



Towards In Silico Photochemistry

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What happens to a molecule once it has absorbed UV or visible light? How does the molecule release or convert the extra-energy it just received? Answering these questions clearly goes beyond a pure theoretical curiosity, as photochemical and photophysical processes are central for numerous domains like energy conversion and storage, radiation damages in DNA, or atmospheric chemistry, to name a few.

In the past two decades, theoretical chemists have devoted a lot of effort to understanding and simulating the dynamics of photoexcited molecules.

A photoexcited molecule will presumably relax in different electronic states as a result of its nuclear motion. This means that the well-known Born-Oppenheimer approximation – which proposes to neglect the coupling between electronic and nuclear motion – is no longer valid, and so-called nonadiabatic effects must be considered. Interestingly, these nonadiabatic effects are not only important in light-triggered processes, but they will likely play a role as soon as the description of a given chemical process requires more than one electronic state, like in electron transfer mechanisms, for example. The loss of the Born-Oppenheimer approximation, however, poses an important number of questions and challenges for theoretical chemists.

The central goal of this presentation is to introduce the non-specialist to the main ideas and methods of theoretical and computational photochemistry. The usefulness of these techniques for chemistry – as well as the challenges in their application – will be highlighted by selected examples on the photochemistry of organic molecules.