O 101: Particles and clusters II

Time: Friday 11:15–13:00 Location: WIL C107

O 101.1 Fri 11:15 WIL C107

Orbital and spin magnetic moments of small, size-selected CoRh alloy clusters, deposited on Ni/Cu(100) — •Torben Beeck, Ivan Baev, Kai Chen, Michael Martins, and Wilfried Wurth — Institute of Experimental Physics, University of Hamburg, Luruper Chaussee 149, 22761 Hamburg, Germany

Besides their high potential for applications in magnetic materials and chemical catalysis, transition metal clusters of few atoms are excellent candidates for comparison with complex theoretical calculations, including correlation effects which become very important on the nanoscale.

X-ray magnetic circular dichroism (XMCD) studies on small, size-selected Co_xRh_y transition metal clusters have been carried out at the Co $L_{2,3}$ absorption edges. Under UHV conditions the clusters were deposited in situ on a remanently magnetized Ni thin film evaporated upon a Cu(100) crystal. All the measurements were performed at the BESSY II, UE52 SGM beamline.

We will show the orbital and spin magnetic moments of the Co_xRh_y clusters which exhibit changes with cluster size and composition. A comparison to other transition metal alloy clusters will be given.

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O 101.2 Fri 11:30 WIL C107

Surface enhanced Raman spectroscopy using tailored noble metal nanoparticles — •Robert Ossig, Frank Hubenthal, and Frank Träger — Institut für Physik and Center for Interdisciplinary Nanostructure Science and Technology – CINSaT, Universität Kassel, Kassel, Germany

Surface enhanced Raman spectroscopy (SERS) is a powerful technique in the field of molecular spectroscopy, which exploits the superior optical properties of metal nanoparticles. In principle SERS allows to detect and to measure spectra of single molecules. However, stable and reproducible SERS substrates, which are necessary for routine applications, are only rarely available. Furthermore, to achieve the optimum enhancement for certain excitation wavelength and molecule combinations, a tailoring of the optical properties is desired. To meet these requirements, our samples were produced by Volmer-Weber growth, in combination with laser tailoring. The combination of both methods allows a tuning of the surface plasmon resonance of the metal nanoparticles in the vicinity of the excitation wavelength for the SERS measurements, independently from the nanoparticle size. Hence, the influence of the wavelength on the SERS spectra can be studied. In this contribution we present SERS measurements of pyrene as a function of the excitation wavelengths. We will show that for all excitation wavelengths the SERS spectra are highly reproducible and strongly enhanced, if tailored nanoparticles serve as substrates. However, only for an excitation wavelength near the infrared, a background free Raman signal with an excellent signal-to-noise ratio is achieved.

O 101.3 Fri 11:45 WIL C107

Stabilization mechanism for cage-like $Si_{16}M^+$ clusters: From global structure optimization to understanding — •Dennis Palagin[1], Matthias Gramzow[2], and Karsten Reuter[1,2] — [1]Technische Universität München — [2]Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin

Doping with endohedral metal atoms appears as a remarkable avenue to tailor the intrinsic properties of silicon clusters, as well as to stabilize cage-like geometries as suitable building blocks for novel engineered materials. A prevalent concept to rationalize this stabilization is that injection of metal electrons into the Si electron gas leads to electronic shell closure. A prominent example is $Si_{16}V^+$, which with 68 valence electrons corresponds to a closed-shell configuration. Intriguingly, $Si_{16}Ti^+$ and $Si_{16}Cr^+$ with 67 and 69 electrons, respectively, are equally believed to stabilize in cage-like geometries [1]. Aiming to further clarify the stabilization mechanism we first use density-functional theory based basin-hopping to ascertain that the cage-like geometry indeed represents the ground-state structure for all three dopant atoms. From this basis we proceed to a detailed analysis of the obtained charge distributions to identify the nature of the bond and the stabilization mechanism in this dopant sequence. [1] J.T. Lau *et al.*, Phys. Rev. A **79**, 053201 (2009).

O 101.4 Fri 12:00 WIL C107

Using STM-Lithography to study interface properties: Footprints of Cu-clusters on single crystalline ZnO($10\bar{1}0$) — •Martin Kroll and Ulrich Köhler — Institut für Experimentalphysik IV / AG Oberflächen, Ruhr-Universität Bochum

As model systems in heterogeneous catalysis Cu clusters on single ZnO crystals grown under UHV conditions are used as a first step to understand complex reactions under real catalytical conditions. STM and STS were used to study the annealing behaviour of Cu clusters deposited by MBE on the nonpolar ZnO($10\bar{1}0$) surface. As already found for the polar ZnO(0001)-Zn surface [1], separated Cu clusters are formed at room temperature and a partial entrenching of Cu into the ZnO substrate at elevated temperatures of $T > 670K$ was found. To investigate what happens at the Cu-ZnO interface in more detail Cu clusters were removed from the ZnO surface after different annealing steps using STM-tip induced diffusion. The remaining footprints of the Cu clusters on the undisturbed ZnO substrate were analysed with STM and STS. The results point to a pure thermally driven interaction of the Cu-clusters with ZnO at the borderline between the cluster and the free ZnO substrate surface.

[1] Kroll, M.; Köhler, U.; Surf. Sci. 601 (2007) 2182

O 101.5 Fri 12:15 WIL C107

Deformation of Ag Clusters Deposited on Au(111) - Experiment and Molecular Dynamics — •Natalie Miroslawski[1], Niklas Grönhagen[1], Bernd von Issendorff[2], Tommi Järvi[3], Michael Moseler[2,3,4], and Heinz Hövel[1] — [1]TU Dortmund, Experimentelle Physik I — [2]Universität Freiburg, Fakultät Physik — [3]Fraunhofer Institut für Werkstoffmechanik, Freiburg — [4]Freiburger Materialforschungszentrum

Mass selected clusters from Ag_{55}^+ to $Ag_{147\pm2}^+$ were deposited with different deposition energies at 77 K on Au(111) and imaged with STM at 77 K. We observed a deformation of the cluster shape due to the strong metallic interaction between the cluster and the substrate. The clusters became epitaxial and developed a structure composed of several Ag monolayers. The number of these monolayers depends on the number of atoms in the cluster and the deposition energy. The larger the cluster mass the more monolayers the cluster develops on Au(111) and the larger the deposition energy the fewer monolayers occur. These results were verified by molecular dynamic simulations. Additionally the behaviour of Ag_N clusters on Au(111) after different annealing steps was investigated.

O 101.6 Fri 12:30 WIL C107

Adsorbate-induced smoothing of Re particles on the atomic scale — •Payam Kaghazchi and Timo Jacob — Universität Ulm, Albert-Einstein-Allee 47, D-89069 Ulm, Germany

Using density functional theory in combination with the *ab initio* atomistic thermodynamics approach we studied the equilibrium shape of Re particles in the presence of strongly interacting O and N adsorbates. At low and intermediate coverages, oxygen adsorption has minor influence on the equilibrium shape of the corresponding clean particles, i.e., truncated polyhedra, while nitrogen adsorption leads to stabilization of spherical-like polyhedra with a large contribution from atomically-rough ($13\bar{4}2$) faces[1]. At very high coverages of O and N, particles are perfect prisms consisting of the (0001) and ($10\bar{1}0$) faces. Since the close-packed surfaces are often less active in O and N-involved reactions than atomically-rough ones, these results offer a possible explanation for the experimentally-observed reduction in the activity of Re particles for ammonia synthesis and also predict a decrease in the activity of this system in oxidation reactions at high coverages. This study suggests that, besides the site-blocking effect, adsorbate-induced smoothing of particles on the atomic scale can reduce catalytic activity of transition metals[2]. [1] P. Kaghazchi and T. Jacob, Phys. Rev. B, **82**, 165448 (2010). [2] P. Kaghazchi and T. Jacob, in preparation.

O 101.7 Fri 12:45 WIL C107

Linear and nonlinear optical properties of supported metal clusters and adsorbed molecules — •Philipp Heister, Martin Thämer, Aras Kartouzian, and Ueli Heiz — Lehrstuhl für Physikalische Chemie, Technische Universität München

Metal clusters in the non-scalable size regime supported on oxide surfaces have unknown optical properties, which are essential for the understanding of photochemical properties of cluster-assembled materials and their use in optical applications. Cavity ring-down spectroscopy (CRDS) and surface second harmonic generation spectroscopy (S-SHGS) have been applied to samples of various metal clusters, in order to investigate their optical properties in the wavelength range from 215 to 700 nm. The performance of the employed experimental apparatus is characterized by measuring organic laser dye molecules adsorbed on surfaces as a model system.

We show that both these highly sensitive spectroscopic methods are applicable and are of complementary nature. CRDS for supported samples is limited to wavelengths above 400 nm. S-SHGS is readily extended into the far UV up to 215 nm but for the interpretation of the results the linear spectra obtained by CRDS are needed.