PhD position

Modeling of chromophore layers on a silica nano-helices for advanced light emitting application.

Location: Laboratoire de Chimie (LCH), ENS de Lyon, France
Duration: 36 months
Starting: autumn 2026
Contact: Tangui Le Bahers (tangui.le_bahers@ens-lyon.fr) and Arnaud Fihey (arnaud.fihey@univ-rennes.fr)

Context:

The ChirExCo project, funded by the PEPR Luma, aims at understanding the mechanism of chiral induction from silica nano-helices to a chromophore layer adsorbed on its surface (Figure 1). The experimental observation made of this phenomenon points toward a role of the supramolecular assembly of the chromophore layer. However, the mechanism of this chirality induction is still unknown. The ChirExCo project brings the expertise in material science and excited states modelling of four teams (LCH (Lyon), CEISAM (Nantes), ISCR (Rennes) and ICR (Marseille)) to unveil this mechanism. The 11 permanents researches involved in the project and the 3 PhD students recruited will work together to build a multi-scale modelling of the system to bring the understanding the chirality induction mechanism.

Objective of the PhD:

The PhD student recruited at the LCH (Lyon) will strongly collaborate with the ISCR (Rennes). Her/his objective will be to build tools to create an atomic model of the silica helices and the chromophore layer adsorbed on them, relying on available experimental characterizations. Different levels of modelling will be used, from molecular mechanics and tight-binding-DFT to DFT. With these tools in hand, the PhD student will have to create several structures of different sizes of silica-helices covered by different kinds of chromophores. Rationalization of the electronic communication between the two parts and of the inter-chromophore interactions will be the first objective, but the simulation of the optical properties of these complex systems will be also considered. These studies will be conducted in parallel with the work of other collaborators of the project focused on the construction of accurate quantum mechanics protocols to simulate the chiroptic responses, and will be refined based on feedback and discussions.

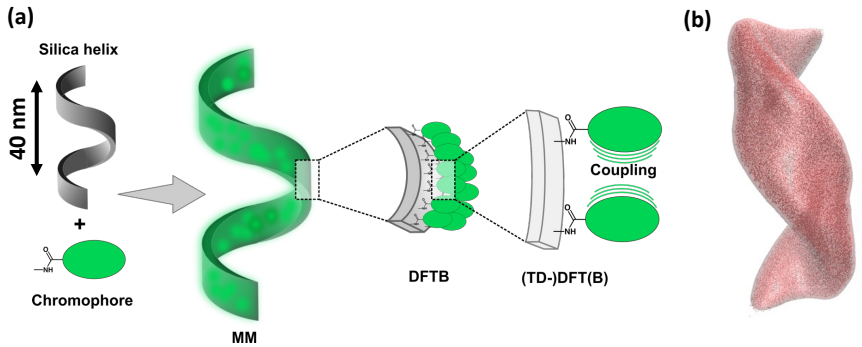

Figure 1: (a) scheme of the system and modeling strategy. (b) first trial of the atomic model of the silica nano-helice.

Candidate skills:
The PhD candidate must have a solid training in physical-chemistry and in computational chemistry as long as a Master degree. Knowledge in programming (Python mainly) is mandatory. The candidate must be able to take initiative and work in a very collaborative manner.

Application process:
Interested candidates can contact Tangui Le Bahers and Arnaud Fihey, providing a CV and a cover letter.