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Charge transfer in DNA: distance-dependence of hole transfer rates

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Charge transport in DNA has been studied intensively the last 15 years due to potential applications in both nanotechnology and biology [1, 2, 3]. Several reviews summarize the results of this effort [4, 5].

Electronic parameters pertinent to charge transfer along DNA are presented. Using a novel LCAO parametrization for π molecular orbitals of planar organic molecules [6], we have calculated the complete set of charge transfer parameters between neighboring bases and also between successive base pairs in DNA, considering all possible combinations between them, for both electrons and holes [7]. These quantities can be used in theoretical models of electron or hole transfer along the DNA double helix, as they provide the necessary parameters for a phenomenological description based on the π molecular overlap.

Using these electronic parameters, we estimate relative reaction rates in order to be compared with corresponding experimental results on hole transfer between guanine radical cations (donors) and GGG traps (acceptors) within appropriately synthesized DNA segments [8, 9]. In these experiments donors and acceptors are separated either by short $(TA)_n$ bridges where the charge transfer rates show an exponential dependence on the length of the bridge for $n = 1 - 3$ [8], or by bridges containing repeating TA,TA double units between single GC units where a weaker distance dependence (power law) appears [9]. Further, in the former experiments a switching behavior to weak distance dependence has been observed for bridges with $n > 3$, attributed to a change of the mechanism of charge transfer [8]. All these experimental observations are reproduced by our simulations, considering only tunneling as the charge transfer mechanism [10].

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