PhD Proposal

MODELING PHOTONASTIC MATERIALS: FROM THE SUPRAMOLECULAR TO THE MESOSCOPIC SCALES.

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.

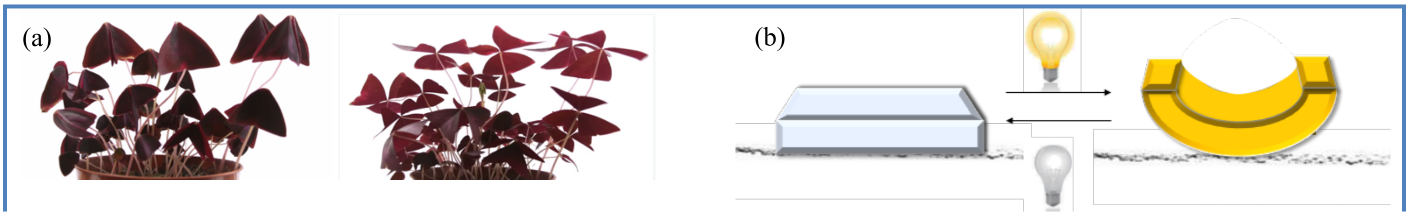

Figure 1 : (a) Illustration of the photonastic motion of Oxalis Triangularis. The leaves open and close in response to sunlight exposure. (b) Schematic representation of a light-responsive shape-changing polymer.

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 supramolecular and mesoscopic 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 objectives of the PhD project are therefore to use the methodology previously set up [1,2] to study the influence of two parameters on the **supramolecular part of the photonastic process**: (1) the type and the strength of the interaction between the photoswitch and the polymer chains because it impacts the energy transfer from the photochrome to its surroundings; (2) the distance between the photochromes in the polymer film, a quantity related to the photochrome/polymer ratio. A last objective of the thesis is to model the **mechanical response** of the polymer over a longer time, up to the microsecond, using **coarse grain methods.**

[1] Lemarchand, C. A.; Bousquet, D.; Schnell, B.; Pineau, N. *J. Chem. Phys*. **2019**, 150 (22), 224902. 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 master/academic degree in Physics, Physical Chemistry or Chemistry. She/he should have a good background in physical chemistry and be interested in physics and continuum mechanics, or have a background in continuum mechanics and be interested in physical chemistry to deal with both the **atomistic and mesoscopic simulations**. She/he must have done a previous research project (Master 1 or Master 2 internship) in mechanical modeling, material modeling, molecular modeling, or computational chemistry.

DATES AND DURATION

The project is funded by French National Research Agency (ANR). The contract will begin in October 2022 for a period of 36 months.

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 and at the CEA DAM Ile-de-France, 91680 Bruyères-le-Châtel, France. The PhD candidate will be supervised by Dr. Claire LEMARCHAND and Dr. Aurélie PERRIER.

CONTACT

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For more information before applying, you can contact:

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