

THE ROLE OF CONICAL INTERSECTIONS IN PHOTOCHEMISTRY, ELECTRONIC ENERGY TRANSFER AND ELECTRON TRANSFER

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Theoretical studies show that real surface crossings (conical intersections) are the central feature of most photochemical processes and lie on the reaction path at the point where the excited state reactant or intermediate is delivered to the ground state via a non-adiabatic transition. We will outline how reaction path computations and the use of non-adiabatic trajectories can be used to obtain mechanistic information that can be used to complement modern spectroscopic data. Applications will be presented to the radiationless deactivation of polymethine cyanines and retinal chromophore models and the creation and annihilation of neutral soliton pairs in photoexcited polyene chains.

Recently we have begun to study the role of conical intersections in electron transfer processes and excited state energy transfer processes. Applications will be presented for intramolecular electronic energy transfer (IEET) in 9-anthryl-1'-naphthyl-alkanes and intramolecular electron transfer (IET): pathways in bis(hydrazine) radical cations.