Molecular electronics of DNA double helices using second order tight-binding modeling

Sadeq Malakooti, Eric R. Hedin, and Yong S. Joe
Center for Computational Nanoscience, Department of Physics and Astronomy, Ball State University, Muncie, IN 47306, USA
E-mail: ysjoe@bsu.edu

Recent observations have disclosed that under various conditions, DNA molecules can act as insulators [1], semiconductors [2], and also conductors [3], which express the immense importance of DNA-based electronic systems and devices. Among the theoretical efforts towards interpreting these fascinating experimental results, model-based Hamiltonian methods are of particular interest due to their ease of application and generality [4, 5].

In this work, an advanced tight-binding model including the next nearest-neighbor effects is proposed, and the characteristics of quantum mechanical electron transport through a gated poly(G)-poly(C) double stranded DNA molecule are investigated. Here the molecule is subjected to a perpendicular gating electric field and so the helix conformation of the strands becomes important [6]. This situation takes place when the trapped molecule is not aligned with the inter-contact electric field, so that there then exists a component of the field perpendicular to the molecule axis. The next nearest-neighbor coupling, or hopping strengths are determined in the form of a Pythagorean relation of two-sided hopping integrals (ie. interbase and interstrand hopping integrals).

We have calculated the overall transmission and current of the system in terms of the contact hopping integrals, and the angle between the tilted molecule and the interconnect electric field, with and without the next nearest-neighbor hopping effects. Here as a sample, for the aligned DNA, the transmission spectra and the average transmission spectra as a function of electron energy for selected symmetrical contact couplings of 0.1 eV (Figs. 1a, 1d and 1g), 0.5 eV (Figs. 1b, 1e and 1h) and 0.9 eV (Figs. 1c, 1f and 1i), with and without the next nearest-neighbor effects are shown.

Also Fig. 2a (2b) shows a contour plot of the room temperature current for a fixed Fermi energy, (5.5 eV), by modulating the applied voltage (V_{sd}) and the symmetrical contact coupling between the leads and the aligned DNA molecule without (with) next nearest-neighbor effects.

It is clearly seen that the inclusion of next nearest-neighbor effects broadens the transmission spectra to include electrons with lower energies. Therefore, we attribute this enhancement of electron transport through DNA molecules to the inclusion of diagonal electron hopping between the sites. This result can be seen even more clearly in the average transmission spectra.

Also in agreement with transmission spectra, the current is enhanced in value when the next nearest-neighbor effects are taken into account. In other words, the current gap (shown as a green color in the contour plots of Fig. 2), which is a typical characteristic of a semiconductor, is decreased by the diagonal electron hopping between the sites.

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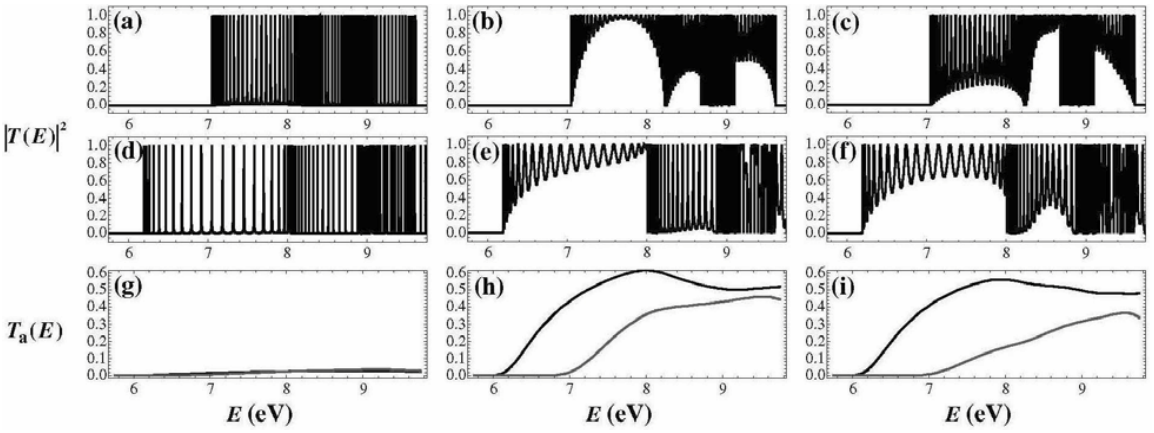

Fig. 1 Transmission spectra as a function of electron energy without (a-c) and with (d-f) the next nearest-neighbor effects (NE). (g-i) average transmission spectra as a function of electron energy: gray line (without NE) and black line (with NE). Plots (a, d and g) have contact hoppings of 0.1 eV, plots (b, e and h) have 0.5 eV, and plots (c, f and i) have 0.9 eV .

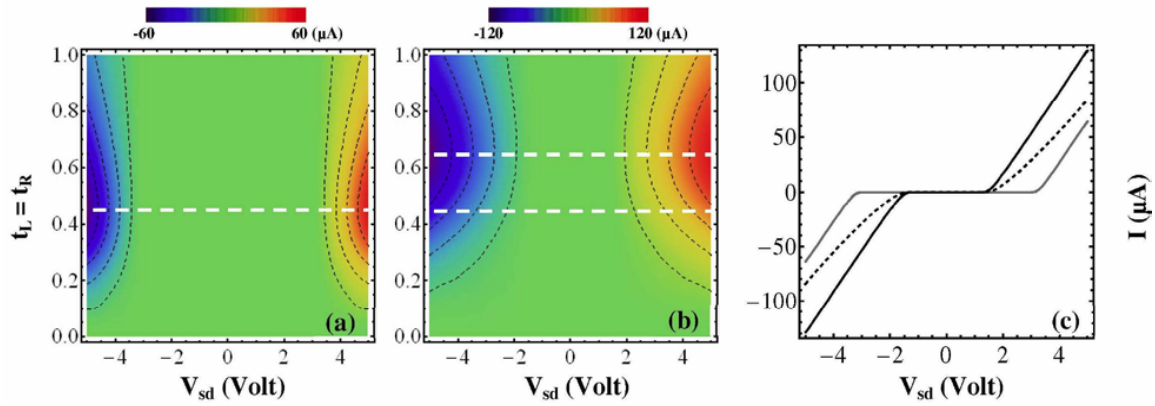

Fig. 2 (Color online) Contour plots of the current as a function of source-drain voltage and contact hopping strengths: (a) without NE and (b) with NE; (c) Current as a function of source-drain voltage without NE and contact hoppings of 0.42 eV (gray solid line), and with NE for two symmetrical contact hopping values of 0.42 eV (black dashed line) and 0.62 eV (black solid line). The Fermi energy is 5.5 eV.