Molecular simulation study of silver nanoparticles on silica substrate

J. Puibasset[a*], C. Andreazza-Vignolle[a], P. Andreazza[a] and C.Mottet[b]

a. Interfaces, Confinement, Matériaux et Nanostructures, UMR7374, CNRS, Université d'Orléans, 1b rue de la Férollerie, 45071 Orléans cedex 02
b. Centre Interdisciplinaire de Nanoscience de Marseille (CINaM), UMR 7325 CNRS-AMU, Campus de Luminy, case 913, 13288 Marseille, Cedex 9, France

* puibasset@cnrs-orleans.fr

Properties of metallic nanoparticles differ from bulk. Moreover, experimental and simulation data show that the support used to produce these nanoparticles, despite weakly interacting like amorphous silica, may have a non-negligible effect, in particular on the morphology and structure of the nanoparticle [1]. We are thus interested in the prediction of the relative stability of the various structures a supported nanoparticle can adopt.

Considering the typical dimensions of the system (few nanometers), a molecular approach based on effective potentials will be considered. The metal-metal interaction is modeled by a tight-binding semi-empirical potential within the second moment approximation (TB-SMA), the interactions between atoms constituting silica are described by the mTTAM potential, and the metal-silica interaction is based on a Lennard Jones potential, with parameters adjusted on experimental and Density Functional Theory calculations. The support will be varied, in particular its surface nature and roughness.

[1] A. C. Ngandjong, C. Mottet, and J. Puibasset, J. Phys. Chem. C 120, 8323 (2016), J. Phys. Chem. C 121, 3615 (2017)

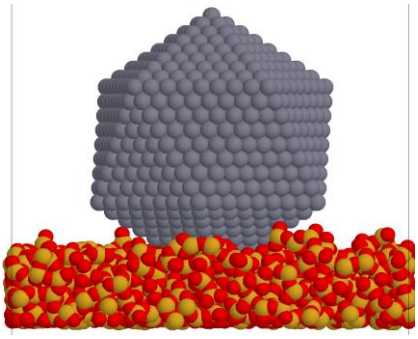

Figure 1 : Silver icosahedron on rough silica support.