





PhD position in photophysics at the Institut des Sciences Moléculaires d'Orsay,
Paris-Saclay University (France)

## PHOTOPHYSICAL INVESTIGATIONS OF MOLECULAR SYSTEMS LEADING TO SINGLET FISSION PROCESS

**Project description:** Singlet fission (SF) is a spin-allowed process involving at least two organic chromophores in which a photo-generated singlet excited state ( $S_1S_0$ ) can spontaneously down-convert to give two lower-energy triplet states ( $T_1+T_1$ ) with a theoretical quantum yield of triplet formation up to 200%. Hence, it offers the possibility to generate two excited states by the absorption of only one photon. SF has thus recently received a strongly growing interest for solar energy conversion. Despite numerous efforts on SF research, the number of chromophores able to generate SF is still limited and actual pathways followed by the system to reach individual triplets remain yet unclear. Understanding such fundamental processes leading to singlet fission stands as the stepping-stone toward the development of more efficient photosystems for solar energy conversion.

The objective of the PhD is to contribute to the elucidation of the SF mechanism within acenes and rylenes which are well known to exhibit SF. Different spectroscopic techniques (steady-state absorption and emission spectroscopies as well as nanosecond/femtosecond transient absorption) will be employed to investigate the nature of intermediate states and photophysical processes upon photoexcitation leading to SF. Several main factors including energetic parameters (endothermic/exothermic processes) and strong/weak coupling between states will be considered. Most studies will be conducted in solution, contribution to gas phase experiments or cross-comparison are planned. In parallel, dedicated theoretical developments will be performed in the group, within the ANR funding project, to support the interpretation.

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**Required Skills**: The candidate should have a background in chemistry or physics, along with experience in spectroscopy and/or photochemistry. She/he should be able to work independently and possess interdisciplinary collaboration skills.

**Duration of the contract:** 3 years, starting from 1 October 2024.

Funding: Doctoral contract will be financed by the French National Agency of Research (ANR)