Research Project

The general aim of the PRIN project “From natural to artificial light harvesting systems: unveiling fundamental processes towards a bio-inspired materials design (HARVEST)” is to reveal the molecular mechanisms of light harvesting in pigment-protein complexes and understand whether quantum coherences in photosynthesis play a biological role, providing the living organisms with a competitive advantage; to test whether similar mechanisms apply also in artificial LH systems, and can be exploited, in a bio-inspired approach, to optimize their performance; to provide a unified and quantitative theoretical description of the role of quantum coherences in LH systems, also using tools of quantum information theory.

In this framework, the hired researcher will perform computational modeling of light harvesting materials in collaboration with the other PRIN partners (Politecnico di MILANO, Università di PISA, Università degli Studi di ROMA "La Sapienza", Università degli Studi di VERONA, Consiglio Nazionale delle Ricerche).

The structure of natural and synthetic light harvesting systems (LHSs) will be obtained by means of classical Molecular Dynamics (MD) simulations, exploiting available experimental results. The task may involve considering an appropriate solvent, solvated membrane or surface, exploring the free energy landscape with adequate sampling techniques and identifying the relevant structural fluctuations in the chromophore region. A further refinement of the resulting trajectories with short QM/MM dynamics of selected pigments might be required to achieve a more accurate description of their geometrical fluctuations as well as of the coupling between their excitations and the intra- and inter-molecular vibrations of the system. The evolution in time of excitation will be used to simulate ultrafast two-dimensional electronic spectroscopy (2DES) spectra, in order to provide an interpretative support of the experimental results obtained by the partners at Politecnico di Milano.

Activity Plan

The post-doctoral researcher will be engaged in the following activities in collaboration with the supervisor and the project team:

1) Prediction of the structure and the nuclear dynamics of LHSs via classical and hybrid MD simulations;
2) Quantum Chemistry calculations of excited and ground state electronic properties of LHSs and of their dynamic fluctuations;
3) Simulations of 2DES spectra;
4) support project implementation both within the local unit and at project level;
5) support the local unit in other activities related to the implementation of the project.