Namur Institute of Structured Matter

UNIVERSITÉ DE NAMUR

**Seminar**


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# « WHEN LIGHT MET MATTERS: A CHALLENGE FOR COMPUTATIONAL CHEMISTRY »

**When and where**:

Friday February 12th 2021 at 16H00
Teams


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# « WHEN LIGHT MET MATTERS: A CHALLENGE FOR COMPUTATIONAL CHEMISTRY »


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Light is at the origin of many natural processes and can be converted into electricity, heat or mechanical energy. If the mechanisms of the conversion of light into electricity (Photovoltaics) and heat (Solar oven) are now well understood, the last one, the conversion into a mechanical energy, is still unclear and most often comes from a cascade of complex mechanisms. Being able to control the matter and its movement with light thus represents a great challenge. Phototropism, actinotropism, photonastism and nyctinastism are as many examples of what light can induce when it meets matters in nature. As the mechanisms behind this light/mechanical energy conversion are complicated, one needs to pave the way with pioneering studies to enable the comprehension of those phenomena at different time and spatial scales. In this sense, computational chemistry and molecular modeling are valuable tools.

We propose here to consider a light-responsive polymer containing embedded photochromic molecules and to develop a tailored computational protocol able to tackle different aspects (explicit description of the environment, photochemistry in a polymer matrix, environmental constraints and deformation, optical properties, etc) of this complex system and phenomenon. By combining quantum mechanical calculations and molecular dynamics simulations we will build a realistic polymeric environment for the photochromic molecules and unravel their mutual influence and interaction. Finally, we will lay the foundation stone for the consideration of optomechanical phenomena from a theoretical point of view[1].

[1] L. Le Bras, C. Lemarchand, S. Aloïse, C. Adamo, N. Pineau, and A. Perrier *J. Chem. Theory Comput.* **2020** *16* (11), 7017-7032