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Single state tight binding model for transport through DNA H. MEHREZ, M.P. ANANTRAM, NASA AMES RESEARCH CTR., Moffett Field, CA 94035 — We develop a new approach to derive the DNA tight binding parameters. Our model is based on *first principles* calculations and can be applied to various DNA configurations with different sequences. These parameters are used to model charge transport through finite length DNA. We investigate (i) the rigor of reducing the full DNA Hamiltonian to a single HOMO-LUMO state to represent charge transport in the vicinity of valence-conduction band (ii) DNA helix symmetry effects on the hopping parameters (iii) on-site energies and tight binding parameters dependence on the DNA sequence. We find that transport characteristics through PolyG-PolyC and PolyA-PolyT can be represented within HOMO-LUMO states. However transmission coefficient spectrum position shifts in energy and is substantially reduced for thymine. This effect can be corrected within 2^{nd} order time independent perturbation theory. Inter-strand charge transport has also been analyzed and it is found to be strongly asymmetric in PolyG-PolyC in the vicinity of the HOMO state. This is attributed to asymmetric hopping parameters between 5'G→5'C and 3'G→3'C. Finally, we have determined on-site energies and inter-bases couplings for DNA structures with different sequences. We find that these parameters have long range dependence as well as helix directional dependence. Hence tight binding model for such structures is not simple. Our derived representation depend strongly on the DNA sequence.

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