Photoinduced processes under constraints: a theoretical insight.

Laura Le Bras,[1] Laure Jourdain de Thieulloy,[1] Aurélie Perrier[1,2]

[1] *Institute of Chemistry for Life and Health Sciences (i-CLeHS), Chimie ParisTech, PSL Research University, CNRS, F-75005 Paris, France*
[2] *Université Paris Cité, F-75006 Paris, France*
Email: aurelie.perrier-pineau@u-paris.fr

Controlling the optical properties of materials is a considerable challenge for high-tech applications. In addition to the choice of efficient molecules (capable of absorbing or emitting in a particular region of the spectrum with high efficiency), it is important to consider the effect of the environment (solution, aggregate, crystalline environment, or polymer matrix) on the targeted properties. We therefore propose to rationalize the interactions that can exist between photo-induced processes (absorption, emission, photochemical reactions) and the environment, with the help of theoretical models based on quantum chemistry (DFT and TD-DFT calculations) and molecular modeling (classical molecular dynamics). In this presentation, we will first be interested in the modelling and the rationalization of the aggregation-induced emission (AIE) and crystallization-induced emission (CIE) photophysical phenomena. [1-4] Then, we will be interested in the properties of photonastic systems. These materials can convert light energy into mechanical energy and are the subject of pre-determined and repeatable deformations in response to light stimuli. This phenomenon is usually associated with plants and flowers, whose petals open in the daylight and close in the evening in response to a light stimulus. Among these materials, light-responsive polymers, composed of photochromic molecules embedded in a polymer matrix, are of high interest and have been recently proposed for a wide range of applications in microfluidics, biomedics, soft robotics and motors. After presenting the tailored computational protocol that we have developed to propose a realistic description of these systems, we will discuss (i) the impact of the polymer matrix on the photochromic properties of the photoswitch and (ii) the impact of the photochromic reaction on the polymer environment. [5]

[1] L. Le Bras, C. Adamo, A. Perrier, *J. Phys. Chem. C,* **2017**, 25603–25616.

[2] L. Le Bras, K. Chaitou, S. Aloïse, C. Adamo, A. Perrier, *Phys. Chem. Chem. Phys*., **2019**, 46-56

[3] L. Le Bras, C. Adamo, A. Perrier, *ChemPhotoChem,* **2019**, 794-803.

[4] L. de Thieulloy, L. Le Bras*, B. Zumer, J. Sanz Garcia, C. Lemarchand, N. Pineau, C. Adamo, A. Perrier, C*hemPhysChem***, 2021**, 1802

[5] L. Le Bras, C. Lemarchand, S. Aloïse, C. Adamo, N. Pineau, A. Perrier, *J. Chem. Theory Comput.* **2020,** 11, 7017–7032