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Influence of vibrational mode on electrical properties of DNA molecules for ladder model

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ABSTRACT: *Based on the tight-binding Hamiltonian for the ladder model of DNA and within the framework of a Generalized Green's function technique, the electronic conduction through the metal/DNA/metal structure has been numerically investigated. Using Landauer formalism, we calculate the current-voltage relation and density of state and conductance perform the study on the effect of vibrational between the electrodes and DNA molecule in ladder model .Our results show that these parameters have significant effect on the conduction properties of the system.*

Keyword:*DNA, tight-binding Hamiltonian, Green's function technique*

I. INTRODUCTION

Within the class of biopolymers, DNA is expected to play an outstanding role in molecular electronics. This is mainly due to its unique self-assembling and self-recognition properties which are essential for its performance as carrier of the genetic code. These properties exploited in the design of nano-electronic circuits used in medical investigations and other hyperfine electronic systems. The nanoelectronic devices have been usually designed in such a way that a single molecule is sandwiched between two electrodes (metallic or organic) [1].

II. METHODOLOGY

In this work 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(eq:1) for the ladder model(figure:1) of DNA and within the framework of a Generalized Green's function technique, the electronic conduction through the metal/DNA/metal structure has been numerically investigated. Using Landauer formalism, we calculate the current-voltage relation(eq:2) and density of state(eq:3) and conductance(eq:4) perform the study on the effect of vibrational between the electrodes and DNA molecule in ladder model [2, 3].

We study electron transport through double stranded DNA wires strongly coupled, both locally and non-locally, to vibrational modes of the DNA [4]. All parameters and equation are explain in references .

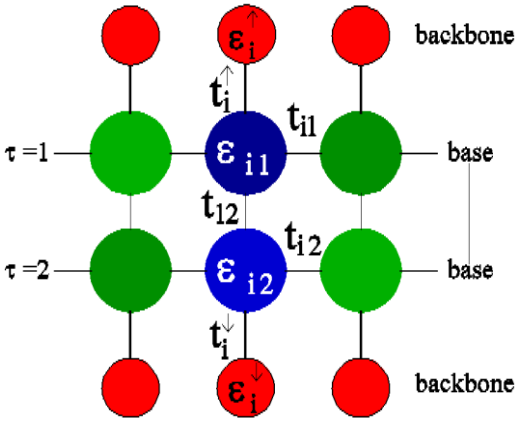

Figure: 1

Equatin1: $$H = H_{el} + H_{vib} + H_{el-vib} + H_L + H_R + H_{T,R} + H_{T,L}$$

Equation2: $$I = \frac{2e}{\pi\hbar}\int_{-\infty}^{\infty} dET(E)\left[f_L(E) - f_R(E+eV)\right]$$

Equation3: $$\rho_i = -\frac{1}{\pi}\mathrm{Im}[G_{ii}]$$

Equation4: $$g(E) = g_0\left|G_{1N}(E)\right|^2\Delta_1(E)\Delta_N(E) \qquad ; g_0 = \frac{2e^2}{h}$$

III. RESULT

We compare the (dos) ,(conductance) and the diagram of (current – voltage) for ladder model of DNA molecules when the numbers of bases pair are 64 and the all of our sites are 1500and all of our parameters are in(ref4). Red diagrams are our results for ladder model when we don't have vibration in system (lead/DNA/ lead), and blue diagrams are our result with vibrational mode in system.

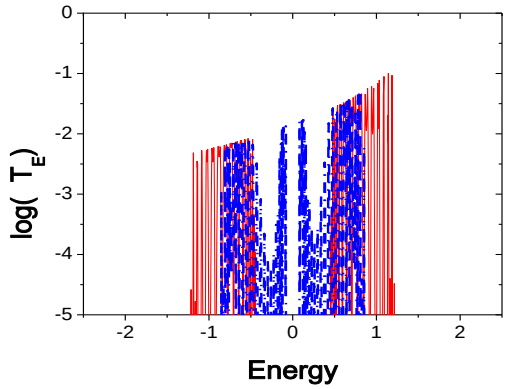

Figure2: when we have vibration in system the energy gap and conductance are considerably decreasing.

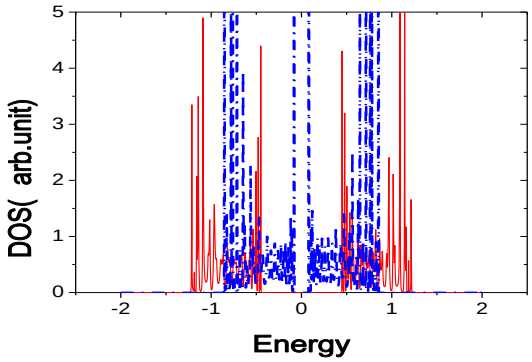

Figure3: when we have vibration in system the energy gap is decreasing and density of state is increasing.

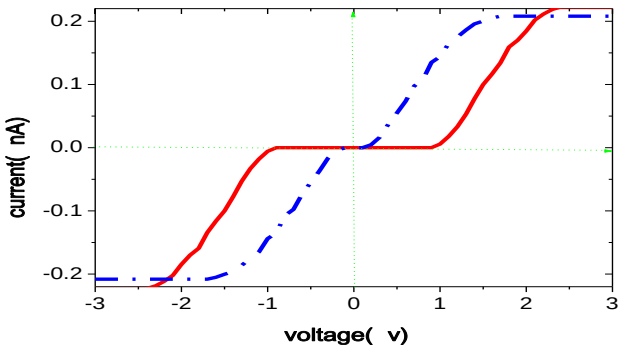

Figure4: when we have vibration in system the energy gap and current-voltage characteristic are decreasing.

IV. CONCLUSION

Some significant electronic conduction properties for DNA molecule in the lead/DNA/lead system have been studied using a presented methodology. Our results suggest a good agreement with the electronic structure of the DNA in the ladder, additional we have presented a technique that allows the computation of electron transport through short sequences of DNA, including local and nonlocal coupling to vibrations. The coupling to vibrations strongly enhances the zero-bias conductance at low temperatures. The current at finite bias above the "semiconducting" gap, however, is only quantitatively modified by the nonlocal electron-vibron coupling. And with vibration we can increase semiconducting state in our system.

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