One Ph.D position (3 years) is open from October 2014 in MACS team/Charles Gerhardt's Institute/Montpellier (MESR Allowance)

Ph.D thesis: Ab initio molecular modelling of bimetallic Au-Pd nanoparticles under reactive gas.

Abstract:

In the field of heterogeneous catalysis, the catalysts optimization depends on the surface composition of bimetallic nanoparticles before and during the reactions. Thus, the understanding of surface segregation phenomenon is crucial especially when this segregation is induced by the presence of gas in the conditions of catalysts preparation and reactions. Indeed, the bonding of adsorbates under reaction conditions may, in some cases, induce modifications of local atomic composition and surface structure, changing the activity and the selectivity of the catalyst. In particular for the AuPd system, in which gold surface enrichment is thermodynamically favored under vacuum conditions, the surface segregation of Pd was reported to occur in the presence of reactive gas such as CO, O_2 [1-2] and atomic oxygen [3].This demonstrates the importance to study structural properties and reactivity of PdAu alloys while considering the gas in the surface environment. Whereas many theoretical works were devoted to the structural characterization of the nanoalloys under vacuum condition, very little is known about the effect of reactive gases on the surfaces [4].

The ambition of the proposed thesis is to identify, on the one hand, the structure and the chemical order of surface nanoalloys in the presence of the adsorbate and on the other hand, to study their reactivity. To this aim, a multi-scale approach based on the combination of Monte Carlo simulation on rigid lattice and atomistic thermodynamics models both based on DFT calculations will be used.

Candidates with Master degree in Chemistry, Physics, Physical-Chemistry, Materials Science Catalysis and motivated by computational chemistry applied to catalysis are invited to send a letter of motivation, CV and 2 letters of recommendation to the contact address.

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