

## DESCRIPTION FOR THE GENERAL PUBLIC

Fluorescent dyes constantly remained in the limelight of science during the past decades due to their numerous technological applications. Indeed, fluorescent dyes pave the way not only to applications in fluorescence microscopy, but can also be used as biomarkers, laser dyes, or as the key building blocks in organic light emitting diodes (OLEDs). Nonetheless, biomedical applications of many popular fluorescent dyes is greatly impeded by their limited range of absorption and/or emission that is typically centered in the visible range, whereas optimal absorption and emission wavelengths are located in the near-infrared (NIR) region, that is in the so-called biological window. In addition dyes presenting large separation between their absorption and emission bands, that is, large Stokes shift are extremely desirable. In this context, excited-state intermolecular proton transfer (ESIPT) can be a valuable phenomenon to help producing more effective fluorescence dyes. Indeed, in these dyes, the absorbing and emitting structures are strongly different, which helps increasing the Stokes shift. Indeed, unlike most organic fluorophores, ESIPT dyes are characterized by unusually large Stokes shifts (exceeding  $5000\text{ cm}^{-1}$ ). These dyes also present large fluorescence yields, that is they are bright, even at high concentrations, which paves the way to numerous applications in optoelectronics and medicine.

Despite numerous studies, the accurate characterization of ESIPT remains a challenge for both experiment and theory. This transfer is ultrafast and takes place in the excited state, and, consequently, experimental means cannot easily probe ESIPT. In turn to optimize the emission signatures of ESIPT dyes, one needs to maintain a specific balance between relative free energies of both tautomeric forms, what is possible only with the use of very refined theoretical approach able to accurately describe all species simultaneously.

The importance of presented topic prompted the applicant of the present proposal to propose a comprehensive theoretical and modeling photophysical studies on ESIPT mechanism in an important series of compounds, the so-called HPIP series for which many experimental characterization have been made, but only a few theoretical characterizations.

This project encompasses many quantum mechanical calculations (mainly with Time-Dependent Density functional Theory, TD-DFT, a very popular method to obtain absorption and emission) aiming at predicting the structural, energetic and spectral properties of ESIPT dyes so as to design of novel dual emitters based on HPIPs dyes.