Potential energy surfaces exploration tools for simulation of molecular photophysics and photochemistry

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In this presentation, we will discuss quantum chemistry methods that enable the simulation of flexible molecules with focus on determining their spectroscopic properties and photochemical reaction mechanisms.

First, state-of-the-art methods in quantum chemistry for conformational sampling will be outlined [1–3] and how these are integrated into a workflow for the simulation of observable properties of molecules in the thermodynamic equilibrium. It will be demonstrated that accounting for the different conformers and their Boltzmann weights appropriately is essential for the simulation of electronic circular dichroism (ECD) spectra, a technique that is used for the determination of the absolute configuration of chiral molecules. [4]

Next, we will turn to the elucidation of photochemical reaction mechanisms and show how potential energy exploration tools can be used for this purpose. In particular, an efficient exploration technique for identifying important state crossing points between the ground and the lowest excited state is presented. [5] At comparably low computational cost, previously unknown photocatalytic processes can be investigated this way, leading to a better understanding of their mechanism. Real-life examples from collaborative research projects will be highlighted. [6, 7]

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