O 52: Nanostructures at Surfaces: Dots, Particles, Clusters

Time: Tuesday 18:30–20:30 Location: P1C

O 52.1 Tue 18:30 P1C

A Neural Network Potential for the Simulation of Copper Clusters on Zinc Oxide — •Martín Leandro Paleico and Jörg Behler — Lehrstuhl für Theoretische Chemie, Ruhr-Universität Bochum, Germany

A catalyst composed of large copper and zinc oxide nanoparticles is utilized in the industrial synthesis of methanol. Studying this system requires a simulation method capable of handling thousands of atoms with ab-initio accuracy, but with computational efficiency comparable to classical force fields. For this purpose Neural Network Potentials (NNP) are trained using DFT reference data, to reproduce the potential energy surface of the system.

The current work focuses on the first results for the ternary copper-zinc oxide system. In particular, the growth of copper clusters on zinc oxide surfaces is studied through combined molecular dynamics and Monte Carlo simulations, utilizing a NNP to provide the energies and forces.

O 52.2 Tue 18:30 P1C

Mobility and apparent height of mass selected copper clusters on well ordered Al_2O_3 layers studied with STM — •Dominik Wolter[1], Raphael Floegel[1], Matthias Bohlen[1,3], Christoph Schröder[1], Conrad Becker[2], and Heinz Hövel[1] — [1]Fakultät Physik / DELTA, Technische Universität Dortmund, 44221 Dortmund, Germany — [2]Aix-Marseille Université, CNRS, CINaM UMR 7325, 13288 Marseille, France — [3]Now at: Physikalisches Institut, Universität Freiburg, 79104 Freiburg, Germany

Oxide layers are commonly used for industrial purposes (e.g. microelectronics) but also a topic of current research. It was shown previously, that an Al_2O_3 film on a clean $Ni_3Al(111)$ surface can provide a template for metal cluster growth [1,2,3]. The quality of the oxidized surface was investigated with LEED and STM. We evaluate the next-neighbor (NN) distances of deposited Cu clusters in order to learn more about their arrangement on the oxidized surface as well as their apparent height, which strongly depends on the applied bias voltage. First Z(V) single point spectroscopy data is shown. Furthermore the mobility of the clusters at various coverages is analyzed by incremental heating procedures. The normalized NN distances are then compared to Monte Carlo simulation data for various lattices to check whether the clusters attach to the oxide's template structure. We found strong indication for the fixation of clusters on the so called dot sites of the surface. [1] S. Degen et al., Faraday Discuss. **125**, 343-356 (2004) [2] A. Wiltner et al., Thin Solid Films **400**, 71-75 (2001) [3] C. Becker et al., New J. Phys. **4**, 75.1-75.15 (2002)

O 52.3 Tue 18:30 P1C

Optische und elektronische Eigenschaften wasserabgesättigter Rutil-Nanopartikel — •Walter Pfäffle — Institute of Physical Chemistry University of Hamburg

Halbleitende Metalloxide in Form von Nanokristallen oder Nanopartikel sind in letzter Zeit unverzichtbar für viele Anwendungen geworden. Mit einer Bandlücke von 3,23 eV für Anatas und 3,0 eV für Rutil ist Titandioxid ein halbleitendes Metalloxid, das insbesondere in Verbindung mit photoktalytischer Wasserspaltung immer häufiger untersucht wird und industriell von großer Bedeutung ist. Man kann sich die Partikel in der Theorie so zurecht bauen, dass sie die gewünschten optischen und elektronischen Eigenschaften besitzen. Der quantum-size Effekt besagt, dass kleine halbleitende Partikel verschiedene Absorptionseigenschaften haben. Wenn also der Radius des Elektron-Loch-Paars größer wird, als die Größe des Partikels verbreitert sich die Bandlücke. Wasser abgesättigte Rutil Nanopartikel werden zunehmend im Hinblick auf ihre photokatalytische Wasserspaltung und elektronische *Fallen* Zustände untersucht. Es wurden in dieser Arbeit strukturelle, optische und elektronische Eigenschaften von verschiedenen mit Wasser abgesättigten Rutil Nanopartikeln mit verschiedenen Methoden berechnet und diese mit dem Festkörper, dessen Oberflächen und nicht abgesättigten Partikeln verglichen. Insbesondere wird auf die Berechnung der absoluten Orbitallagen und die Visualisierung der Grenzorbitale Wert gelegt, da sie für photokatalytische Wasserspaltung von großem Interesse sind. Dabei benutzte ich zur Strukturoptimierung, dass semi empirische Programm MSINDO , GPAW und CRYSTAL.

O 52.4 Tue 18:30 P1C

Formation and stabilization of silver and gold nanoparticles in room temperature ionic liquids. — •Alexander Kononov, Stefanie Roese, Florian Lippert, and Heinz Hövel — Fakultät Physik/DELTA, TU Dortmund, Otto-Hahn-Str. 4, 44221 Dortmund, Germany

Room temperature ionic liquids (RTILs) are chemically stable salts in the liquid phase at room temperature (RT) with negligible vapour pressure, which makes them suitable for vacuum applications. RTILs form a self organized structure of cations and anions by hydrogen bonds, which allow steric and electronic stabilization of metallic nanoparticles (NPs) [1].
Deposition of metal atoms on the RTIL surface leads to the formation of metal NPs in the RTIL [2,3]. For a better understanding of the formation mechanism of silver and gold NPs, several samples were prepared by magnetron sputter deposition into an RTIL (BMIM PF_6) under different sputter conditions. Formation and aggregation processes of NPs stored at different temperatures were detected (after sputtering at RT) by UV/Vis absorption measurements. Afterwards the sputtered Ag RTIL samples are compared to samples produced by deposition of clusters preformed in a supersonic expansion [4].
[1] J. Dupont, J. D. Scholten, Chem. Soc. Rev. **39**, 1780, (2010). [2] K. Richter, A. Birkner, A. Mudring, Phys. Chem. Chem. Phys. **13**, 7136, (2011). [3] T. Torimoto, K. Okazaki, T. Kiyama, K. Hirahara, N. Tanaka, S. Kuwabata, Appl.Phys.Lett. **89**, 243117, (2006). [4] D. C. Engemann, S. Roese, H. Hövel, J. Phys. Chem. **120**, 6239, (2016).

O 52.5 Tue 18:30 P1C

Metal-enhanced fluorescence of oriented emitters in plasmonic nanostructures — •Fabian Gossler[1], Matthias Stöter[2], Thorsten Schumacher[3], Markus Lippitz[3], Josef Breu[2], Andreas Fery[1], and Tobias A.F. König[1] — [1]Institute of Physical Chemistry and Polymer Physics, Leibniz Institute of Polymer Research (IPF), Hohe Str. 6, 01069 Dresden — [2]Dept. of Inorganic Chemistry 1, University of Bayreuth, Universitätsstr. 30, 95440 Bayreuth — [3]Dept. of Experimental Physics 3, University of Bayreuth, Universitätsstr. 30, 95440 Bayreuth

For implementation of nanophotonic devices, a tunable life-time and controllable enhancement of the spontaneous emission is necessary. We fabricate a gold film coupled anisotropic silver nanocube cavity to systematically study the fluorescence enhancement of oriented fluorophores. For a rational design, the plasmonic properties of the silver nanocubes are designed to match with the emission spectrum of a selected fluorophore. Silicate bilayers with intercalated fluorophores are used as emitting spacer due to their regular height of 4 nm on large scales and orientation of the dye molecules. Finite-difference time-domain (FDTD) simulations, atomic force microscopy (AFM), dark field spectroscopy, confocal and time-resolved photoluminescence measurements have been used to characterize the tailormade nanocavity. Significant emission enhancement and a strong influence on life-times are observed inside the nanocavity. FDTD simulations support the results and demonstrate the potential of this cavity enhancement as building block for application in plasmonic lasers or metamaterials.

O 52.6 Tue 18:30 P1C

Deposition and temperature dependent surface interaction of Co nanoparticles on W(1 1 0) — •Jens Schubert, Hendrik Bettermann, and Mathias Getzlaff — Institute of Applied Physics, Heinrich-Heine-Universität Düsseldorf

Our research involves supported nanoparticles of 3d-metal alloys. Temperature dependent behavior is interesting for fundamental research and possible technological applications. These properties depend strongly on the nanoparticles' size.

The nanoparticles are produced under UHV conditions by a magnetron sputter source (Haberland-type), which gives access to sizes ranging from 3nm to >12nm.

Our approach is to measure surface structure and cleanliness with LEED (low energy electron diffraction) and the temperature dependent interaction of cobalt nanoparticles on a W(110) surface with spatial resolution by scanning tunnelling microscopy (STM) before and after heating.

O 52.7 Tue 18:30 P1C

Nanoparticle Adhesion and Optical Particle Motion Control — •Michaela Schmid[1], Daniel Geiger[1], Clara Wanjura[1], Irina Schrezenmeier[1], Matthias Roos[2], and Othmar Marti[1] — [1]Institute of Experimental Physics, Ulm University, Albert-Einstein-Allee 11, 89081 Ulm, Germany — [2]Carl Zeiss SMT GmbH, Rudolf-Eber-Strasse 2, 73447 Oberkochen, Germany

The adhesion of nanoparticles on substrates like silicon wafers is of high interest for a variety of scientific and industrial applications. To determine adhesion, a method based on lateral pushing of nanoparticles by an atomic force microscope (AFM) tip was used. The lateral force acting on the cantilever by the particle is then a function of its adhesion force to the substrate.

However, the nature of the detachment and moving process remains unclear. Additional experiments are necessary to distinguish between rolling, sliding or jumping motion. These processes are investigated by simultaneous optical observation. Using total internal reflection (TIR) illumination, the scattering intensity of the bead contains the distance information from bead to substrate. Partially fluorescent particles allow to distinguish between rolling and sliding motion [1].

[1] S. Schiwek et al, Evidence of a rolling motion of a microparticle on a silicon wafer in a liquid environment, J. of Appl. Phys. 119, 194304 (2016)

O 52.8 Tue 18:30 P1C

Nanoparticle Adhesion on Flat Surfaces - an AFM Lateral Force Study — •Clara Wanjura[1], Daniel Geiger[1], Michaela Schmid[1], Irina Schrezenmeier[1], Matthias Roos[2], and Othmar Marti[1] — [1]Institute of Experimental Physics, Ulm University, Albert-Einstein-Allee 11, 89081 Ulm, Germany — [2]Carl Zeiss SMT GmbH, Rudolf-Eber-Strasse 2, 73447 Oberkochen, Germany

Understanding how nanoparticles adhere to surfaces is relevant, since in many applications, as for example in photolithography, such nanoparticles can already cause defects. In other settings, the adhesion of nanoparticles might be desirable. In all of these cases, it is important to understand how strongly particles stick to the surface and how to influence that interaction.

The lateral force needed to move nanoparticles with an AFM tip is sampled at discrete points in time over several weeks for probes stored in different environments to understand the aging process of silicon surfaces decorated by nanoparticles. As well as an increase in lateral force in certain environments, the formation of layers of a hard material, possibly silicon oxide, around the particles is shown. In addition, the height of these layers is examined with an AFM and compared to a published model for the growth of silicon oxide layers through oxidation, the Deal-Groves model [1].

[1] General Relationship for the Thermal Oxidation of Silicon, Deal, B. E. and Grove, A. S., Journal of Applied Physics, 36, 3770-3778 (1965), DOI:http://dx.doi.org/10.1063/1.1713945

O 52.9 Tue 18:30 P1C

Noncollinear spin arrangement in size-selected FeV clusters on Cu(100) — •Fridtjof Kielgast[1], Ivan Baev[1], Friederike Albrecht[1], Christina Ossig[1], Michael Martins[1], and Wilfried Wurth[1,2] — [1]Physics Department, University of Hamburg — [2]DESY Photon Science, Hamburg

Deposited clusters constitute interesting model systems for fundamental as well as applied research, as their electronic and magnetic properties tend to change nonlinearly with cluster size and composition. Here, we present investigations on small, size-selected V_nFe_m adsorbates produced by high energy sputtering. The clusters were deposited onto a Cu(100) surface using a soft landing scheme to avoid fragmentation. X-Ray magnetic circular dichroism (XMCD) measurements were carried out up to sizes of n+m=3. The XMCD signal was obtained by switching an external magnetic field (±7T) and scanning the $L_{2,3}$ edges of V and Fe respectively with circular polarized light at the P04 beamline at PETRA III, DESY. By changing the incidence angle between the incoming light and the sample, the axis of easy magnetization could be found. This work is supported by the DFG in the framework of the SFB 668.

O 52.10 Tue 18:30 P1C

Synthesis of transition metal oxide nanoparticles by thermal decomposition of metal oleate precursors — •Aladin Ullrich, Mostafizar Mohammad Rahman, and Siegfried Horn — Institut für Physik, Universität Augsburg, D-86159 Augsburg, Germany

Iron oxide nanoparticles are currently one of the most interesting materials due to unique properties and potential applications. The size, shape and size distribution of iron oxide nanoparticles have great influence on their physical properties and therefore on their application potential.

We have investigated the influence of synthesis parameters like the heating rate or surfactants on particle size, shape and size distribution of iron oxide nanoparticles applying the method of thermal decomposition of iron oleate precursor. The particle size varies from 14-24 nm for different heating rates (from 1 to 35°C/min) in our experiments. Spherical nanoparticles were obtained in the presence of oleic acid as surfactant, cubic nanoparticles were obtained using a mixture of oleic acid and Na-oleate as surfactants. Different size distributions are observed for different heating rates. Magnetic properties of different sized particles were investigated using SQUID magnetometry. In addition, manganese ferrite nanoparticles with varying Fe:Mn ratio were synthesized. The influence of the Fe:Mn ratio on the Curie temperature and saturation magnetization of the nanoparticles was investigated.

O 52.11 Tue 18:30 P1C

Characterization of Ag clusters in ionic liquids with DLS — •Florian Lippert, Stefanie Roese, and Heinz Hövel — Fakultät Physik / DELTA, TU Dortmund, Otto-Hahn-Str. 4, 44221 Dortmund

Ag clusters produced in a supersonic expansion [1] can be deposited without coalescence into room temperature ionic liquids (RTILs), which are salts of weakly coordinating cations and anions being liquid at room temperature controlled by UV/Vis spectroscopy [2].

To get an insight into the process of stabilization and aggregation, we investigate Ag clusters in EMIM-FAP and BMIM-PF_6 by dynamic light scattering (DLS) [3].

The time-dependent change of the scattered light intensity depends on the Brownian motion of the nanoparticles. By means of that it is possible to receive the size distribution of the particles given by their hydrodynamic radius.

For proper measurement the material properties as viscosity and refractive index are indispensable. To determine the refractive index of the RTIL an Abbe refractometer and extrapolation to other wavelengths is used.

Measurements for storage at different temperatures show how stable the clusters in the ionic liquid are over time scales of several days.

[1] H. Hövel, S. Fritz, A. Hilger, U. Kreibig and M. Vollmer, Phys. Rev. B 48, 18178, 1993 [2] D. Engemann, S. Roese and H. Hövel, J. Phys. Chem. C 120, 6239, 2016 [3] B.J. Berne and R. Pecora, Dynamic Light Scattering, Dover Publications, New York, 2000

O 52.12 Tue 18:30 P1C

Ultrafast vibration and cooling of ultrathin gold nanotriangles studied by ultrafast X-ray Diffraction — •J. Pudell[1], A. von Reppert[1], R. M. Sarhan[1], F. Stete[1], M. Reinhard[1,4], M. Rössle[1], W. Koopmann[1], F. Zamponi[1], N. Del Fatti[2], A. Crut[2], J. Koetz[3], F. Liebig[3], C. Prietzel[3], and M. Bargheer[1,4] — [1]Institut für Physik, Universität Potsdam, Karl-Liebknecht-Str. 24-25, 14476 Potsdam, Germany — [2]FemtoNanoOptics group, Institut Lumière Matière, Univ Lyon, Université Lyon 1, CNRS, 69622 Villeurbanne, France — [3]Institut für Chemie, Universität Potsdam, Karl-Liebknecht-Str. 24-25, 14476 Potsdam, Germany — [4]Helmholtz-Zentrum Berlin, Wilhelm-Conrad-Röntgen Campus, BESSY II, Albert-Einstein-Str. 15, 12489 Berlin, Germany

We study the vibrations and subsequent thermalization of ultrathin gold nanotriangles upon optical excitation of the electron gas by ultrafast x-ray diffraction (UXRD). Our measurements yield an accurate determination of the structural response of an asymmetric nanoparticle including amplitude and phase of the excited vibrational motion. The amplitude of the fastest mode with 3.6 ps period measures the instantaneous rise of electronic pressure and the phonon-pressure rising within 6 ps. Slower symmetric in-plane modes of the particle contribute less to the signal. The nanosecond relaxation time of the expansion yields a direct measure of heat flow out of the nano-object, which is limited by the molecular connection to the substrate. We report data recorded at the laser-driven Plasma X-ray Source (PXS) in Potsdam and at the XPP-KMC3 Beamline at the synchroton radiation facility Bessy II.

O 52.13 Tue 18:30 P1C

Selective nucleation of MnSb Islands on GaAs Substrates — •Christian Klump[1], Bo Zhang[1], Julian Ritzmann[2], Arne Ludwig[2], Andreas Wieck[2], and Ulrich Köhler[1] — [1]Experimentalphysik IV, AG Oberflächen, Ruhr-Universität Bochum, Germany — [2]Lehrstuhl für Angewandte Festkörperphysik, Ruhr-Universität Bochum, Germany

For future spintronic semiconductor devices, spin polarization and injection is one important prerequisite. Ferromagnetic or half-metallic materials can be used as efficient spin-injectors. As with the underlying semiconductor quantum dots, it is necessary to be able to grow the spin-injector material site-selectively. Prestructuring the substrate and strain-driven nucleation are two approaches for site-selective growth.

Prestructuring the substrates introduces defects to the surface and may deteriorate the quality of subsequent island growth. Examples of growth on a prestructured substrate are shown.

Strain-driven nucleation, on the other hand, opens the prospect of pin-pointing exactly one spin-injector island to one semiconductor QD by using the inherent strain induced by the underlying semiconductor QD, so spin-injection can be studied for each QD, individually.

MnSb is an interesting material for spin-injection with its high Curie temperature of 587 K and its compatibility with semiconductor substrates. The strain induced pairing of MnSb islands with InAs QDs is studied. MnSb islands were grown on different GaAs substrates by MBE. Structural and magnetic properties have been studied by STM, LEED and MOKE.