Thesis Proposition

Molecular dynamics and electronic structure simulations of photoexcited chromophores in the gas-phase and complex environments

Laboratory: Institut de Chimie Radicalaire, ICR, UMR 7273
Facultés des sciences, Aix Marseille Université, Marseille

Thesis supervisor: Pr Mario Barbatti

Contact person: mario.barbatti@univ-amu.fr

A major challenge in the twenty-first century is to increase global food production. Central to this problem is the necessity to increase the yield of numerous important crop species and to find ways to extend geographical locations suitable for agriculture. Cold stress is an environmental extreme that hampers crop yield. This project is part of the BoostCrop FET-OPEN consortium, which aims at developing a novel approach to improve crop yields by protecting plants from cold stress. The approach is based on 'molecular heaters'; nature-inspired molecules that absorb light at wavelengths that are either harmful to the plant or not used in photosynthesis and converting this light energy to heat.

The goal of this research project is to develop models for nonadiabatic excited state dynamics of chromophores in isolation and in complex environments. Comparison of computer simulations with experimental data will establish structure-dynamics-function relationships, and thus a molecular rationale for photon-to-molecule heaters. Such knowledge will also enable tuning the absorption profiles to be compatible with leaf photosynthetic machinery.

The doctorate work will focus on electronic structure calculations of chromophores in the gas-phase and in complex environments. These calculations will run in tandem with the experiments by our coworkers. The doctorand will also help develop models for the nonadiabatic relaxation of the photon energy absorbed by the chromophore. These calculations will be carried out through a two-pronged strategy involving: i) static techniques for determining conical intersections, excited state critical points, and reaction pathways connecting them; and ii) nonadiabatic dynamics simulations. The nonadiabatic relaxation models will determine how the photon energy is converted into ground state vibrational energy (heat) and how possible chemical functionalization will aid retention of excess vibrational energy near the cellulose wall.

Duration: 36 months
Contract: AMU
Funding: FET-OPEN BoostCrop
Starting date: 1 October 2019