Photodynamical Simulations in Biology: The Photostability of DNA Bases and DNA Models

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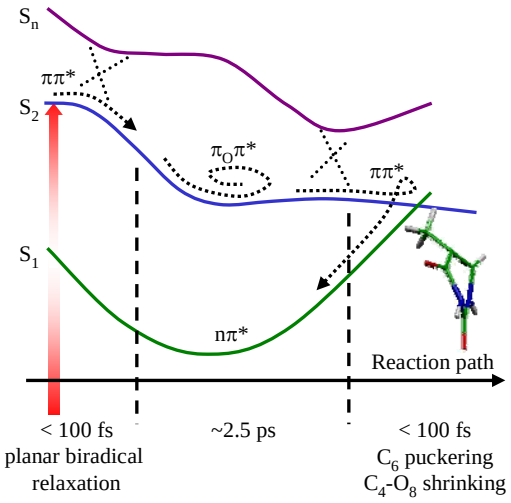
The simulation of photochemical processes is an extremely fascinating and challenging field. Very high demands are posed on the quantum chemical methods to be used since the energy surfaces of several electronic states have to be computed including nonadiabatic coupling between different states. The present work is based on the MCSCF and MRCI methods as implemented in the program package COLUMBUS using analytic energy gradients and nonadiabatic couplings and on Tully surface hopping by means of the program system NEWTON-X.

In this talk an overview of ultrafast deactivation mechanisms for DNA will be given and the importance of ππ* and nπ* states will be discussed. As an example, the figure below shows a summary of the



photodynamics of thymine explaining the relatively long lifetimes in the S_2 and S_1 states.

First modeling of defect transport through π-stacking by means of surface hopping is presented for interactions in the system ethylene/ethylene$^+$ and the relation to Marcus theory is discussed.