Theoretical investigation of molecular switch properties of several quinoline compounds

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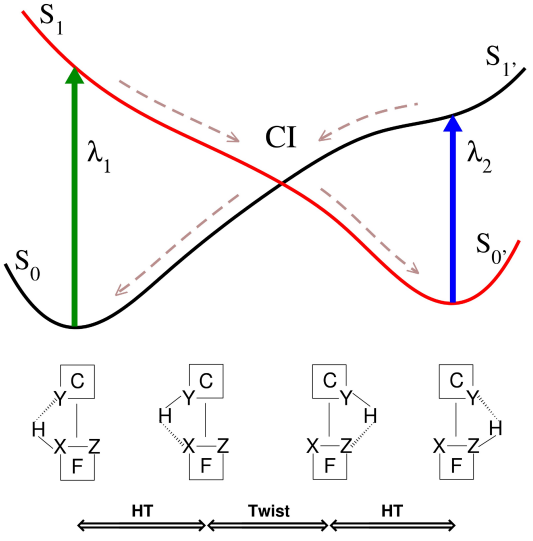
Molecular switches, being the simplest molecular level devices, are of great interest nowadays [1]. They have wide range applications, maybe the most important is in informatics: by representing an elementary bit memory unit they allow high density data storage on molecular level [2].

In this study we investigate the effect of chemical substitutions on the functional properties of a molecular photoswitch [3] by means of theoretical tools. Molecular switches are known to be consisting of so-called frame and crane components. Several functional groups are substituted to the 7-hydroxyquinoline molecular frame at position 8 as crane fragments. The impact of π-electron donating NH_2 groups attached to the frame is also investigated. Excited state intramolecular hydrogen transfer mediated by the frame-crane torsion has been considered as a possible reaction mechanism.

For all the investigated systems, we present the resulting CC2 potential energy profiles of the ground and first excited states. The presence of conical intersections around the 90 degree twist was shown using the CASSCF method. Vertical excitation energies and oscillator strengths of the 5 lowest-lying excited electronic states calculated at the two terminal points of the reaction path are also presented [4].



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