PhD Position

Encapsulation of metal transition complexes
in supramolecular cages for tuning luminescence or catalytic properties.

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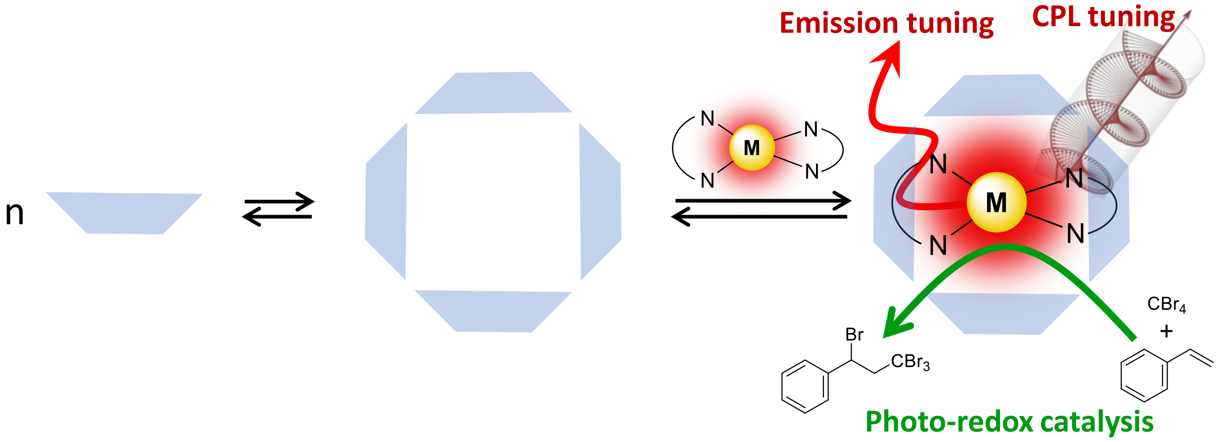
Context.
Molecular capsules and cages are structures enable to encapsulate organic molecules or coordination complexes. They received increasing attention of supramolecular chemists since their cavity provides a bio-inspired confined environment mimicking the reactive pocket of enzymes. Those capsules show large cavities suitable for encapsulation of cations, in particular coordination complexes. Providing confined and controlled environment around a complex owing to capsules, is a promising strategy to tune its luminescence property that can be ultimately enhanced inside the capsule and maintained in the solid state. Besides the interest of solid-state emission for applications in material science, the control of the encapsulated complex reactivity opens application in catalysis. Indeed, confinement of substrates is known to modify a reaction selectivity and to enhance its reactivity. Among the large panel of catalyzed reactions, photoredox catalysis based on an encapsulated coordination complexes, appears promising. Finally, intrinsic chirality of capsules upon introducing chiral bias, opens route towards asymmetric photoredox catalysis and circularly polarized luminescence (CPL). Emitting complexes located in a chiral environment should display CPL, a barely harnessed property that shows applications in CP-OLED, bio-imaging or secured papers.



Objectives. The objectives of this thesis are to study the parameters for a successful encapsulation and the influence of the encapsulation of a complex on its luminescence and photocatalytic properties. Chiral version of capsules will be synthetized and harnessed to implement circularly polarized luminescence or asymmetric catalysis.
Work plan. Following some preliminary results, the first task will include synthesis of ligands, complexes (Cu(I), Cr(III)…) and cages (achiral and chiral versions). Then encapsulation of the synthetized complexes will be studied harnessing a large panel of methods (NMR, EPR, UV-Visible spectrocopies), which will afford understanding of the parameters controlling encapsulation. The emissive properties of the encapsulated complexes will be compared to their non-encapsulated parents in solution and in solid state. Encapsulation effect of photocatalytic activity will be also studied. Finally effect of chiral bias will be investigated (Circular dichroism) focusing in particular on the cage chirality induction, on photocatalysis and on the CPL outcome.

Funding: obtained for 3 years after a competitive examination (programmed on the 1 and 2 of June 2023) in front of the board of the Doctoral School (https://ed563.u-paris.fr/financement/contrats-doctoraux-ed-563/).

To apply, send to benoit.colasson@u-paris.fr and benjamin.doistau@u-paris.fr your **CV**, the **name of two former advisors** and the **transcript of the marks** of your Master degree (1st and 2nd years).
The academic record is one of the main criteria for the final selection.

Online application after acceptance until 3rd of May 2023