Laboratoire de Chimie Théorique - UMR 7616 UPMC/CNRS
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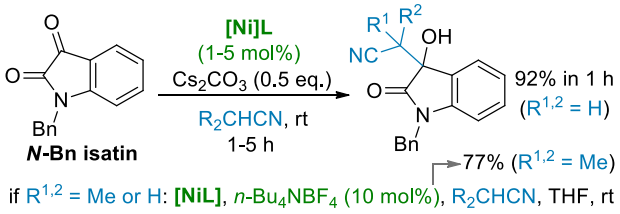
Post-doctoral position

Nickel ate-complexes as ion pairs in catalysis: Computational study of solution structure, synthesis, stability and catalytic activity

Context and objectives:

Nickelate project intends to explore the catalytic behavior of Nickel derived ate-complexes in diastereo- and enantioselective transformations through various C-H functionalization and addition reactions. A cooperative action of ion-pairing species is envisaged with organic cations, as well as a metal complexes, including dual-metal. From a computational point of view, the reaction mechanisms will be tackled based on DFT molecular modelling approaches. This study will be backed to a mass spectrometry determination of reaction intermediates (C Afonso, COBRA, Rouen) and carried out in collaboration with organic chemists experts in ion-pairing (JF Brière, COBRA, Rouen) and in metal catalyzed methodology (I Gillaizeau, ICOA, Orléans). Starting with a model reaction recently developed by the experimental teams (see figure below, *Adv. Synth. Catal.* **2023**, *365*, 156), the DFT investigations aim at describing the complete catalytic cycle at stake in this cyanoalkylation reaction, in order to define kinetically and thermodynamically relevant intermediates and transition states (TS). As the reactant is an ate complex, a special attention will be paid to the description the intra and intermolecular interactions, in order to better understand the factors responsible for activation and selectivity.



Keywords:

DFT, organometallic, reaction mechanisms, ion-pairs, selectivity, nickel

Candidate profile:

The candidate should have a PhD in theoretical chemistry including an expertise in applications of quantum chemistry, and more precisely DFT, to the determination of reaction mechanisms, with a preference for an experience in organometallic reactivity. Additional knowledge or experience in interaction with experimentalists would an asset.

Post-doctoral grant:

The position is a 18 months grant as a Sorbonne University post-dostoral researcher, starting beginning October 2024 financed in the framework of ANR project NICKELATE.

Contact and application procedure:

A full CV and a motivation letter, including the names and information to contact 2 persons who accept to recommend the candidate, should be sent by e-mail to**: helene.gerard@sorbonne-universite.fr.** The same address can be used for further information.