M2R internship in molecular modelling :
Catalytic properties of some specific organocatalysts

Work place : IPREM, Université de Pau et des Pays de l'Adour, Pau, Nouvelle-Aquitaine, France
Keywords: computational chemistry, molecular modelling softwares, organocatalysts
Occupation: Research training

Context

The position is a part of the four year project **HCO_for_LLAC** (Low Loading Asymmetric Catalysis with Helical Chiral Oligoureas) funded by the **ANR** (Agence Nationale de la Recherche). The main aim of the project is to explore metal-free catalysis at (very) low catalyst loading using helically folded ureido oligomers as chiral components of new catalytic systems and to develop the potential of these organocatalysts for challenging asymmetric transformations including carbon-carbon bond forming reactions and enantion-asymmetric polymerization as well as for catalysis in-flow.

Concerning the part devoted to molecular modelling, the objectives are to elucidate the mechanism(s) of action of the catalyst on the reactants and to propose further improvments of its catalytic capabilities. Accessibility to the substrate, electronic and structural features that control the reaction and stereocontrol, as well as energetic profiles, are the informations that can be provided at the QM (Quantum Mechanical) level.

Position and assignment

The position concerns the investigation of the strength of the hydrogen bonds that make the interaction between reactants and catalyst. Theoretical determination of pKa, NBO, QTAIM as well as other indexes to assess the strenghts of the interactions will be carried out on several and different type of organocatalysts. This work will be driven in strong connection with experimentalists of LCPO (Laboratoire de Chimie des Polymères Organiques, Bordeaux) and UPV (University of Pais Vasco, San Sebastian)

Among all, this M2 internship have to be considered as an initiation to the investigation of physico-chemical properties from computational chemistry. Moreover this will provide experiences in bash script coding and data parsing, HPC (High Performance Computing) and bibliographic search.

The selection will be based on excellent academic background in Universities and/or Engineering schools.

Contact advisor

Candidates are requested to address their CV and cover letter to **philippe.carbonniere@univ-pau.fr** and **jean-marc.sotiropoulos@univ-pau.fr**