"JOURNEY IN EXCITED STATES OF DYES AND PHOTOCHROMES"

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May 07, 2021 (Friday)
12pm (BRT time) - Google Meet

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with the words "Adèle Laurent – Virtual" on the "subject"
Deadline: May 05, 2021 (Wednesday), 06pm (BRT time)

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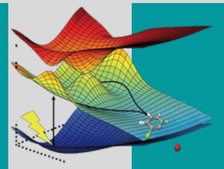

ABSTRACT

Journey in excited states of dyes and photochromes

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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 this communication, I will present several applications of Time-Dependent Density Functional Theory (TD-DFT) with a first focus on dyes undergoing excited state intramolecular proton transfer (ESIPT).[1,2] Second, solvatochromism effects will be analyzed using a set of complementary approaches, including empirical solvent parameters, high-level calculation of the excited-state dipole and polarizability, several flavors of the implicit and explicit solvent models.[3,4] Third, I will illustrate the recent investigations on donor–acceptor Stenhouse adducts (DASA) and Iminothioindoxyl (ITI) new photochromes which have been performed in close collaboration with spectroscopists.[5,6] DFT and TD-DFT calculations succeed to get a deeper insights to ultrafast time-resolved pump-probe spectroscopy in both the visible and IR region for both photochromes. Such an interplay allowed us to understand their mechanism aiming at tuning their optical properties. ITI being the most promising photochrome operates with fully visible light, exhibits a large separation of absorption bands between the two isomers, and is soluble in water. Such features makes ITI promising switches to photo-controlled systems for a wide variety of biological applications that require fast responsive functions.

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