

Photoinduced Charge Transfer processes in oligonucleotides: from base pairs up to DNA duplexes

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Processes involving the creation or the migration of charges play an important role in the photoactivated dynamics of DNA.[1] Charge transfer (CT) excited states are formed in substantial yield via electron transfer (ET) between π -stacked bases in both single and double DNA strands.[2, 3, 4, 5] In duplexes, base pairing provides the necessary reaction coordinate for interstrand proton transfer, giving rise to Proton Coupled Electron Transfer (PCET) processes,[3, 6] which can occur also in simple hydrogen bonded pairs in low-polarity solvents.[7, 8, 9] On the ground of our Quantum Mechanical calculations on realistic DNA models, we shall analyse what are the most important chemical physical effects ruling these processes. We shall focus, in particular, on the influence of environmental effects on such processes and on the methodological challenges to be tackled to treat a strong coupling between electronic and solvent dynamics.

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