

## INFLUENCE OF VIBRATIONAL MODE ON THE ELECTRONIC PROPERTIES OF DNA MOLECULE IN LADDER MODEL

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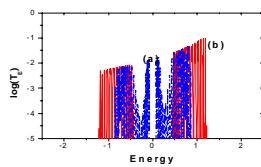
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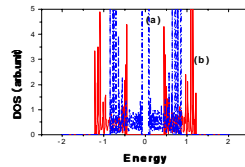
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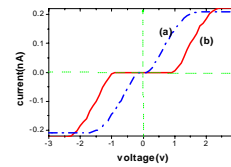
Within the class of biopolymers, DNA is expected to play an outstanding role in molecular electronics. We studied the electron transport properties in single DNA molecules considering a metal/DNA/metal system using model Hamiltonian method based on the tight-binding Hamiltonian for the ladder model of DNA [1]. Now Current-voltage relation, density of state and conductance study with vibration (a diagrams) and without vibration (b diagrams) and compare with together [2, 3].



(Figure1)



(Figure2)



(Figure3)

Figure1: with vibration the energy gap and conductance are considerably decreasing.

Figure2: with vibration the energy gap is decreasing and density of state is increasing.

Figure3: with vibration the energy gap and current-voltage characteristic are decreasing.

Our results suggest a good agreement with the electronic structure of the DNA in the ladder model, additionally presented a technique that allows the computation of electron transport in DNA, including local and nonlocal coupling to vibrations. And with vibration we can increase semiconducting behavior in our system.

### References:

[1] G. Cuniberti, F. Gromann, and R. Gutiérrez. The Role of Contacts in Molecular Electronics, *Adv. in Solid State Phys.* **42**, pp. 133. , (2002)

[2] V. Mujica, M. Kemp, and M. A. Ratner " current- voltage characteristics of tunneling molecular junctions for off-resonance injection," *J. Chem. Phys.*, **104**(18)365-370, (1996)

[3] B. Schmidt, M.H. Hettler, and G. Schön, Influence of vibrational modes on the electronic properties of DNA , *PHYS. REV. B* **75**, 115125 ( 2007)