

O 58: Poster Session III (Solid-liquid interfaces; Scanning probe and other methods; Electronic structure theory; Spin-orbit interaction)

Time: Wednesday 18:15–21:45

Location: Poster B1

O 58.1 Wed 18:15 Poster B1

Temperature dependent wear experiments on the nanoscale — ●JOHANNES SONDHAUSS¹, HARRY MÖNIG¹, HARALD FUCHS¹, and ANDRÉ SCHIRMEISEN² — ¹Institute of Physics, University of Münster, Germany — ²Institute of Applied Physics, University of Giessen, Germany

The importance of wear effects on small scales, e.g. with regard to moving mechanical components in MEMS, motivated increased efforts to analyze the basic mechanisms of wear at the nanoscale. Especially the atomic force microscope (AFM) has been proved useful to study wear effects on the atomic scale [1, 2]. Typically, the models used to describe the observed wear characteristics are based on Arrhenius kinetics and therefore a thermally activated characteristic is expected. However, a complete picture of the fundamental wear processes is still under debate. In this work we performed wear experiments as a function of temperature. We used Si-tips to wear single step edges on a KBr(001)-crystal. The measurements were conducted under UHV-conditions in a temperature range between 100 K and 300 K. We investigated the effect of different loads and, as a further important channel, we simultaneously measured the friction force acting between tip and sample during the wear process. With our results we are able to make an assessment if nanoscale wear can be described by an Arrhenius type model. In addition the influence of the different components of the acting normal and frictional stresses inside the contact area is discussed.

[1] Sheehan, Chem. Phys. Lett. 410, 151-155 (2005)

[2] Gotsmann and Lantz, Phys. Rev. Lett. 101, 125501 (2008)

O 58.2 Wed 18:15 Poster B1

Friction force microscopy on activated silicon surface — ●JOHANNA BLASS¹, FLORIAN HAUSEN^{1,2}, MATTHIAS LESSEL², PETER LOSKILL², MARCEL ALBRECHT³, NITYA NAND GOSVAMI¹, GERHARD WENZ³, KARIN JACOBS², and ROLAND BENNEWITZ^{1,2} — ¹INM - Leibniz-Institute for New Materials Campus D2 2, 66123 Saarbrücken, Germany — ²Department of Experimental Physics, Saarland University, D-66041 Saarbrücken, Germany — ³Organic Macromolecular Chemistry Campus C4 2, Saarland University, D-66123 Saarbrücken, Germany

Surfaces with defined friction and adhesion properties are often required for technical applications such as strong mechanical links with high shearing but low peeling resistance. Therefore, we currently develop a novel surface material based on cyclodextrin assemblies with controlled anisotropy friction and adhesion characteristics. The interaction of two surfaces is based on host-guest interactions which are investigated by single molecule force spectroscopy and high resolution friction force microscopy. Immobilization results of cyclodextrin assemblies on activated silicon and gold are presented. Additionally, FFM experiments are presented which reveal an influence of the sub-surface on an activated silicon surface. We found that friction forces on octadecyltrichlorosilane (OTS) self assembled monolayers as well as on siliconoxide decrease with a thicker oxide layer. The effect is attributed to a change in the van der Waals part of the effective interaction potential [1]. [1] P. Loskill, H. Hähl, T. Faidt, S. Grandthyll, F. Müller, and K. Jacobs, Adv. Coll. Interf. Sci. 107 (2012) 179182

O 58.3 Wed 18:15 Poster B1

Investigation of Tribological Properties of Mesoporous Alumina Membranes With Water Lubrication — ●FLORIAN KRÄMER¹, FELIX WÄHLISCH², ANDREAS TSCHÖPE¹, RAINER BIRRINGER¹, and ROLAND BENNEWITZ² — ¹Universität des Saarlandes, Saarbrücken — ²INM - Leibniz-Institut für Neue Materialien

Nanoporous membranes are interesting substrates for tribological applications because their porous structure allows to carry liquid lubricants into the friction interface directly.

In the present study, alumina templates with hexagonally arranged pores were synthesized by two step anodization of aluminum. The alumina-layer was separated by a voltage reversal technique. The barrier oxide at the pore-bottom was dissolved by chemical etching resulting in free-standing mesoporous membranes with complete open pore morphology (pore diameter about 60 nm). The membranes were mounted on a sample holder which allowed the direct contact with a water reservoir. Upon contact, the pores were filled with water by

capillary forces to provide a thin water-layer on top of the membrane surface, where the tribological measurements were carried out.

The friction of a 500 μm ruby sphere on the membrane was characterized in the dry and the water-lubricated state by a reciprocal sliding tribometer. The wear track of the tribometer measurement was investigated by atomic force microscopy and scanning electron microscopy.

O 58.4 Wed 18:15 Poster B1

EC-STM study of the influence of gas adsorbates on the structure and morphology of Cu-monolayers on Au(111) and Pt(111) electrodes — ●CHRISTIAN SCHLAUP and SEBASTIAN HORCH — Center for Individual Nanoparticle Functionality (CINF), Department of Physics, Technical University of Denmark (DTU), DK-2800 Kongens Lyngby, Denmark

The electrodeposition of metals adlayers in general, and the underpotential deposition (upd) of metal (sub)monolayers in particular, is a major topic in interfacial electrochemistry and has been studied extensively. Often a strong dependence of the atomic structure of such metal upd layers on both, the substrate and the involved anionic species in the deposition electrolyte, was found.

In the present work, we studied the influence of neutral gas coadsorbates, such as dissolved CO_2 and CO , on the structure and morphology of Cu-upd layers on Au(111) and Pt(111) electrodes by means of cyclic voltammetry and EC-STM. Contrary to the case of purely anionic adsorbates, these gas adsorbates may not only influence the structure of the metal upd layer directly by coadsorption, but also indirectly due to attractive interactions with the underlying substrate. In order to be able to distinguish between these effects, we studied both, the Cu deposition in presence of gas adsorbates and the reaction of Cu-films on the introduction of gas adsorbates after their deposition from a *blank* electrolyte.

O 58.5 Wed 18:15 Poster B1

Two-dimensional metal-organic complexes as catalyst for the oxygen reduction reaction — ●BENJAMIN WURSTER¹, DORIS GRUMELLI¹, SEBASTIAN STEPANOW¹, and KLAUS KERN^{1,2} — ¹Max-Planck-Institut für Festkörperforschung, D-70569 Stuttgart, Germany — ²Institut de Physique de la Matière Condensée, Ecole Polytechnique Fédérale de Lausanne, CH-1015 Lausanne, Switzerland

Two-dimensional metal-organic coordination networks (2D-MOCNs) consist of arrays of organic ligands coordinated with metal atoms self-assembled on metal surfaces. Due to the similarity with catalytically active sites in biological systems, the low-coordinated metal centers are considered to have promising properties in catalysis.

In this work, we will present the electrochemical characterization of 2D-MOCNs. The networks were prepared under ultra-high vacuum (UHV) conditions on Au(111). As organic ligands we used trimesic acid (TMA) and biphenyl-4,4'-dicarboxylic acid (BDA). The metal centers were single atoms of iron or manganese. The composition and structure of the networks were controlled and characterized by scanning tunneling microscopy in UHV. The sample is brought from UHV to the electrochemical cell through a transfer chamber in a controlled environment. Cyclic voltammetry experiments show that the networks catalyze the complete oxygen reduction towards H_2O and change the mechanism on Au(111) in alkaline media from a $2e^-$ pathway to a $4e^-$ ($2e^- + 2e^-$) pathway.

O 58.6 Wed 18:15 Poster B1

Growth of imidazolium-based ionic liquid films on gold at low temperatures — MARCEL MARSCHEWSKI¹, CORNELIA KUNZ¹, ●OLIVER HÖFFT², WOLFGANG MAUS-FRIEDRICHS¹, and FRANK ENDRES² — ¹Institut für Energieforschung und Physikalische Technologien, TU Clausthal, Leibnizstr. 4, 38678 Clausthal-Zellerfeld, Germany — ²Institut für Elektrochemie, TU Clausthal, Arnold-Sommerfeld-Str.6, 38678 Clausthal-Zellerfeld, Germany

Room temperature Ionic Liquids (RT-ILs) are a class of materials, which has recently gained enormous interest. Due to their exciting combination of properties they are of interest for numerous applications. Here we present our results for the growth of monolayers of imidazolium-based ionic liquid (ILs) films on gold at low temperatures. This was studied by electron spectroscopy using ultraviolet

photoelectron spectroscopy (UPS, HeI) and metastable induced electron spectroscopy (MIES). We have prepared monolayers of 1-octyl-3-methyl-imidazolium bis(trifluoromethylsulfonyle)imide ([OMIm]Tf₂N) on gold by vapour deposition at 140K. In contrast to the preparation of the monolayers at room temperature we observe an ordered growth of [OMIm]Tf₂N beyond the first monolayer. Heating up to room temperature, results in the formation of a disordered film. In addition we present the interaction of cesium with thin films of imidazolium based ILs. Here we will focus on the solvation of cesium in these ionic liquid films. For the IL monolayers, grown on Si(100), we find a shift of the IL valence band states to higher binding energies during Cs adsorption.

O 58.7 Wed 18:15 Poster B1

Atomic resolution under ambient conditions with a qPlus force sensor — •DANIEL S. WASTL, ALFRED J. WEYMOUTH, and FRANZ J. GIESSIBL — University of Regensburg, Regensburg, 93053, Germany

Frequency modulation atomic force microscopy (FM-AFM) is the preferred method to obtain high resolution AFM. So far, FM-AFM has mainly been employed in ultrahigh vacuum, but recently, atomic resolution has been obtained by FM-AFM in liquid [1] under ambient conditions with silicon cantilevers and by the qPlus sensor [2] in liquid [3]. The qPlus sensor is attractive, because it is self-sensing and thus does not require optical deflection measurements. Moreover, it has a higher quality factor in ambient conditions and should be competitive to silicon cantilevers in its noise performance [4, 5, 6]. However, we observed severe challenges due to a large change in cantilever damping on its transition from air to the adsorption layer / sample interface. Here, we provide atomic resolution on cleaved KBr (001) and of cleaved muscovite mica(001) under ambient conditions in a quality similar to data obtained in ultrahigh vacuum.

- [1] T. Fukuma et al, Appl. Phys. Lett., 87, 034101 (2005)
- [2] F. J. Giessibl, Appl. Phys. Lett., 76, 1470 (2000)
- [3] T. Ichii et al, Jpn. J. Appl. Phys. 51 (2012)
- [4] F. J. Giessibl et al, Phys. Rev. B 84, 125409(2011)
- [5] E. Köstner, PhD thesis (2012)
- [6] E. Wutscher et al, Rev. Sci. Instrum. 82, 093703 (2011)

O 58.8 Wed 18:15 Poster B1

Epitaxial order of self-assembled monolayers with attached molecular switches on Si(111), investigated by X-ray diffraction — •CHRISTOPHER WEBER¹, MICHAEL AXMAN PETERSEN², and STEFAN KOWARIK¹ — ¹Institut für Physik, Humboldt-Universität zu Berlin, 12489 Berlin — ²Institut für Chemie, Technische Universität Berlin, 10623 Berlin

Self-assembled monolayers (SAMs) can be used to chemically attach molecular switches to metal or semiconductor surfaces. The structure of the underlying linker SAM is often crucial for the switching efficiency of the system. In this case carboxyl-terminated alkyl-SAMs are used to couple molecular switches to a hexagonal Si(111) surface. The thickness, electron density and area per molecule of the SAM have been determined by X-ray reflectivity (XRR). The XRR results indicate that every second accessible Si-bond is occupied by an alkyl chain, in agreement with simulations. In addition to the out-of-plane information, the in-plane SAM structure and the epitaxial orientation of the SAM with respect to the Si(111) surface has been analyzed with grazing incidence X-ray diffraction (GIXD). We show that the alkyl-molecules form a highly stable SAM with a well-defined in-plane structure and epitaxial orientation relative to the Si(111) surface.

O 58.9 Wed 18:15 Poster B1

Work function change introduced by water on a halogen covered Pt(111) surface — •FLORIAN GOSSENBERGER and AXEL GROSS — Institute of Theoretical Chemistry, Ulm University, D-89069 Ulm/Germany

Anion adsorption on metal electrodes plays an important role in electrochemistry. Still, the knowledge about the microscopic structure of the interface between anion-covered electrodes and the electrolyte is still limited. We have used periodic density functional theory calculations to address the adsorption of halogen atoms (F, Cl, Br, I) on Pt(111). Typically, one expects that the adsorption of electronegative adsorbates will increase the work function. Interestingly enough, we find that the adsorption of halogens on a clean Pt(111) may lead to a significant decrease in the work function. According to our calculations, this behavior is due to a reduction in the surface dipole moment which itself depends on the charge distribution around the adsorbed halogen atoms.

Furthermore, we have studied the interaction of the adsorbed halogen atoms with single water molecules and whole water layers. We will in particular discuss the influence of the water molecules on the halogen-induced work function change of Pt(111).

O 58.10 Wed 18:15 Poster B1

Hierarchical self-assembly of polycyclic heteroaromatic stars into snowflake patterns: A route towards very large lattice constants — •STEFAN-S. JESTER, EVA SIGMUND, LISA M. RÖCK, and SIGURD HÖGER — Kekulé-Institut für Organische Chemie und Biochemie, Universität Bonn, Gerhard-Domagk-Strasse 1, 53121 Bonn, Germany

The self-assembly of rigid molecules with long alkyl/alkoxy side chains at the solution/solid interface allows an efficient approach towards 2D supramolecular crystalline surface patterns.[1,2] Scanning tunneling microscopy yields a submolecularly resolved insight into the adlayer structures and thus a conclusion on the driving forces for their formation. Of particular interest is how the nanoscale architectures depend on the design of the molecules, and how large unit cells can be derived. Here we present the two-dimensional self-assembly of polycyclic heteroaromatic star molecules with alkoxy side chains of distinct lengths on graphite. Depending on the chain length different dense and porous adsorbate patterns are observed. For $n = 12$ the frustrated self-assembly leads to hierarchically organized superstructures. Up to 10 molecules form triangular aggregates which pack densely into hexagonal patterns with very large (15.5 nm) lattice constants.[3]

[1] S.-S. Jester, N. Shabelina, S. M. Le Blanc, S. Höger, *Angew. Chem. Int. Ed.* **2010**, *49*, 6101. [2] S.-S. Jester, E. Sigmund, S. Höger, *J. Am. Chem. Soc.* **2011**, *133*, 11062. [3] S.-S. Jester, E. Sigmund, L. M. Röck, S. Höger, *Angew. Chem. Int. Ed.* **2012**, *51*, 8555.

O 58.11 Wed 18:15 Poster B1

Nanoscale surface patterning by molecular polygons: Can shape-persistent molecules behave like geometric tiles? — •STEFAN-S. JESTER, NINA SCHÖNFELDER, EVA SIGMUND, and SIGURD HÖGER — Kekulé-Institut für Organische Chemie und Biochemie, Rheinische Friedrich-Wilhelms-Universität Bonn, Gerhard-Domagk-Str. 1, 53121 Bonn, Germany

Shape-persistent macrocycles are formed by cyclooligomerization of respective acetylene-terminated half-ring structures under oxidative coupling conditions and subsequent separation of the crude product by recycling gel permeation chromatography. Self-assembled monolayers of the resulting monodisperse compounds are investigated by scanning tunneling microscopy at the interface of 1,2,4-trichlorobenzene and highly oriented pyrolytic graphite. The macrocycles ($3 \leq n \leq 6$) can be viewed as equilateral molecular polygons (triangles, squares, pentagons, hexagons) that consist of rigid backbones and long flexible alkoxy side chains. We particularly focus on dithiophene corner units linked by p-phenylene-ethynylene-butadiynylene rods. The length of the latter can be systematically increased, and the related polygon sizes define the pattern periodicities. Cocrystallization - for example after mixing triangles and hexagons - increases the complexity of the resulting patterns. One fundamental question is how and to which extent the concepts of discrete geometry can be transferred to design patterns with unit cells far beyond 20 nm. [1] S.-S. Jester, E. Sigmund, S. Höger, *J. Am. Chem. Soc.* **2011**, *133*, 11062.

O 58.12 Wed 18:15 Poster B1

Self-assembled monolayers of molecular spoked wheels: Scanning tunneling microscopy — •STEFAN-S. JESTER¹, VIKAS AGGARWAL¹, ALISSA IDELSON¹, ALEXANDER THIESSEN², DANIEL KALLE¹, DOMINIK WÜRSCH³, THOMAS STANGL³, FLORIAN STEINER³, JAN VOGELANG², JOHN M. LUPTON^{2,3}, and SIGURD HÖGER¹ — ¹Kekulé-Institut für Organische Chemie und Biochemie, Universität Bonn, Gerhard-Domagk-Str. 1, 53121 Bonn, Germany — ²Department of Physics and Astronomy, University of Utah, Salt Lake City, UT 84112, USA — ³Institut für Experimentelle und Angewandte Physik, Universität Regensburg, 93040 Regensburg, Germany

Shape-persistent molecular polygons can be viewed as a combination of rigid molecular rod units and corners. The stiffness of the molecules is related to the persistence length of the sides, arylene-alkynylene rods, and the rotational degree of freedom of the corner units. For corner/side numbers $n < 3$ such molecules can deform out of their plane by rotation of the corner joints. Nevertheless, shape-persistence can be established by intraannular rigid spoke units to yield molecular spoked wheels.[1,2] STM investigation of adlayers of these molecules

and its smaller subunits at the solid/liquid interface (e.g. 1-octanoic acid/graphite) yields a submolecularly resolved insight into the molecular architectures and their adsorbate pattern formation.

[1] D. Mössinger, D. Chaudhuri, T. Kudernac, S. Lei, S. De Feyter, J. M. Lupton, S. Höger, *J. Am. Chem. Soc.* **2010**, *132*, 1410. [2] D. Mössinger, J. Hornung, S. Lei, S. De Feyter, S. Höger, *Angew. Chem. Int. Ed.* **2007**, *46*, 6802.

O 58.13 Wed 18:15 Poster B1

Two-photon photoemission of thin CoO-Films on Ir(100)-(1x1) — ●SEBASTIAN OTTO and THOMAS FAUSTER — Lehrstuhl für Festkörperphysik, Universität Erlangen-Nürnberg, D-91058 Erlangen, Germany

Two-photon photoelectron spectroscopy is used to study unoccupied states on thin CoO films grown epitaxially on Ir(100)-(1x1). Unoccupied states were found on various reconstructions of one Co-monolayer thick films with different oxygen amounts [1] and CoO(111) films [2] with thickness of up to ten bilayers. Ultrathin CoO films with a Co amount of about one monolayer show an increasing energy of the unoccupied state from 2.36 to 4.03 eV and an increase of the work function from 5.18 to 6.12 eV with increasing oxide content. For low coverages the observed states are in good agreement with scanning tunneling spectroscopy measurements [3]. On thicker CoO(111) films an increase of the energy from 3.36 to 3.62 eV with film thickness is found, while the work function decreases from 6.01 to 5.69 eV. A comparison with calculations for bulk CoO [4] suggests that the observed states correspond to unoccupied Co 3d orbitals.

[1] M. Gubo, C. Ebensperger, W. Meyer, L. Hammer and K. Heinz. *Phys. Rev. B* **83** (2011) 075435.

[2] K. Biedermann, M. Gubo, L. Hammer and K. Heinz. *J. Phys.: Condens. Matter* **21** (2009) 185003.

[3] C. Tröppner. Dissertation, Universität Erlangen-Nürnberg (2011).

[4] V. I. Anisimov, F. Aryasetiawan and A. I. Lichtenstein. *J. Phys.: Condens. Matter* **9** (1997) 767.

O 58.14 Wed 18:15 Poster B1

Photon energy and polarization dependent photoemission from Ag(001) using a laboratory light source with time-of-flight setup — ●MICHAEL HUTH¹, CHENG-TIEN CHIANG^{1,2}, JÜRGEN KIRSCHNER¹, and WOLF WIDDRA^{1,2} — ¹Max-Planck-Institut für Mikrostrukturphysik, Weinberg 2, D-06120, Halle(Saale), Germany — ²Institute of Physics, Martin-Luther-Universität Halle-Wittenberg, Von-Danckelmann-Platz 3, D-06120, Halle(Saale), Germany

We use a high-harmonic generation light source for time-of-flight angle-resolved photoemission spectroscopy at 4 MHz on Ag(001). With 17 eV and 20 eV photon energy we observed dispersive features of the bulk electronic structure starting from 7 eV below the Fermi level. The dispersion depends on the chosen linear polarization of the incident light due to symmetry selection rules. Our results demonstrate efficient application of momentum-resolved high-repetition rate time-of-flight spectroscopy [1].

[1] C.-T. Chiang, A. Blättermann, M. Huth, J. Kirschner, and W. Widdra, *Appl. Phys. Lett.* **101**, 071116 (2012)

O 58.15 Wed 18:15 Poster B1

Reduced Ceria Surfaces: Ab initio computation of the electronic structure with the GGA+U method — ●ALEXANDER HAMPEL, DANIEL GRIEGER, and FRANK LECHERMANN — 1. Institut für Theoretische Physik, Universität Hamburg, Germany

This work deals with the investigation of the atomic and electronic structure of oxygen reduced ceria (111) surfaces within the *GGA+U* formalism as implemented in the Vienna ab initio Simulation Package (VASP). Within the *GGA+U* formalism one can take account of the strongly correlated *f*-states. The ab initio investigation starts with the determination of the correct lattice constant and the choice of the Hubbard-U value in the bulk to reproduce a correct insulating band gap. Using periodic supercells the electronic structure of the surface is calculated and the main properties of the clean surface are pointed out. This leads to the investigation of the oxygen vacancies. The change of the ceria structure by the lack of an oxygen atom on the surface and in the sub-surface are investigated. Surface energies give a good estimation of the probability for the (111) surface to appear and formation energies estimate the stability of the defects. Finally, we have a look on the change of electronic structure initiated by the vacancies, mainly the density of states. So one can see the advantages of the *GGA+U* treatment of the *f*-states and where the strongly correlated electrons are located.

O 58.16 Wed 18:15 Poster B1

Scanning tunneling spectroscopy of the highly correlated electron system Sn on Si(111) — ●JOCHEN SETTELEIN¹, PHILIPP HÖPFNER¹, JÖRG SCHÄFER¹, GANG LI², WERNER HANKE², and RALPH CLAESSEN¹ — ¹Physikalisches Institut, Universität Würzburg — ²Inst. für Theoret. Physik und Astronomie, Universität Würzburg

Two-dimensional electron systems can be realized at the surface of semiconductors by metal atom adsorption. A particularly intriguing scenario emerges for submonolayer coverages, since strong electron correlations come into play. At the same time, if a triangular lattice symmetry is chosen, any concomitant spin order faces the problem of geometric frustration. Here we address these intriguing questions by studying the reconstruction of Sn on Si(111) which, contrary to naive expectation of a metallic state, is suggestive of a Mott-Hubbard insulator at low temperatures [1].

We have studied the electronic properties by scanning tunneling microscopy and spectroscopy (STS). The tunneling spectra at low temperature show a characteristic dip around the Fermi level, indicative of insulating behavior. The spectral features on either side can well be interpreted in terms of lower and upper Hubbard band, respectively. Above 40 K the differential conductivity at the Fermi level increases gradually. The results are consistent with advanced many-body modeling by a dynamical cluster approximation. The STS results support the view as Mott insulator without a sharp transition as a function of temperature, and point at the role of longer-ranged correlations.

[1] S. Modesti *et al.*, *Phys. Rev. Lett.* **98**, 126401 (2007).

O 58.17 Wed 18:15 Poster B1

Scanning tunneling microscopy and spectroscopy of the phase change alloy Ge₂Sb₂Te₅ — ●JENS KELLNER¹, CHRISTIAN PAULY¹, MARCUS LIEBMANN¹, ALESSANDRO GIUSSANI², RAFFAELLA CALARCO², and MARKUS MORGENSTERN¹ — ¹II. Phys. Inst. B, RWTH Aachen University and JARA-FIT, Germany — ²Paul Drude Institut für Festkörperelektronik, Berlin, Germany

We use scanning tunneling microscopy (STM) in ultrahigh vacuum (UHV) to probe the local atomic structure and the electronic properties of the phase change alloy Ge₂Sb₂Te₅(0001) grown on Si(111) by molecular beam epitaxy. In order to obtain a clean surface, the mixed native oxides on the GST surface were removed by dipping the sample in de-ionized water followed by annealing at 200°C in UHV [1]. We realized images with atomic resolution in constant-current mode at different voltages in order to distinguish different chemical elements on the surface. Local variations in the atomic corrugation and lattice constants are found and analyzed in detail. Using the spectroscopy mode, we find a band gap of about 500 meV. A p-type doping becomes apparent in agreement with photoelectron spectroscopy data.

[1] Z. Zhang *et al.*, *Appl. Surf. Sci.* **256**, 7696 (2010).

O 58.18 Wed 18:15 Poster B1

Characterization of single crystalline phase change materials by angular-resolved photoemission spectroscopy: Evidence for topological band inversion — ●CHRISTIAN PAULY¹, MARCUS LIEBMANN¹, ALESSANDRO GIUSSANI², JENS KELLNER¹, SVEN JUST¹, JAIME SÁNCHEZ-BARRIGA³, ANDREI VARYKHALOV³, OLIVER RADER³, RAFFAELLA CALARCO², and MARKUS MORGENSTERN¹ — ¹II. Phys. Institut B, RWTH Aachen University and Jara Fit, Germany — ²Paul Drude Institut für Festkörperelektronik, Berlin, Germany — ³Helmholtz-Zentrum für Materialien und Energie, Berlin, Germany

Phase change materials based on Ge-Sb-Te ternary alloys have been widely used as optical rewritable data storage media. They are also regarded as a promising candidate for a nonvolatile storage system (PCRAM), which exploits the high electrical contrast between the amorphous and the crystalline phase. Using angular-resolved photoemission spectroscopy (ARPES) we probe the band structure of epitaxially grown single crystalline phase change materials, Ge₂Sb₂Te₅ and GeTe. The samples are either transferred in-situ using a home-made UHV shuttle or cleaned by dipping in de-ionized water for 1min and annealing to 250°C in UHV [1]. ARPES maps show well defined bands for both materials. Interestingly, the band structure of Ge₂Sb₂Te₅ reveals a prominent bulk valence band which crosses E_F , forming two maxima around the $\bar{\Gamma}$ -point. According to recent DFT calculations [2], this is a hint for a spin-orbit induced band inversion which is a requirement for topological properties. [1] Z. Zhang *et al.*, *Appl. Surf. Sci.* **256**, 7696 (2010) [2] J. Kim *et al.*, *Phys. Rev. B* **82**, 201312 (2010)

O 58.19 Wed 18:15 Poster B1

Van der Waals adsorption of Xe on Cu(100) — ●ANUSCHKA

SCHAFFNER, ALEXANDER POTZUWEIT, HAGEN ALLMRODT, LARS KRAFT, and HEINZ J. JÄNSCH — AG Oberflächen, Fachbereich Physik, Philipps-Universität Marburg, Deutschland

We employ Nuclear Magnetic Resonance (NMR) of ^{129}Xe to investigate the adsorption of Xenon on metal single crystal surfaces, here Cu(100). On various metals Xe shows a reasonably strong shift in the work function and in the TPD desorption temperature. Calculations show the mixing of the Fermi-level electrons with the wavefunctions of Xenon. This local density of states (LDOS) manifests itself in the NMR chemical shift (Knight shift) and/or T_1 relaxation (Korringa relaxation). The such visible hyperfine interaction is a pure ground state property and is thus accessible to theoretical treatment in a LDOS determination in DFT or other appropriate calculation.

Experimentally Xe is adsorbed in a constant flux of atoms impinging on the surface, typically 4 ML/s or 40 ML/s. By controlling the crystal's temperature the formation of either a bulk or an equilibrium of ad- and desorbing atoms can be established. To achieve the necessary sensitivity, spin exchange optical pumping of Rubidium/Xenon mixtures is employed, resulting in a signal gain of 5 orders of magnitude.

In first experiments the chemical shift σ of ^{129}Xe on Cu(100) is determined and will be contrasted to the shift on Cu(111). The shift of Xe/Cu(100) is substantially smaller as compared with Xe/Cu(111). This is attributed to the narrow surface state at the Fermi level of Cu(111) which is missing at the Cu(100) surface.

O 58.20 Wed 18:15 Poster B1

Dielectric Properties of Functional Oxide thin-films from First Principles — ●JAWAD ALSAEI¹, NEAL ALFORD², PAUL TANGNEY¹, and ARASH A. MOSTOFI¹ — ¹Departments of Materials and Physics, Imperial College London, SW7 2AZ, United Kingdom. — ²Department of Materials, Imperial College London, SW7 2AZ, United Kingdom.

Perovskite oxide materials show a wide range of physical properties that make them interesting both technologically and scientifically. Particular attention has been drawn to perovskites in thin-film form in order to meet the demand of manufacturing smaller industrial components such as advanced integrated electronic devices.

The optical properties of thin-film perovskite oxides can differ significantly from those of the bulk due to several factors, such as the mismatch strain imposed by the substrate, cation substitution, point defects, etc. We investigate, from first principles, the effect of some of these factors on the optical properties of functional oxide materials (BaTiO_3 and SrTiO_3).

First, it is found that the refractive index, at (400-1600 nm), increases with applied uni-axial strain. Second, the optical properties of $\text{Ba}_x\text{Sr}_{1-x}\text{TiO}_3$ (BSTO) solid solutions are studied using both the supercell and the virtual-crystal approximation (VCA) approaches. It is found, surprisingly perhaps, that the two methods agree remarkably well. Third, the effect of Sr content in BSTO is investigated. It is found that the refractive index decreases almost linearly as the Sr:Ba ratio increases. Finally, the effect of Oxygen vacancies is studied.

O 58.21 Wed 18:15 Poster B1

Tb on Bi thin films - Conductivity and surface diffusion — ●P. KRÖGER¹, D. LÜCKERMANN¹, S. SOLOGUB², H. PFNÜR¹, M. HORN VON HOEGEN³, C. KLEIN³, and C. TEGENKAMP¹ — ¹Inst. f. Festkörperphysik, Leibniz Universität Hannover, Appelstr. 2, 30167 Hannover — ²Nat. Acad. of Science, Nauky Av. 46, 03028 Kyiv, Ukraine — ³Dep. of Physics and CeNIDE, Uni Duisburg-Essen, Lotharstraße 1, 47057 Duisburg

The semimetal bismuth has attracted a lot of interest because of its unique electronic properties such as a low carrier concentration and a large mobility. Furthermore, the surface states reveal a pronounced Rashba splitting and the conductivity can be well discriminated from bulk contributions if thin films are grown epitaxially on Si(111) substrates, making surface related effects accessible even in macroscopic conductance measurements. In this conclusion the adsorption of various adsorbates on Bi(111) will be discussed. Adsorption of magnetic atoms (Fe, Co and Tb) at low T is accompanied by a transition from Weak Anti- to Weak Localization in magneto-transport measurements, related to the break of time reversal symmetry. Furthermore there a significant increase of carrier concentration due to hybridization effects has been found. [1] For Tb, additionally, surface diffusion of Tb-atoms even at $T \approx 10$ K needs to be considered. Visible as a low coverage minimum in conductance during adsorption. A simple nucleation theory approach describes the data very well. Tb turns out to be an even stronger scatterer than the other magnetic atoms like Co or Fe. [1]

Lükermann et. al, PRB 84 (2012), accepted.

O 58.22 Wed 18:15 Poster B1

Barrier free sub-surface incorporation of magnetic impurities into the Bi(111) surface: Manipulation of the protected surface state — ●C. KLEIN¹, P. ZAHL², N. VOLLMERS³, U. GERSTMANN³, D. LÜCKERMANN⁴, D.P. ACHARYA², P. SUTTER², H. PFNÜR⁴, C. TEGENKAMP⁴, W.-G. SCHMIDT³, and M. HORN-VON HOEGEN¹ — ¹Faculty of Physics and CENIDE, University of Duisburg-Essen, Lotharstr. 1, 47057 Duisburg, Germany — ²CFN, Brookhaven National Laboratory, Upton, New York 11973, USA — ³Department of Physics, University of Paderborn, Warburger Str. 100, 33098 Paderborn, Germany — ⁴Institut für Solid State Physics, University of Hannover, Appelstr. 2, 30167 Hannover, Germany

Due to the large spin orbit coupling electron backscattering in the Bi(111) surface state is strongly suppressed: the surface state is protected. In order to identify possible scattering mechanism we performed low temperature scanning tunneling microscopy (LT-STM) measurements in which sub-monolayer amounts of Fe and Co were deposited into the STM at 5K. After deposition the metal atoms are immediately embedded in a sub-surface site, as they are not present in topology. In dI/dV images the embedded impurities, however, become apparent as they are surrounded by a pronounced anisotropic threefold electronic scattering pattern with lateral dimensions of more than 10 nm. Calculations indeed confirm a barrier free incorporation of the impurities into the first Bi-Bilayer even at such low temperatures. Large changes of the scattering pattern as function of the tunneling bias reflects the dispersion of the occupied and unoccupied surface state of Bi(111).

O 58.23 Wed 18:15 Poster B1

Barrier free sub-surface incorporation of magnetic impurities into the Bi(111) surface: Manipulation of the protected surface state — ●C. KLEIN¹, P. ZAHL², N. VOLLMERS³, U. GERSTMANN³, D. LÜCKERMANN⁴, D.P. ACHARYA², P. SUTTER², H. PFNÜR⁴, C. TEGENKAMP⁴, W.G. SCHMIDT³, and M. HORN-VON HOEGEN¹ — ¹Faculty of Physics and CENIDE, University of Duisburg-Essen, Lotharstr. 1, 47057 Duisburg, Germany — ²CFN, Brookhaven National Laboratory, Upton, New York 11973, USA — ³Department of Physics, University of Paderborn, Warburger Str. 100, 33098 Paderborn, Germany — ⁴Institut für Solid State Physics, University of Hannover, Appelstr. 2, 30167 Hannover, Germany

Due to the large spin orbit coupling electron backscattering in the Bi(111) surface state is strongly suppressed: the surface state is protected. In order to identify and tune possible scattering mechanisms we performed low temperature STM (LT-STM) measurements in which sub-monolayer amounts of Fe and Co were deposited into the STM at 5K. After deposition the metal atoms are immediately embedded into a sub-surface site, as they are not present in topology. In dI/dV images the embedded impurities, however, become apparent as they are surrounded by a pronounced anisotropic threefold electronic scattering pattern with lateral dimensions of more than 10 nm. DFT calculations indeed confirm a barrier free incorporation of the impurities into the first Bi-Bilayer even at such low temperatures. Large changes of the scattering pattern as function of the tunneling bias reflects the dispersion of the occupied and unoccupied surface states of Bi(111).

O 58.24 Wed 18:15 Poster B1

Band bending in the unoccupied electronic structure of Bi_2Se_3 — ●CH. LANGENKÄMPER¹, A. ZUMBÜLTE¹, A. B. SCHMIDT¹, M. DONATH¹, T. FÖRSTER², P. KRÜGER², M. BIANCHI³, R. C. HATCH³, P. HOFMANN³, J. MI⁴, B. B. IVERSEN⁴, G. MUSSLER⁵, and D. GRÜTZMACHER⁵ — ¹Physikalisches Institut, Universität Münster, Germany — ²Institut für Festkörpertheorie, Universität Münster, Germany — ³Department of Physics and Astronomy, Aarhus University, Denmark — ⁴Department of Chemistry, Aarhus University, Denmark — ⁵Peter Grünberg Institut, Forschungszentrum Jülich, Germany

We report on angle- and spin-resolved inverse photoemission measurements on the topological insulator Bi_2Se_3 .

Vacancies and adsorbates on surfaces of topological insulators are known to modify the charge density at the surface. The resulting band bending leads to an energetic shift of the bandstructure and the evolution of Rashba-split surface states. With regard to possible future applications and the interpretation of surface reactions, the influence of this band bending on the unoccupied electronic structure plays an important role. Here, we examine the time evolution of the band structure for two different sample systems: an MBE-grown thin film and

a bulk crystal. Especially the evolution of new structures due to surface reactions will be discussed on the basis of theoretical calculations. Additionally, we investigate the influence of the threefold crystal symmetry, which causes differences between the surface states in $\bar{\Gamma}\bar{M}$ - and $\bar{\Gamma}\bar{M}$ -direction.

O 58.25 Wed 18:15 Poster B1

Imaging the local transport field of a Bi₂Se₃ surface — •SEBASTIAN BAUER, ALEXANDER M. BERNHART, MARK R. KASPER, ROLF MÖLLER, and CHRISTIAN A. BOBISCH — Faculty of Physics, Center of Nanointegration Duisburg-Essen, University of Duisburg-Essen, 47048 Duisburg, Germany

Since the prediction of the unique properties of topological insulators in 2007 [1] those new material class has become one of the most studied materials in condensed matter physics. To study the lateral variation of the electrochemical potential we performed scanning tunneling potentiometry (STP) [2] on the surface of thin films of Bi₂Se₃ grown on a Si(111) substrate. The films were prepared according to Zhang et al. [3]. All experiments, the preparation as well as the analysis, were carried out in situ under UHV conditions. For the STP measurements two tips of a four probe scanning tunneling microscope (STM) are contacted to the surface to apply an electric field parallel to the surface. A third tip simultaneously maps the topography and the local electrochemical potential of the surface [4]. We present first STP results showing a spatial variation of the electrochemical potential of the Bi₂Se₃ surface. In addition, to the transport field the thermovoltage of the tunneling barrier is detected. The two signals can be disentangled by reversal of the lateral current, because that changes the sign of the transport field leaving the thermovoltage unchanged. [1] L. Fu, C. Kane, and J. Mele, Phys. Rev. Lett. 98, 106803 (2007)[2] P. Murali, D. Pohl, Appl. Phys. Lett. 48, 514 (1986)[3] G. Zhang, et al., Appl. Phys. Lett. 95, 053114 (2009)[4] J. Homoth, et al., Nano Letters 9, 1588 (2009)

O 58.26 Wed 18:15 Poster B1

Unoccupied Surface States of Si(111)($\sqrt{3} \times \sqrt{3}$)R30°-Bi — •F. RÜHL¹, D. NIESNER¹, TH. FAUSTER¹, P. SESSI², M. BODE², M. TRIONI³, S. ACHILLI³, G. BIHLMAYER⁴, and E. V. CHULKOV⁵ — ¹Universität Erlangen-Nürnberg, Staudtstr. 7, D-91058 Erlangen, Germany — ²Experimentelle Physik II, Universität Würzburg, Am Hubland, D-97074 Würzburg, Germany — ³Dipartimento di Scienza dei Materiali and CNISM, Università degli Studi di Milano-Bicocca, Via Cozzi 53, 20125 Milano, Italy — ⁴Institut für Festkörperforschung, Forschungszentrum Jülich, 52425 Jülich, Germany — ⁵Donostia International Physics Center, 20018 San Sebastián, Basque Country, Spain

The ($\sqrt{3} \times \sqrt{3}$)R30°-reconstructed trimer phase Bi on Si(111) shows giant Rashba spin-splitting in UV photoemission [1]. In the present study, the unoccupied states were investigated by monochromatic ($h\nu=3.1, 4.65$ eV) and bichromatic ($h\nu=1.55+4.65$ eV) two-photon-photoemission. From the photon energy and polarization dependence, surface states are identified and a downward dispersing band 3.28 eV above the Fermi level was found. In addition, surface states exist at 2.58 eV and 2.23 eV at the $\bar{\Gamma}$ -point and at the \bar{M} -Point at 2.5 eV. The workfunction is 4.64 eV. The photovoltage for flatband conditions was determined to 70 meV. The Fermi level is located 0.22 eV above the valence band maximum. A long-lived feature with a lifetime >15 ps was identified at 0.73 eV. The results are compared with scanning tunneling spectroscopy data and density functional theory calculations.

[1] K. Sakamoto *et al.*, Phys. Rev. Lett. **103**, 156801 (2009)

O 58.27 Wed 18:15 Poster B1

Adsorption of organic layers on the giant spin orbit split BiAg₂ surface alloy — •MAREN C. COTTIN¹, JOHANNES SCHAFFERT¹, JORGE LOBO-CHECA², J. ENRIQUE ORTEGA^{2,3,4}, ANDREW L. WALTER⁴, CHRISTIAN A. BOBISCH¹, and ROLF MÖLLER¹ — ¹Faculty of Physics, Center for Nanointegration Duisburg-Essen, University of Duisburg-Essen, 47048 Duisburg, Germany — ²Centro de Física de Materiales CSIC/UPV-EHU-Materials Physics Center, Manuel Lardizábal 5, E-20018 San Sebastián, Spain — ³Departamento Física Aplicada I, Universidad del País Vasco, E-20018 Donostia-San Sebastián, Spain — ⁴Donostia International Physics Center, Manuel Lardizábal 4, E-20018 San Sebastián, Spain

The emerging field of spintronic devices has recently triggered a lot of research effort on materials exhibiting a spin-splitting of their electronic states. Recently, surface alloys such as PbAg₂, BiCu₂ or BiAg₂ have gathered a lot of attention due to the giant spin orbit splitting of

their surface states. At the same time organic molecules have already become important electronic building blocks of modern electronic devices.

To study the effect of the adsorption of organic layers on such giant spin split surface states, scanning tunneling microscopy (STM) experiments have been performed, e.g. on the archetype organic molecule 3,4,9,10 - perylene tetracarboxylic dianhydride acid (PTCDA) adsorbed on BiAg₂. The STM images show ordered layers exhibiting different molecular superstructures.

O 58.28 Wed 18:15 Poster B1

Unoccupied surface states of p-type topological insulators — •VOLKER HERMANN¹, DANIEL NIESNER¹, THOMAS FAUSTER¹, EUGENE V. CHULKOV², ZIYA S. ALIEV³, MAHAMMAD B. BABANLY³, and IMAMADDIN R. AMIRASLANOV⁴ — ¹Lehrstuhl für Festkörperphysik, Universität Erlangen-Nürnberg, Staudtstr. 7, D-91058 Erlangen, Germany — ²Donostia International Physics Center (DIPC), 20018 San Sebastián/Donostia, Basque Country, Spain — ³General and Inorganic Chemistry Department, Baku State University, Baku, AZ1148, Azerbaijan — ⁴Institute of Physics, Azerbaijan National Academy of Science, Baku, AZ1143, Azerbaijan

Density functional theory calculations predict a topological surface state (TSS) for SnSb₂Te₄ [1]. No Dirac point was found in UV photoemission. The material therefore is doped p-type.

Two-photon photoemission was used to investigate the unoccupied band structure. The Dirac point is found 0.3 eV above the Fermi level with a group velocity of 3.4 eVÅ. A work function of about 5.25 eV was measured. Time-resolved experiments show that the TSS is not only populated optically by the pump pulse but also indirectly by refilling from the bulk conduction band similar to the case of Bi₂Se₃ [2]. From a rate-equation model a lifetime of about 45 fs was found. A small lifetime is explained by scattering to the partly depleted bulk valence band.

[1] T.V. Menshchikova *et al.*, Appl. Surf. Sci., in press

[2] J.A. Sobota *et al.*, Phys. Rev. Lett. **108**, 117403 (2012)

O 58.29 Wed 18:15 Poster B1

Relaxation dynamics in laser-excited metals under non-equilibrium conditions — •BENEDIKT Y. MUELLER and BÄRBEL RETHFELD — Technical University Kaiserslautern, Germany

When an ultrashort laser pulse irradiates a metal, energy is absorbed by the electron system which is driven out of thermal equilibrium on a femtosecond timescale. Due to electron-electron collisions a new thermodynamical equilibrium state within the electron system is established in a characteristic time, the so-called thermalization time. The absorbed energy of the electrons will be further transferred to the phononic system. The thermalization time as well as the electron-phonon coupling strength [1] both strongly depend on the material properties and the excitation type. Furthermore, a non-thermalized electron gas couples differently to the phononic system as a thermalized one [2]. In order to follow the relevant microscopic dynamics without the need to assume thermalized electrons, we apply complete Boltzmann collision integrals to describe the transient electron distribution due to excitation, thermalization and relaxation. We implement the density of states of real materials in our approach [3]. As a result of our simulations, we extract the electron thermalization time and the electron-phonon coupling under non-equilibrium conditions. Examples are given for aluminum, gold and nickel.

[1] Z. Lin *et al.*, Phys. Rev. B **77**, 075133 (2008)

[2] B. Rethfeld *et al.*, Phys. Rev. B **65**, 214303 (2002)

[3] B. Y. Mueller *et al.*, AIP Conf. Proc. **1461**, 609 (2012)

O 58.30 Wed 18:15 Poster B1

Dynamical Simulation of Photoinduced Electron Transfer in Nitrile-Substituted Alkanethiolate Self-Assembled Monolayers Adsorbed at the Au(111) Surface — •VERONIKA PRUCKER¹, PEDRO B. COTO², ÓSCAR RUBIO-PONS¹, MICHEL BOCKSTEDTE¹, HAOBIN WANG³, and MICHAEL THOSS¹ — ¹Institut für Theoretische Physik, Interdisziplinäres Zentrum für Molekulare Materialien, Friedrich-Alexander-Universität Erlangen-Nürnberg, Staudtstr. 7/B2, D-91058 Erlangen, Germany — ²Departamento de Química-Física, Universidad de Alcalá, Alcalá de Henares, Madrid, Spain — ³Department of Chemistry and Biochemistry, MSC 3C, New Mexico State University, Las Cruces, New Mexico 88003, USA

Photoinduced electron transfer dynamics in self-assembled monolayers consisting of nitrile substituted short-chain alkanethiolate molecules

adsorbed at the Au(111) surface is studied. The method employed is based on a model Hamiltonian, which is determined by first-principles electronic structure calculations [1], and dynamical simulations. In comparison with experimental results [2], we analyze the influence of the orbital-symmetry of the donor state and the length of the aliphatic spacer chain of the monolayer on the electron transfer process. Moreover, the mechanisms controlling the electron transfer times are discussed.

- [1] I. Kondov *et al.*, J. Phys. Chem. C 111, 11970 (2007).
 [2] F. Blobner *et al.*, J. Phys. Chem. Lett. 3, 436 (2012).

O 58.31 Wed 18:15 Poster B1

Electronic lifetimes in a 2D electron gas in Bi/Cu(111): Screening effects and consequences for the spin structure — ●SVENJA VOLLMAR, ANDREAS RUFFING, SEBASTIAN JAKOBS, ALEXANDER BARAL, STEFFEN KALTENBORN, MIRKO CINCHETTI, STEFAN MATHIAS, MARTIN AESCHLIMANN, and HANS CHRISTIAN SCHNEIDER — University of Kaiserslautern

We compare energy resolved lifetimes in the quantum-well system Bi/Cu(111) as obtained from time- and angle-resolved 2-photon photoemission spectroscopy with the results of a Rashba model for the quantum-well bands with parameters extracted from the experiment.

Since the bulk screening constants for Bi and Cu are very different, we derive the correct statically screened potential for the Coulomb interaction of the electrons in the Bi-layer on the Cu-substrate.

We find that the measured lifetimes plateau around the intersection point cannot even qualitatively be explained on the basis of the Rashba model. Only by the ad-hoc introduction of a more complicated spin structure by assuming a k-dependent spin mixing, the calculated lifetimes qualitatively agree with experiment. Our results indicate that the spin-orbit coupling leads to band-structure effects beyond those described in a pure Rashba model.

O 58.32 Wed 18:15 Poster B1

Temporal Evolution of Excited Electrons in the Ni(111) Image-Potential States — ●BEATRICE ANDRES¹, PAUL WEISS¹, MARKO WIETSTRUK¹, ANKE B. SCHMIDT², MARKUS DONATH², and MARTIN WEINELT¹ — ¹Fachbereich Physik, Freie Universität Berlin, 14195 Berlin — ²Physikalisches Institut, Westfälische Wilhelms-Universität Münster, 48149 Münster

In ferromagnetic materials electronic relaxation times differ for electrons with majority and minority spin. Besides spin-conserving decay, which mainly occurs through inelastic electron-electron scattering, relaxation is also caused by spin-flip processes. Additionally the interaction of electrons with phonons and defects give rise to spin-dependent dephasing rates.

In spin- and time-resolved two-photon-photoemission experiments (2PPE) we populate the $n = 1$ and $n = 2$ image-potential states on Ni(111) with the third harmonic ($3h\nu \approx 5.0$ eV) of our Ti:Sa laser. We can excite electrons from different initial states by changing the photon energy and thus modify the spin polarization created in the image states. Probing the electronic structure after a variable time delay with the fundamental ($1h\nu \approx 1.67$ eV) enables us to study spin-dependent differences in image-state lifetimes and temporal evolution of linewidths. Our results indicate diversities in the decay channels and dephasing processes for majority- and minority-spin electrons.

O 58.33 Wed 18:15 Poster B1

Combined XPS and XAS Analysis Using the Software UNIFIT 2013 — ●RONALD HESSE, REINHARD DENECKE, and MARTIN WELKE — Universität Leipzig, Wilhelm-Ostwald-Institut, 04103 Leipzig, Linnéstr. 2

A combination of X-ray absorption spectroscopy (XAS) and x-ray photoelectron spectroscopy (XPS) using synchrotron radiation with variable energy and polarized soft x-rays with high resolution and high flux is a powerful technique to observe atomic compositions and electronic state of surfaces of materials. In order to extract the maximum of information of the studied material a spectrum fit for both methods has to be done. The newest version of the software UNIFIT allows the combined spectrum processing and peak fit of XPS and XAS measurement data. The different theoretical description of the spectral background of XA spectra was implemented in the software. Additionally, the input routine was expanded for the reading of four special XAS data formats (NEXAFS, BESSY-EMP/2, LUND-MAXlab Scan Zeiss, 1. Column: Photon Energy - 2. Column: Intensity). The peak fit of a XA and XP spectrum of Ti 2p as well as a XMCD study of a thin Co film on BaTiO₂ demonstrate the new possibilities of the

improved software UNIFIT 2013.

O 58.34 Wed 18:15 Poster B1

Numeric atom-centered basis set with valence correlation consistency from H to Ar — ●IGOR YING ZHANG, XINGUO REN, PATRICK RINKE, VOLKER BLUM, and MATTHIAS SCHEFFLER — Fritz-Haber-Institut der MPG, Berlin

Numeric atom-centered orbitals are appealing for electronic structure theory, particularly density-functional theory (DFT), because the occupied effective single-electron orbitals required to construct the density can be represented by rather efficient, compact, yet transferable NAO basis sets [1]. It is well known, however, that for perturbative approaches beyond DFT (RPA, MP2, GW, etc.) the basis set convergence is much slower. We here present a prescription for numeric atom-centered correlation consistent basis sets, coined NAO-VCC-XZ (X=D,T,Q,5). Like their Gaussian based counterparts [2], these NAO-VCC-XZ basis sets provide a much more systematic convergence to the complete basis set limit, reducing the basis set superposition error and giving rise to extrapolation techniques for total energies, binding energies, etc. The advantage of NAOs over Gaussians is that the shape of basis function tails is not analytically constrained. In practice, we use hydrogen-like basis function tails, and explicitly control their radial extent. This prescription recovers the complete basis set convergence properties of the largest available quantum chemical basis sets for perturbation theory, but with significantly smaller basis sets and numerical efficiency. [1] V. Blum, et al., Comp. Phys. Comm. 180, 2175 (2009); [2] H. Eshuis, F. Furche, J. Chem. Phys. 136, 084105 (2012).

O 58.35 Wed 18:15 Poster B1

Ordering in two dimensional amorphous atomic sheet — TAKAHIRO SUZUKI^{1,2}, KIYOSHI KOYANAGI¹, YASUMASA TANISHIRO^{1,2}, and ●KUNIO TAKAYANAGI^{1,2} — ¹Tokyo Institute of Technology — ²Crest, JST

Amorphous film is an issue of nano-surface science, because the local ordering of atoms/ions determines electronic properties. We used an aberration corrected electron microscopy (AbC-EM) to find a local order/disorder of atoms/ions in amorphous thin films. An amorphous carbon mono-sheet is found to have a specific "local ordering" in the atomic sheet. Local order of metal ions in an amorphous InGaZnO film, a transparent amorphous oxide semiconductor (TAOS), is found to be seen also by AbC-EM. The electron transport via overlapping between neighboring metal s-orbitals in TAOS is discussed in terms of the local ordering.

O 58.36 Wed 18:15 Poster B1

ROSE: RObotable Spin-polarized Electron source — ●SEBASTIAN D. STOLWIJK, HENRY WORTELEN, ANKE B. SCHMIDT, and MARKUS DONATH — Physikalisches Institut, Westfälische Wilhelms-Universität Münster

Surfaces of non-magnetic materials may exhibit surface states with complex spin structures in reciprocal space. To understand the fundamental mechanisms of the underlying effects, it is crucial to obtain as complete information as possible on the polarization of the electronic states. So far, current spin- and angle-resolved inverse photoemission experiments are limited to one polarization direction. Here, we introduce a recently developed RObotable Spin-polarized Electron source (ROSE). Briefly, this is based on a GaAs spin-polarized electron source, which is modified by embedding a variable rotation of the source chamber. It produces a transversally spin-polarized electron beam, whose polarization direction lies either in the plane of incidence or is perpendicular to it. With ROSE, the inverse photoemission experiment is sensitive to at least two in-plane polarization directions. Furthermore, by rotating the sample, one gains sensitivity to the out-of-plane component. In-situ measurements of the unoccupied electronic structure of Ti/Si(111) demonstrate the beauty of the ROSE.

O 58.37 Wed 18:15 Poster B1

Combined STM/AFM study on cyclic trimeric perfluoro-ortho-phenylene mercury — ●FLORIAN ALBRECHT¹, JOHN McMANUS¹, MARTIN FLEISCHMANN², MANFRED SCHEER², and JASCHA REPP¹ — ¹Institute of Experimental and Applied Physics, University of Regensburg, 93053 Regensburg, Germany — ²Institute of Inorganic Chemistry, University of Regensburg, 93053 Regensburg, Germany

Despite the fact that cyclic trimeric perfluoro-ortho-phenylene mer-

cury (TPM) molecules have a relatively large void at their center, their lowest unoccupied molecular orbital (LUMO) was calculated to have highest density just there [1]. To verify this experimentally, we studied TPM by means of low-temperature combined scanning tunneling (STM) and atomic force microscopy (AFM). From combining the structural information obtained in the AFM with the electronic information in the STM channel, we indeed confirm this picture. The molecule has the tendency to attract electron rich ligands at its center. We directly mapped out the interaction of a prototype ligand to the TPM molecule by attaching the ligand to the tip and measuring its interaction with the molecule adsorbed on the sample surface.

[1] M. R. Haneline and F. P. Gabbaï, *Inorg. Chem.*, 44, 6248, (2005)

O 58.38 Wed 18:15 Poster B1

FIM meets AFM: Quantification of Long-Range Forces in Non-Contact Atomic Force Spectroscopy using Field Ion Microscopy Characterized Tips — ●JENS FALTER^{1,2}, GERNOT LANGEWISCH², HENDRIK HÖLSCHER³, HARALD FUCHS², and ANDRÉ SCHIRMEISEN¹ — ¹Institute of Applied Physics (IAP), Justus-Liebig-University Giessen — ²Center for Nanotechnology (CeNTech) and Institute of Physics, University of Muenster (WWU) — ³Karlsruhe Institute of Technology (KIT), Karlsruhe

Non-contact Atomic Force Microscopy (ncAFM) is capable to measure interaction forces between the probing tip and the sample with atomic precision. Although the sample can be imaged with atomic resolution, the structure of the tip remains unknown in most ncAFM experiments. Therefore, a quantitative comparison to models from theory is often impossible. Here we present long range ncAFM force spectroscopy experiments with FIM characterized tungsten tips on Ag(111) [1]. With the additional information about the tip geometry, the measured forces can be compared to analytical models. Our analysis shows a quantitative agreement between experiment and theory for the van der Waals- and electrostatic forces [2, 3]. Even more interestingly our approach provides a value for the absolute tip sample distance. Furthermore, an additional force contribution of long range character can be separated and assigned to arise from so called "patch charges" [4].

[1] J. Falter et al, submitted to PRB (2012) [2] S. Hudlet et al, *Eur. Phys. J. B* 2, 5-10 (1998) [3] C. Argento and R.H. French, *J. Appl. Phys.* 80 (11), (1996) [4] N.A. Burnham, *Phys. Rev. Lett.* 69, 1 (1992)

O 58.39 Wed 18:15 Poster B1

Dynamic Friction Force Microscopy: Imaging via control of nonlinear cantilever oscillation — ●FELIX MERTENS, THOMAS GÖDDENHENRICH, and ANDRÉ SCHIRMEISEN — Institut für Angewandte Physik, Justus-Liebig-Universität Gießen, D-35392 Gießen

A dynamic friction force microscopy technique is presented, which uses the nonlinear cantilever oscillation response to control the sample modulation amplitude. A periodic stick-slip motion of the tip at higher modulation amplitudes leads to an additional cantilever resonance frequency signal due to a self-excited cantilever oscillation. Using a lock-in amplifier together with a modulation amplitude feedback control system, friction contrast in terms of the modulation amplitude near the nonlinear-to-linear regime can be obtained. Applying this technique on HOPG, the observed friction images clearly reveal higher friction at step edges as well as an area contrast otherwise unseen in the topography.

O 58.40 Wed 18:15 Poster B1

Surface investigation of Topological Insulators with STM and STS: From local defects and aging processes. — ●SEBASTIAN FIEDLER^{1,2}, PETER LUTZ^{1,2}, HENRIETTE MAAS^{1,2}, CHRISTOPH SEIBEL^{1,2}, HENDRIK BENTMANN^{1,2}, and FRIEDRICH REINERT^{1,2} — ¹Experimentelle Physik VII, Universität Würzburg, 97074 Würzburg, Germany — ²Gemeinschaftslabor für Nanoanalytik, Karlsruher Institute für Technologie KIT, 76021 Karlsruhe, Germany

Topological Insulators (TIs) are presently one of the most promising topics in solid state physics. Theoretical calculations predict a spin polarised current on the surface of the TI without electrical resistance, which should be robust since the involved states are protected by time reversal symmetry. This dissipation-less transport of a spin polarised current requires an insulating bulk and a band gap with two crossing bands, one for spin up and one for spin down states [1]. However, defects are the main reason, why the bulk is not insulating thus destroying this effect. We investigate the surface of TIs with Scanning Tunneling Microscopy (STM) and Spectroscopy (STS). We observe local defects and measure the local electron density, which helps un-

derstanding the influence of defects. Moreover, we demonstrate that aging of the TI results in a broadening of the band gap. This effect can also be mimicked by adsorption of alkali metals.

[1] arXiv:0801.0901v1 [cond-mat.mes-hall] 7 Jan 2008

O 58.41 Wed 18:15 Poster B1

A scanning tunneling microscope exhibiting 120 ps time resolution — ●CHRISTIAN SAUNUS, MARCO PRATZER, and MARKUS MORGENSTERN — II. Physikalisches Institut B and JARA-FIT, RWTH Aachen University, D-52074 Aachen, Germany

Short tunneling voltage pulses are used in a pump-probe set-up to increase the time resolution of the current STM measurements, thereby beating the bandwidth limit of the current preamplifier.[1] Using a home built radio frequency STM, we apply voltage pulses as short as 120 ps to the tunneling junction between tip and sample. This is verified by measuring the overlap of pump and probe visible due to the non-linearity of the I - V characteristic of the junction measured independently. Atomic resolution on HOPG is achieved in the pump-probe mode exploiting differences in the non-linearity of $I(V)$ which basically corresponds to a d^2I/dV^2 mapping on HOPG.

[1] S. Loth, M. Etzkorn, C. P. Lutz, D.M. Eigler, and A. J. Heinrich, *Science* 329, 1628 (2010).

O 58.42 Wed 18:15 Poster B1

4-Tip STM Transport Measurements on Si(111)-7x7 — ●MARCUS BLAB, MATTHIAS WUNDE, VASILY CHEREPANOV, PETER COENEN, and BERT VOIGTLÄNDER — Forschungszentrum Jülich, Peter Grünberg Institut, 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 on the nanoscale. An n-doped Si(111)-7x7 sample was chosen as a first test sample. We will present atomic resolution images with all four tips and distance dependent 4-tip transport measurements of this surface. These measurements are compared with finite elements calculations, which show a strong tip distance dependence of the current density. Furthermore the calculations show a possibility to suppress the bulk in order to measure the surface conductance of Si(111)-7x7.

O 58.43 Wed 18:15 Poster B1

A combined LT-STM/FIM for tip specific tunnelling experiments — ●MATTHIAS MÜLLER, BEN WORTMANN, and ROLF MÖLLER — Faculty of Physics, Center of 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 characterisation of the tip is possible without transfer to a different position in the UHV system, so that the characterised tip is identical to the one used in the STM experiment. The geometry of the microscope resembles a cylinder with a height of 13 cm and a diameter of 4 cm. The STM is screwed directly onto a commercially available continuous flow cryostat which allows cooling to about 5-7 K. The very compact design minimises helium consumption to about 1 litre/hour. Insulation from vibration is provided by a combination of springs and eddy current damping. 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 slider holding the tip. The slider can be easily exchanged in vacuum. The performance of the STM setup has already been shown for an almost identical system [1]. [1] (H. Karacuban, M. Lange, J. Schaffert, O. Weingart, Th. Wagner and R. Möller, *Surf. Sci. Lett.*, 603, Issue 5, L39 (2009).

O 58.44 Wed 18:15 Poster B1

Development of a low-temperature scanning tunneling microscope for spin-polarized measurements in high magnetic fields — ●OLIVER STORZ, PAOLO SESSI, and MATTHIAS BODE — Institute of Experimental Physics II, University Würzburg, Am Hubland, 97074 Würzburg

The discovery and characterization of new phenomena in surface science calls for advanced experimental techniques which combine ultra-high spatial and energy resolution with extreme environments. Here we present a new Scanning Tunneling Microscope (STM) designed for

spin-polarized measurements at low temperatures and in high magnetic fields. Cooling is achieved by pressing the STM head against a pumped liquid He bath with a base temperature $T \leq 1.2$ K. A superconducting magnet supplies a vertical field up to 12.5 T. The microscope design and the materials used have been optimized to achieve high resonance frequencies, resulting in an excellent stability of the instrument. A piezo-driven x, y -sample stage allows for a lateral travel range of ± 2 mm. By means of a linear transfer system the STM head can be moved between the measurement position inside the cryostat and a position for tip and sample exchange as well as for in-situ deposition onto the cold sample surface.

O 58.45 Wed 18:15 Poster B1

Atomic Resolution on KBr (100) Achieved by Means of KPFM and nc-AFM — ●TIMM VOLKMANN, AARON GRYZIA, ARMIN BRECHLING, and ULRICH HEINZMANN — Molecular and Surface Physics, Bielefeld University

We modified an Omicron UHV AFM/STM for Kelvin Probe Force Microscopy (KPFM). The modified setup consists out of a nanoSurf easy PLL plus Controller/Detector for AFM, and a Signal Recovery DSP Lock-in Amplifier and SRS Analog PID Controller for KPFM. Cleaving potassium bromid (KBr) under ambient conditions and consecutive heating provides a clean surface for atomic imaging. We did research regarding different baking parameters. Annealing reduces contamination and electrostatic forces on the sample surface. Finally, cleaving the crystal in-situ provides a significant improvement of the image quality in the contact potential difference (CPD) and topography data.

O 58.46 Wed 18:15 Poster B1

Combination of Tuning Fork Non-Contact Atomic Force Microscopy with Field Ion Microscopy — ●SÖREN ZINT¹, ANDREAS NEJBERT¹, DIRK DIETZEL¹, JENS FALTER¹, ANDRÉ SCHIRMEISEN¹, and HARALD FUCHS² — ¹Institute of Applied Physics (IAP), Justus-Liebig-University Giessen — ²Center for Nanotechnology (CeNTech) and Institute of Physics, University of Muenster (WWU)

Non-contact atomic force microscopy (ncAFM) has proven to be a valuable tool for surface characterization with atomic-resolution. For a quantitative comparison between force spectroscopy experiments and corresponding analytical models, knowledge of the true tip geometry is required. One method for determining the tip geometry is the field ion microscopy (FIM) technique. Thus we combined a tuning fork sensor based low temperature AFM with the field ion microscopy technique, in one ultra-high vacuum chamber. With this AFM we can acquire atomically resolved AFM images (e.g. on NaCl) together with force spectroscopy data, while the FIM allows for tip reconstruction of electrochemical etched tungsten tips. This setup enables us now to approach the problem of correlating specific features of force spectroscopy experiments with corresponding tip geometries.

O 58.47 Wed 18:15 Poster B1

Infrared subsurface imaging of nanoparticles embedded in textile fibres — ●ALFRED VAN MUNSTER^{1,3}, BENEDIKT HAUER¹, BENJAMIN GLAUSS², WILHELM STEINMANN², MARKUS BECKERS², THOMAS GRIES², and THOMAS TAUBNER^{1,3} — ¹I. Institute of Physics (IA), RWTH Aachen University, Sommerfeldstraße 14, 52074 Aachen, Germany — ²Institut für Textiltechnik ITA, Otto-Blumenthal-Straße 1, 52074 Aachen, Germany — ³Fraunhofer-Institut für Lasertechnik ILT, Steinbachstraße 15, 52074 Aachen, Germany

The mechanical and electrical properties of polymer based materials (e.g. fibres) are affected by additives like nanoparticles [1]. However, it is difficult to detect the location of embedded nanoparticles beneath the surface without damaging the sample. Scattering-type scanning near-field optical microscopy (s-SNOM) offers the opportunity to characterize a sample in such a non-destructive way. The evanescent field at the apex of a sharp, illuminated tip is used to probe the dielectric properties of a material with a sub-wavelength resolution given by the tip radius.

In our sample system siliconcarbide nanoparticles are embedded in polypropylene fibres. At mid-infrared wavelengths the phonon polaritons in SiC resonantly enhance the near-field interaction [2]. We compare the experimental data to reference measurements on bulk SiC and to the calculated predictions of a layered system model [3].

- [1] W. Steinmann et al., Text. Res. J. 82, 1846 (2012).
- [2] R. Hillenbrand et al., Nature 418, 159 (2002).
- [3] B. Hauer et al., Opt. Express 12, 13175 (2012).

O 58.48 Wed 18:15 Poster B1

The detection of light emitted from the tunneling junction of a low temperature STM — ●EBRU ÖZEN, 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

The decrease in size of the building blocks used in modern electronic devices requires the understanding of electronic transport phenomena down to the atomic level. Beside the elastic tunneling processes in a scanning tunneling microscope (STM) experiment, also inelastic processes take place. This leads to an excitation of the sample. The relaxation may decay e.g. by emission of photons [1]. The spectral analysis of the emitted light from the tunneling junction in the STM experiment provides valuable information about radiative decay channels, e.g. within an adsorbed organic molecule [2]. We implemented an experimental setup for the detection of photons which are emitted during the decay of the excitation of the sample. During first measurements light from the tunneling junction either during field emission or tunneling could efficiently be detected.

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

O 58.49 Wed 18:15 Poster B1

Study of protein DNA interaction by simultaneous atomic force and fluorescence microscopy — ●SÖREN GRANNEMANN, VOLKER WALHORN, and DARIO ANSELMETTI — Bielefeld University, Bielefeld, Germany

Atomic force microscopy (AFM) and fluorescence microscopy are in each case valuable tools for affinity studies at the single molecule level. A combination of both might even provide further insights in intermolecular binding and dissociation processes.

We combined AFM with total internal reflection microscopy (TIRFM) to study the affinity of a fluorescently labeled Protein DNA receptor ligand pair. The fluorescence markers were chosen such that Fluorescence Resonant Energy Transfer (FRET) can occur at close proximity of the dye molecules. Consequently, receptor-ligand binding should be correlated with FRET.

In first proof of principle experiments we used the DNA-binding Domain of the transcriptionfactor PhoB from *E. coli* and the associated DNA containing the PhoB recognition sequence as receptor-ligand system. Simultaneously acquired force and acceptor fluorescence data showed a correlation between the decrease of acceptor fluorescence intensity and molecular dissociation events of the Protein-DNA complexes. In present experiments, the donor fluorescence is measured additionally to prove the anti-correlation of donor and acceptor fluorescence intensity as well.

O 58.50 Wed 18:15 Poster B1

A simple design to convert an UHV-STM into an AFM — ●STEFAN BORGS DORF and ULRICH KÖHLER — Experimentalphysik IV, Ruhr-Universität Bochum, Germany

A simple design of an atomic force microscope (AFM) is presented, by which an ultra high vacuum scanning tunneling microscope (UHV-STM) is converted into an UHV-AFM. For this purpose piezoresistive Cantilevers with bimorph actuator are used. Under these conditions it is less complicated to build up an AFM in vacuum than with an optical readout. In our setup the cantilever is scanning. Therefore the tip is located in the middle of the piezo tube to minimize the crosstalk between different scanning directions as in STM. Another requirement is that it should be able to exchange the sensor in the vacuum chamber and also to create a layout to exchange the sensor type, for example to a qPlus Sensor.

O 58.51 Wed 18:15 Poster B1

Nanosecond scanning tunneling microscopy — ●SHICHAO YAN^{1,2}, DEUNG-JANG CHOI^{1,2}, and SEBASTIAN LOTH^{1,2} — ¹Max Planck Research Group-Dynamics of Nanoelectronic Systems, Center for Free-Electron Laser Science, Hamburg — ²Max Planck Institute for Solid State Research, Stuttgart

The scanning tunneling microscope (STM) can provide very high spatial resolution down to the atomic scale. One of the usual limits of the STM technique is its limited time resolution which is typically milliseconds because of the bandwidth of the control electronics. Yet, many processes on the nanoscale occur at nanosecond speed or faster. We present the instrumentation and test of a scanning tunneling microscope system that combines sub-Kelvin operation with high-frequency electronic circuitry. Nanosecond or picosecond electric pump-probe

pulses can be introduced into the tunneling junction with high fidelity to study the dynamics of the nanostructures. The design of the high bandwidth circuitry and the cooling mechanism of the semi-rigid cables will be presented. With this instrument, we have reached nanosecond time resolution while maintaining atomic spatial resolution. We apply this technique to measure the spin relaxation time of iron nanostructures on copper nitride. In principle, the electric pump-probe STM technique can also be used to study long lifetime vibrational excitations and conformational changes of molecules.

O 58.52 Wed 18:15 Poster B1

Investigation of single Co atoms on Mn/W(001) — ●ARNE KÖHLER, ALEXANDER SCHWARZ, and ROLAND WIESENDANGER — Institute of Applied Physics, University of Hamburg, Germany

Recently, the magnetic coupling between single Co atoms and the antiferromagnetic spin-spiral of Mn/W(110) has been studied with Scanning Tunneling Microscopy [1]. Using the ferromagnetic spin-spiral of Mn/W(001) [2] as a further complex magnetic template for Co atoms, our final goal is to investigate local magnetic properties of Co adatoms using Magnetic Exchange Force Microscopy [3] and Spectroscopy [4].

To inhibit aggregation of Co atoms on the substrate, they are deposited and investigated at low temperature. In our particular set-up, Co atoms are deposited from a miniature evaporator inserted into the cantilever holder. After deposition, different atomic scale contrast features are found on the substrate, indicating several adsorbed species. The origin of these adsorbates can be twofold: coadsorption during Co evaporation, i.e., CO, or formation on the surface after deposition, i.e., H:Co complexes. The latter is of particular interest, as it can be expected that H:Co behave magnetically different than single Co atoms.

Therefore, it is necessary to differentiate between Co atoms and other species on the surface.

- [1] D. Serrate et al., Nat. Nanotech. 5, 350 (2010).
- [2] P. Ferriani et al., Phys. Rev. Lett. 101, 027201 (2008).
- [3] U. Kaiser et al., Nature 446, 522 (2007).
- [4] R. Schmidt et al., Phys. Rev. Lett. 106, 257202 (2011).

O 58.53 Wed 18:15 Poster B1

Heat transfer through a single molecule — ●NILS KÖNNE, LUDWIG WORBES, DAVID HELLMANN, KONSTANTIN KLOPPSTECH, and ACHIM KITTEL — EHF, Fak. V, Physik, Carl von Ossietzky Universität Oldenburg

The measurement of the molecular heat transfer at the single molecule level has attracted a lot of interest in recent years [1]. To measure this phenomenon with high spatial resolution we use our self-developed near field scanning thermal microscope (NSThM). Hence we are able to simultaneously detect the electron and heat transfer through a single molecule under ultra-high vacuum conditions. The conduction measurements are done for different temperature and potential differences within an Au-octanedithiol-Au junction using the NSThM-break junction technique. We have proven our concept by repeatedly retract the tip from the octanedithiol covered surface and record the distance dependency of the conductance which partially exhibit a step like behaviour. The histogram of these conduction steps reveals the commonly known [2] low conduction value of 1 nS for a single octanedithiol. [1] Yonatan Dubi and Massimiliano Di Ventra, Rev. Mod. Phys. 83, 131 (2011). [2] Wolfgang Haiss et al, J. Phys. Chem. C 113, 5823-5833 (2009).

O 58.54 Wed 18:15 Poster B1

In situ characterization of thermal resistance of sensor tips of a near-field scanning thermal microscope (NSThM) — ●KONSTANTIN KLOPPSTECH, NILS KÖNNE, LUDWIG WORBES, and ACHIM KITTEL — EHF, Inst. f. Physik, CvO Universität Oldenburg

The experimental analysis of near-field heat transfer by means of absolute fluxes is based on accurate knowledge of the thermal resistance of the thermocouple sensor. We present an accurate in situ method for the determination of the sensor's thermal resistance which can be applied for each sensor right before the scanning procedure. Therefore a sample holder consisting of a 5 μ m thin and 3-10mm long tungsten wire which is glued to an isolated copper block is realized. The wire itself is mechanically pre-tensioned to minimize thermal vibrations because it is heated via a high frequency current. By this a temperature profile will develop along the wire resulting in a measurable change in electric resistance. Parasitic heat-drain channels can be neglected, because the experiment is performed in UHV. The determination of the thermal resistance of the tip is performed in two steps. First, the mean temper-

ature rise is calculated for various values of heating power. Thermal resistance of the wire is determined by fitting the curve of temperature change versus heating power. Second, the tip is being approached to the wire resulting in a second channel for heat drain. The thermal resistance of the tip is then calculated from the resulting temperature change for different heating powers of the coupled system. This can be done by means of solving a 1d heat transfer equation, which describes the coupled systems of wire and tip.

O 58.55 Wed 18:15 Poster B1

Highly controlled electron bombardment of SPM-tips for cleaning — DAVID HELLMANN, LUDWIG WORBES, KONSTANTIN KLOPPSTECH, NILS KÖNNE, and ●ACHIM KITTEL — EHF, Faculty V, Department of Physics, C. v. O. University of Oldenburg, 26129 Oldenburg, Germany

In the field of scanning probe microscopy, it is of great importance to operate with a well defined state of sample and probe with respect to unintentionally adsorbed molecules. There are many techniques for tip cleaning described in literature; among others the use of accelerated electrons as an energy source is reported. So far, all of the setups described, yielded either no or only indirect information about the probe's temperature reached during the cleaning procedure, which is an important quantity to control the process. The Near-Field Scanning Thermal Microscopy probe not only serves as scanning tunneling microscope tip, but also includes a thermosensor in the vicinity of the probe's apex. These sensors are very delicate because they combine different kind of materials. We use electron bombardment for cleaning these unique sensors, while the thermosensor is used as a sensor in the loop which is controlling the procedure. We observed probe temperatures up to 1800 K for a few tens of milliseconds without causing any damage to the tip function. We describe here the device as well as experimental data concerning the relation between the energies used for cleaning and the resulting temperature of the probe. The presented data might serve as an indicator for other setups where a direct measurement of the temperature of the apex is impossible.

O 58.56 Wed 18:15 Poster B1

Fabrication of gold nanocone near-field scanning microscope probes — ●OMAR TANIRAH¹, ALEXANDER WEBER-BARGIONI², STEFANO CABRINI², DIETER P. KERN¹, and MONIKA FLEISHER¹ — ¹Institute for Applied Physics, Eberhard Karls University Tübingen, Auf der Morgenstelle 10, 72076 Tübingen, Germany — ²Molecular Foundry, Lawrence Berkeley National Laboratory, 1 Cyclotron Road, Berkeley, California 94720, United States

Gold nanostructures have fascinating plasmonic properties. Hence, they are promising for a vast field of cutting edge nanophotonics technology. Our special interest is focused on developing near-field scanning optical microscopy (NSOM) probes by combining scanning probes with gold nanostructures. NSOM probes with plasmonic nanocones are expected to enable simultaneously ultrahigh resolution spectroscopy and topography measurements [1]. This is possible since the nanocone has an outstanding shape which can restrict the localized surface plasmon to subwavelength dimensions. Here, we report the fabrication of gold nanocones on top of both atomic force microscope (AFM) cantilevers and optical fibre tips. The fabrication method depends mainly on focused ion beam, electron beam induced deposition, and ion milling techniques. This method provides precise control over size and shape of the gold nanocones, and accordingly their plasmonic properties. Their optical properties were investigated by means of dark field spectroscopy, and their morphology was studied using AFM and scanning electron microscopy. Results of both fabrication and characterization will be shown. [1] M. Fleischer et al., ACS Nano 5, 2570 (2011).

O 58.57 Wed 18:15 Poster B1

Enhanced heat transfer by nanoscale NaCl-Islands on Au(111) observed by Near-field Scanning Thermal Microscopy (NSThM) — ●LUDWIG WORBES, DAVID HELLMANN, KONSTANTIN KLOPPSTECH, NILS KÖNNE, and ACHIM KITTEL — EHF, Faculty V, Department of Physics, C. v. O. University of Oldenburg, 26129 Oldenburg, Germany

Due to the advance in nanoscience heat transport at small length scales is receiving more attention as a field of fundamental research as well as one influencing future technologies. The Near-field Scanning Thermal Microscope (NSThM) is a tool to investigate heat transport on the nanoscale [1]. It is based on a UHV-STM, featuring a tunneling probe with an integrated miniaturized thermocouple temperature sensor. Therefore, we can measure the temperature change of the tip due

to heat flux between a heated or cooled sample and the probe in the range of distances between (tunnel-) contact and a few nanometers with high spatial resolution.

In this poster we present measurements of the heat-flow above one monolayer thick islands of NaCl prepared by physical vapor deposition on top of Au(111). We observe a distinct enhancement due to the NaCl-layer. For future applications such measurements are important for designing the heat flow management of nanoscaled devices. Such measurements may also trigger new theoretical approaches, because they show a distinct effect at length scales below the ones described by the established macroscopic theories.

[1] Uli F. Wischnath et al., *Rev. Sci. Instrum.* 79, 073708 (2008)

O 58.58 Wed 18:15 Poster B1

Measurements of elastic properties of surfaces with nanometer resolution — ●MARINA SARMANOVA, ERIK THELANDER, ALEXANDER MALWIN JAKOB, JÜRGEN W. GERLACH, STEFAN G. MAYR, and BERND RAUSCHENBACH — Leibniz-Institut für Oberflächenmodifizierung e. V., Permoserstr. 15, D-04318 Leipzig

Quantitative and qualitative measurements of local mechanical properties on nano and ultra-fine scale are useful for both fundamental research of physical properties of the surface and quality control of modern nano-scale devices. The experimental arrangement of mechanical measurements with nanometer resolution is demonstrated. Measurements of Young's modulus of surfaces could be performed with high resolution by means of contact resonance force microscopy (CR-FM) [1]. It is shown that CR-FM technique is suitable for measurements of materials with Young's modulus in a wide range. The local elastic properties of Ge₂Sb₂Te₅, a phase change material well known for its data storage application based on the well-pronounced difference of optical and electrical properties between amorphous and crystalline phases, were investigated. GaN, a semiconductor with wide band-gap, famous for production of high-efficiency diodes and lasers, yields high values of local Young's modulus. This project is funded by Leibniz Association. [1] Rabe U., Arnold W., *Appl. Phys. Lett.* Vol.64, P1493-1495 (1994)

O 58.59 Wed 18:15 Poster B1

Time of Flight X-Ray Photoelectron Spectroscopy — ●STEPHAN HANNIG¹, ULF BERGES^{1,2}, and CARSTEN WESTPHAL^{1,2} — ¹E1-TU Dortmund, Otto-Hahn-Straße 4, D-44227, Germany — ²DELTA-TU Dortmund, Maria-Goeppert-Mayer-Straße 2, D-44227, Germany

X-ray Photoelectron Spectroscopy (PES) reveals the electronic structure of surfaces by detecting the energy distribution of short mean-free path photo-emitted electrons. Conventional setups consist of a channeltron-detector attached to a concentric hemispherical analyzer. A disadvantage of this technique is the limited lifetime of the electron multiplier inside the detector. In addition to that, measurements are rather time-consuming if large angle scans have to be performed as in photoelectron diffraction experiments. Here we present the first tests of the applicability of a delay-line detector at the synchrotron DELTA and its performance. In the next step the setup will be compared to the existing conventional detector described above.

O 58.60 Wed 18:15 Poster B1

Fully Controlled, High Flux Electrospray Ion Beam Deposition of Nonvolatile Molecules in Vacuum — ●STEPHAN RAUSCHENBACH¹, GORDON RINKE¹, MATTHIAS PAULY¹, and KLAUS KERN^{1,2} — ¹Max-Planck-Institute for Solid State Research, Stuttgart, Germany — ²Institut Physique de Matière Condensée, École Polytechnique Fédérale de Lausanne, Switzerland

The inherent chemical purity and the ability to control the growth make vapor deposition in vacuum an extremely successful technology with applications from food packaging to semiconductor devices. Large functional molecules of either natural or synthetic origin, however, tend to be thermally labile, which hinders the conventional vacuum processing by evaporation. Alternative approaches to evaporation often do not reach the performance of vapor deposition in vacuum terms of purity, control, versatility, or deposition rate.

We developed electrospray ion beam deposition (ES-IBD) as a method for the vacuum deposition of non-volatile molecules. ES-IBD is based on electrospray ionization, a soft ambient ionization method, creating intact molecular gas phase ions of even fragile molecules. The deposition apparatus is differentially pumped and contains ion optics in each stage, conveying the ion beam to the target in UHV, as well as current detectors and mass spectrometers, together providing full

control over the deposition process. In addition our newly designed, hydrodynamically optimized electrospray ion source provides high flux and high efficiency, which demonstrates the potential of ES-IBD for commercial applications.

O 58.61 Wed 18:15 Poster B1

Fast XPS - monitoring surface reactions in the microsecond regime — ●OLIVER HÖFERT, MAX AMENDE, STEFAN SCHERNICH, CHRISTOPH GLEICHWEIT, CHRISTIAN PAPP, and HANS-PETER STEINRÜCK — Lehrstuhl für Physikalische Chemie II, Universität Erlangen-Nürnberg, Egerlandstr. 3, 91058 Erlangen

High temperatures and low coverages are hard to handle in reaction studies under surface science conditions and the respective analytical methods, due to the short characteristic reactions timescales. In this study, we show that by improving the time resolution of photoelectron spectroscopy, we can follow surface reactions at high temperatures in the microsecond regime. This is realized by recording the signal at selected (and characteristic) binding energies as function of time. By using a periodic dosing procedure and subsequent adding up of the resulting data sufficient signal to noise ratio is obtained. Further improvements towards an even better time resolution are envisioned. As a first test case the adsorption and desorption of CO on Pt(111) was studied at temperatures between 460 K and 500 K with a time resolution of 500 μ s. The experiments have been performed at the synchrotron facility BESSY II.

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

O 58.62 Wed 18:15 Poster B1

Characterization of an Effusive High Flux Metal Source — HAN ZHOU, BENEDIKT KLEIN, HANS-JÖRG DRESCHER, and ●J.MICHAEL GOTTFRIED — Philipps-Universität, Marburg

The here presented pulsed molecular / atomic beam source and signal detector are designed for Nanojoule Adsorption Calorimetry (NAC), which is a technique especially suitable for the characterization of non-reversible molecular or atomic adsorption enthalpies on well defined substrates in ultrahigh vacuum. Similar to previous adsorption calorimeters by Černý, King and Campbell, NAC relies on the direct measurement of microscopic temperature changes induced by incremental adsorption utilizing pyroelectric detectors. NAC requires long-term stable fluxes at high evaporation rates leading to special requirements on the deposition source, e.g. high volume and constant evaporation temperature established by specially designed evaporator with relatively higher capability of heat generation and proportional-integral-derivative controlling which enables sensitive and non-linear evaporator self-administration. Inspired by the investigations on interfaces between low work-function metals and semi-conducting organic molecules, we here present the characterization of the evaporator regarding the most important parameters as well as the performance of additional pulse-defining devices using Magnesium as adsorbate. In addition the degrading, i.e. the loss of sensitivity, of the pyroelectric detectors due to thermal exposure during bake-outs and the effect of corresponding compensation techniques, i.e. electrical inducement during thermal treatment, were systematically studied.

O 58.63 Wed 18:15 Poster B1

Characterization of an Effusive High Flux Metal Source and of Pyroelectric Detectors for Nanojoule Adsorption Calorimetry — ●HAN ZHOU, BENEDIKT KLEIN, HANS-JÖRG DRESCHER, and J. MICHAEL GOTTFRIED — Fachbereich Chemie, Physikalische Chemie, Philipps-Universität Marburg, 35032 Marburg, Hans-Meerwein-Str.

The here presented pulsed molecular / atomic beam source and signal detector are designed for Nanojoule Adsorption Calorimetry (NAC), which is a technique especially suitable for the measurement of non-reversible molecular or atomic adsorption enthalpies on well defined substrates in ultrahigh vacuum. Similar to previous adsorption calorimeters by Černý, King and Campbell, NAC utilizes pyroelectric detectors for the direct measurement of temperature changes in the μ K range induced by incremental adsorption. NAC requires long-term stable fluxes at high evaporation rates leading to special requirements on the deposition source, e.g., high volume and constant evaporation temperature established by proportional-integral-derivative controlling. Motivated by the general interest in interfaces between low work-function metals and semi-conducting organic molecules, we here present the characterization of the evaporator regarding the most important parameters as well as the performance of additional pulse-

defining devices using Magnesium as an adsorbate. In addition, the sensitivity of the pyroelectric detectors and its dependence on thermal stress and other factors are systematically studied.

O 58.64 Wed 18:15 Poster B1

Surface segregation of FePt investigated by STM, XPS and PAES — ●SAMANTHA ZIMNIK¹, CHRISTOPH HUGENSCHMIDT^{1,2}, and FLORIAN LIPPERT¹ — ¹TU München, Lehrstuhl E21, James-Franck Straße, 85748 Garching — ²ZWE FRM-II, Lichtenbergstr. 1, 85747 Garching

Segregation processes are of high importance for the understanding of the macroscopic properties of thin films or nano particles such as the magnetization in the system FePt. Positron annihilation induced Auger Electron Spectroscopy (PAES) is a powerful technique to gather information about the elemental composition of only the top-most atomic layer of a sample. Time dependent PAES allows the observation of the segregation process in-situ. The results are compared with X-ray induced Photoelectron Spectra (XPS). The Scanning Tunneling Microscope (STM) is used as a complementary method to investigate the electron density with atomic resolution of the same sample before and after the segregation process. PAES, XPS and STM allow the characterization of both, the elemental composition and the surface topology. The new experimental setup at NEPOMUC at the FRMII in Munich enables the preparation as well as the characterization of the sample using PAES, XPS and STM. Financial support within the project no. 05KI0WOB by the BMBF is gratefully acknowledged.

O 58.65 Wed 18:15 Poster B1

Combining High-Resolution Scanning Probe Studies with Reactivity Experiments — ●HENDRIK RONNEBURG, STEFANIE STUCKENHOLZ, CHRISTIN BÜCHNER, GERO THIELSCH, MARKUS HEYDE, and HANS-JOACHIM FREUND — Fritz-Haber-Institut der Max-Planck-Gesellschaft, Faradayweg 4-6, 14195 Berlin, Germany

In our group we use noncontact atomic force microscopy (nc-AFM) and scanning tunneling microscopy (STM) for the analysis of metal supported thin oxide films. This custom built instrumentation gives us the opportunity to gain a deeper understanding of oxide surfaces at the atomic level, e.g. MgO [1].

These scanning probe measurements should ideally be accompanied by reactivity studies. Therefore, we are setting up a new temperature programmed desorption (TPD) experiment.

In this setup the adsorption of CO on MgO surfaces will be studied. This reaction serves as a model for the interaction of CO with an ionic surface [2, 3].

Plans for the integration of a low temperature TPD setup with the existing ultra high vacuum chamber will be presented.

- [1] T. König, *et al.*, Beilstein J. Nanotechnol. **2**, 1 (2011)
- [2] R. Wichtendahl, *et al.*, Phys. Status Solidi A **173**, 93 (1999)
- [3] M. Sterrer, *et al.*, Surf. Sci. **596**, 222 (2005)

O 58.66 Wed 18:15 Poster B1

Helium Ion Microscopy as tool to investigate thin layer thicknesses — ●HENNING VIEKER, KARSTEN ROTT, UDO WERNER, ANDRÉ BEYER, GÜNTER REISS, and ARMIN GÖLZHÄUSER — Bielefeld University, Faculty of Physics, Germany

The recently developed helium-ion microscope allows remarkable surface resolution with the secondary-electron (SE) detector. Simultaneously, backscattered ions can be detected that allow imaging with a substantially higher elemental contrast. This Rutherford backscattered ion (RBI) contrast depends mainly on the elemental composition of the investigated sample surface. The escape depth of backscattered ions is much larger than for secondary electrons. Thus whole layers with a wide range of thicknesses will contribute to a RBI image, whereas the SE image is far more surface sensitive, i.e. insensitive to buried parts under the sample surface.

In this contribution we examine RBI imaging as tool to characterize thickness variations of layered samples with well defined compositions. In a model example the homogeneity of gold layers on silicon substrates is investigated and compared to simulation data. Achievable spatial resolutions as well as the possibilities in using a reference sample to measure layer thicknesses will be addressed. Furthermore, buried layers are investigated.

O 58.67 Wed 18:15 Poster B1

Angular and Energy Resolved Measurement of Reemitted Positrons from W, Pt and Ni Single Crystals —

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Monoenergetic positron beams are applied for a variety of non-destructive experiments in surface- and solid state physics. In order to create monoenergetic positrons, so called (re-)moderating materials with negative positron work functions are used, such as W, Pt and Ni. After thermalisation and diffusion to the surface, moderated positrons leave the solid with an energy according to the absolute value of the positron work function. In this work the angular distribution of reemitted positrons from W(100), W(110), Pt(100), Pt(110), Ni(100) and Ni(110) is being measured. In addition, low-temperature measurements are performed to study the thermal spread. Financial support within the project no. 05KI0WOB by the BMBF is gratefully acknowledged.

O 58.68 Wed 18:15 Poster B1

Effects of electron-phonon coupling on excitation spectra — ●HONGHUI SHANG, CHRISTIAN CARBOGNO, PATRICK RINKE, and MATTHIAS SCHEFFLER — Fritz-Haber-Institut der MPG, Berlin

The electron-phonon interaction plays a crucial role in many areas of physics. The main purpose of our study is to investigate the effect of the electron-phonon coupling on the excitation spectra of (organic) molecules and solids. For example, the phonon induced renormalization of electronic excitations can be as large as a few tenths of an eV for diamond and similar magnitudes are expected for other materials such as SiC, GaN, ZnO. To incorporate electron-phonon effects from first principles we employ a Green function/self-energy framework. Here we present an implementation for the electron-phonon coupling matrix elements in the all-electron Fritz Haber Institut *ab initio* molecular simulations (FHI-aims) package [1]. For the calculations of the first-order density response, both the coupled-perturbed self-consistent field method and density functional perturbation theory have been implemented. By comparing with the results from finite differences, the accuracy of the first-order response in the Hamiltonian and the density is demonstrated for both methods. With the first-order density response, the electron-phonon coupling matrix elements are then calculated using numeric atom-centered orbital (NAO) basis sets. Due to the spatial locality of the NAO basis set, we anticipate our approach to be applicable to large systems up to hundreds of atoms.

[1] <https://aimsclub.fhi-berlin.mpg.de/>

O 58.69 Wed 18:15 Poster B1

Monte Carlo simulations of growth processes on prepatterned surfaces — ●OLEG BULLER and ANDREAS HEUER — Institut für Physikalische Chemie, Westfälische Wilhelms-Universität Münster

The creation of desired structures after molecule deposition processes on prepatterned surfaces by using self-organization is a developing technique. Experiments with deposited organic molecules on prepatterned geometries display a multitude of different growth mechanisms. Here we use lattice Monte Carlo simulations to study the growth behavior in dependence of the interaction strength, the initial properties of the prepatterned surface as well as the chosen flux. It turns out that in particular the chosen interaction strength is of crucial importance for the characterization of the resulting structure.

O 58.70 Wed 18:15 Poster B1

Evaporation of nanosized droplets on heated substrates — ●JIANGUO ZHANG, FREDERIC LEORY, and FLORIAN MÜLLER-PLATHE — Theoretical Physical Chemistry, Technische Universität Darmstadt, Germany

The evaporation of nanometer scale droplets (about 10 nm in diameter) on flat heated substrates has been studied. The systems were modeled by means of Lennard-Jones potentials. The interaction between the liquid and the substrate atoms was varied to reproduce a range of equilibrium contact angles from 120 to 60 degrees. The evaporation process in a closed fixed volume was followed in terms of time variations of the contact angle. It was observed that the contact angle is a monotonic decreasing function of time. However, for large equilibrium contact angles (weak solid-liquid interactions), the respective time decays are characterized by larger characteristic times than for small contact angles (strong solid-liquid interactions). The evaporation has also been characterized with spatial resolution. It was observed that the evaporation process preferentially occurs in the vicinity the three-

phase contact line in the case of weak solid-liquid interactions. This observation is more contrasted in the case of the strongest solid-liquid interactions.

O 58.71 Wed 18:15 Poster B1

Representation of the 42-dimensional DFT Potential-Energy Surface of R,R-Tartaric Acid by Neural Networks — ●SINJA KLEES and JÖRG BEHLER — Lehrstuhl für Theoretische Chemie, Ruhr-Universität Bochum, D-44780 Bochum, Germany

The development of accurate interatomic potentials is a prerequisite to study complex systems, but often several physical approximations are indispensable to reduce the computational costs. Neural Networks (NNs) are a class of flexible mathematical functions, which allow to construct accurate interatomic potentials for systems with an arbitrary number of atoms without the introduction of any constraints on the functional form. Instead, a systematic construction of the potential-energy surface (PES) is carried out by interpolation of energies and forces obtained from first-principles reference calculations. To date, most NN PESs refer to inorganic solids and molecules up to six atom. We use R,R-Tartaric Acid to demonstrate that the method is equally applicable to organic molecules. We show that the PESs obtained from DFT reference calculations and NN interpolation are in a very good agreement.

O 58.72 Wed 18:15 Poster B1

Kondo effects in inelastic spin transitions — ●RICHARD KORYTÁR¹, NICOLÁS LORENTE², and JEAN-PIERRE GAUYACQ³ — ¹Institut für Nanotechnologie, Karlsruher Institut für Technologie, Germany — ²Centro de investigación en nanociencia y nanotecnología CIN2, Barcelona, Spain — ³Institut de Sciences Moléculaires d'Orsay, Unité Mixte CNRS-Université, Orsay, France

Electron currents can induce magnetic excitations in molecular nanostructures. Magnetic inelastic electron tunneling spectroscopy (IETS) shows sharp increases in conductance when a magnetic excitation is induced by the incident electron. A previous one-electron theory successfully explained both the conductance thresholds and the magnitude of the conductance variation. The elastic spin flip of conduction electrons by a magnetic impurity leads to the well known Kondo effect. In the present work, we compare the theoretical predictions for inelastic magnetic tunneling obtained with a one-electron approach and with a many-body theory including Kondo-like phenomena. We apply our theories to a singlet-triplet transition model system that contains most of the characteristics revealed in magnetic IETS. We use two self-consistent treatments (non-crossing approximation and self-consistent ladder approximation). One of the main findings is that many-body effects translate into sharp peaks that appear close to the inelastic thresholds; the peaks being more robust than the Kondo resonance. Another consequence of the interaction with underlying electron gas is the reduction of the inelastic gap. This may render more difficult the extraction of magnetic anisotropy features for IETS experiments.

O 58.73 Wed 18:15 Poster B1

Electronic transport in carbon nanotubes: the role of water and long-range electrostatics — ●ROBERT A. BELL¹, ARASH MOSTOFI², and MIKE PAYNE¹ — ¹TCM Group, Cavendish Laboratory, University of Cambridge, UK — ²Dept. of Materials & the Thomas Young Centre for Theory and Simulation of Materials, Imperial College London, UK

Understanding interactions between carbon nanotubes and environmental adsorbants is vital for the use of nanotube devices under ambient conditions. Previous theoretical studies have concluded water n-dopes the nanotube, providing a mechanism to increase conductivity.

In this work, we show that the use of short nanotube supercells in these calculations is inappropriate in the presence of long-range electrostatic interactions. Using large-scale DFT calculations with ONETEP, we study long (>60 Å) nanotube segments, and conclude that negligible charge is transferred between the water and the nanotube. Weak long-range charge-redistribution in the nanotube is observed, however, which is explained using a simple classical electrostatic model for the polarisation of the nanotube by the water dipole. Conclusions derived from local charge transfer methods such as Mulliken analyses are unable to capture this behaviour and are potentially misleading.

Electron transport calculations, using the Landauer-Büttiker approach, on large nanotube segments with many adsorbed water molecules show only weak scattering at the nanotube valence band edge. No evidence is observed to support an increase in conductivity.

O 58.74 Wed 18:15 Poster B1

HSE06 and G_0W_0 for Pyrite- and Marcasite-type compounds — ●TIMO SCHENA, PENGXIANG XU, MARTIN SCHLIPF, GUSTAV BIHLMAYER, MARKUS BETZINGER, CHRISTOPH FRIEDRICH, and STEFAN BLÜGEL — Peter Grünberg Institut and Institute for Advanced Simulation, Forschungszentrum Jülich & JARA, D-52425 Jülich, Germany

The accuracy of density functional theory (DFT) depends only on the choice of a suitable approximation for the *xc*-functional. The local *xc*-functionals LDA and PBE can result in a severe underestimation of band gaps in insulators and semiconductors. The prediction of the band gap is usually improved considerably by employing hybrid functionals (*e.g.* HSE06) or many-body-perturbation-theory (*e.g.* G_0W_0). Recently, these methods have been implemented in the Jülich-all-electron DFT code FLEUR [1,2]. However, in this work we present material systems, for which no considerable improvement of the band gaps is obtained in comparison to the experimental values. In opposite sometimes even a worsening is found. Amongst others, we present a detailed analysis of the electronic structure of Pyrite-like compounds FeS₂, RuS₂, OsS₂, NiP₂ and Marcasite-type compounds FeS₂, FeSe₂, FeTe₂ and CrCl₂. By detecting similarities and differences, we can draw some hypotheses of what is causing the shortcomings of HSE06 and G_0W_0 for these systems. We gratefully acknowledge funding from BMBF of the NADNum project 03SF0402A.

[1] www.judft.de, [2] C. Friedrich *et al.* JPCM 24 293201 (2012)

O 58.75 Wed 18:15 Poster B1

Representing Complex Potential Energy Surfaces by Artificial Neural Networks — ●CHRISTOPHER HANDLEY, TOBIAS MORAWIETZ, and JÖRG BEHLER — Lehrstuhl für Theoretische Chemie, Ruhr-Universität Bochum, D-44780 Bochum, Germany

Simulations of large systems using ab initio methods are computationally costly, and in many cases intractable. An alternative is approximate interatomic potentials. These potentials are typically constructed from computationally simple functions, chosen to be representative of particular atomic interactions. Fitting of these potentials is not straightforward, as many different selections of functions and their parameters are valid, with varying accuracy. Neural Networks (NNs) recently have been shown to provide interatomic potentials that are comparable to the accuracy of quantum mechanical calculations[1,2]. NNs are flexible enough to fit complex functions, interpolating, from quantum mechanical training data, accurate energies and forces. A major drawback of the method is the non-physical functional form of the NNs. Here, we present the first steps towards a more transferable NN based upon electronic structure methods.

[1] C. M. Handley and P. L. A. Poplier, J. Phys. Chem. A, 114, 3371-3383, (2010).

[2] J. Behler, PCCP, 13, 17901-18232 (2011).

O 58.76 Wed 18:15 Poster B1

Bandgap Engineering of Layered Perovskites for Single- and Two-Photon Water Splitting — ●IVANO CASTELLI, KRISTIAN THYGESEN, and KARSTEN JACOBSEN — Department of Physics, Technical University of Denmark, Kgs. Lyngby, Denmark

The conversion of solar light into electrons and holes and the subsequent use of their energy to create fuels like hydrogen is one of the possible ways to address the world's pressing energy supply and storage problem. The properties determining the usefulness of a material to be used as light harvester in a photochemical cell include a narrow band gap well positioned with respect to the redox potentials of water and chemical/structural stability.

We have recently screened for one- and two-photon water splitting materials[1,2] in the cubic perovskite structure. We have found 20 promising materials for one-photon water splitting and an additional 12 for the two-photon process. We have applied the screening procedure to the double perovskite oxides and we have extracted some rules to combine two materials for obtaining a bandgap in the desired region.

We currently investigate the layered perovskite structure, consisting of 2D slabs of cubic perovskite separated by some motif, with a general formula of $A_{n-1}B_nO_{3n+1}$. We focus on finding new combinations for one- and two-photon water splitting and on designing new rules to tune the bandgap by changing the interlayer motif.

References [1] I.E. Castelli, *et al.*, Energy Environ. Sci., 5, 5814 (2012). [2] I.E. Castelli, *et al.*, Energy Environ. Sci., 5, 9034 (2012).

O 58.77 Wed 18:15 Poster B1

Benchmarking G_0W_0 for small metal clusters using exact frequency treatment — ●FERDINAND KAPLAN¹, MICHIEL VAN SETTEN¹, and FERDINAND EVERS² — ¹Institute of Nanotechnology, Karlsruhe Institute of Technology, Germany — ²Institute of Theoretical Condensed Matter, Karlsruhe Institute of Technology, Germany

One of the most used approaches for the computational study of solids, nanoscale systems and molecules is the density functional theory (DFT). However, as is well known, DFT calculations of single particle excitation spectra, e.g. ionization potentials and electron affinities, often suffer from approximations in exchange correlations potentials. More importantly, even fundamental difficulties exist with the common practice to identify the Kohn-Sham particles of ground-state DFT with the genuine quasi-particles.

To systematically improve the estimation of quasi-particle energies for molecular system, we have implemented the so called GW method into a standard quantum chemistry package (G_0W_0 -level). The approach represents a perturbative expansion of the many-body Green's function with respect to the screened interaction, W .

Here, we present applications of the method to small metal cluster systems. First, we show that our implementation works well also in the metallic case where the HOMO-LUMO gap is relatively small, so that one might expect problems for standard perturbative results. Second, we find that deviations from experimental ionization potentials and electron affinities can be reduced against those of Kohn-Sham-DFT using PBE functionals.

O 58.78 Wed 18:15 Poster B1

Quasiparticle Spectra from Self-Consistent GW Calculations for Transition-Metal Monoxides — ●MERZUK KALTAK and GEORG KRESSE — University of Vienna, Computational Physics, Vienna, Austria

We present calculations for the transition-metal monoxides MnO, FeO, CoO and NiO within the framework of many-body perturbation theory, specifically using a self-consistent GW approximation with vertex corrections. Using a maximally localized Wannier projection, the band structure seems to be predicted reasonably well in the antiferromagnetic phase AFII at $T = 0$. The stacking of ferromagnetic planes in the [111] direction causes a reduction of the symmetry, which consequently leads to a splitting of the t_{2g} bands into a_g and energetically more favourable e_g states. We show that self-consistent GW quasiparticle band gaps are closer to experiment than previously published results obtained from conventional ab-initio methods using a nonlocal exchange-correlation functional with a subsequent not self-consistent G_0W_0 calculation. In addition to the electronic structure we investigate the optical properties of the compounds. To this end, the Bethe-Salpeter equation in the independent particle picture for the irreducible polarizability is solved and the optical spectrum is calculated.

O 58.79 Wed 18:15 Poster B1

A self-consistent dynamical embedding — ●Wael CHIBANI, XINGUO REN, PATRICK RINKE, and MATTHIAS SCHEFFLER — Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, Germany

We present an embedding scheme that facilitates the treatment of the physically important part of a system with electronic structure methods, that are typically computationally too expensive for periodic systems, whereas the rest of the periodic system is treated with computationally less demanding approaches in a self-consistent manner. Our embedding scheme is based on Green functions within the concept of dynamical mean-field theory (DMFT) [1] and allows the embedded region to exchange particles with its environment, a feature that distinguishes the current approach from conventional embedding schemes. In contrast with the original DMFT formulation for correlated model Hamiltonians, we consider here the unit cell as embedded cluster in an *ab initio* way, that includes all electronic degrees of freedoms. We implemented our scheme in the all-electron code FHI-aims [2]. To demonstrate the performance of the scheme we first stay within density functional theory and treat the embedded region with hybrid functionals and the environment with generalized gradient approximations, although in principle any Green functions method can be used. Preliminary tests for simple solids show that the total energy and the density of states converge well with respect to the computational parameters. The convergence with respect to the cluster size will also be addressed. [1] A. Georges *et al.*, Rev. Mod. Phys. **68**, 14 (2006). [2] V. Blum *et al.*, Comp. Phys. Comm. **180**, 2175 (2009).

O 58.80 Wed 18:15 Poster B1

Thermal transport in Graphite and related materials from

general third order density functional perturbation theory. — ●LORENZO PAULATTO, MICHELE LAZZERI, FRANCESCO MAURI, and GIORGIA FUGALLO — IMPMC - UPMC/CNRS, Paris, France

We use a novel generic implementation of the third order anharmonic density-functional perturbation theory to study the phonon-phonon interaction in monolayer and bilayer graphene and in bulk graphite. We describe the anharmonic effects in terms of widening of the phonon linewidth and as a phonon mean free path in the medium. We discuss the temperature and q-point dependency of the linewidth.

We estimate the phonon-driven thermal transport in the single-mode relaxation time approximation, for room temperature and higher, and compare it to graphene and pyrolytic graphite experiments.

O 58.81 Wed 18:15 Poster B1

Electrochromic coatings based on an electron-conducting vapour-deposited organic semiconductor — ●JULIANE WEISSBECKER and DERCK SCHLETTWEIN — Institute of Applied Physics, Justus Liebig University of Giessen, Heinrich Buff-Ring 16, 35392 Giessen, Germany

Thin films of phthalocyanine molecules are interesting for applications as electrochromic layers because of their strong light absorption and the strong change of colour upon oxidation or reduction. Because of instable cycling during oxidation, molecules are sought that are easily reduced (high electron affinity). The redox behaviour of vapour-deposited thin films (50 nm) of $F_{16}PcCu$ was studied using simultaneous cyclic voltammetry and UV/Vis-spectroscopy. Upon electrochromic charging of the films electroneutrality has to be preserved by intercalating ions. The measurements were performed in contact to different electrolyte solutions and the influence of K^+ , Na^+ or Li^+ ions is discussed. During an initial conditioning cycle a decrease of the crystallinity of the thin films was found and correlated with the ion diameter. An influence of ion diffusion on the overall current was not found. Almost constant potentials independent of the electrolyte were seen for the first reduction but differences were observed in subsequent waves. These differences are again correlated to the ion diameter and, hence, the interaction potential with the reduced molecules in the films.

O 58.82 Wed 18:15 Poster B1

Impedance Spectroscopy performed to measure and modify the oxide thickness on aluminum wires in an aqueous solution — ●FELIX FIEHLER and DERCK SCHLETTWEIN — Institute of Applied Physics, Justus-Liebig-University Giessen, Germany

Metal wires are of interest as electrode materials in different applications also, e.g., in solar cells like dye-sensitized solar cells (DSC). Electron back transfer from the metal collector electrode to the iodine electrolyte or, even worse, corrosion of the metal can be a major problem. Some metals (including aluminum) are covered with a thin oxide layer, which is formed in contact with air providing a thin tunneling barrier, protecting the electrode from further corrosion by the electrolyte. This oxide layer, however, also can present a barrier in the electrodeposition of an active semiconductor and, in the DSC, an injection barrier for charge injection from the semiconductor to the metal. The thickness of the oxide therefore has to be controlled in detail for a successful application of aluminum wires in DSC. It is well known that electrochemical impedance spectroscopy (EIS) offers such a possibility to determine the thickness of the passivating oxide layer in situ during different applied potentials. The latter are of interest since the oxide thickness can be tuned by applying different positive or negative potentials relative to the standard electrode potential. Impedance spectra were measured for planar sheets and for wires of aluminum under variation of the applied DC potentials. The experimental results in the different potential ranges were discussed by use of established equivalent circuits.

O 58.83 Wed 18:15 Poster B1

III-V semiconductors for photoelectrolysis and their interface to the electrolyte — ●MATTHIAS M. MAY^{1,2}, WOLF-DIETRICH ZABKA^{1,2}, OLIVER SUPPLIE^{1,2}, HELENA STANGE^{1,2}, CHRISTIAN HÖHN¹, HANS-JOACHIM LEWERENZ^{1,3}, and THOMAS HANNAPPEL^{1,4,5} — ¹Helmholtz-Zentrum Berlin, Institute of Solar Fuels — ²Humboldt-Universität zu Berlin, Institut für Physik — ³California Institute of Technology, Pasadena, USA — ⁴TU Ilmenau, Institut für Physik, Fachgebiet Photovoltaik — ⁵CiS Forschungsinstitut für Mikrosensorik und Photovoltaik, Erfurt

III-V semiconductors such as the dilute nitride GaP(N) represent an

interesting material class for photoelectrolysis, especially in multi-junction approaches [1]. Corrosion and the charge-transfer efficiency towards the electrolyte [2] are challenges that have to be addressed by growth and/or electrochemical processing of the semiconductor surfaces. We prepare GaP(N) by metalorganic vapour phase epitaxy under in situ control with reflection anisotropy spectroscopy (RAS). Applying RAS and photoelectron spectroscopy at the semiconductor-liquid interface, we aim to improve the microscopic insight into the interface and to achieve in situ control of electrochemical processing. To this end, we perform H₂O adsorption in UHV as model-experiments, which we compare with results for the electrochemical environment.

[1] Döscher et al., *ChemPhysChem* **13**:2899 (2012). [2] Kaiser et al., *ChemPhysChem* **13**:3053 (2012).

O 58.84 Wed 18:15 Poster B1

Scanning tunneling microscopy (STM) studies on the self-assembly of a twin monomer at the liquid-solid interface controlled by sonication time. A first step to the study of twin polymerization — NGUYEN DOAN CHAU YEN¹, •NGUYEN THI NGOC HA¹, PATRICK KEMPE², STEFAN SPANGE², and MICHAEL HIETSCHOLD¹ — ¹Institute of Physics, Solid Surfaces Analysis Group, Chemnitz University of Technology, D-09107 Chemnitz, Germany — ²Institute of Chemistry, Polymer Chemistry Group, Chemnitz University of Technology, D-09111 Chemnitz, Germany

Twin polymerization has been used as an elegant method for synthesizing nanostructured hybrid materials. Twin polymerization is a polymerization process which creates two different polymers out of a so-called twin monomer. The polymerization of a monomer 2,2*-spirobi[4H-132-benzodioxasilin](SBS) is initiated by cleavage of the Si-O-C bonds. Here self-assembly of this SBS at the undecanol/HOPG interface is investigated by STM. It reveals a co-adsorption of SBS and undecanol solvent molecules in a regular pattern at ambient conditions. The non-planar twin monomer can be clearly identified in the linear pattern with undecanol molecules oriented with their zig-zag plane orthogonally to the HOPG surface. Sonication has been proven to be a simple and powerful method to control the polymorphism of molecular adsorbates out of a solution. It is demonstrated that by sonicating SBS/undecanol solutions with different sonication time the co-adsorption of SBS and undecanol on HOPG can be controlled.

O 58.85 Wed 18:15 Poster B1

Influence of electrochemical adsorption on the conductive properties of thin platinum films in sulfuric acid — •DAMIAN BÜRSTEL and DETLEF DIESING — Universität Duisburg - Essen, Fakultät für Chemie, Universitätsstrasse 2, D - 45141 Essen, Germany

The electrochemical hydrogen and oxygen reactions on platinum surfaces in acidic solution are still of great interest for electrocatalytic as well as for energy conversion research. In modern applications platinum is used in form of a few tens of nanometer thick metal films or as nanoparticles. At these dimensions one must be aware of the conductive properties of the metal film and particle and the influence of the changing metal-electrolyte interface on these properties during the electrochemical reactions.

The conductance of a thin platinum film on glass was measured by DC methods as well as AC methods at different frequencies simultaneously to cyclic voltammetric experiments in 0.5 M sulfuric acid. For the oxidation region the film conductance is mainly affected by the volumetric oxidation and reduction of the film and less affected by the

metal-liquid interface properties. At hydrogen free platinum surfaces in the oxidation as well as in the electrochemical double-layer region a considerably high phase shift of the conductance with respect to the driving voltage across the film exists in AC measurements. In the course of hydrogen adsorption at $E_{\text{HESS}} < 0.4 \text{ V}$ a conduction parallel to the metal-liquid interface sets in with a low phase shift.

O 58.86 Wed 18:15 Poster B1

Investigation of spin-polarized transmission for electrons through Co/diamond/Co junctions — •FELIX HUERKAMP, PETER KRÜGER, and JOHANNES POLLMANN — Institut für Festkörpertherorie, Universität Münster, Germany

We investigate the transmission properties of spin-polarized electrons at the interfaces of the metal-semiconductor hybrid system cobalt/diamond/cobalt within density-functional theory employing the generalized gradient approximation. The considered open system consists of three parts: the left and right semi-infinite cobalt leads, as well as the scattering region build by N layers of carbon atoms in a diamond structure. We use a Greens function technique which is based on the representation of the wave functions by Gaussian orbitals. This enables us to treat the scattering problem as a localized perturbation of a Co crystal. We have investigated junctions of hexagonal Co with C layers grown in (111) direction, as well as junctions of fcc Co with C layers oriented in (001) direction. We have identified different mechanisms, such as transmission resonances and overlapping interface states, that cause for specific energies and wave vectors a high transmission through the diamond layers. On the other hand, we find a vanishing transmission for energies within the Co bands and the diamond band gap at particular wave vectors even for thin C barriers. The results are discussed in dependence on the spin-direction and the number of carbon interlayers for hcp, as well as fcc Co leads.

O 58.87 Wed 18:15 Poster B1

Pulsed spray evaporation CVD of metal thin films: Role of reactor and precursor conditions — •FEDOR STRIGUNOV, VOLKMAR ZIELASEK, and MARCUS BÄUMER — Universität Bremen, Institut für Angewandte und Physikalische Chemie, Leobener Str. NW2, 28359 Bremen, Deutschland

A widely employed method to deposit thin films of metals and their compounds is chemical vapor deposition (CVD). A recently developed hydrogen-free approach to metal-CVD uses pulsed spray evaporation (PSE) delivery of simple and commercially available non-toxic metal-organic precursors dissolved in alcohols [1] and ease of use.

We have designed a compact PSE-CVD reactor that is attached to a UHV system for direct transfer to thin film analysis techniques such as XPS, STM, LEED or IR spectroscopy. We will present demonstrate the growth of thin Ni films on various substrates, including silicon oxide, without incubation time and without the need for any metallic seed layer. The efficiency of growth process and the quality of the resulting film strongly depend on several deposition parameters such as concentration of the precursors, deposition pressure, carrier gas flow rate, substrate temperature, deposition duration, spray pulse frequency and pulse width which have to be optimized for each new material and selected precursor. Besides the substrate temperature we have identified the concentration of water in the alcohol-carrier of precursor as very critical for the growth rate and deposition mechanism.

[1] P. A. Premkumar et al., *Chem. Vap. Deposition*, **13** (2007) 219