PhD position in computational modeling of higher-order light-molecule interactions

Molecules can both absorb or emit light, as governed by the laws of quantum mechanics. These provide useful understanding of light-molecule interactions in terms of dipole allowed/forbidden transitions, a key concept of photochemistry. Recently, the field of photonics has seen the development of picocavities, which offer unprecedented control of light with highly confined fields and effective wavelengths that shrink down to the nanometer-scale. When a molecule is placed in the vicinity of a picocavity, new physico-chemical effects arise and activate a whole set of usually 'forbidden' transitions. Consequently, photochemistry can now be explored beyond the dipolar order. Moreover, hybrid light-matter states (polaritons) can emerge and redefine the whole reactivity of the molecule. This triggers the new and vivid field of polaritonic chemistry.

Nonetheless, the study of such advanced nanostructures is hampered by a lack of efficient and available theoretical methods. In this project, the PhD candidate will implement novel modeling methods to describe higher order photonic transitions in molecules, beyond the standard dipolar approach. Subsequently, the candidate will apply this framework to innovative structures, with an eye towards new chemical applications.

This research is carried out in the context of a 4-year project. The task of the PhD candidate is mainly theoretical and numerical: designing, understanding and evaluating structures.

You are expected to carry out both independent and collaborative research, to disseminate research findings via publications in international peer-reviewed journals and to participate in international conferences. If interested, you can also benefit from a teaching experience at the University of Mons.

Skills & Qualifications:

- The candidate should hold an MSc in physics, chemistry, nanophysics, photonics, materials science, engineering physics (or similar/equivalent).
- Experience in numerical methods for quantum electrodynamics (QED) and/or quantum chemistry is an asset.
- You have a good knowledge of English.
- You are a dynamic and enthusiastic team player.
- You have problem solving skills and are motivated to do PhD research.

Contract:

Temporary contract at full-time (38hours/week).

Contact:

If you are interested in the project, please contact colin.vandyck@umons.ac.be along with your CV and a motivation letter before 05/04/2021 included.