

O 69: Symposium: Size-Selected Clusters at Surfaces III

Time: Thursday 14:00–15:00

Location: MA 042

O 69.1 Thu 14:00 MA 042

Size-dependent structure and bonding of Ir clusters on Graphene / Ir(111) — ●CARSTEN BUSSE¹, ALPHA T. N'DIAYE¹, JOHANN CORAUX¹, PETER J. FEIBELMAN², and THOMAS MICHELY¹ — ¹II. Physikalisches Institut, Universität zu Köln, Germany — ²Sandia National Laboratories, Albuquerque, USA

Small Ir clusters are grown by deposition of Ir onto a graphene moiré on Ir(111) and analyzed using scanning tunneling microscopy (STM). The clusters are arranged in a hexagonal lattice with perfect ordering and exhibit a narrow, tunable size distribution.

The apparent cluster height for monolayer clusters shows a pronounced increase with cluster size from 1.8 Å for trimers to 2.5 Å for 11-clusters. Density functional theory (DFT) calculations rule out a geometric explanation of this effect, so we attribute it to differences in electronic structure. The majority of clusters are stable and immobile at room temperature, but for certain cluster sizes we observe a jiggling motion (trimer to heptamer) or rapid shape changes (tetramer).

For the experimentally observed binding sites of the clusters within the moiré unit cell, DFT reveals that the bonding of the clusters to the substrate induces a rehybridization of the C directly underneath the particles. The bonding changes from a graphene-like (sp^2) into a diamond-like (sp^3) arrangement, thus explaining the strong binding of the clusters to the substrate.

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O 69.2 Thu 14:15 MA 042

Density functional modeling of supported clusters: on the road to an understanding of nanoscale catalysis — ●MICHAEL MOSELER^{1,2} and BERND HUBER² — ¹Fraunhofer Institute for Mechanics of Materials IWM, Wöhlerstr. 11, 79108 Freiburg — ²Freiburg Materials Research Center, Stefan-Meier-Str. 21, 79104 Freiburg

Understanding and predicting heterogeneous catalysis remains one of the main motivations underlying the science of supported nano-cluster. Surface science experiments provide important insights into nano-particles catalysed reactions [1]. Often however, this progress is only achieved in combination with quantum-chemical atomistic simulations. Here we show how density functional theory can be used to understand experimental size evolutionary patterns in the activity of metal-oxide supported Pd clusters [2,3]. We provide theoretical as well as experimental evidence that the reaction of supported Pd clusters with molecular oxygen results in the formation of nano-oxides which are in epitaxy with the ceramic support. These oxides serve as a Mars-van-Krevelen oxygen reservoir and therefore play an important role in the catalyzed combustion of carbon monoxide.

[1] U.Heiz, E.L.Bullock, Mater. Chem. 14, 564 (2004)

[2] B.Huber, P.Koskinen, H.Häkkinen, M.Moseler, Nature Materials 5, 44 (2006)

[3] B.Huber, M.Moseler, Eur. Phys. J. D online-First (2007)

O 69.3 Thu 14:30 MA 042

X-ray photoelectron spectroscopy on deposited noble metal clusters — ●MATTHIAS NEEB, BARIS BALKAYA, NICOLETTA FERRETTI, and WOLFGANG EBERHARDT — BESSY, Albert-Einstein Str. 15, 12489 Berlin

Noble metal clusters (Cu, Ag, Au) were produced in a magnetron sputter source and mass-selected by a magnetic sector field prior to soft-landing on a p-doped Si-wafer. XPS, XANES, UPS and Auger spectra of the supported metal clusters at a surface coverage of $\sim 1\%$ have been measured with soft X-ray synchrotron radiation. The cluster spectra are compared with the respective bulk spectra of an evaporated metal film. In general, the core binding energies of the clusters vary with size and are blue shifted with respect to the bulk value. Similarly, the L_3 absorption edge of Cu-clusters up to 70 atoms is blue shifted with respect to Cu-bulk. For larger Cu-clusters (≥ 13) a multiple-scattering NEXAFS-feature is detected behind the L_3 absorption edge, indicating an icosahedral structure. The Auger energy of the clusters shows a red shift with respect to the bulk value. Moreover, the kinetic energy of the Auger electron is influenced by post-collision interaction (PCI) and varies with cluster size.

O 69.4 Thu 14:45 MA 042

Electrospray Ion Beam Deposition of Nonvolatile Molecules and Nanoparticles in High- and Ultrahigh Vacuum — ●STEPHAN RAUSCHENBACH, THOMAS WEITZ, ALICIA FORMENT, JENS BOETTCHER, GIOVANNI COSTANTINI, NICOLA MALINOWSKI, and KLAUS KERN — Max-Planck-Institute for Solid State Research, Stuttgart, Germany

Electrospray Ionization is a soft ionization technique with which non-volatile molecules or nanoparticles from a solution can be transferred into the gas phase. Based on this technique we developed a novel vacuum deposition apparatus, which is capable to transfer these ions into high- or ultrahigh vacuum, mass select them and deposited them on a surface [S.Rauschenbach et. al., Small 4 (2006)]. Destruction free deposition (soft landing) can be achieved, since the kinetic energy of the ions can be controlled. An UHV-STM/AFM is connected to the system for in-situ analysis.

The capability to deposit the large organic molecules, clusters and nanoparticles is demonstrated with a variety of systems. Soft landing of molecules is proven by fluorescence spectroscopy and TOF-SIMS identification of deposited dye molecules. Au-nanoparticles (5 - 20 nm) and carbon nanotubes deposited from ion beams were found intact on the surface identified by atomic force microscopy (AFM). *CdS* nanorods (30 nm diameter) and V_2O_5 nanowires (5 nm diameter) observed in AFM after deposition are identified by TOF-SIMS. Estimations of the charge state and the mass-to-charge-ratio show that the nanoparticle ion beams mainly consist of very highly charged particles.