Service Interdisciplinaire sur les Systèmes Moléculaires et Matériaux
SÉMINAIRE

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Lundi 09/09/2013, 14h30-15h30

CEA-Saclay ¡b¿¡font color ='red'¿SIS2M¡/font¿¡/b¿ Bât 125, pièce 157

An efficient many-body potential for the interaction of transition and noble metal nano-objects with an environment

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Metallic nanoparticles (NPs) have been extensively investigated in view of their shape- and size-dependent electronic, surface, catalytic, magnetic and optical properties. In order to engineer NPs with a wide variety of shapes, wet-chemical methods are routinely used because of their large-scale cost effective production capabilities [1]. However, the detailed microscopic mechanism behind nucleation and growth of NPs in solvation is far for being completely understood. Gold nanorods (NRs) in particular, i.e. NPs with aspect ratio ¿ 1, provide the perfect example of the delicate interplay of thermodynamic and kinetic effects that occurs in such experiments. These effects include stabilisation of lateral open facets by the environment and the mechanism responsible for the evolution of highly-symmetric crystals into anisotropic structures. Even though it is not clear at the moment if such symmetry breaking mechanism is due to kinetic or thermodynamic effects, simulations based on semi-empirical potentials provide an excellent compromise between efficiency and accuracy in the context of growth simulations [2].

In this talk, we present a semi-empirical model for a generic description of transition metal nano-objects interacting with an environment, which includes a many-body metal-metal interatomic potential given by the second-moment approximation to the tight-binding Hamiltonian, and an additional many-body coordination-dependent potential that affects only the nano-object outer atoms [3]. The model does not refer to a specific type of chemical conditions, but rather provides trends as a function of a limited number of parameters. A large variety of vicinal gold surfaces are considered and their surface energy calculated as a function of these parameters. The study of relative stability of selected monocrystalline and multitwinned gold NPs suggests that the model is robust enough to account for environments in which particles exhibiting different facets and structures stabilise. Finally, the thermodynamic stability of elongated equilibrium shapes is discussed.

References
[1] Viswanath, et.al., J. Phys. Chem. C 113, 16866 (2009)
[2] Jelea, et. al., Phys. Rev. B 79, 165438 (2009)

[3] Cortes-Huerto, Goniakowski, Noguera, J. Chem. Phys. 138, 244706 (2013)

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Le cafe sera servi 10 minutes avant
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