THEMIS1000 with an Wide Angle Lens - SPECS) and an especially for coincident measurements designed time- and position-sensitive detector (HEX90 - RoentDek), we will be able to measure coincident electrons with +/- 30° emission angle and a resolution comparable to state of the art hemispherical analyzers. The data analysis plays a crucial role in the experiment, since the electrons are expected to hit the detector at the same time. We present the results of a new method for pulse analysis and other experimental improvements in order to achieve nearly dead-time free detection efficiency.

O 35.131 Tue 18:15 Poster B

Towards NMR of buried interfaces — •Anuschka Schaffner, Hagen Allmrodt, Lars Kraft, Richard Kastelik, Alexander Potzuweit, and Heinz Jänsch — Fachbereich Physik, Philipps-Universität Marburg, D-35032 Marburg

We employ Xe-NMR to investigate surface phenomena by adsorbing hyperpolarized ^{129}Xe onto a helium-cooled single crystal and studying the electronic interactions of substrate and adsorbate. The high nuclear spin polarization of the adsorbed Xe-film could be transferred to buried interfaces within the substrate (which then would be accessible for further NMR experiments) via dipolar near distant-field transfer. The proposed distant-field transfer [1] will be discussed. As a test of the here proposed polarization transfer, we use a system of an absorbed hyperpolarized ^{129}Xe-film beneath a layer of unpolarized ^{129}Xe in a matrix of CO_2, geometrically and spectrally separated. Here, we present the experiments and discuss the transfer mechanism.

[1] Desvaux et al. Eur. Phys. J. Appl. Phys. Vol. 36, No. 1, 2006

O 35.132 Tue 18:15 Poster B

Construction of a Neural Network Potential-Energy Surface for R,R-Tartaric Acid — •Sinja Klees, Tobias Morawietz, and Jörg Behler — Lehrstuhl für Theoretische Chemie, Ruhr-Universität Bochum, D-44780 Bochum, Germany

The availability of accurate interatomic potentials is a necessary condition for studying complex systems for example by molecular dynamics simulations. Typically, a number of physical approximations are introduced to obtain potential-energy surfaces (PESs), which are sufficiently efficient to study large systems. Artificial Neural Networks (NN) offer a very general way to construct accurate PESs without the introduction of any constraint on the functional form. They are extremely flexible and allow to interpolate reference energies and forces obtained from first-principles calculations. To date, most NN potentials for molecules have been reported only for very small systems containing up to six atoms. Using R,R-tartaric acid as a benchmark system we show that also high-dimensional NN PESs for larger molecules can be constructed in a systematic way.

O 35.133 Tue 18:15 Poster B

Excitons of pure and functionalized carbon nanotubes studied by many-body perturbation theory — •Ferdinand Schulz and Michael Rohlfing — Fachbereich Physik, Universität Osnabrück

We discuss excitonic states in semiconducting carbon nanotubes from first principles. Based on structural data from density-functional theory, band structures and optical excitations are obtained from many-body perturbation theory (GW approximation and Bethe-Salpeter equation, BSE). We employ a simplified, perturbative LDA+GdW version of the theory, which is numerically much more efficient than conventional GW and BSE realizations. This enables us to discuss both pure and functionalized nanotubes, with functionalization given by point defects and adsorbates (like hydrogen).

O 35.134 Tue 18:15 Poster B

Method for solving the N-point Hedin equations — •Falk Tandetzky, Sangeeta Sharma, Kay Dewhurst, and Hardy Gross — Max-Planck-Institut für Mikrostrukturphysik (Theory Dep.), Weinberg 2, D-06120 Halle, Germany

The *GW* approximation is a state-of-the-art method for band structure calculations but there are still some cases for which *GW* fails [1]. Towards the goal of improving on this situation, we present a new method for solving the Hedin equations which, expressed perturbatively, includes an infnite subset of vertex corrections. We further provide conditions for guaranteeing convergence of the algorithm to a unique solution. This is an important point since it has recently been pointed out that there is danger of running into unphysical solutions, when using vertex corrections [2].

All these findings are supported by numerical calculations for $N = 1$ which compare the exact $\Sigma[G, W]$ to that obtained from our approximate algorithm as well as a Borel resummation of the linearised Hedin equations [2,3]. As our method has a favourable scaling with N we envisage that it can be applied to physical problems, albeit with discretized degrees of freedom and be useful for band structure calculations beyond the *GW* approximation.

[1] M. Guzzo, G. Lani, F. Sottile, P. Romaniello, M. Gatti, J. J. Kas, J. J. Rehr, M. G. Silly, F. Sirotti and L. Reining, Phys. Rev. Lett. 107, 166401 (2011). [2] G. Lani, P. Romaniello and L. Reining, arXiv:1103.1630v1 (2011). [3] Y. Pavlyukha and W. Hübner, J. Math. Phys. 48, 5 (2007).

O 35.135 Tue 18:15 Poster B

Electronic and optical properties of tin oxides computed from first principles with different levels of approximation — •Anna Miglio, Martin Stankovski, Matteo Giantomassi, and Xavier Gonze — NAPS-IMCN Université catholique de Louvain, Louvain la Neuve, Belgium

SnO2 is a wide-gap semiconductor of considerable industrial interest as a transparent conductor. Depending on deposition conditions a SnO phase might coexist with SnO2. In this work, we apply the standard DFT approach and the more accurate many-body formalism in the GW approximation to compute the electronic and optical properties of SnO2 and SnO. One-shot G0W0 calculations performed with the plasmon pole approximation[1]and the more accurate contour deformation technique[2] improves the agreement of the computed band gap with the experimental value. The effect of self-consistency in GW is then investigated by using two different methods: a one-shot G0W0 iteration performed on top of self-consistent COHSEX results[3] and the quasi particle self-consistent GW method proposed in [4]. Finally we analyze the importance of excitonic effects by comparing the absorption spectrum computed within the RPA with the results obtained by solving the Bethe Salpeter equation. [1] R. W. Godby and R.J. Needs, Phys. Rev. Lett. 62, 1169 (1989). [2] S. Lebegue et al. PRB 67, 155208 (2003). [3] F. Bruneval, N. Vast, and L. Reining, Phys. Rev. B 74, 045102 (2006). [4] T. Kotani, M. van Schilfgaarde, S. V. Faleev, Phys. Rev. B 76, 165106 (2007).

O 35.136 Tue 18:15 Poster B

Nucleation Growth: Occupation Probability Field Ansatz as an Approximation of a Lattice Monte Carlo Simulation — •Tanja Mues and Andreas Heuer — Institut für Physikalische Chemie, Westfälische Wilhelms-Universität Münster

Molecular nucleation growth on surfaces was studied numerically with different simulation models on microscopic and macroscopic scale. The adaption of a macroscopic method without loss of accuracy is the topic of this work. Regarding the occupation probability of a site by a molecule as the key observable we can simulate nucleation growth on larger time and length scales as compared to a Lattice Monte Carlo (LMC) simulation. To prevent loss of information on macroscopic scale, we import three main parameters: the diffusion constant, the critical nucleus size and a nucleation pre-factor from our LMC simulation. By means of the cluster density and their radial distribution we compare the results of both methods and find very good agreement.

O 35.137 Tue 18:15 Poster B

DFT-Calculations of NEXAFS spectra of small alkanes and alkanethiols — •Katharina Diller[1], Klaus Hermann[2], Florian Klappenberger[1], and Johannes V. Barth[1] — [1]Physik Department, E20, Technische Universität München, James- Franck-Str. 1, 85748 Garching, Germany — [2]Fritz-Haber-Institut der Max-Planck-Gesellschaft, Faradayweg 4-6, 14195 Berlin, Germany

We simulate near-edge x-ray absorption fine structure (NEXAFS) spectra of different small alkanes and alkanethiols in gas phase using the density functional theory (DFT) package StoBe. Since alkanethiols are widely used as building blocks for self-assembled monolayers (SAMs) their properties are of great interest. However, the interpretation of the experimental NEXAFS data, especially the peak assignment, can be challenging as vibrational features dominate the spectra of small alkane(thiol)s and are still present for larger molecules. In this work we examine the performance of StoBe using (i) the implemented transition potential method and (ii) ΔSCF calculations to determine the first transitions for the peak assignment and interpretation of NEXAFS spectra of saturated hydrocarbons. Additionally we address the problems arising when progressing from the analysis of small alkanes in gas phase to the examination of adsorbed long-chained alkanethiols.

O 35.138 Tue 18:15 Poster B

Systematic Construction of High-Dimensional Potential-Energy Surfaces by Neural Networks — Tobias Morawietz, Nongnuch Artrith, and •Jörg Behler — Lehrstuhl für Theoretische Chemie, Ruhr-Universität Bochum, D-44780 Bochum, Germany

Artificial neural networks (NNs) have become a promising method for the development of reliable potential-energy surfaces (PESs) for a wide range of systems including molecules, solids and surfaces [1,2]. Due to their high flexibility NNs are able to accurately represent energies and forces obtained from quantum chemical calculations, which makes them ideal tools to extend the length and time scale of molecular dynamics simulations. An important aspect for the constructing of high-dimensional NN PESs is the choice of the reference configurations. Here we present a systematic approach to build up NN potentials in an iterative fashion by identifying poorly represented parts of the configuration space.

[1] J. Behler, PCCP **13**, 17930 (2011).
[2] N. Artrith, T. Morawietz, and J. Behler, PRB **83**, 153101 (2011).

O 35.139 Tue 18:15 Poster B

Description of Rabi oscillations in density-functional theory: The effect of spin — •Jeiran Jokar and Nicole Helbig — Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich and JARA, 52425 Jülich, Germany

Applying a monochromatic laser with a frequency close to resonance leads to Rabi oscillations between the initial and an excited state of the system. These oscillations are a prototype for the nonlinear interaction of light with matter and one of the few analytically solvable cases of nonlinear electron dynamics where the population of states changes dramatically in time. Due to these dramatic changes a description within density-functional theory needs to go beyond the use of adiabatic functionals. Here, we investigate the influence of the spin of the initial state as well as the polarization of the laser on the quality of a DFT description in order to gain more insight into how to construct non-adiabatic approximations. Through the exact solution of one and two-dimensional two-electron systems interacting with a monochromatic laser of either linear or circular polarization we are able to assess the quality of a local density approximation and the exact exchange approximation.

O 35.140 Tue 18:15 Poster B

Magnetism and unusual Cu valence in correlated perovskites — •Paola Alippi[1] and Vincenzo Fiorentini[2] — [1]CNR-ISM, Rome, Italy — [2]CNR-IOM and University of Cagliari, Italy

The interplay of the valence states of Cu and of the X cation determines the magnetic and conduction properties of the $A\mathrm{Cu_3X_4O_{12}}$ quadruple perovskites. $\mathrm{CaCu_3Ti_4O_{12}}$ (CCTO) should be a Mott-like insulator due to the nominal 4+ valence of Ti and 2+ valence of Cu. As Fe and Co prefer greatly a 3+ valence to a 4+ one, $\mathrm{LaCu_3Fe_4O_{12}}$ (LCFO) and $\mathrm{YCu_3Co_4O_{12}}$ (YCCO) will be insulating if Cu is 3+. It was suggested that the nominally 3+ Cu state may actually be a “Zhang-Rice singlet” bound state of a ligand hole and a native Cu hole, coupled antiferromagnetically. If however Cu is 3+ and unmagnetized along with its neighbors, neither Mott nor Zhang-Rice physics are at play.

Based on ab initio calculations using several beyond-local density-functional approaches (GGA+U, HSE hybrid, self-interaction correction, $\mathrm{G_0W_0}$) we confirm the Mott-like nature of CCTO, and show that LCFO is an antiferromagnetic (on the Fe lattice) insulator, while Co adopts a low-spin state and produces a non-magnetic and insulating YCCO. Unexcitingly, neither LCFO or YCCO are Mott or Zhang-Rice-like systems, as Cu therein is strictly non-magnetic and effectively 3+ in valence. CCTO may instead exhibit Zhang-Rice type behavior upon hole doping, progressively emptying its flat Cu-like top valence band.

O 35.141 Tue 18:15 Poster B

Reversible switching process of spiropyran on Au(111) — F. Lorbeer[1], •P. Stoll[1], I. Fernandez Torrente[1], T. R. Umbach[1], C. Maity[2], S. Hecht[2], J.I. Pascual[1], and K.J. Franke[1] — [1]Institut für Experimentalphysik, Freie Universität Berlin, Berlin — [2]Department of Chemistry, Humboldt-Universität zu Berlin

The isomerisation process of molecules adsorbed on a metal surface can be very different from the one in solution or gas phase. The prototypical light induced ring-opening reaction of spiropyran (SP) to its isomer merocyonine (MC) and the thermally induced ring-closing back-reaction in gas phase is not easily reproduced on the surface due to the electronic coupling of molecular orbitals with the substrate states. We study 5’,6,8 Tri-tertbutylindolinospirobenzopyran on Au(111) with low temperature scanning tunneling microscopy and spectroscopy. The molecule is functionalised with the three tertbutyl groups to reduce the interaction with the substrate and enable reversible switching. An ordered structure is obtained by mixing SP with thermally isomerised MC. In this ordered structure we can excite a ring-opening reaction of SP by electric field and illumination with 445nm laser light. This change is visible as an upward pointing tertbutyl group and is completely reversible by individually adressing the molecule with a voltage pulse. A complete unfolding into the MC form however does not take place due to steric hindrance in the ordered structure.

O 35.142 Tue 18:15 Poster B

In situ metalation of 2H-tetraphenylporphyrins with copper substrate atoms on Cu(111): a scanning tunneling microscopy study — •Martin Drost, Stefanie Ditze, Michael Stark, Florian Buchner, Hans-Peter Steinrück, and Hubertus Marbach — Lehrstuhl für Physikalische Chemie II, Universität Erlangen-Nürnberg, Egerlandstr. 3, D-91058

The development of functional nanostructures requires a detailed understanding of the physical and chemical properties of the involved species. In this regard porphyrinoids appear to be ideal candidates. They can bear various peripheral ligands, which enables control over molecule/molecule and molecule/substrate interactions, and their reactivity can be modified by inserting specific metal atoms at the center of the macrocycle. Herein, we studied the in situ coordination reaction of 2H-tetraphenylporphyrin molecules (2HTPP) with copper substrate atoms under ultra high vacuum conditions with scanning tunneling microscopy. The experiment reveals that 2HTPP molecules deposited on Cu(111) react to form metaloporphyrins (CuTPP) at 400K, by incorporation of substrate Cu atoms. While at room temperature, 2HTPP shows a specific 1D diffusion behavior of individual molecules, after partial metalation the coexistence with an ordered 2D CuTPP phase is found. To obtain detailed insight, a kinetic analysis of the metalation behavior as a function of time and temperature was performed.

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DFT study of the attachment of silane linker molecules to hydroxylated Mg surfaces — •Steffen Seiler and Bernd Meyer — Interdisziplinäres Zentrum für Molekulare Materialien und Computer-Chemie-Centrum, Universität Erlangen-Nürnberg

The prospect of using magnesium and its alloys as biodegradable implants has triggered much interest in finding suitable processes for functionalization of their surfaces with biomolecules. In recent experimental work it was shown that by surface hydroxylation and the use of appropriate linker molecules (3-aminopropyltriethoxysilane, APTES) self-assembled monolayers of proteins can be formed on Mg surfaces [1].

DFT calculations have been used to explore the binding mode and the most favorable binding configuration of silane molecules on hydroxylated magnesium. Attachment of the silane molecules via hydrogen bonding or covalent bond formation have been considered. Special attention was given to the role of water recombination and association to the surface in the silane adsorption process. Also the influence of van der Waals contributions to the adsorption energy will be discussed.

[1] M.S. Killian, V. Wagener, P. Schmuki, S. Virtanen, *Langmuir* 26 (2010) 12044

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Probing gas ligation of surface anchored porphyrins through an experiment-theory IETS study — •Knud Seufert[1], Willi Auwärter[1], Shiri Burema[2], Marie-Laure Bocquet[2], Johannes V. Barth[1], David Écija[1], and Saranyan Vijayaraghavan[1] — [1]Physik Department E20, TU München, Germany — [2]CNRS, Université de Lyon, France

The response of metalloporphyrins towards small gas molecules is of fundamental interest as it plays a key role in both biological systems as the transport of respiratory gases and artificial nanostructures as sensors. STM and STS investigations combined with DFT-calculations turned out to be a good method to get insight into such systems. Here we present the ligation of NO to Co-TPP, immobilized onto a metallic substrate. The molecular interaction with the substrate is weakend by the binding of the bent NO radical to the metal-center. This results in a changed appearance and electronic structure. IETS spectra of this system were performed and the measured signal was assigned to an unique vibration mode on the NO-complex, namely the Co-N-O Rocking mode lying in a plane perpendicular to the metallic surface. Furthermore the experimental extension to other porphyrins and diatomic gases is shown.

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Switching of an industrial dye-molecule on Au(111) and Ag(111) — •Marcel Müller[1], Gerald Dräger[2], Konrad Boom[1], Friederike Matthaei[1], and Karina Morgenstern[1] — [1]Leibniz Universität Hannover, Institut für Festkörperphysik, Abteilung ATMOS, Appelstraße 2, 30167 Hannover — [2]Leibniz Universität Hannover, Institut für Organische Chemie, AK Dräger, Schneiderberg 1B, 30167 Hannover

Molecular switches are an essential part of future ideas in molecular electronics. We investigated a possible candidate, the cyanine astraphloxine, on Au(111) and Ag(111) with a low-temperature STM. We deposit a coverage of $0,022\,\mathrm{molecules/nm^2}$ at a sample temperature of 113 K on Au(111) and $0,014\,\mathrm{molecules/nm^2}$ at a sample temperature of 83 K on Ag(111). Astraphloxine exists in two different sizes on both surfaces. On Ag(111), the molecule forms smaller clusters while on Au(111) it adsorbs as single molecule. The molecule's size and shape are changed by manipulation via inelastic tunneling electrons. In this presentation we will show different switching processes and discuss possible interpretations of these processes, in particular which isomerisations are induced. Finally, we will discuss these results in light of a combustion analysis of the molecule.

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Tuning the interaction between carbon nanotubes and dipole switches: influence of the change of the nanotube-spiropyran distance — •Pascal Bluemmel[1], Antonio Setaro[1], Chandan Maity[2], Stefan Hecht[2], and Stephanie Reich[1] — [1]Department of Physics, Freie Universität Berlin, Arnimallee 14, 14195 Berlin — [2]Department of Chemistry, Humboldt Universität zu Berlin, Brook-Taylor-Str. 2, 12489 Berlin

The non-covalent functionalization of carbon nanotubes with spiropyran molecules, serving as optically addressable dipole switches, is reported. Two types of pyrene-spiropyran based dyads with spacers of different lengths resulting in different switch-tube distances were investigated. While both surfactants were able to form stable carbon nanotube suspensions, the different distances between the switch and the tube affect both of the components' optical properties. In the case of the shorter spacer, the nanotubes' luminescence as well as the merocyanine absorption band were red-shifted and furthermore, the rate of the merocyanine to spiropyran thermal back isomerization was decreased.

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Efficient energy transfer in perylene-nanotube complexes — •Friederike Ernst[1], Timm Heek[2], Antonio Setaro[1], Rainer Haag[2], and Stephanie Reich[1] — [1]Institut für Physik, Freie Universität Berlin — [2]Institut für Chemie, Freie Universität Berlin

Carbon nanotubes are interesting for biomedical applications because they emit in the IR part of the spectrum; establishing nanotube-adsorbant energy transfer complexes in aqueous solution is thus a key step towards the complex non-covalent functionalization of nanotubes in biocompatible environments. We demonstrate direct energy transfer in perylene-imido-diester nanotube complexes in water: upon excitation of the adsorbed perylene unit we observe an emission from the carbon nanotubes, which indicates a successful excitation transfer. The efficiency of the indirect excitation via the adsorbant is of the same order of magnitude as the direct excitation of the nanotubes. Furthermore the perylene-imido-diester compound simultaneously serves as a surfactant for the nanotubes with a strong chirality preference for tubes with a small E11 transition energy, obliterating the need for a supplementary surfactant. We thus created a self-sufficient excitation transfer complex which is stable in an aqueous medium over many months.

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Chirality Enrichment of Carbon Nanotubes by Amphiphile Replacement — •Marcus Ulf Witt, Antonio Setaro, Frederike Ernst, Pascal Bluemmel, Michael Gegg, and Stephanie Reich — Frei Universität Berlin, Institut für Experimentalphysik, Arnimallee 14,14195 Berlin

We present suspensions with selected enriched chiralities of carbon nanotubes. Such a suspension of selected chirality has well defined photoluminecence spectra and conductive properties. The chirality enrichment is achieved by the replacement of amphiphiles. The solvatochromic shift of the carbon nanotubes during the replacement was monitored with the photoluminescence excitation (PLE). From this PLE measurements we calculated the required concentration of the second amphiphile to replace the first one applying the Hill-model. The achieved enrichment was verified by the PLE. The use of amphiphiles with different morphologies leads to the enrichment of different chiralities depending on the coupling between amphiphiles and carbon nanotubes. This will help understanding the fundamental mechanisms of coupling between carbon nanotubes and aromatic moieties.