SEMINAIRE ISMO (LCAM - LIXAM – LPPM)

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Structure prediction of free and supported metal nanoparticles

Determining the most favourable structures of nanoparticles is a challenging task. In fact, depending on their nature and environment, nanoparticles can present an enormous variety of possible structures, whose number increases exponentially with size. Here we describe a predictive computational methodology for structure determination. This methodology relies on the combination of global optimization searches with *ab-initio* structural relaxation. Results are presented for both gas-phase binary systems (AgCu, AgNi) and oxide-supported metal clusters (Ag, Au, Ni and PtCo/Mg0(001)). The results are compared to available experimental data.

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