Simulation of ultrafast dynamics and their experimental signatures

Klaus B. Møller

Department of Chemistry, Technical University of Denmark, DK-2800 Kgs. Lyngby, Denmark
kbmo@kemi.dtu.dk

Our fundamental understanding of the light-induced ultrafast events determining photochemical properties of molecules has undergone significant advancements thanks to time-resolved studies. Modern femtosecond X-ray techniques are particularly suited for such investigations. Yet, the analysis and the interpretation of the experimental outcomes necessitate support from detailed simulations of the ultrafast dynamics as well as their experimental signatures. In this talk, I will give an overview of some of our recent efforts using quantum and semiclassical methods to simulate photoinduced non-adibatic dynamics and our own developments to calculate time-resolved X-ray scattering signals and spectra. Examples will include organic photo-switches,[1,2] electronic relaxation processes,[3,4] and transition-metal systems.[5-8]

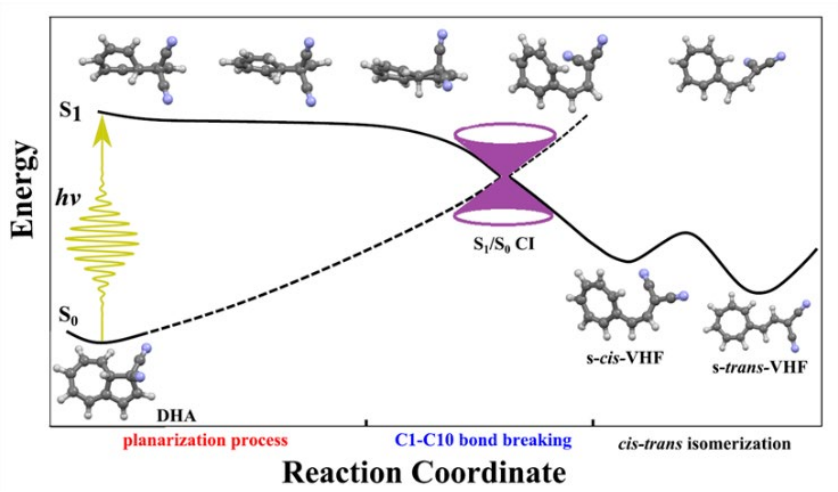

Figure 1: Reaction path for dihydroazulene ring-opening from the FC region through the S1/S0 CI toward the cis-trans isomerization process, from [1].

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