MASTER DE PHYSIQUE ET APPLICATIONS - 2ème année
Spécialité Sciences des Matériaux et Nano-objets
International Nanomat Master Program

Internship proposal 2009-2010

Laboratory : Uppsala University, Department of Physics and Astronomy, Division for Materials Theory

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Supported gold nano-clusters as heterogeneous catalysts for oxidation reactions

Scientific project : The imperfect combustion of carbon hydrides produces not only carbon dioxide but a number of other oxides as well, i.e. NOx and CO. Those account for acid rain or are poisonous. Using catalysts to further oxidize these by-products does substantially decrease the negative environmental impacts that come along with these combustion processes. Nowadays palladium and platinum are commonly used catalytic materials. The cheaper and more abundant gold on the other hand is known to be chemically inert in bulk. But two decades ago the catalytic potential of nanometer sized gold clusters was first discovered for the oxidation of carbon monoxide at low temperatures. This finding initiated a wide range of theoretical and experimental work both by physicists and chemists alike, trying to understand the underlying principles, improve the performance, and widening the range of catalytically enhanced chemical reactions. These affords already led to a number of industry-scale applications of gold as a catalyst.

In our ongoing research on the catalytic activity of gold clusters towards CO oxidation we study, for instance, cluster-size effects, the influence of different support materials and co-adsorption of different molecules, e.g. water, on the electronic structure level. Our knowledge of these systems helps to create tailor-made nano-catalysts that lack some of the draw-backs of today's catalysts, such as the need for high temperatures and the sensitivity to moisture.

In the proposed scientific project the student will investigate metal-oxide and metal-oxide/metal supported gold clusters by means of state-of-the-art density functional theory computer codes, running on Sweden's fastest research computer clusters. Depending on the student's interests and previous knowledge a wide range of interesting and challenging problems can be addressed in the project, ranging from solid state physics to surface chemistry. For the time of the project the student will work in one of Europe's biggest and most competitive research groups within computational condensed matter physics. An individual and comprehensive supervision of the student will be guaranteed during his or her stay.

Techniques in use : density functional theory computer codes, e.g. the Vienna Ab-Inition Simulation Package (VASP)

Applicant skills : We expect enthusiasm for computational physics in general, a profound knowledge of quantum physics, a basic understanding of solid state physics and chemistry, and experience with Unix-like operating systems. English is our working language.

Granted internship : no
Possibility for a thesis : yes