PhD Proposal

Quantum Mechanical Investigation of Light-to-Mechanical Energy Conversion in Molecular Photoswitches.

DESCRIPTION

Polymer-Based PhotoActuators (**PPA**s) are polymer matrix materials doped with molecular photoswitches. Upon irradiation, **PPA** films undergo a reversible macroscopic mechanical deformation, making them attractive systems for the **transduction between light and mechanical energy,** with possible applications in motors, drug delivery devices, textiles and electrical generators. Recent experimental studies demonstrated a **quantitative correlation between the molecular photoswitch properties and the photomechanical effect**.[1] In addition, material structuration plays a crucial role both at the supramolecular scale (through interactions between the photoswitch and the polymer chains) and at the microscale, enabling the conversion of molecular deformation into local strain and ultimately macroscopic actuation.

The SIMULACTOR project aims to develop an integrated multiscale approach to model the mechanical behavior of PPAs. Its objective is to understand and optimize PPA properties using a simulation strategy that spans from the molecular scale (*ab initio* calculations) to continuum approaches, thereby accounting for the different levels of complexity present in real materials. The PhD student will focus on the **molecular scale** to model and optimize the optical and mechanical properties of both the **photoswitch** and the **photomorphon** (the photoswitch and its neighboring polymer chains**)**, the latter governing how the photoinduced strain is transmitted to the surrounding material through photochrome/polymer interactions.

To this end**, quantum mechanical (QM)** methods will be employed. The PhD student will first) assess the efficiency of light-to-mechanical energy conversion by adapting **excited-state mechanochemical analyses**[2] to quantify the fraction of absorbed light energy effectively converted into mechanical work. In parallel, the influence of the local polymer environment (the "photomorphon") on photoswitch performance will be investigated using **non-adiabatic molecular dynamics**[3] and **QM/MM simulations**. By comparing isolated molecules with polymer-embedded systems, the project will clarify how intermolecular interactions influence photoreactivity and mechanical output. Overall, this work will enable the screening and rational design of optimized photoswitch/polymer combinations[4] and will lay the groundwork for future PPA materials design.

[1] Arroyo, I et al. *Small* 2024, *20* (46), 2402131. [2] Stauch, T.; Dreuw, A. *J. Phys. Chem. Lett*. 2016, 7 (7), 1298–1302. [3] Oruganti, B.; Wang, J.; Durbeej, B. *J. Org. Chem.* 2022, 87 (17), 11565–11571. [4] (a) 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. (b) Villegas, O.; Serrano Martínez, M.; Le Bras, L.; Ottochian, A.; Pineau, N.; Perrier, A.; Lemarchand, C.. *Macromolecular Theory and Simulations* 2024, 33 (6), 2400033. https://doi.org/10.1002/mats.202400033 (c) Serrano Martínez, M.; Pineau, N.; Lemarchand, C.; Perrier, A. *Phys. Chem. Chem. Phys.* 2025, *27* (44), 23669–23684. https://doi.org/10.1039/D5CP02807H.

SKILLS

The candidate should hold a master's degree in chemistry, physical chemistry, or physics. A strong background in physical chemistry is required, and prior experience in computational chemistry would be an asset. The candidate must have completed a research project (Master's internship) in theoretical chemistry, molecular modeling or computational chemistry.

CONTEXT

This PhD proposal is part of the SIMULACTOR project, funded by **the Agence Nationale de la Recherche (ANR) under the PEPR LUMA program.** The SIMULACTOR consortium is made up of specialists in quantum calculation applied to photochromic systems (LIED, U. Paris Cité), specialists in classical atomistic simulations (molecular dynamics and coarse-graining, LMCE, CEA/DAM/DIF), and specialists in continuous media simulations (Finite Element Method, Discrete Element Method, IML, Université de Lille).

The research will be carried out at the "Laboratoire Interdisciplinaire des Energies de Demain – LIED", Université Paris Cité, 75013 Paris. The LIED ("Interdisciplinary Energy Research Institute", CNRS, Univ. Paris Cité) aims at developing fundamental and applied science in response to the challenges of the energy and climate transitions. In this context, the LIED favors a global approach by a unique multi-disciplinary method with researchers working in biology, chemistry, physics, informatics as well as in social sciences. The LIED offers a unique and stimulating scientific environment, structured around team meetings, laboratory seminars, and interdisciplinary public seminars focused on energy and transition-related topics.
The PhD candidate will join the "Climate and Energy in Urban Environments" team, which brings together chemists and physicists (6 permanent members) with complementary expertise. Within this group, the PhD candidate will work directly with Prof. Aurélie Perrier, specialist in computational photochemistry, and will interact closely with all members of the SIMULACTOR consortium. The quantum chemistry codes required for the project are available, along with access to both local and national computing resources.

CONDITIONS

Three-year contract starting on October 1st, 2026. The gross salary is at least €2,300 per month.

APPLICATION

Candidates must apply via the CNRS dedicated job platform (offer available in French and English version):

https://emploi.cnrs.fr/Offres/Doctorant/UMR8236-AURPER-002/Default.aspx

Required documents for application:

- A cover letter outlining the candidate's research interests and motivation
- A CV including relevant academic and research experience, as well as contact details for at least one reference