Internship M2 Chemistry or Physics
2022/2023

- Period of the internship: February 1– July 31

- Gratification of the internship : yes

- Laboratory : **Institut des Sciences Moléculaires d'Orsay (ISMO) UMR 8214 Bâtiment 520, Université Paris-Saclay**.

- Responsable for the internship:

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- Proposal:

Tittle : Quantum Dynamics in condensed phase:
Charge transfer in biological systems and organic photovoltaics (Theory)

Summary :

Industrial processes involving chemical reactions are typically controlled by macroscopic parameters, such as temperature or pressure, which often results in a huge waste of energy and the massive production of unwanted by-products. These mentioned drawbacks feature two major societal issues: non-renewable energy consumption and pollution. For instance, most energy production relies on fossil fuels, which are limited sources and generate CO_2, a greenhouse-effect gas that induces perturbations of planet's climate.

On the other hand, it is well-known that **photosynthetic organisms** absorb solar photons, the energy of which they employ to live and multiply. In order to harvest and utilize efficiently this energy, photosynthetic organisms have developed a sophisticated apparatus. The absorption of an incoming solar photon by light-harvesting pigments is followed by a rapid transfer of the resulting excitation energy to the reaction centers, in which photo-initiated electron transfer reactions and proton transfers achieve the ultimate transduction of the solar energy into chemical potential energy. A fascinating property of these **natural systems is that they perform this task with a very high efficiency**, even with defects and energy traps due to static and dynamic disorder, a property, which has not yet been achieved in artificial systems. **The success rate of the process is amazing and probably due to the optimization of quantum effects.**

The goal of the internship will be, in collaboration with Prof. Xiang Sun (Shanghai) to simulate the quantum dynamics of the charge transfer in several organic and biological systems, inspired by nature, in solvent. We will use the ML-MCTDH (Heidelberg package, collaboration with Prof. Oriol Vendrell) approach to perform quantum simulation of the full systems. **We will make a link between quantum effects and chemical structure-function (relative positions of the electronic states, strength of coupling), i.e. to formulate general principles that govern the efficiency on the basis of quantum interference in artificial photosynthesis.**

The goal is to try to mimic photosynthesis to propose to chemists to synthesize new systems that could greatly optimize photovoltaics.

- Fields :

Theory Chemical Physics Biophysics