

## O 54: Particles and clusters I

Time: Wednesday 15:00–16:15

Location: WIL C307

O 54.1 Wed 15:00 WIL C307

**Gold clusters at finite temperature: influence of fluxionality on ligand adsorption** — ●LUCA M. GHIRINGHELLI, ELIZABETH C. BERET, JÖRG MEYER, and MATTHIAS SCHEFFLER — Fritz-Haber-Institut der Max-Planck-Gesellschaft, Faradayweg 4-6, 14195 Berlin, Germany

Metal clusters, in particular in relation with their catalytic properties, have been the object of intensive experimental and theoretical studies, in the recent years. A great deal of effort has been devoted by many theoretical groups to understanding the zero kelvin properties of such clusters. Here, by focusing on small gas phase  $Au_N$  clusters ( $3 \leq N \leq 20$ ) and their interaction with CO and O<sub>2</sub> as a showcase, we illustrate a methodology for the study of small clusters and their interaction with atoms and molecules at finite temperature. We combine all-electron density functional theory, including scf-density dependent van-der-Waals tail corrections, with finite temperature sampling techniques, like Biased MD and Parallel Tempered MD. We find an unusual flexibility of the clusters, at room and lower temperature. At certain sizes,  $Au_N$  clusters at room temperature are liquid droplets. This has an important implication, when accounting for the dynamics of ligand adsorption. One has to consider that the energy released by an exothermic ligand adsorption heats up the newly formed complex, and the equilibration with the environment is much longer than the typical timescale for conformational rearrangement. In this respect, the very concept of a preferred adsorption site in the bare cluster might be meaningless.

O 54.2 Wed 15:15 WIL C307

**Small-Angle X-ray Scattering (SAXS) for metrological size determination of nanoparticles** — ●GUDRUN GLEBER<sup>1</sup>, MICHAEL KRUMREY<sup>1</sup>, ARMIN HOELL<sup>2</sup>, LEVENT CIBIK<sup>1</sup>, STEFANIE MARGGRAF<sup>1</sup>, and PETER MÜLLER<sup>1</sup> — <sup>1</sup>Physikalisch-Technische Bundesanstalt, Abbestr. 2-12, 10587 Berlin — <sup>2</sup>Helmholtz-Zentrum Berlin, Albert-Einstein-Str. 15, 12489 Berlin

To measure the size of nanoparticles, different measurement methods are available but their results are often not compatible. In the framework of an European metrology project we use Small-Angle X-ray Scattering (SAXS) to determine the size and size distribution of nanoparticles in aqueous solution, where the special challenge is the traceability of the results.

The experiments were performed at the Four-Crystal Monochromator (FCM) beamline in the laboratory of Physikalisch-Technische Bundesanstalt (PTB) at BESSY II using the SAXS setup of the Helmholtz-Zentrum Berlin (HZB). We measured different particles made of PMMA and gold in a diameter range of 200 nm down to about 10 nm. The aspects of traceability can be classified in two parts: the first is the experimental part with the uncertainties of distances, angles, and wavelength, the second is the part of analysis, with the uncertainty of the choice of the model used for fitting the data. In this talk we want to show the degree of uncertainty, which we reached in this work yet.

O 54.3 Wed 15:30 WIL C307

**Control of ultrafast photoinduced processes at graphene-supported metal clusters** — ●KIRA HINRICHS, MIHAI VAIDA, and THORSTEN MARCO BERNHARDT — Institute of Surface Chemistry and Catalysis, University of Ulm, Albert-Einstein-Allee 47, 89069 Ulm, Germany

A new experimental setup is presented which enables the control of the laser-induced photodissociation of molecules on graphene supported

metal cluster nano-structures. Graphene is employed as a substrate providing a geometric template to obtain a regular array of clusters with equal size and distance for the investigation of field localization effects.

The temporal control of the processes at this system is achieved by photodissociation and detection of the adsorbed probe molecule methyl bromide via femtosecond laser pump-probe mass spectrometry with resonance enhanced multi-photon ionization.

For the additional spatial resolution the fate of the photodissociation products on the surface after the reaction is analyzed by scanning tunneling microscopy. The combination of methyl product mass spectrometry and local surface analysis opens new possibilities to optimize laser pulse shapes for enhanced photoreaction and selective field localization at the surface.

O 54.4 Wed 15:45 WIL C307

**Reactive forcefield for simulating gold surfaces and nanoparticles** — ●DONATO FANTAUZZI, JOHN KEITH, JOSEF ANTON, and TIMO JACOB — Ulm University, Albert-Einstein-Allee 47, D-89069 Ulm, Germany

Due to its special physicochemical properties Gold has reached a wide range in modern-day applications, e.g. in electronics, nanotechnology, and catalysis. This has stimulated many experimental and theoretical studies in the past decades. Unfortunately, theoretical contributions on the QM level of theory are restricted by the computational expense, motivating the development of empirical atomistic interaction potentials to rapidly simulate atomic-level phenomena on larger-scale systems [1]. However, the parametrization of these (semi-)empirical potentials to specific physical data often limits their transferability.

In our work we report how to construct a ReaxFF (reactive force-field) potential from first-principles for broad material applications. After comparing this reactive forcefield to other available forcefields reported in literature, we show that this potential is capable of reproducing qualitatively and quantitatively binding energies and diffusion barrier profiles for surface processes, as well as bulk equations of state. A strict transferability test on effective cohesive energies of molecular clusters indicated the capability to not only study bulk and single crystal surfaces, but also the morphology of Au nanoparticles [2].

[1] M. S. Daw, and M. I. Baskes, *Phys. Rev. Lett* **50**, 1285 (1983)  
[2] J. A. Keith, D. Fantauzzi, T. Jacob, A. C. T. van Duin, *Phys. Rev. B* **81**, 235404 (2010)

O 54.5 Wed 16:00 WIL C307

**CO adsorption on neutral iridium clusters** — ●CHRISTIAN KERPAL, DANIEL HARDING, GERARD MEIJER, and ANDRÉ FIELICKE — Fritz-Haber-Institut der Max-Planck-Gesellschaft, Faradayweg 4-6, 14195 Berlin

The adsorption of carbon monoxide on neutral iridium clusters in the size range of  $n = 3$  to 21 atoms is investigated with infrared multiple photon dissociation spectroscopy. The spectra are obtained by irradiating a molecular beam containing  $Ir_nCO$  complexes with intense, tunable IR radiation from the Free Electron Laser for Infrared eXperiments (FELIX) and measuring the changes induced in the mass distribution. For each cluster size only a single  $\nu(CO)$  band is present with frequencies in the range between  $1962\text{ cm}^{-1}$  ( $n = 8$ ) and  $1985\text{ cm}^{-1}$  ( $n = 18$ ) which can be attributed to an atop binding geometry. This behaviour is compared to the CO binding geometries on clusters of other group 9 and 10 transition metals as well as to that on extended surfaces. The preference of Ir for atop binding is rationalized by relativistic effects on the electronic structure of the later  $5d$  metals.