Séminaire LIONS

Mercredi 26 Septembre à 11h, pce. 157, bât. 125

MOLECULAR DYNAMICS SIMULATIONS OF METAL NANOSTRUCTURES: DYNAMICAL STRAIN, INTERACTION WITH A SUBSTRATE AND ENVIRONMENT EFFECTS

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Computer simulations are routinely used to extract quantitative properties of materials that complement and/or support experimental investigations. Several computational approaches have been developed to describe materials at the nanoscale. On the one hand, ab-initio methods stand as highly accurate but are computationally demanding and thus restricted to system of less than few hundred atoms. On the other hand, the interplay of precision, efficiency and flexibility makes of semi-empirical methods a successful strategy to study structure, dynamics and thermodynamics of a wide variety of nanosystems.
In this talk, we discuss some recent extensions and applications of a semi-empirical potential based on the second-moment approximation (SMA) to the tight binding Hamiltonian. First, temperature effects on the breaking and formation of gold mono-atomic chains. Second, the influence of the morphology of MgO substrates on the shape of supported Ag nanoparticles. Finally, we focus our attention to the study of growth of anisotropic nanoparticles in solution.