The effects of molecular elongation on defective DNA electronics

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

DNA defects may explain the origin of many serious diseases in human body. A recently reported study of DNA flaws shows an increased blood cancer risk from type 2 diabetes [1]. It has also been shown that electrical charge transport properties of DNA molecules are dramatically changed by the presence of any structural defect, which makes an intriguing field of study for researchers. Therefore, we investigate quantum mechanical electron transport along DNA molecules of poly (dG) and poly (dC) base pairs with a single defect.

For this purpose, we deal with a 30 base-pairs ds-DNA molecule coupled between two semi-infinite metallic leads (Fig. 1a). Here, the Hamiltonian for a ds-DNA molecule is described by a summation over all base-pair sites as follows:

$$H_{DNA} = \sum_{\substack{m=1 \\ i=1}}^{\substack{i=15 \\ m=8}} \varepsilon_m |i,m\rangle\langle i,m|$$
$$+ \sum_{i,m\neq n} \left(\begin{array}{c} t_{mn} |i,m\rangle\langle i,n| \\ + \bar{t}_{mn} |i,m\rangle\langle i+1,n| + h.c. \end{array} \right). \quad (1)$$

in which ε_m is the on-site energy of the m-th site, t_{mn} are the hopping integrals between inner unit-cell sites and $\bar{t}_{mn}$ are ones between two adjacent cells. The unit cell is bounded by a dashed line (Fig. 1b).

By taking the advantage of semi-empirical Slater-Koster theory [2] which relates the hoppings to the inter-orbital distance, the hopping integrals for the system are determined as follows:

$$t = -\eta_{pp\pi} \left(\hbar^2 / m_e d_0^2 \right) e^{-d/R_c}, \quad (2)$$

where d is the inter-orbital distance, m_e is the mass of electron, and $\hbar^2 / m_e d_0^2 = 7.62$ eV for $d_0 = 1$ Å.

For guanine and cytosine sites, $\eta_{pp\pi} = 2.26$ and $R_C = 0.87$ Å, and for the backbone sites, $\eta_{pp\pi} = 0.65$ and $R_C = 0.87$. Further, in the small strain regime, the DNA molecule has a negative Poisson's ratio, around -0.5 [3].

For the numerical calculation, we study a point defect as an energy perturbation in the onsite energies of the ds-DNA molecule which is assumed to have unperturbed on-site energies of 8.85 eV for sugar-phosphate backbone sites, 7.75 eV for guanine, and 8.87 eV for cytosine sites. The energy perturbation is defined as follows:

$$\varepsilon_m = \xi_m \varepsilon_{m0}, \quad (3)$$

where ε_{m0} is the unperturbed onsite energy and ξ_m is the perturbing coefficient of the m-th site.

Figure 2 shows a contour plot of the electron transmission spectrum of the molecule when the defect is applied to the guanine onsite energy. The result was calculated for different guanine defect locations and no difference was observed. It is clearly seen that the inclusion of a very small perturbation ($\xi_m = 0.8$) leads to vanishing of the entire guanine transmission band. In addition, molecular stretching (strain) causes localization of the guanine and cytosine bands from each other, which eventually creates a natural band gap of width approximately 0.2 eV.

REFERENCES

[1] A. Bonnefond, B. Skrobek, S. Lobbens, E. Eury, D. Thuillier, S. Cauchi, O. Lantieri, B. Balkau, E. Riboli, M. Marre, G. Charpentier, L. Yengo, and P. Froguel, Nature Genetics **45**, 1040 (2013).
[2] J. C. Slater, and G. F. Koster, Phys. Rev. **94**, 1498 (1954).
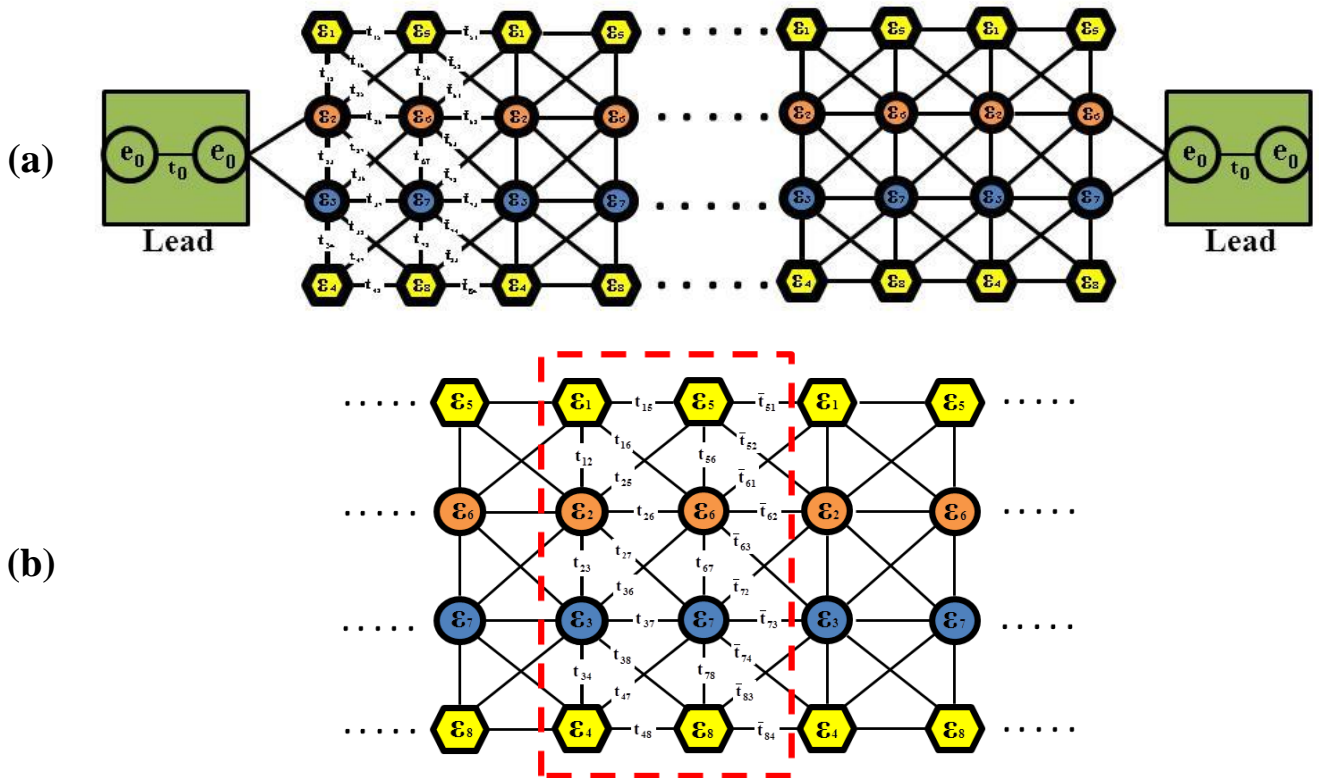[3] S. Malakooti, E. R. Hedin, and Y. S. Joe, J. Appl. Phys. **114**, 014701 (2013).

Fig. 1 (a) Schematic of a 30 base-pairs DNA chain coupled between two semi-infinite lead electrodes. (b) The molecule repeating unit-cell is bounded by a dashed line.
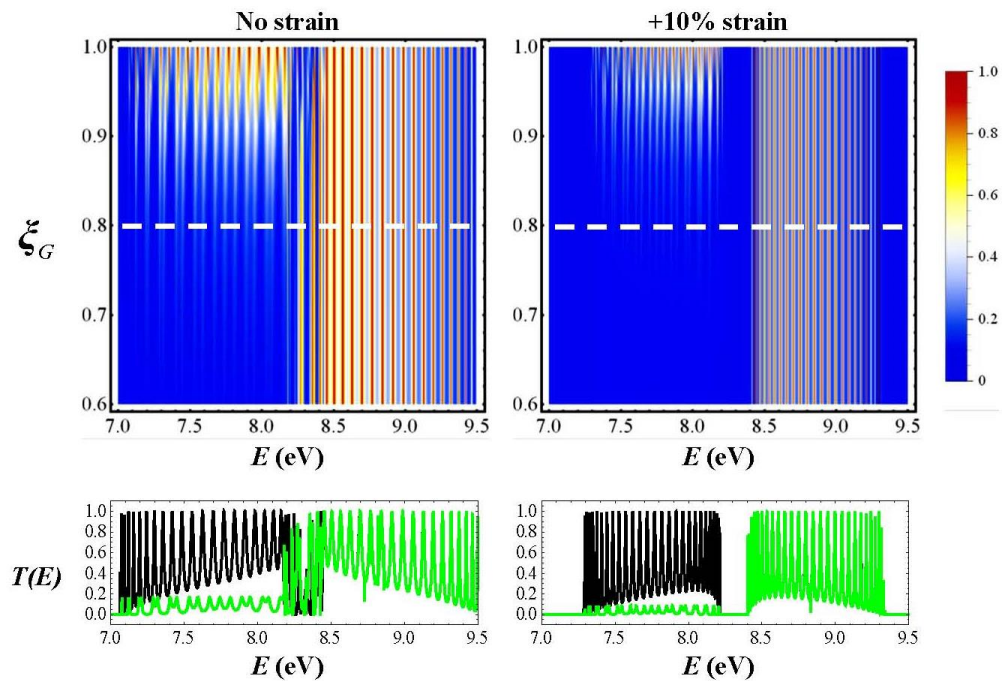

Fig. 2 Contour plots of the electron transmission spectrum of the molecule as a function of incoming electron energy and onsite energy perturbation for no strain and 10% strain. The bottom graphs show the transmission spectra with the perturbation $\xi_m = 0.8$.