O 24: Particles and clusters

Time: Tuesday 10:30–12:30 Location: H34

O 24.1 Tue 10:30 H34

Not so loosely bound: temperature dependent vibrational fingerprints of Au_NKr_M clusters — •Luca M. Ghiringhelli, Philipp Gruene, Gerard Meijer, Andrè Fielicke, and Matthias Scheffler — Fritz-Haber-Institut der Max-Planck-Gesellschaft, Faradayweg 4-6, 14195 Berlin, Germany

In order to interpret the vibrational spectra of *neutral* Au_NKr_M clusters, as measured in a Multiple Photon Dissociation Far-IR experiment (P. Gruene *et al.*, Science **321**, 674 (2008)), we calculated their finite temperature vibrational spectra, by means of all electron density functional theory, including the Tkatchenko-Scheffler van der Waals correction. We surprisingly find that Kr forms weak chemical bonds (binding energy around 0.2 eV per Kr atom) with 1- to 3-fold coordinated Au atoms belonging to small Au_N clusters ($N \leq 4$). Such Au_NKr_M clusters have a vibrational spectrum which is different from the related Au_N clusters. For bigger Au_N clusters, Kr physisorbs to the clusters, forming a complex whose vibrational spectrum is practically identical to the spectrum of the bare cluster. Anharmonicities affect the spectrum by changing (with respect to the harmonic spectrum) the relative intensity of the peaks and by showing new peaks, due to interactions among eigenmodes.

O 24.2 Tue 10:45 H34

RHEED Study of Au-induced Surface Reconstructions and 3D AuSi Nanoparticles — •Stephan Bartling, Ingo Barke, Kristian Sell, Stefan Polei, Viola von Oeynhausen, and Karl-Heinz Meiwes-Broer — Institut für Physik, Universität Rostock, 18051 Rostock, Germany

The contribution focuses on *in situ* reflection high energy electron diffraction (RHEED) of Au/Si(111). Three different surface reconstructions can be observed in recorded RHEED patterns during Au evaporation in the sub-monolayer regime. Recently, the ideal Au coverage for the Si(111)5×2-Au reconstruction has been revised [1]. The result of $\Theta = 0.6$ML is confirmed by the coverage-dependent intensity of spots.

After Au deposition of >1ML on vicinal Si(111) three-dimensional gold-rich AuSi nanoparticles are formed via Stranski-Krastanov growth. A mean particle height of 5.8nm has been determined from large-scale STM images for ≈ 3ML Au. The RHEED diffraction pattern can be modeled by a quasi close-packed structure with rhombohedral unit cell. We do not observe flat top facets reported for similar preparation conditions [2]. This is in agreement with the crystal orientation determined by RHEED.

[1] I. Barke et al., Phys. Rev. B 79, 155301 (2009)
[2] E. Moyen et al., Appl. Phys. Lett. 94, 233101 (2009)

O 24.3 Tue 11:00 H34

Orbital and spin magnetic moments of small, deposited CoPd alloy clusters on Ni/Cu(100) — •Steffen Fiedler[1], Ivan Baev[1], Kai Chen[1], Leif Glaser[1], Paolo Imperia[2], Stephan Klumpp[1], Michael Martins[1], and Wilfried Wurth[1] — [1]Institut für Experimentalphysik, Universität Hamburg — [2]Institute of Materials and Engineering Science, Australian Nuclear Science and Technology Organisation New Illawarra Road, Lucas Heights, NSW Australia

It has been shown that the orbital magnetic moments of Co clusters can be exceptionally large on a platinum substrate [1]. Together with a strong induced spin-orbit-coupling this leads to a high magnetic anisotropy.

We examine the magnetic moments of transition metal elements in small, mass selected alloy clusters on ferromagnetic substrates with the method of X-ray circular magnetic dichroism (XMCD). The measurements are performed at the storage ring of the synchrotron radiation source Bessy II in Berlin. Starting with Co_xPt_y clusters we proceeded with the investigation of Co_xPd_y clusters. We will classify the results in the light of the previous measurements also including pure Co_x clusters as a reference.

This work was funded by the DFG through the SPP 1153.

[1] P. Gambardella et al., Science 300, 1130 (2003)

O 24.4 Tue 11:15 H34

Structural properties of individual mass-filtered *3d*-metal nanoparticles deposited on W(110) — •Wolfgang Rosellen[1], Christian Kleinhans[1], Volker Hückelkamp[1], Furkan Bulut[1], Joachim Bansmann[2], Armin Kleibert[3], and Mathias Getzlaff[1] — [1]Institute of Applied Physics, University of Düsseldorf — [2]Dep. of Surface Chemistry, Ulm University — [3]Swiss Light Source, Paul Scherrer Institute

Nano-sized clusters and particles are regarded as a new class of material because their physical and chemical properties can significantly change with size. Thus, new features are accessible and additionally tunable by size-selection. Due to the high surface-to-volume ratio and the reduction of the coordination numbers the properties also differ from the respective bulk material such as melting point, conductance or electronic and, for magnetic particles, magnetic behavior. Fe, Co and FeCo alloy nanoparticles were produced by a continuously working arc cluster ion source (ACIS), mass-filtered by means of an electrostatic quadrupole and subsequently deposited on a W(110) surface. We discuss the structural properties of *individual* nanoparticles with diameters between 3 nm and 15 nm. High-resolution transmission electron microscopy (HR-TEM) is used to estimate the size and the crystallographic structure of the nanoparticles before deposition. The height and shape after deposition is investigated by scanning tunneling microscopy (STM). Additionally, the melting behaviour of the nanoparticles at elevated temperatures will be discussed.

O 24.5 Tue 11:30 H34

Molecular Dynamics Studies on the Morphology of PtNi-alloy Particles — •Donato Fantauzzi and Timo Jacob — Ulm University, Albert-Einstein-Allee 47, D-89069 Ulm, Germany

Platinum-based catalysts supported on carbon still serve as the preferred electrocatalyst for the oxygen reduction reaction (ORR), which is one of the most important reactions in basic electrochemistry but also in various applications such as low-temperature polymer electrolyte fuel cells. In order to find a more active catalyst than pure Pt, in the past years various platinum alloys such as PtNi, PtCo, etc. with different atom ratios were synthesized and investigated [1]. Since Pt is limited and rather expensive, these multi-metallic catalysts are not only saving precious metal but also show enhanced reactivity and selectivity.

Motivated by recent experimental work on the morphology of Pt_xNi_1 *(x=1,2,3)* nanoparticles, we investigated the bulk and surface structure as well as the segregation behavior of differently sized (1.0-3.0 nm) alloy nanoparticles using ReaxFF [2], a reactive molecular dynamics (MD), with a self-optimized forcefield. By applying subsequent simulated annealing cycles to particles of variable size and bulk composition direct comparison to the experimental results was possible [3].

[1] U. A. Paulus *et al.*, *J. Phys. Chem. B*, **106**, 4181 (2002).
[2] A. C. T. van Duin, S. Dasgupta, F. Lorant, W. A. Goddard III., *J. Phys. Chem. A*, **105**, 9396 (2001).
[3] E. Favry, D. Wang, D. S. Su, N. Alonso-Vante, D. Fantauzzi, T. Jacob, *to be published.*

O 24.6 Tue 11:45 H34

X-ray absorption fine-structure spectroscopy of bimetallic Pt nanoparticles — •Torsten Laurus[1], Ardalan Zargham[1], Edyta Piskorska-Hommel[1,2], Jan Ingo Flege[1], Sarah Röhe[3], Patrick Sonström[3], Xiaodong Wang[3], Marcus Bäumer[3], and Jens Falta[1] — [1]Institute of Solid State Physics, University of Bremen, Otto-Hahn-Allee, 28359 Bremen, Germany — [2]Institute of Physics, Polish Academy of Science, Al. Lotnikow 32/46, 02-668 Warsaw, Poland — [3]Institute for Applied and Physical Chemistry, University of Bremen, Leobener Straße, 28359 Bremen, Germany

Bimetallic nanoparticles have generated great interest in recent years because of their huge number of possible applications, e. g., in future electronic and magnetic devices as well as in heterogeneous catalysis. Since the physical and chemical properties of the nanoparticles significantly depend on both their atomic structure and chemical composition, their material characteristics may individually be tailored provided that these parameters can be controlled.

Several Pt-containing bimetallic nanoparticles, produced by wet chemical synthesis, have been studied by means of fluorescence x-ray absorption fine-structure spectroscopy (XAFS), which was performed at beamlines C and E2 at the Hamburg Synchrotron Radiation Laboratory (HASYLAB/DESY). Our data allow the identification of the crystalline structure of the nanoparticles and the quantification of the local atomic coordination of the constituents. Furthermore, the analysis reveals details on their compositional inhomogeneity and the concomitant oxidation states of the individual components.

O 24.7 Tue 12:00 H34

Structural metastability of endohedral M@Si$_{20}$ cages: A first-principles sampling study — Alexander Willand[1], •Matthias Gramzow[2], Stefan Goedecker[1], and Karsten Reuter[2,3] — [1]Univ. Basel (Switzerland) — [2]Fritz-Haber-Institut Berlin (Germany) — [3]Technische Universität München (Germany)

Cage-like clusters are considered as appealing building units for nanoscale materials. Their hollow structure facilitates the incorporation of guest atoms, which can either be viewed as an atomic-scale tailoring of the materials properties of the cage through doping or as a perfect shielding of the encapsulated moiety. With Si in general favoring tetrahedral sp^3-coordination, corresponding endohedral metal doping appears as a primary avenue to accomplish the stabilization of Si cage geometries at all. C$_{20}$ is the smallest known fullerene cage and Si$_{20}$ cages are building blocks of clathrate materials. We therefore investigate the structural stability of endohedral Si$_{20}$ structures for a large variety of metal dopants. For this purpose we combine global optimization within minima hopping [1] with a DFT potential energy surface using different levels of xc approximation (LDA, GGA, hybrid functionals). In contrast to previous work proposing endohedral M@Si$_{20}$ cages as ground state (e.g. [2]) we find for all investigated systems largely more stable isomers, in which the cage structure is broken into smaller cages with additional surface atoms or into completely exohedral isomers. [1] S. Goedecker, JCP **120**, 9911 (2004) [2] Q. Sun *et al.*, PRB **65**, 235417 (2002).

O 24.8 Tue 12:15 H34

Magnetic coupling and anisotropy of Fe nanoclusters deposited onto Cu(111) — •Christian Praetorius[1], Greg A. Ballentine[2,4], Armin Kleibert[3,5], Norman Wilken[3], Andris Voitkans[3], Karl-Heinz Meiwes-Broer[3], and Kai Fauth[1,2] — [1]Physikalisches Institut, Universität Würzburg, Am Hubland, 97074 Würzburg, Germany — [2]MPI für Metallforschung, Heisenbergstr. 3, 70689 Stuttgart, Germany — [3]Physikalisches Institut, Universität Rostock, 18051 Rostock, Germany — [4]Dpt. of Physics, Brandon University, 270 18th street, Brandon, Canada R7A 6A9 — [5]Swiss Light Source, Paul Scherrer Institute, 5232 Villigen, Switzerland

Magnetization and magnetic response of Fe nanoclusters is studied by temperature and density dependent in situ X-ray magnetic circular dichroism after deposition onto Cu(111). At particle diameters of 6 nm, ferromagnetic response is obtained at ambient temperature for nanocluster densities well below percolation threshold. Both, enhanced intrinsic magnetic anisotropy energy (MAE) density as well as collective effects contribute to this effect. This enhancement of MAE is not accompanied by enhanced orbital magnetic moments. At elevated cluster densities we observe sizeable macroscopic magnetic in plane anisotropy. This anisotropy can quantitatively be understood as the effect of a demagnetizing field, and thus the average effect of diplar interactions of the nanoclusters.