Properties of metal clusters and nanoparticles

« Experiment and simulation in the quest of a complete understanding of the outstanding properties of metal clusters and nanoparticles »

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An astounding number of applications, ranging from plasmonic and biomedical applications to catalysis, are based on the exceptional *properties* of metal nanoparticles, which are very different from the bulk materials. The constant development and refinement of experimental and theoretical tools enables today the treatment of increasingly complex systems, many of which had been until now mostly out of reach due to technical limitations, and their likewise *increasingly complex properties.* Fabrication and characterization now allow for larger quantities, better definition, including better control of structures and properties. At the same time, progress in theoretical methods as well as in computational tools allows for increasingly accurate descriptions of metal clusters.

The mini-colloque proposes to unite theorists and experimentalists who aim to further the understanding of metal clusters' and nanoparticles' properties, based on the study of structure-property relations, the production of benchmark results, and the extension of computations to realistic systems. Questions comprise but are not limited to:

- Methods for an increasingly predictive description of the metal clusters' properties;
- Description of the clusters' surfaces and interfaces which influence their optical, magnetic, and catalytic properties;
- The potential of machine learning techniques in the framework of these studies

The community susceptible to participate comprises notably participants of the GDRs or-nano and « Plasmonique Active » and the IRN Nanoalloys. In addition, the *inherently multidisciplinary field* of metal nanoparticles and structures comprises likewise chemists studying clusters for, in particular, catalysis, as well as some participants of IAMAT.

We propose a mini-colloque with one invited speaker, Hazar GUESMI, ICGM, UMR5253, Montpellier (DFT calculations for surfaces effects in metal clusters) as well as contributions of 15-20 minutes.