Intitulé du Sujet de Thèse :

Complexes of the First Transition Series : Properties and Reaction Mechanisms

Laboratoire : iSm2, UMR-CNRS-7313

Equipe : CTOM

Directeur de thèse : Pr. Stéphane Humbel

Co-directeur : Dr. Paola Nava

email : paola.nava@univ-amu.fr

Contexte de l'étude

In catalysis today, chemists aim to reduce the use of metals of the second and third transition series, in order to develop the chemistry of the more available and cheaper elements of the first transition series.
This project continues recent efforts that have been made in our group on the catalytic activity analysis of metal complexes, within established collaborations with the experimentalists of our department.

Descriptif du projet

From a computational point of view, the treatment of systems containing these elements elements of the first transition series is not trivial. The aim of this project is to identify a methodological protocol to study properties and reactivities of metal complexes of the first transition series, in particular iron, cobalt and copper. A first aspect to deal with is the possibility to have a multi-state reactivity, as for the case of several cobalt(I) complexes, which are supposed to switch between singlet and triplet states. A second aspect is related to the theoretical treatment of the chemical environment around the metal center. The existence of elaborated molecular architecture has indeed an influence on the spectroscopy, on the accessibility of substrates to the catalytic centers and their reactivity.
These theoretical studies will allow the PhD student to use a large panel of computational methods, ab-initio and DFT, and to manipulate several computing codes (for instance: Gaussian, TURBOMOLE, Molpro).
Beside those applications in theoretical chemistry, our group is involved in some method development projects. An access to this expertise is therefore open.

Références Bibliographiques

1. M. Delorme *et al.*, *Dalton Trans.* **2019**, 48, 15767-15771.
2. P. Nava *et al.*, *Dalton Trans.* **2019**, 48, 17605 - 17611.
3. P. Nava *et al.*, *ChemCatChem* **2015,** 7, 3791.
4. P. Nava, D. Hagebaum-Reignier, S. Humbel, *ChemPhysChem* **2012**, 13, 2090-2096.