Photochemistry from a theoretical and computational perspective

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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 to numerous domains like energy conversion and storage, radiation damages in DNA, or atmospheric chemistry. A plethora of theoretical tools have been developed over the past decades to address these questions by simulating the excited-state dynamics of molecules. These methods are often tested and theoretically validated on reduced-dimensionality models or rather simple molecules.

In this seminar, I will show a series of examples where studying the photophysics and photochemistry of real-life molecules helped spotlight the limitations of current theoretical methodologies and stimulate the development of new strategies for excited-state dynamics. In particular, I will focus on the sunlight-induced reactivity of volatile organic compounds in the troposphere, as well as athermal ground-state processes following passage through a conical intersection.