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Monte Carlo Simulation of Supported Silver Nanoparticles on Amorphous Silica Substrate

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Extended Abstract

Metallic nanoparticles, especially transition metals, have a number of exciting potential applications in various fields such as optics, catalysis, electronics and magnetism. Size, morphology and structure of these nanoparticles give them remarkable properties that are not found in bulk materials. We are particularly interested in the case of metallic nanoparticles obtained experimentally by physical vapor deposition on a substrate interacting weakly such as amorphous silica and carbon. Up to now, theoretical studies and experimental data analysis have neglected the influence of this substrate because of its relatively weak interaction with the deposited metal nanoparticles. However, experimental observations show that there is a truncation effect on the nanoparticles.

The context of this work is the thermodynamics of supported metal nanoparticles using Molecular modeling. Monte Carlo simulations were carried out for silver nanoparticles (Ag NPs) supported on amorphous silica substrates using tight-binding potential within the second moment approximation (TBSMA) (Rosato et al., 1989). for the metal-metal interaction. The mTTAM potential is used for silica substrate (Guissani and Guillot., 1996) and Lennard-Jones potential adjusted on DFT calculations and experimental results for Ag-silica interaction.

For free Ag NPs it is known that Icosahedron (Ih) is favorable for small size, monitoring by Decahedron and Truncated Octahedron (TOh) for large size as show by Baletto et al. (2002). Here we performed simulations to study the influence of amorphous silica surface on the structural stability of Ag NPs at zero temperature according to the size, structure, aspect ratio and orientation. We obtain the move of crossover points among structural motifs. The effect of surface roughness in the equilibrium structure is also study for size range of 2 to 5 nm.

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