Playing with ESIPT dyes and embedded bilirubine thanks to computationnal tools

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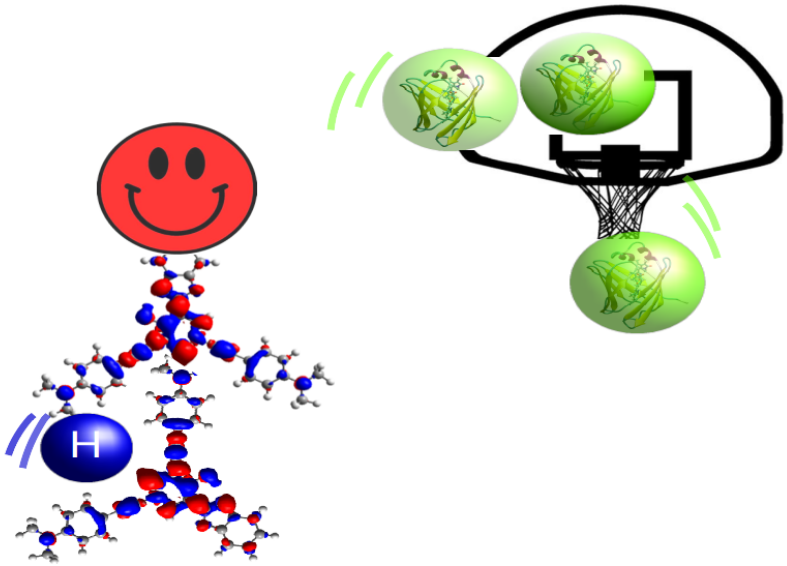
Light-sensitive compounds are playing a central role for establishing precise control over the properties and functions of chemical, material and biological systems. In the present talk, I will present two different systems were are dealing with using computational methods, and more particularly Time-Dependent Density Functional Theory (TD-DFT), Molecular Dynamics simulations, and hybrid quantum mechanics and molecular mechanics (QM/MM) methods. Firstly, dyes undergoing excited state intramolecular proton transfer (ESIPT) will be presented showing how theoretical works can help chemists to design new compounds. [1,2] Secondly, the first critical steps towards the understanding of the impact of a single mutation in a protein onto fluorescence intensity will show you how the global structural change tune the optical properties.[3]



[1] Y. Houari, A. Charaf-Eddin, A. D. Laurent, J. Massue, R. Ziessel, G. Ulrich, D. Jacquemin, *Phys. Chem. Chem. Phys.* **2014**, 16, 1319.

[2] Y. Houari, S. Chibani, D. Jacquemin and A. D. Laurent *J. Phys. Chem. B*, **2015,** 119, 2180.
[3] M. Asad and A. D. Laurent, *Phys Chem Chem Phys*, **2021**, submitted.