PhD Thesis 2026-2029

CHIRAL PROPERTIES OF ACHIRAL MOLECULES ON CHIRAL SURFACES

DESCRIPTION: PhD position in theoretical chemistry for 3 years starting Oct 1st 2026.
Financed by the PEPR LUMA – **ChirExCo** project

LOCATION: Principal **ModES:** *Modelling & Spectroscopy* — CEISAM, UMR CNRS 6230 Nantes University
Secondary **CTI:** *Theoretical Inorganic Chemistry* — ISCR, UMR CNRS 6226 Rennes University

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PROJECT OVERVIEW

This PhD thesis is part of the **ChirExCo project which aims to develop a multiscale modelling procedure to understand the origin of the chirality induction from chiral surface** (e.g., helical silica) **to achiral adsorbed molecules.** The induction of chirality in achiral chromophores via adsorption on helical silica has been demonstrated experimentally by several groups and applied, for instance, in circularly polarized light (CPL) emission. It has also been observed that the efficiency of this induction is related to the packing density of the adsorbed molecules. While the phenomenon is well documented, the underlying mechanism of this chirality induction is still unknown. The proposed PhD thesis will take place in the framework of this project involving theoretical chemistry teams in Lyon, Marseille, Rennes and Nantes.

RESEARCH PROGRAM

The recruited PhD student will be involved in the second work-package of the program, which aims to **develop a reliable computational protocol to predict, for organic chromophores, both chirality quantifying factors (g_{abs} and g_{lum}) resulting from excitonic couplings**. This will require the student to adequately select the computational approaches needed for all computational steps. More details on the three envisaged steps (ca. 1/PhD year) are listed below.

The first task will be to define a TD-DFT protocol for obtaining accurate g_{abs} and g_{lum} values for nearly-isolated (i.e. solvated in apolar media) intrinsically chiral dyes. In a first phase, the PhD student will perform vertical calculations of chiroptical properties of a series of experimentally-relevant chromophores using several TD-DFT schemes and compare the responses to those obtained with reference wavefunction approaches. A few adequate functionals will be selected, with a special focus on long-range effects, essential for the following. In a second phase, the PhD student will use experimentally available values for chiroptical spectra and responses (g_{abs} and g_{lum}) and model them accounting for vibronic effects inspired by literature. Various vibronic schemes will be assessed using not only band shapes but also absolute response values as metrics.

Since the experimental response to be modelled originates from a collective chiral response of intrinsically achiral molecules, likely due to an excitonic effect, the PhD student will design an approach to tackle this scenario. In this context, two types of dimers should likely be considered: homodimers of chiral molecules so as to ensure perfectly degenerate excited states and heterodimers composed of one chiral molecule and one achiral dye yet presenting similar excitation energies. Various relative geometries corresponding to, e.g., *H* and *J* aggregates will be modelled. For all cases, reference calculations will be achieved using the model resulting from the first task. It is likely that using heterodimers will offer first insights into chiral induction: can the response of such a dimer exceed that of a single chiral molecule? In the second stage, the PhD candidate will build an excitonic coupling model suited for the larger (real) systems. The performances of TD-DFT, sTD-DFT, and TD-DFTB will be compared so as to evaluate the performances of the two latter.

In this final step, the PhD students will use realistic systems coming from partners of the project to evaluate chiral induction by the surface on a cluster of achiral dyes. Again, two steps will be considered, each requiring embedding strategies. First, electrostatic embedding will be used for the absorption since such techniques are available, allowing effective comparisons between an actual dimer and excitonic models. Second, for emission (g_{lum}), the PhD student will next design an approach allowing self-consistently obtaining the environmental charges for the considered excited state. In both cases, the environmental parameters will be provided by the Partner in Lyon.

During the course of the PhD, several stays in the ISCR laboratory in Rennes will take place in order for the PhD student to gain/increase their expertise in multi-reference calculations and TD-DFTB approaches.

CANDIDATE PROFILE

- A recent Master's degree (or equivalent) in Chemical Physics, Physical Chemistry, Theoretical Chemistry, Theoretical Physics, or a related discipline.
- Experience with at least one recognized computational molecular chemistry software (e.g., Gaussian, TurboMole, ORCA…) is an asset.
- Analytical and problem-solving skills, with a proactive and motivated mindset.
- Ability to work both in a research team and independently.
- Excellent communication skills, both written and verbal.

APPLICATION PROCESS

Interested candidates can contact direct Denis.Jacquemin@univ-nantes.fr and boris.leguennic@univ-rennes.fr for additional information. If possible, please send the following:

1. A cover letter outlining their research interests and motivation
2. A CV with relevant academic and research experience
3. Contact details of two references

Note that the actual applications will have to be carried out through the Nantes University portal, once open for the next PhD call.