PhD position at Laboratoire de Physique et Chimie Théoriques, Nancy, FRANCE

MODELLING THE MOLECULAR MOTION IN AGGREGATES: NANOMATERIALS FOR PHOTOTHERMAL THERAPY

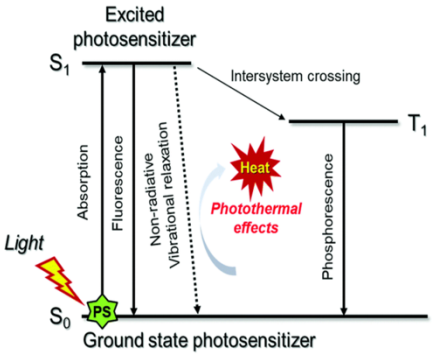

Figure 1. PTT scheme

Photothermal therapy (PTT) uses photosensitizing agents that accumulate in the tumor site to generate heat from light, causing the ablation of tumor cells by rapidly increasing the local temperature. As depicted in Figure 1, following light absorption, the photosensitizer (PS) undergoes rapid internal conversion to the lowest excited singlet state (S1). This latter state can decay back to the ground state by a radiative mechanism (fluorescence) or through nonradiative relaxation pathways. Intersystem crossing to a triplet state, typically T1, is also possible. Photothermal effects (i.e., heat generation) generally arise as the result of nonradiative relaxation processes. Various inorganic materials have been used as photothermal agents, including golden nanorod, graphene, and MoS_2 nanosheet. Interestingly, the supramolecular assembly of organic dyes can also be applied as PTT materials, offering the advantages of low long-term biosafety risk, high biocompatibility, and high biodegradability. The PhD project, in collaboration with an experimental group which will prepare and test the PTT agents, will focus on the application and generalization to the case of PTT aggregates of a multilevel computational strategy, recently developed in the framework of the collaboration between LPCT and ICCOM-CNR in Italy, capable to tackle the variations of the photophysical properties going from the molecule in solution to the supramolecular aggregates. In this mixed quantum-classical approach, the electron-vibrational coupling, the effect of interstate couplings among low energy quasi-degenerate states, the non-bonded electrostatic interactions among the chromophores and with the environmental solvent molecules and the dynamical effects are simultaneously accounted for.

Duration and start date: 3 years, starting from 01/10/2022

The candidate should possess or should be about to obtain a Master's degree in Physical Chemistry, Physics, Chemistry or Engineering with at least merit or distinction (passing grade >= 12/20 in the French system). It is highly desirable to have skills in numerical simulation/molecular simulation or a high motivation to learn, skills in programming (Fortran, Python) or a high motivation to learn.

Applicants should send a complete CV as well as the contact information of at least two references to Mariachiara Pastore mariachiara.pastore@univ-lorraine.fr