

O 59: Poster Session III (Nanotribology; Polymeric biomolecular films; Organic electronics and photovoltaics, Covalent networks on surfaces; Phase transitions; Particles and clusters; Transparent conductive oxides)

Time: Wednesday 17:30–21:00

Location: P3

O 59.1 Wed 17:30 P3

Nanoscale hotspot formation in an energetic material during friction — ALEXANDER KOVALEV and HEINZ STURM — BAM - Federal Inst. Mat. Res. Testing, FG "Scanning Probe Microscopy, Tribology and Wear Protection", 12200 Berlin

The chemical-mechanical decomposition of energetic materials is not fully understood, and the initial decomposition steps are not firmly established yet. The nanoscale formation of the hot-spot on 2,4,6-trinitrophenol (TNP) single crystal has been studied using atomic force microscopy (AFM). Indentation and plowing AFM techniques were used for destructive modification of TNP crystal surface. Micro-crystals of TNP were grown on a gold substrate by fast evaporation from aqueous saturated solution. During friction we observed features of TNP crystal at the nanoscale which are difficult to explain from the macroscopic point of view of explosion. Occasionally, the hotspot has occurred spontaneously during the scanning process. According to the accepted knowledge of chemical reaction/decomposition of energetic materials the main decomposed substances are gases CO₂ and NO₂. But, in our experiments, agglomerated solid particles have been occurred on a surface of TNP crystal. It is known that TNP has two polymorph structures. Additionally, partially decomposed TNP may have still a phenyl ring, so pi-pi-complexes may be formed. However, we observed that friction at the nanoscale does not stimulate spontaneous decomposition. The observed behaviours of energetic materials at the nanoscale need further elucidation.

O 59.2 Wed 17:30 P3

Transition from Static to Kinetic Friction of Nanoparticles — MICHAEL FELDMANN¹, DIRK DIETZEL¹, UDO D. SCHWARZ², and ANDRÉ SCHIRMEISEN¹ — ¹Institute of Physics and Center for Nanotechnology, University of Münster, Germany — ²Department of Mechanical Engineering, Yale University, New Haven, USA

On macroscopic scales a phenomenological difference between static and sliding friction forces is routinely observed for contacts between solid surfaces. But does this hold true for nanoscopic contacts as well? We investigated this fundamental question through manipulation of thermally evaporated antimony nanoparticles over atomically flat HOPG substrates with the tip of a friction force microscope (FFM) [1]. In contrast to direct measurements with the FFM tip the manipulation of nanoparticles has important advantages of providing very well defined contact areas as well as enabling the precise measurement of static friction. A novel approach to nanoparticle manipulation, called 'tip-on-top' technique, allowed us to vary the lateral forces exerted on individually chosen particles in very small increments. This was achieved by scanning the FFM tip on top of the particle while slowly increasing the applied normal force. The results clearly show a transition between frictional states, corresponding to static and sliding friction. Interestingly, we observe a hysteresis when switching from the static friction to the sliding friction regime and back. We found that the ratio between the static and kinetic friction forces for individual particles is 1/2 independent of their size, in agreement with theoretical predictions. [1] Dietzel et al., Appl. Phys. Lett. 95, 53104 (2009)

O 59.3 Wed 17:30 P3

Simulations of friction force microscopy on KBr(001) based on ab-initio forces — CHRISTINE WIEFERINK, PETER KRÜGER, and JOHANNES POLLMANN — Institut für Festkörpertheorie, WWU Münster

We report on ab-initio based simulations of friction force microscopy on the KBr(001) surface at zero and nonzero temperature. To simulate sliding friction we employ an extended three-dimensional Prandtl-Tomlinson model. The microscopic part of the tip is modeled by K⁺ and Br⁻ terminated tips. We use a tip-surface interaction potential, which is calculated within the local-density approximation of density-functional theory and supplemented by long-range van der Waals interaction resulting from the macroscopic part of the tip. The loading force acting on the tip enters the equation of motion separately from all other forces so that it can be changed at will. We find smaller sliding friction for the K⁺ compared to the Br⁻ tip. Especially we observe a

very low sliding friction for the K⁺ tip at loading forces up to 1.5 nN.

O 59.4 Wed 17:30 P3

Wear experiments on the nanoscale — JOHANNES SONDHAUS^{1,2} and ANDRÉ SCHIRMEISEN^{1,2} — ¹Institute of Physics, University of Münster, Münster, Germany — ²Center for Nanotechnology (CeN-Tech), University of Münster, Münster, Germany

The basic mechanisms of wear at the nanoscale are of large interest, e.g., for the lifetime limitations of moving mechanical components in MEMS. So far it was not possible to derive macroscopic wear behavior from fundamental processes on small scales. The atomic force microscope (AFM) has been recently proved useful to model a single sliding asperity in order to study wear processes on the atomic scale [1]. It was found that nanoscale wear is dominated by an atom-by-atom loss process which can be modeled by a thermally activated bond breaking process. In this work we performed several wear experiments using different Si-tips sliding for distances from a few hundreds of μm to about 2m on a silicon oxide surface. We varied the applied normal load and performed measurements under ambient conditions and in UHV. The change of the tip radius due to wear was determined from the adhesion force at different sliding distances. As a further channel we simultaneously measured the friction force acting between tip and sample. Our results seem to agree with the model, that frictional stresses lower the barrier for breaking an atomic bond and thus are jointly responsible for the observed characteristic wear rates at the nanoscale.

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

O 59.5 Wed 17:30 P3

Wear measurement by friction force and dynamic force microscopy — ÖZHAN ÜNVERDİ¹, TOBIAS MEIER¹, JAN-ERIK SCHMUTZ^{2,3}, and HENDRIK HÖLSCHER¹ — ¹Institute for Microstructure Technology (IMT), Karlsruhe Institute of Technology, P.O. box 3640, 76021 Karlsruhe, Germany — ²Center for Nanotechnology (CeNTech), Heisenbergstr. 11, 48149 Münster, Germany — ³Physikalisches Institut Westfälische Wilhelms Universität Münster, Wilhelm-Klemm-Str. 10, 48149 Münster, Germany

For measuring nano-scale wear, we introduce a new technique using friction force and dynamic force microscopy. As the cantilever resonance frequency depends on mass of the tip, we can measure the increase or decrease of the tip's worn mass down to some picograms due to the resonance frequency shift of the cantilever. By attaching a small sphere to the upper end of the cantilever's tip we can detect the nano-wear of several material combinations with this approach.

O 59.6 Wed 17:30 P3

Self-assembly of pyridine-substituted alkanethiols on gold — HICHAM HAMOUDI¹, KATRIN DÖRING², HEINRICH LANG², and MICHAEL ZHARNIKOV¹ — ¹Angewandte Physikalische Chemie, Universität Heidelberg, Im Neuenheimer Feld 253, 69120 Heidelberg, Germany — ²Lehrstuhl für Anorganische Chemie, Technische Universität Chemnitz, Straße der Nationen 62, 09111 Chemnitz, Germany

High-resolution X-ray photoelectron spectroscopy, near-edge X-ray absorption fine structure spectroscopy, and infrared reflection absorption spectroscopy were used to study the properties of SAMs of aminomethyl-di(2-pyridyl)-11-mercaptopundecanamide (C10AP1), 4-(aminomethyl)pyridine-11-mercaptopundecanamide (C10AP2), and 2-(aminomethyl)pyridine-11-mercaptopundecanamide (C10AP3) prepared on Au(111) substrates. Whereas all molecules formed well-defined SAMs, their structural and electronic properties were found to be noticeably different depending on (i) either ortho- or para-attachment of the terminal pyridine moiety to the molecular chain and (ii) the number of the pyridine units in the tail group. The highest order was found in the C10AP3 SAM where the alignment of the SAM constituents seemed to be additionally strengthened by intramolecular interaction. Further, the branching of the characteristic pre-edge absorption resonances in the C K-edge spectra of the SAMs is distinctly different for the cases of the ortho- or para-attachment of pyridine, which could be explained by the different coupling of the electronic and vibrational excitations in both cases.

O 59.7 Wed 17:30 P3

On the surface tension of ionic liquids — ●CLAUDIA KOLBECK¹, JULIA LEHMANN³, KEVIN R. J. LOVELOCK⁴, TILL CREMER¹, NATALIA PAAPE², PETER WASSERSCHIED², ANDREAS P. FRÖBA³, FLORIAN MAIER¹, and HANS-PETER STEINRÜCK¹ — ¹LS Physikalische Chemie II, FAU Erlangen, D — ²LS Chemische Reaktionstechnik, FAU Erlangen, D — ³SAOT, FAU Erlangen, D — ⁴School of Chemistry, University of Nottingham, UK

The interface between ionic liquids (ILs) and gases plays a vital role in many applications such as gas separation and heterogeneous catalysis. An understanding of the surface properties of ILs is thus essential for developing new and commercially favourable systems for industrial applications. To probe the influence of the cation and anion on the surface tension of ILs nine [Tf₂N]⁻-based and twelve [C₈C₁Im]⁺-based ILs were measured with the pendant drop method. When increasing the alkyl chain length in the [C_nC₁Im][Tf₂N] series (n = 1, 2, 4, 6, 8, 10, 12), an initial decrease in surface tension is observed whereas for alkyl chain lengths greater than n = 8 the surface tension reaches a plateau. Functionalizing the alkyl chains with ethylene glycol groups results in a higher surface tension. For the dependence of surface tension on the chemical nature of the anion, relations are only found for subgroups of the studied ILs. Surface tension values are discussed with respect to intermolecular interactions and surface composition as determined by angle resolved X-ray photoelectron spectroscopy. - Supported by the DFG through SPP 1191 and by the Cluster of Excellence - Engineering of Advanced Materials.

O 59.8 Wed 17:30 P3

Azobenzene thin film growth on surfaces of layered materials — ERIC LUDWIG¹, ●TORBEN JOHANNSEN¹, THOMAS STRUNSKUS², ALEXEI NEFEDOV³, CHRISTOF WÖLL³, LUTZ KIPP¹, and KAI ROSSNAGEL¹ — ¹Institut für Experimentelle und Angewandte Physik, Universität Kiel, D-24098 Kiel — ²Institut für Materialwissenschaft, Universität Kiel, D-24098 Kiel — ³Institut für Funktionelle Grenzflächen, Karlsruher Institut für Technologie, D-76344 Eggenstein-Leopoldshafen

NEXAFS and ultraviolet photoelectron spectroscopy have been used to determine the layer growth and structural properties of azobenzene adsorbed on layered compounds. We used metallic TiTe₂ and semiconducting HfS₂ as substrates to elucidate the influence of different electronic structures. Due to weak van der Waals-like coupling between the layers both materials serve as excellent substrates for the analysis of adsorbed photoswitches and their possible switching behavior. NEXAFS measurements were performed at BESSY (beamline HE-SGM). UPS measurements were done with a He gas-discharge lamp (hν = 21.22 eV) and a hemispherical photoelectron analyzer.

Results indicate different growth modes on semiconducting and metallic substrates. Partial reversible photoswitching of the multilayer system was observed on the semiconducting substrate. On the metallic substrate no switching was observed, presumably due to stronger adsorbate-substrate interactions. This work was supported by the DFG through SFB 677.

O 59.9 Wed 17:30 P3

Combined study of interface and device properties of a solid state dye sensitized solar cell — ●JULIA MAIBACH, RENÉ HOCK, THOMAS MAYER, and WOLFRAM JAEGERMANN — Technische Universität Darmstadt, Department of Material Science, Surface Science Division, Petersenstr. 32, 64287 Darmstadt

We present the combined photoelectron spectroscopic and photoelectric characterization of a solid state dye sensitized solar cell (SDSC). The aim of this study is the development of a model system that allows a direct correlation of PES determined interface properties to global IV-measurements of the complete optoelectronic device.

The samples consist of a nanoporous TiO₂ layer on FTO, which was sensitized with a metal free organic dye developed by BASF. As a hole transport material spiro-OMeTAD doped with the organic salt Li-TFSI was used. Both the dye and the hole conductor were applied via drop coating at normal pressure under clean Ar atmosphere within a glass cell integrated to the UHV system. The TiO₂/dye and the TiO₂/dye/spiro-OMeTAD interfaces were characterized using synchrotron induced photoelectron spectroscopy (SXPS) at BESSY. From these measurements the band diagram of the energy converting interface is derived which shows that driving forces for the relevant charge transfer processes are given in the investigated TiO₂/dye/spiro-OMeTAD system. To perform the IV-measurements a gold contact was

sputtered on top of the hole conductor of the SXPS-sample. Despite the unusual preparation for a SDSC the resulting solar cell shows a photo current density of 0,72 mA/cm² under AM1,5 illumination.

O 59.10 Wed 17:30 P3

Multi-plasmon enhancement of thin film organic solar cells — ●ADAM WILLIAMSON¹, ERICH RUNGE¹, EADAON MCCLEAN², and DOMINIC ZERULLA² — ¹Institut für Physik and Institut für Mikro- und Nanotechnologien, Technische Universität Ilmenau, 98693 Ilmenau, Germany — ²University College Dublin, Belfield, Dublin 4, Ireland

A theoretical, two-dimensional (2D), periodic nano-structured design for thin film organic solar cells is presented. In this design the superposition of two periodic silver plasmonic gratings is seen to strongly increase the absorptive dissipation around two selectable wavelengths in the sub bandgap region. Finite-difference time domain (FDTD) calculations were found to be comparable to analytical predictions of the plasmon dispersion relation for the system which were calculated with an averaged dielectric permittivity. A method for tuning the strength of the generated plasmons is demonstrated by controlling the ratio of silver to active material within the grating layer. Profile cross-sections illustrate areas of the active layer exhibiting an increase of 40 times the absorptive dissipation compared to a non-grating cell structure. The areas of strongest increase in absorptive dissipation are visible next to the cell exit interfaces, as desired for a reduction in recombination losses.

O 59.11 Wed 17:30 P3

Adsorption Calorimetry of Conjugated Organic Molecules on Metal Surfaces — ●OLE LYTKEN, HANS-JÖRG DRESCHER, FABIAN BEBENSEE, HANS-PETER STEINRÜCK, and J. MICHAEL GOTTFRIED — Universität Erlangen-Nürnberg, Lehrstuhl für Physikalische Chemie II

Traditional experimental methods for determining adsorption energies, such as temperature programmed desorption (TPD) and equilibrium adsorption isotherms, rely on desorption. However, on many metal surfaces large conjugated organic molecules, such as PTCTDA and pentacene, decompose at elevated temperatures before or simultaneously with desorption. Discussions about relative bond strengths are, therefore, typically based on indirect arguments, such as the height of the adsorbed species above the surface as measured with normal incidence X-ray standing waves (NIXSW) or chemical shifts in spectroscopic techniques such as X-ray photoelectron spectroscopy (XPS). Unlike the more traditional methods, nanojoule adsorption calorimetry does not require desorption of the molecules; instead, the heat of adsorption is measured directly as an adsorption-induced temperature change of the sample. We will describe the construction of such a calorimeter at the Universität Erlangen-Nürnberg. Support from the Alexander von Humboldt Foundation is gratefully acknowledged.

O 59.12 Wed 17:30 P3

Preparation and spectroscopic study of self-assembled monolayers of a functionalized perylene dye on SiO₂ — ●DEB KUMAR BHOWMICK¹, NABI AGHDASSI¹, STEFFEN LINDEN¹, ANDRÉ DEVAUX², LUISA DE COLA², and HELMUT ZACHARIAS¹ — ¹Westfälische-Wilhelms Universität, Physikalisches Institut, Wilhelm-Klemm Straße 10, 48149 Münster, Germany — ²Westfälische Wilhelms-Universität, Physikalisches Institut, Mendelstrasse 7, 48149 Münster, Germany

Polyaromatic hydrocarbons (PAHs) are the focus of our attention because of their characteristically high fluorescence quantum yield, their sensitivity properties of their local environment and ability to access a wide range of photophysical and electrochemical properties. A perylene derivative, N-benzyl perylene-3,4,9,10-tetracarboxylic-3,4-anhydride-9,10-imide was synthesized. A self-assembled monolayer of this dye was prepared on the aminopropyl triethoxy silane (linker molecule) modified quartz (SiO₂) surface by an imide bond between the NH₂ group of the linker molecule and the acid anhydride group of the dye. The covalent attachment on the surface was verified by X-ray photo emission spectroscopy and FT-IR spectroscopy. UV absorption and steady-state fluorescence were measured both in the adsorbate and in the solution phase of the dye. Characteristic differences in both phases of the UV absorption, fluorescence spectrum and fluorescence lifetime are observed and will be discussed.

O 59.13 Wed 17:30 P3

Coherent phonons: an ultrafast probe of the VO₂ phase transition — ●LAURA FOGLIA¹, SIMON WALL¹, DANIEL WEGKAMP¹, JOY-EETA NAG², RICHARD F. HAGLUND², JULIA STÄHLER¹, and MARTIN

WOLF¹ — ¹Fritz-Haber Institut der MPG, Dep. of Physical Chemistry, Berlin, Germany — ²Dep. of Physics and Astronomy, Vanderbilt University, Nashville, TN, USA

The nature of the insulator to metal transition in VO₂ at 340 K has been a matter of controversy, since both lattice distortion and electronic correlations play a crucial role. Understanding the ultrafast dynamics of the *photoinduced* phase transition (PPT) may elucidate the contributions of electrons and lattice to the process. We present transient reflectivity data showing a strong change in the coherent phonon spectrum crossing the critical fluence $\Phi_c = 6.2$ mJ/cm², which can be explained by two scenarios: (i) The PPT is driven by the increase of the lattice temperature due to energy transfer from the photoexcited electrons. (ii) The sudden electronic excitation is sufficient to alter the symmetry of the lattice potential, even before ionic motion occurs. In a pump-pump-probe experiment we excite coherent phonons to monitor the changes of the lattice symmetry on a femtosecond time scale. Below Φ_c , we are able to coherently control the amplitude of the oscillations by changing the delay between the two pump pulses. Above threshold, this is not possible; on the contrary, the dynamics after the 2nd pump pulse is comparable to the one of the thermally induced metallic phase. These results suggest that the PPT begins with a lattice potential symmetry change due to the strong electronic excitation.

O 59.14 Wed 17:30 P3

Time-resolved core-level photoelectron spectroscopy — ●CHRISTIAN OBERER, MARTIN MICHELWIRTH, HATEM DACHRAOUI, JOCHEN VIEKER, TOBIAS MILDE, NORBERT MÜLLER, and ULRICH HEINZMANN — Molecular and Surface Physics, University of Bielefeld
An experimental setup based on a combination of few femtosecond EUV pulses from high-harmonic generation, with time-of-flight (TOF) analysis of the emitted photoelectrons. A selection of the 61th harmonic 95 eV from the harmonic spectrum of the light source is achieved with a multilayer Mo/Si double mirror monochromator. Our data present a clear demonstration of the potential of femtosecond time-resolved core-level photoelectron spectroscopy to directly study ultrafast dynamical processes at surfaces and in condensed matter systems.

O 59.15 Wed 17:30 P3

Post-deposition annealing induced reduction of γ -Fe₂O₃ ultra thin films studied by XRD — ●FLORIAN BERTRAM¹, CARSTEN DEITER¹, KATHRIN PFLAUM¹, MATRIN SUENDORF², CHRISTIAN OTTE², and JOACHIM WOLLSCHLÄGER² — ¹Hamburger Synchrotronstrahlungslabor am Deutschen Elektronen-Synchrotron, Notkestr. 85, 22607 Hamburg — ²Fachbereich Physik, Universität Osnabrück, Barbarastr. 7, 49069 Osnabrück

Due to their magnetic and catalytic properties iron oxide thin films are of interest for both applications and fundamental research. In both cases precise control of the oxide phase is crucial. Here, we present the effect of the post deposition annealing (PDA) in high vacuum on a 8nm γ -Fe₂O₃ film epitaxially grown by molecular beam epitaxy on MgO(001). The reduction from γ -Fe₂O₃ to FeO could be monitored by *in-situ* XRD measurements at the MgO (002) bulk reflection. By these measurements we could show that the reduction is occurring in two steps. First the film is reduced to Fe₃O₄ with the phase transition completed around 360°C. Afterwards the film is reduced to FeO which is completed at about 410°C.

O 59.16 Wed 17:30 P3

Nanoparticle impact on a W(110) surface — ●WOLFGANG ROSELLEN, HENDRIK BETTERMANN, and MATHIAS GETZLAFF — Institute of Applied Physics, University Duesseldorf

Deposited clusters and nanoparticles become more and more interesting from a technological point of view due to their size dependent electronic and magnetic properties. Therefore it is important to have access to the structure of these deposited particles. We will show that the deposition event itself is primarily responsible concerning the shape of the particles. In molecular dynamical simulation by Haberland et al. different kinetic energies result in a softlanding process of the particles without deformation due to thermalization up to an implantation of particles into the substrate surface. In our experiments we investigate nanoparticles with different sizes and deposition energies. The particles are performed in the gas phase by a UHV compatible Arc Ion Cluster Source (ACIS) being developed for softlanding condition. The kinetic energy of the particles are far below 1eV/atom. For mass and therefore size selection an electrostatic quadrupole is used at the

exit of the particle source. This is possible due to 50% of all particles are positively or negatively charged. Our investigations are carried on a bare W(110) surface. The deposited nanoparticles, mainly Fe, Co and their alloy are investigated by the means of Scanning Tunneling Microscope under UHV conditions. To gain a deeper insight into the landing process we will discuss the resulting shape of charged nanoparticles after accelerating the particles in an electrostatic field to prevent the nanoparticles from softlanding.

O 59.17 Wed 17:30 P3

Thermally activated decay of size selected clusters on thin C₆₀ films — ●STEFANIE DUFFE¹, NIKLAS GRÖNHAGEN¹, LUKAS PATRYARCHA¹, BENEDIKT SIEBEN¹, CHUNRONG YIN², BERND VON ISSENDORFF², MICHAEL MOSELER^{2,3,4}, and HEINZ HÖVEL¹ — ¹TU Dortmund, Experimentelle Physik I — ²Universität Freiburg, Fakultät für Physik — ³Fraunhofer Institute for Mechanics of Materials IWM — ⁴Freiburg Material Research Center

Metal nanoparticles supported by thin films are important for molecular electronics, biotechnology and catalysis, among other fields. Here we demonstrate a mechanism for the penetration of thin films and other nanoscopic barriers which is different from mere diffusion. Mass selected clusters from Ag₅₅⁺ to Ag_{923±9}⁺ were soft landed at 165 K on graphite (HOPG) and Au(111) covered with 1 and 2 monolayers (ML) C₆₀. Imaging by STM at 77 and 5 K showed that the clusters have extremely narrow cluster height distributions at low temperature [1]. Using C₆₀/HOPG or 2 ML C₆₀/Au(111) the cluster heights are stable for more than 12 h at room temperature, whereas for 1 ML C₆₀/Au(111) Ag_{309±3} clusters decayed and penetrated the C₆₀ film [2]. Atomistic calculations reveal a process by which the clusters decay atom by atom through 1 ML C₆₀/Au(111). These results demonstrate that a metallic substrate exerts attractive forces on metallic nanoparticles which are separated from the substrate by a single monolayer of C₆₀ molecules.

[1] S. Duffe et al., Eur. Phys. J. D **45**, 401 (2007)

[2] S. Duffe et al., Nature Nanotechnology **5**, 335 (2010)

O 59.18 Wed 17:30 P3

The height of Ag_N clusters on C₆₀ films studied for N=55 to N=147 — ●NIKLAS GRÖNHAGEN¹, NATALIE MIROSLAWSKI¹, KOLJA MENDE¹, STEFANIE DUFFE¹, BERND VON ISSENDORFF², MICHAEL MOSELER^{2,3,4}, and HEINZ HÖVEL¹ — ¹TU Dortmund, Experimentelle Physik I — ²Universität Freiburg, Fakultät für Physik — ³Fraunhofer Institut für Werkstoffmechanik, Freiburg — ⁴Freiburger Materialforschungszentrum

Mass selected clusters from Ag₅₅⁺ to Ag_{138±2}⁺ were soft landed at 77 K on C₆₀/Au(111) and imaged with STM at 77 K. Up to 9 deposition spots were imaged on a single sample using a new cluster focusing device. We were able to separate the spots clearly. The cluster heights are constant up to Ag₈₀⁺ which can be explained assuming an icosahedral shape for Ag₅₅⁺ and the formation of caps of silver atoms at the rim of the clusters for larger sizes. Every single height between Ag₈₀⁺ and Ag₈₈⁺ has been deposited and analysed. However the resolution of our cluster machine had to be taken into account. A remarkable change in height occurs between Ag₈₄⁺ and Ag₈₇⁺. An additional monolayer formed at the top cluster facet might be responsible. Ag₈₇⁺, Ag₈₈⁺ and Ag₉₅⁺ have the same height, Ag_{110±2}⁺ and Ag_{138±2}⁺ are larger and approach the height of the closed shell icosahedral cluster Ag_{147±2}⁺.

O 59.19 Wed 17:30 P3

Ag clusters in polymer PDMS: UV-VIS absorption and XANES — ●KAMIL LATUSEK¹, SABRINA HOFFMANN¹, STEFANIE DUFFE¹, CHRISTIAN STERNEMANN¹, RALPH WAGNER², and HEINZ HÖVEL¹ — ¹TU Dortmund, Experimentelle Physik I, Otto-Hahn-Str. 4, 44221 Dortmund, Germany — ²BU Wuppertal, Fachbereich C - Fachgruppe Physik - Materialwissenschaften, Gaußstraße 20, 42097 Wuppertal, Germany

Optical properties of noble metal clusters and nanostructures such as their UV-VIS absorption band alter significantly with size, shape and interparticle spacing as well as with the properties of the local environment. The possible amount of noble metal clusters deposited on a SiO₂ substrate is limited by the process of beginning coalescence to larger particles and electromagnetic coupling. Depositing these clusters into a matrix such as a polymer yields the possibility to investigate a much higher amount of separated particles. The plasmon resonance of Ag clusters in PDMS before and after exposure to air is examined using optical spectroscopy [1]. Then the same clusters are examined with

XANES at the Ag L₃ edge [2].

[1] U. Kreibitz et al., Optical Investigations of Surfaces and Interfaces of Metal Clusters, In: Advances in Metal and Semiconductor Clusters Vol. 4, (ed. M.A. Duncan), JAI press Inc., 345 (1998).

[2] P. Behrens et al., Z. anorg. allg. Chem. 625, 111 (1999).

O 59.20 Wed 17:30 P3

Heterostructural Interfaces: Structural and Electronic Properties of ZnO/Si from First Principles — •BENJAMIN HÖFFLING, ANDRÉ SCHLEIFE, and FRIEDHELM BECHSTEDT — IFTO and ETSEF, FSU Jena, Germany

The growth in computational power has greatly increased the possibilities and applications of parameter-free calculations. Ever more complex systems can be accurately modeled using ab-initio computational methods. One of the great challenges that remains is the construc-

tion of realistic geometric models of these systems. Interfaces between materials of different crystal structures are particularly challenging to model within the confines of repeated-supercell methodology. Since ZnO is being widely used as a transparent electrode in Si-based photovoltaics, the interface with silicon is of particular interest.

We present a method based on coincidence lattices and Density Functional Theory (DFT) calculations to create geometric models for heterostructural interfaces and construct a model structure for the interface between diamond structure Si and wurtzite ZnO. We then use this model to predict electronic properties using both DFT and modern quasiparticle theory based on hybrid functionals within the HSE03+GW approach. We predict band level alignment and the nature and location of electronic interface states. Our results concerning structural and electronic properties are compared to experimental and theoretical findings.