Postdoctoral position

MODELING PHOTONASTIC MATERIALS: INSIGHTS FROM THE MOLECULAR SCALE.

DESCRIPTION

Photonastic materials 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.

Researchers have recently proposed bio-inspired photoactuator devices based on crystals, liquid crystals, metal-organic framework, or polymers. In this project, we are interested in bio-inspired polymeric photoactuator devices which can have applications in microfluidics, biomedics, soft robotics and motors. The keystone of these systems is the **insertion of photoactive molecule within polymer films**. These molecules can undergo reversible photochemical reactions between two isomers that present different physico-chemical properties and, most often, significant structural modifications that can stimulate a large macroscopic shape-change in disordered or amorphous materials. While the number of experimental studies dedicated to photonastic materials, and more specifically to light-responsive polymers, is exploding, only few theoretical studies are dedicated to their investigation. Yet, their macroscopic behavior is likely dictated by atomistic/molecular scale processes, making computational chemistry the appropriate tool for understanding the unequivocal correspondence between the state of the photochrome and the shape of the film.

In this project, the aim is to identify the key parameters at the molecular and supramolecular scales involved in the mechanical response of a photoresponsive polymeric thin film. The challenge is to rationalize the multiscale mechanisms underlying these phenomena, namely the ultrafast photochromic reactions at the molecular level, the momentum transfer to the surrounding matrix, and after a cascade of processes, the long-term polymer relaxation which yields the macroscopic experimental deformation. The postdoctoral fellow will be responsible for describing the coupling between the photochromic reaction and the consequent behavior of the polymer matrix up to ~ 10 ps. To this purpose, he/she will rely on quantum chemistry and classical molecular dynamics. More precisely, to simulate the photochemical reaction and the polymer intramolecular relaxation simultaneously, we propose to derive a purely classical molecular mechanics model for the photoswitches under investigation in both their ground and first excited states. Electronic excitations and decay will then be mimicked in the course of MD simulations by switching between these two potential energy surfaces. The postdoctoral fellow will be involved in the implementation of this coupling strategy in STAMP, a MD code developed at the CEA/DAM, in collaboration with the developpers.

[1] Lemarchand, C. A.; Bousquet, D.; Schnell, B.; Pineau, N. J. Chem. Phys. 2019, 150 (22), 224902. https://doi.org/10.1063/1.5065785. https://doi.org/10.1063/1.5065785.

[2] Le Bras, L.; Lemarchand, C.; Aloïse, S.; Adamo, C.; Pineau, N.; Perrier, A. *J. Chem. Theory Comput.* **2020**, *16* (11), 7017–7032. https://doi.org/10.1021/acs.jctc.0c00762.

SKILLS

The candidate should have a PhD in Computational Chemistry and a good experience in the application of theoretical methods for photochemical processes. The postdoctoral fellow will mainly use Time-Dependent DFT (TD-DFT) and Molecular Dynamics simulations. Experience in the Force Field parametrizations would be highly appreciated, and programming skills are expected.

DATES AND DURATION

15 to 18 months of post-doctoral position, depending on the experience of the candidate.

The research will be carried out at the Institute of Chemistry for Life and Health sciences (i-CLeHS), Chimie Paris Tech, 11 rue Pierre et Marie Curie, 75 005 Paris, France

The project is funded by French National Research Agency (ANR). The contract will begin in February 2022.

CONTACT

Send CV + motivation letter + recommendation letter to:

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