EXPLORING ELECTRONIC EFFECTS IN SELECTIVE HYDROGENATIONS BY SINGLE-ATOM CATALYSTS (SACs)

Start : 1st October 2022

Keywords: Density Functional Theory, Single Atom Catalysis, Surface Science techniques

Candidate Profile: Strong background in physics or chemistry or materials science with an interest for atomistic simulations. Good knowledge of quantum mechanics. Experience with Linux environment and python programming will be appreciated. Please send a motivation letter, CV and transcripts, along with names and contact information of two referees.

Context and objectives :

Electronic effects are known to have a great impact on the catalytic properties. While such effects have largely been investigated in traditional catalysts (pure metals and simple alloys), little is known in Single Atoms Catalysts (SACs), i.e. catalysts where the active site (usually a transition metal) is isolated in a solid. The first objective of the work is thus to investigate electronic effects in selective hydrogenations by SACs. The second objective is to design optimal SACs within a given system, by tuning both the active metal M, its loading, and the support in interaction with M. Hydrogenation reactions have been selected for their applied interest, their relative simplicity enabling deep mechanistic understanding, and their need for noble metals as catalysts.

Expected results include a thorough understanding of the relationship between the structure/composition and the catalytic properties, as well as the drawing of a general picture rationalizing the behavior of SACs in several systems to guide the discovery of new low-cost and efficient catalysts.

Methods :

Understanding the atomic-scale surface structure of single atom catalysts is a crucial step on the path toward designing optimal heterogeneous catalysts. We plan to combine surface science experiments and theoretical calculations to facilitate the design and development of single atom materials with fine-tuned catalytic properties. Density Functional Theory will be used to model the systems, guide the SAC selection through high-throughput predictions of SAC reactivity, and help in the interpretation of experimental data (see next paragraph). The theoretical work described above will be completed by an experimental study, consisting in the elaboration of single-atom based systems and investigation by low and variable temperature Scanning Tunnelling Microscopy (STM) and Spectroscopy (STS).

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Location :

The Institut Jean Lamour (IJL, Univ. Lorraine & CNRS) is a lab for fundamental and applied research in materials science; it brings together scientists from different disciplines. The lab is located in Nancy (France), a nice city in the heart of Europe (close to Germany, Belgium, Luxembourg) and direct from Paris by TGV.

This project has an international dimension and takes place within the *Integrated European Center for the Development of New Alloys and Metallic Compounds (https://ecmetac.eu/)*, the research network *Open space between aperiodic order and physics & chemistry of materials* and the International Lab between IJL and the Joseph Stefan Institute (JSI, Ljubljana, Slovenia).