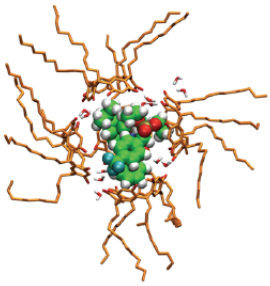
CMC - UMR 7140 Strasbourg

PHD Proposal
Molecular modelling of organometallic catalysts in a self-assembled capsule

Keyword: Supramolecular chemistry, molecular modelling, quantum chemistry, organometallic catalysis



Project: The project ANR HEXCAPS, **will combine experimental studies and molecular modelling of organometallic catalysts hosted in a self-assembled capsule in order to understand the influence of the second coordination sphere of the metal, the cavity walls on catalytic reactions in terms of chemo-, regio- or enantioselectivity.** The catalytic reaction pathways will be computed by means of DFT calculations in the absence of the cage. Additionally, MD simulations will be performed to study the dynamics and complementarity of the catalytic species (capsule + catalyst) and to determine its accessibility to the reactants in solution. Finally, both approaches will be combined through DFT/MM methods to extract the impact of the capsule on the mechanism. Solvent effects on the catalytic mechanism such as the presence of solvent molecules contained inside the capsule will also be explored. Theoretical spectroscopic calculations (such as UV-visible, infra-red, differences in NMR shifts) will be computed and compared to the experimental ones for interpretation, especially for proving that the catalyst is encapsulated inside the cage and not interacting with its surface. The experimental differences induced by the cage on the catalyst spectroscopic properties will be confronted to the computed ones in different situation/conformation extracted from MD simulations which will serve as input for the QM calculations.

Preliminary work can be found in: *Encapsulated neutral ruthenium catalyst for substrate-selective oxidation of alcohols*" S. Hkiri, M. Steinmetz, R. Schurhammer, D. Sémeril, *Chem. Eur. J.*, **2022**, *28*, e202201887

Project context: The PhD (36 months) will start in October in Strasbourg and is funded by the ANR HEXCAPS Project. The "Modélisation et Simulations Moléculaires (MSM)" team is part of the UMR7140 - Chimie de la Matière Complexe (CMC) of the Université de Strasbourg. We are specialized in molecular modelling (classical molecular dynamics and quantum chemistry) applied in the context of complex systems chemistry (new green solvents, supramolecular assemblies, reactivity, spectroscopy). The project is in close connection with the SOCAT team of the Institut de Chimie UMR 7177.

Candidate profile: Master 2 in chemistry or 3rd year of chemistry engineer school with a specialization, if possible, in the field of computational chemistry. Basic knowledge of unix/linux, in atomistic modelling (force field, DFT) and programming are desirable.

Please apply by sending a CV to:
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