

Abstract Submitted
for the MAR06 Meeting of
The American Physical Society

Inter-strand coupling and base pairing sequences in DNA charge transport.¹ EFTA YUDIARSAH, Ohio University, SERGIO ULLOA, Ohio University — The electronic transport properties of double-stranded DNA are studied using a tight-binding Hamiltonian. Transfer and scattering matrix methods for double strands are employed simultaneously in the calculation, guaranteeing numerical stability. Realistic on-site energies [1] and hopping constants are used in the model [2]. The role of inter-strand coupling is shown to be extremely important for random sequences typical of genetic DNA. In contrast, inter-strand coupling only changes slightly the charge transport properties for more periodic sequences. The effect of base-pairing across strands and details of the sequences were investigated. Our model shows that the resistance of DNA depends on the sequences and the ratio of the bases. This agrees with previous results by Roche [3]. The resistance is also shown to increase with the concentration of different bases in a homogenous strand, and we find that for certain sequences only short-range electronic transport is possible.

[1] H. Sugiyama and I. Saito, J. Am. Chem. Soc. 118, 7063 (1996).

[2] A. A. Voityuk, J. Jortner, M. Bixon, and N. Rosch, J. Chem. Phys. 114, 5614 (2001).

[3] S. Roche, Phys. Rev. Lett. 91, 108101 (2003).

¹Supported by NSF-NIRT.

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Date submitted: 30 Nov 2005

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