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Extra Carrier Transfer Oscillations in DNA Monomers, Dimers and Trimers

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Abstract: The study of charge transfer (CT) in biologically important molecules is recently a great scientific challenge. Specifically, CT plays a central role in DNA damage and repair [1], it might be an indicator to discriminate between pathogenic and non-pathogenic mutations at an early stage [2] and it may be used as a building block in molecular electronics [3]. We study, theoretically, CT oscillations of an extra carrier (electron or hole) in DNA monomers (base pairs), dimers and trimers. To examine such oscillations we employ two variations of the Tight-Binding (TB) approach: (I) TB I, at the base-pair level, using on-site energies of base pairs and hopping parameters between successive base pairs [4,5,6], and (II) TB II, at the single-base level, using on-site energies of bases and hopping parameters between neighboring bases. For monomers, i.e., adenine-thymine and guanine-cytosine and for dimers we also employ Real-Time Time-Dependent Density Functional Theory (RT-TDDFT). With TB II, for monomers, we predict periodic carrier oscillations with frequency $f \approx$ 50-550 THz. For dimers, TB I gives oscillations with $f \approx$ 0.25-100 THz. For trimers made of identical monomers, with TB I the frequencies are $f \approx$ 0.5-33 THz. TB I and TB II show similar frequency content, giving complementary aspects of the oscillations. RT-TDDFT also predicts oscillations in a similar range.

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