



Nanoparticles and their environment: an intimate relationship

A talk by Michael Walter

Freiburg Materials Research Center, Albert-Ludwigs-University of Freiburg i. Br., Germany
Fraunhofer IWM Freiburg, Germany

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Michael Walter | michael.walter@mf.uni-freiburg.de

The controlled manipulation of structures on the nanometer scale is one of the key pathways for future technology. Moores' empirical law of the constant downscale in structural features in electronic devices keeps true since nearly 50 years, but will come soon to an end as we will reach the sizes where every atom counts.

Metal clusters represent such systems, where their properties are not anymore similar to the bulk, but are largely determined by strong electronic effects and the shell structure of the delocalized electrons. There is a long history in studies of gas-phase clusters, that produced the basis of understanding for protected clusters, which can be produced by wet chemistry are stable under ambient conditions. These are strongly influenced by their environment, the protection layer, however.

With the help of efficient computers and the corresponding codes the calculation of structural and electronic properties of nanoscale systems based on density functional theory are possible. I will present our studies of interactions between nanoscaled systems in such different environments like the gas-phase, chemically bound ligands, oxide support, explicit ionic liquids as well as in classical polarizable media.