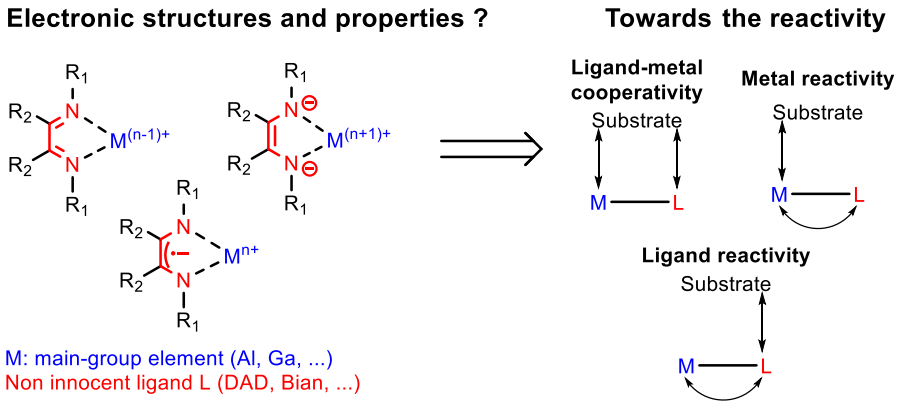
PhD position

Structures, Properties, and Reactivities of Main Group Complexes with Redox-Active Ligands: A Theoretical Study.

Location: Laboratoire de Chimie Théorique, Sorbonne Université, Paris 5e (http://www.lct.jussieu.fr/)
Starting date: October 1st, 2025, during 3 years
Funding: Doctoral contract provided by ED388
Level of education: M2 or equivalent

Summary of the PhD project:

Redox-active ligands (often qualified as "non-innocent" ligands), which act as electron reservoirs capable of donating or accepting one or more electrons, are widely used in catalysis with transition metal complexes. This electronic versatility provides a powerful approach to extend the electronic flexibility of the central element, enabling a broader range of reactions involving multiple oxidation states and diverse coordination environments. In this context, the use of non-innocent ligands can also be extended to **p-block elements**, offering a promising and increasingly explored alternative to conventional transition metal-based catalysts, due to their distinct modes of reactivity.



This PhD project aims to investigate the structures and properties of main group element complexes featuring redox-active ligands using quantum chemistry methods and chemical bonding analysis tools, particularly during reduction processes, in order to better understand the observed reactivities. The M–L or L–M–M–L systems of interest (where *L* is a redox-active ligand of the type X=C–C=Y, with X/Y = O, NR; and *M* is a main group element), whose reactivity is already known, will be investigated using methods for both open-shell systems (doublet, triplet, … states) and closed-shell systems (singlet state) taking account the environmental effects. Descriptors, such as the Lewis acidity of the metal center, the electrophilic/nucleophilic character of these systems, will be considered and correlated with their known reactivity. The reactivity of M-L or L-M-M-L may involve the ligand either directly or indirectly. Investigations of different reaction mechanisms will therefore be considered in order to rationalize the experimental results.

Profile and skills required:

We seek a highly motivated student to join our multidisciplinary research project at the interface of quantum chemistry and molecular chemistry. The successful candidate will conduct innovative computational studies with strong connections to experimental chemistry, requiring regular interaction with experimental collaborators.

The ideal applicant should be currently enrolled in a Master's degree (or equivalent) in computational chemistry, physical chemistry, molecular chemistry or closely related fields. A solid background in molecular chemistry is expected and prior experience with quantum chemistry software (such as Gaussian) would be welcome but not mandatory.

How to apply:

Submit your application via ADUM (https://adum.fr/candidature/) **no later than May 11, 2025**. The application should include a **cover letter**, a **CV** with the names of people to contact for a recommendation and **grades** from the Master's degree (or equivalent).

In parallel, candidates must also contact Dr. Gilles FRISON (gilles.frison@cnrs.fr) et Dr. Stéphanie HALBERT (stephanie.halbert@sorbonne-universite.fr).