

## Electronic conduction of poly(dG)-poly(dC) DNA in SWNT/DNA/SWNT structure

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### Abstract

In this work, using a tight-binding Hamiltonian model, a generalized Green's function method and Löwdin's partitioning techniques, some of the significant properties of the conductance of poly(dG)-poly(dC) DNA molecule in SWNT/DNA/SWNT structure are numerically investigated. In Fishbone model, we consider DNA as a planar molecule which contains  $M$  cells and 3 further sites (one base pair site and two backbone sites) in each cell sandwiched between two semi-infinite single-walled carbon nanotubes (SWNT) as the nano-electrodes. Relying on Landauer formalism as the basis for investigating the conductance properties of this system, we focus on the studying of the electron transmission and the current-voltage characteristics of DNA in the foregoing structure. In addition, in the presence of the electric potential between DNA molecule ends, our results suggest that the increasing of the value of applied bias give rise to the large enhancement in the conductance of the system. We also find that, as the tube radius increases, the conductance of the system considerably increases.

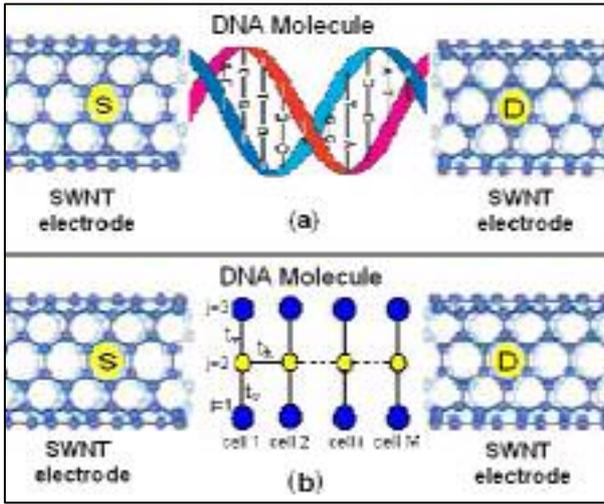
**Keywords:** DNA, electronic transmission, carbon nanotube, Fishbone model, Green's function

### 1. Introduction

The discovery that Deoxyribose Nucleic Acid (DNA) can conduct an electrical current has made it an interesting candidate for the roles that nature did not intend for this molecule. In particular, DNA could be useful in nanoelectronics for design of electric circuits, which could help to overcome the limitations that silicon-based electronics is facing in the recent years. However, DNA electronics does not aim to make something new. Its immediate goal is to improve old concepts in a new manner, although in the process it may create entirely new ideas in nanoelectronics [1-3]. The nanoelectronic devices have been usually designed in such way that a single molecule is sandwiched between two electrodes (metallic or organic). Considering the immense progresses in the field of the nanofabrication, attempts have also been made towards other structures, such as carbon nanotubes (CNTs), as the conducting metallic reservoirs [4-7]. The significantly improved switching characteristics of the short organic FETs with CNT electrodes compared to the metallic one are attributed to the excellent electrostatics attainable with the nanotube electrode geometry [8, 9].

A number of experimental groups have reported

measurements of the current-voltage characteristics of DNA molecule which are, however, quite controversial [10, 11]. It has been characterized that DNA may be an insulator [12, 13], semiconductor [14] or metallic [15, 16]. In particular, according to the Porath et al experiments [14], DNA molecule as a 10.4 nm long (30 base-pairs) poly(dG)-poly(dC) sequence has electrical characteristics similar to that of a semiconductor diode, that allows current to flow in one direction only. This stimulated intense research interest in the transport properties of DNA. Accordingly, DNA may be an excellent candidate for molecular electronics and may serve as a molecular wire, transistor, switch or rectifier depending on its electronic properties [10, 17]. Also several theoretical models which range from quantum mechanical approaches mostly use strictly one-dimensional tight-binding models [18-21] to density functional theory [22] have been developed for investigating the electron transport properties of DNA molecule. In present work, we numerically investigate the electronic transport properties of DNA in the SWNT/DNA/SWNT model structure. In our model, the typical system is considered as a planar DNA molecule sandwiched between two semi-infinite armchair( $l, l$ )



**Figure 1.** (Color online) Panels (a) and (b) show schematically representations of the SWNT/DNA/SWNT structure. As described in the text, in panel (b) the suggested model for DNA contains of  $M$  cells in Fishbone model is drawn.

single-walled carbon nanotubes (SWNT) as nano-electrode (figure 1). The model and description of the computational methods for investigating the conductance properties of the model structure are introduced in section 2. The results and discussion are presented in section 3, followed by conclusion in section 4.

## 2. Model and methodology

As it is well-known, the nature of charge transfer and electron transport through DNA molecule depends on the understanding of its structural parameters. DNA consists of a double-helix with an aromatic  $\pi$ -stack core where four types of nucleobase (thymine, T; cytosine, C; adenine, A; guanine, G) participate in Watson-Crick base pairing (A:T; G:C) [23]. A schematic representation of the double-helix structure of DNA is illustrated in figure 1(a). A detailed understanding of DNA structure suggests that the  $\pi$ - $\pi$  interaction between the stacked base pairs in DNA could support extended charge transport. Density-functional calculations [22] have shown that the bases, especially Guanine, are rich in  $\pi$ -orbitals. The double-strand DNA could offer pathways for long-range charge transport. The electronic coupling through a duplex stack of nucleobases is expected to involve both intrastrand and interstrand pathways [24]. Here we consider a model which includes the backbone structure of DNA explicitly and exhibits a semiconducting gap, the Fishbone model. As shown in figure 1(b), DNA molecule in Fishbone model, has one central conduction channel in which individual sites represent a base-pair (bp) which are interconnected and further linked to upper and lower sites, representing the backbone, but are not interconnected along the backbone [17]. In our model the DNA structure as a 2-dimensional layer which consists of  $M$  cells and 3

further sites in each cell is set between two semi-infinite armchair ( $l, l$ ) SWNTs as nano-electrodes and then the conductance properties of the system are numerically investigated based on well-known procedures particularly suitable to treat the electron transmission through the mesoscopic structures, Landauer formalism and a generalized Green's function method. As illustrated in figure 1(b), the cell of number  $i$  connects to the cells of number  $(i-1)$  and  $(i+1)$  only through one horizontal hopping integral,  $t_h$ . Also in a typical cell the base-pair site connects to upper and lower backbone sites via vertical hopping integrals,  $t_v$ . In addition, the cell of number 1( $M$ ), via the linker groups, may be connected to the left(right) semi-infinite armchair ( $l, l$ ) SWNT as nanocontact. In this study we consider a DNA molecule with 30 bps and so a layer consists of  $N=90$  sites. Here the nanocontacts are considered to be the armchair (5, 5).

To proceed, we use the following generalized Hamiltonian for the description of the SWNT/DNA/SWNT structure,

$$H = H_{SWNT} + H_{DNA} + H_C, \quad (1)$$

where  $H_{SWNT}$ ,  $H_{DNA}$  and  $H_C$  describe the semi-infinite SWNT nanocontacts, the DNA Hamiltonian and the couplings of the contacts to DNA molecule, respectively. The SWNTs (electron reservoirs) are modeled within the tight-binding approximation with only one  $\pi$ -orbital per atom. Accordingly,  $H_{SWNT}$  can describe the band structure of a nanotube reasonably well, especially near the Fermi level which is considered zero in this case since the onsite energy is assumed to be zero and each orbital is half-filled,

$$H_{SWNT} = \sum_i \varepsilon_i |i\rangle\langle i| - \sum_i t_{i,i+1} |i\rangle\langle i+1| + h.c., \quad (2)$$

where  $|i\rangle$  denotes the electron state in the reservoirs. For the semi-infinite SWNT contacts we set  $\varepsilon_i = 0$  for all  $i$  and  $t_{i,i\pm 1} = t_{SWNT}$  between all  $i$  and  $i\pm 1$  for the nearest-neighbor hopping.  $H_C$  denotes the interacting Hamiltonian between DNA molecule and nanotube contacts and is given as,

$$H_C = -t_C (|i\rangle\langle 1| + |M\rangle\langle i|). \quad (3)$$

Here  $t_C$  denotes the interaction strength between single electron state of cell 1( $M$ ) in DNA molecule and the electron state in the left(right) electrode. Using the Löwdin's matrix partition technique [25] we may rewrite the Hamiltonian of the total system as follow:

$$H_{eff} = -\Sigma^L |1\rangle\langle 1| + H_{DNA} - \Sigma^R |M\rangle\langle M|, \quad (4)$$

where  $\Sigma^L (\Sigma^R)$  is the self-energy matrix resulting from the coupling of the DNA molecule to the left(right) electrode. Now considering the Fishbone model for DNA molecule, according to figure 1(b), the effective Hamiltonian (4) can be expressed in matrix form as follow,

$$H_{eff} = \begin{bmatrix} \mathbf{H}_1 & \mathbf{T}_1 & 0 & \dots & \dots & \dots & \dots & \dots & 0 \\ \mathbf{T}_1^\dagger & \mathbf{H}_2 & \mathbf{T}_2 & 0 & \vdots & \vdots & \vdots & \vdots & \vdots \\ 0 & \mathbf{T}_2^\dagger & \mathbf{H}_3 & \ddots & 0 & \vdots & \vdots & \vdots & \vdots \\ \vdots & 0 & \ddots & \ddots & \ddots & 0 & \vdots & \vdots & \vdots \\ \vdots & \vdots & 0 & \ddots & \mathbf{H}_{i-1} & \ddots & 0 & \vdots & \vdots \\ \vdots & \vdots & \vdots & 0 & \mathbf{T}_{i-1}^\dagger & \mathbf{H}_i & \mathbf{T}_i & 0 & \vdots \\ \vdots & \vdots & \vdots & \vdots & 0 & \ddots & \mathbf{H}_{i+1} & \ddots & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots & 0 & \ddots & \ddots & \mathbf{T}_{M-1} \\ 0 & \dots & \dots & \dots & \dots & \dots & 0 & \mathbf{T}_{M-1}^\dagger & \mathbf{H}_M \end{bmatrix}, \quad (5)$$

where  $\mathbf{H}_i$  is a  $3 \times 3$  matrix describing the 3 sites within the  $i$ th cell (see figure 1(b)) and  $\mathbf{T}_{i-1}^\dagger$  and  $\mathbf{T}_i$  are  $3 \times 3$  matrices describing the hopping to and from cell  $i$ , thus,

$$\mathbf{H}_1 = \begin{bmatrix} E_{11} & t_v & 0 \\ t_v & E_{12} - \Sigma_{12} & t_v \\ 0 & t_v & E_{13} \end{bmatrix},$$

$$\mathbf{H}_M = \begin{bmatrix} E_{M1} & t_v & 0 \\ t_v & E_{M2} - \Sigma_{M2} & t_v \\ 0 & t_v & E_{M3} \end{bmatrix},$$

$$\mathbf{H}_i = \begin{bmatrix} E_{i1} & t_v & 0 \\ t_v & E_{i2} & t_v \\ 0 & t_v & E_{i3} \end{bmatrix}, \quad 1 < i < M,$$

$$\mathbf{H}_i = \begin{bmatrix} E_{i1} & t_v & 0 \\ t_v & E_{i2} & t_v \\ 0 & t_v & E_{i3} \end{bmatrix}, \quad 1 < i < M,$$

$$\mathbf{T}_i = \begin{bmatrix} 0 & 0 & 0 \\ 0 & t_h & 0 \\ 0 & 0 & 0 \end{bmatrix}. \quad (6)$$

Here  $\Sigma_{12} = \Sigma_{M2} = \Sigma$  is considered. For poly(dG)-poly(dC) DNA, the hopping integrals  $t_h = 0.37$  eV and  $t_v = 0.74$  eV are set [1]. Also  $E_{ij} = \varepsilon_{ij} - z$  ( $i=1, \dots, M$  and  $j=1, 2, 3$ ) where  $\varepsilon_{ij}$  are the onsite energies within the  $i$ th cell and  $z = E + i0^+$  is the complex number whose real part,  $E$ , is the energy at which the transfer occurs. It is to be noted that the matrix of  $H_{DNA}$  differs from the matrix of  $H_{eff}$  only in both the elements (1,2) and (M,2), so that,

$$\begin{aligned} (H_{DNA})_{12} &= (H_{eff})_{12} + \Sigma, \\ (H_{DNA})_{M2} &= (H_{eff})_{M2} + \Sigma, \\ (H_{DNA})_{ij} &= (H_{eff})_{ij} \quad ; \quad (i,j) \neq (1,2) \text{ and } (M,2), \end{aligned} \quad (7)$$

where the number of sites in the DNA structure  $N = 3M$  and  $M$  is the number of the cells, as shown in

figure 1(b). The matrices of self-energy are also defined as,

$$\Sigma^L = \Sigma^R = \begin{pmatrix} 0 & 0 & 0 \\ 0 & \Sigma & 0 \\ 0 & 0 & 0 \end{pmatrix}. \quad (8)$$

Based on the suggested model Hamiltonian, we proceed to calculate the conductance of the SWNT/DNA/SWNT structure. The most commonly used computational schemes for calculating the (coherent) conductance  $g$  are the Landauer theory [26] and the Green's function formalism [27, 28]. The conductance  $g$  at zero temperature is simply proportional to the transmission coefficient,  $T(E)$ , for injected electrons at the Fermi energy,

$$g = g_0 T(E) \quad , \quad g_0 = \frac{2e^2}{h}. \quad (9)$$

The transmission coefficient can be calculated from the knowledge of the molecular energy levels, the nature and the geometry of the contacts. Using the Fisher-Lee formalism [29] the differential conductance may be expressed as,

$$g = g_0 |G_{1M}(E)|^2 \Delta_{12}(E + eV) \Delta_{M2}(E), \quad (10)$$

where  $G_{1M}(E)$  is the (1,  $M$ ) element of the retarded Green's function matrix of the DNA molecule and  $\Delta_{12}(= \Delta_{M2}) = \Delta$ , the spectral density matrix is related to the semi-infinite left(right) electrode Green's function matrix. For details of how  $\Delta$  and  $G_{1M}(E)$  may be calculated, we refer to Ref. [30]. Introducing the self-energy corrections into the bare molecule Green's function, then the DNA molecule electronic Green's function in the SWNT/DNA/SWNT sandwich is define as,

$$G^{-1} = G_m^{-1} - \Sigma^L - \Sigma^R, \quad (11)$$

where  $G_m^{-1}$  and  $\Sigma^{L(R)}$  are the retarded Green's function of bare DNA molecule and the left(right) SWNT self-energy matrix, respectively. The operator of the retarded Green's function of the bare molecule is given by,

$$G^m = (1z - H_{DNA})^{-1}, \quad z = E + i0^+, \quad (12)$$

in which  $H_{DNA}$  represents the Hamiltonian of the bare molecule and 1 stands for the identity matrix. In order to calculate the Green's function matrix element  $G_{1M}(E)$ , in eq. (10), which carries all the information about the molecular structure needed to calculate the conductance, we generalize the partitioning algorithm proposed by Mujica et al [27] to our layer model for DNA structure. Accordingly we find  $G_{1M}(E)$  in matrix form as follow,

$$G_{1M}(E) = [G_{eff}]_{1M}^{-1} = \begin{bmatrix} \mathbf{G}_1 & \mathbf{T}_1 & 0 & \dots & \dots & \dots & \dots & \dots & \dots & 0 \\ \mathbf{T}_1^+ & \mathbf{G}_2 & \mathbf{T}_2 & 0 & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ 0 & \mathbf{T}_2^+ & \mathbf{G}_3 & \ddots & 0 & \vdots & \vdots & \vdots & \vdots & \vdots \\ \vdots & 0 & \ddots & \ddots & \ddots & 0 & \vdots & \vdots & \vdots & \vdots \\ \vdots & \vdots & 0 & \ddots & \mathbf{G}_{i-1} & \ddots & 0 & \vdots & \vdots & \vdots \\ \vdots & \vdots & \vdots & 0 & \mathbf{T}_{i-1}^+ & \mathbf{G}_i & \mathbf{T}_i & 0 & \vdots & \vdots \\ \vdots & \vdots & \vdots & \vdots & 0 & \ddots & \mathbf{G}_{i+1} & \ddots & \vdots & \vdots \\ \vdots & \vdots & \vdots & \vdots & \vdots & 0 & \ddots & \ddots & \mathbf{T}_{M-1} & \vdots \\ 0 & \dots & \dots & \dots & \dots & \dots & 0 & \mathbf{T}_{M-1}^+ & \mathbf{G}_M & ]_{1M}^{-1} \quad (13)$$

where  $\mathbf{G}_i$  describes the Green's function of  $i$ th cell.

Thus,

$$\mathbf{G}_I = \begin{bmatrix} \varepsilon_{11} & t_v & 0 \\ t_v & \varepsilon_{12} + i\Delta & t_v \\ 0 & t_v & \varepsilon_{13} \end{bmatrix},$$

$$\mathbf{G}_M = \begin{bmatrix} \varepsilon_{M1} & t_v & 0 \\ t_v & \varepsilon_{M2} + i\Delta & t_v \\ 0 & t_v & \varepsilon_{M3} \end{bmatrix}, \mathbf{G}_i = \begin{bmatrix} \varepsilon_{i1} & t_v & 0 \\ t_v & \varepsilon_{i2} & t_v \\ 0 & t_v & \varepsilon_{i3} \end{bmatrix};$$

$i \neq 1, M$  (14)

in which  $\Delta_{12} = \Delta_{M2} = \Delta$ , the imaginary part of self-energy  $\Sigma$  is defined through eq. (11), and  $\varepsilon_{ij}$  are the onsite energies within the  $i$ th cell.

According to the foregoing procedure, we may also find an expression for the electronic density of states (DOS) of the system. So the DOS at site  $i$  is given by,

$$\rho_i(E) = -\frac{1}{\pi} \text{Im}\{G_{ii}(E)\}. \quad (15)$$

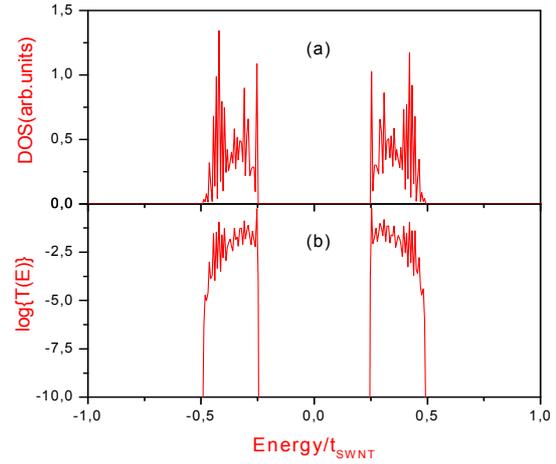
Using the eqs. (13) and (14) we obtain the diagonal elements of the Green's function matrix as follow,

$$G_{ii}(E) = \mathbf{G}_K, \quad K \neq 1, M$$

$$G_{11}(E) = \mathbf{G}_I, \quad G_{MM}(E) = \mathbf{G}_M. \quad (16)$$

### 3. Results and discussion

Based on the formalism described in section 2, we have investigated some of the significant properties of electronic conduction of SWNT/DNA/SWNT structure. To proceed, first we study the electronic density of states (DOS) and the electron transmission coefficient,  $T(E)$ , through DNA molecule in the foregoing structure. Panels (a) and (b) in figure 2 illustrate the DOS and the logarithm of  $T(E)$  for the SWNT/DNA/SWNT structure, respectively. DNA molecule has  $N=30$  base pairs (bps) and the SWNT electrodes are considered to be armchair (5, 5). Here the SWNT/molecule coupling strength and the hopping integral in the SWNT structure are set  $t_C = 0.3\text{eV}$  and  $t_{SWNT} = -3\text{eV}$ , respectively. Figure 2 displays the semiconducting behaviour of DNA molecule in the model with  $\approx 1.45\text{eV}$  energy gap,



**Figure 2.** (Color online) Panels (a) and (b) show the electronic density of states (DOS) and the logarithm of the transmission coefficient versus the dimensionless parameter  $energy/t_{SWNT}$  for the SWNT/DNA/SWNT system. Using the model parameters as mentioned in the text, we set  $t_{SWNT} = -3\text{eV}$ ,  $t_C = 0.3\text{eV}$  and 30 bps for DNA molecule. In addition the SWNTs are considered to be armchair (5, 5).

clearly. The semiconducting gap is principally induced by the vertical coupling strength between base pairs and the back bone in DNA structure.

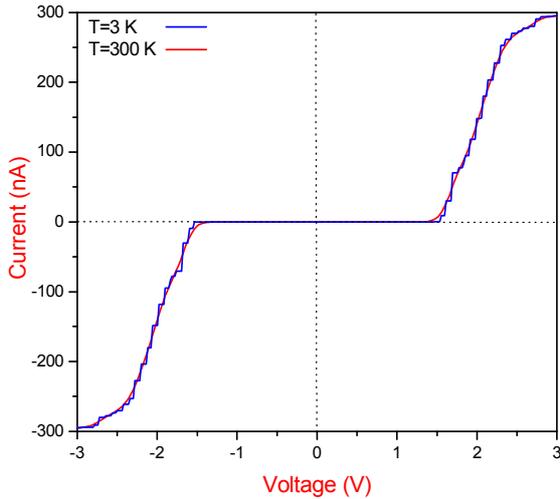
The current-voltage (I-V) characteristic of the system is investigated in figure 3. In order to calculate the current through SWNT/DNA/SWNT structure, we consider the standard transport formalism of electric current under an applied potential bias of  $V$  [24, 31],

$$I = \frac{2e}{h} \int_{-\infty}^{+\infty} dE T(E) W(E - E_f; eV), \quad (17)$$

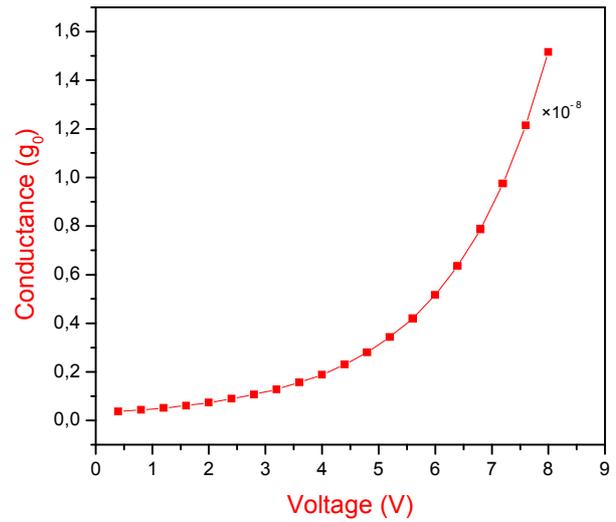
where  $T(E)$  denotes the electron transmission coefficient of DNA molecule in the SWNT/DNA/SWNT structure and  $E_f$  is the Fermi energy of the nano-electrodes,

$$W(E, eV) = f(E) - f(E + eV), \quad (18)$$

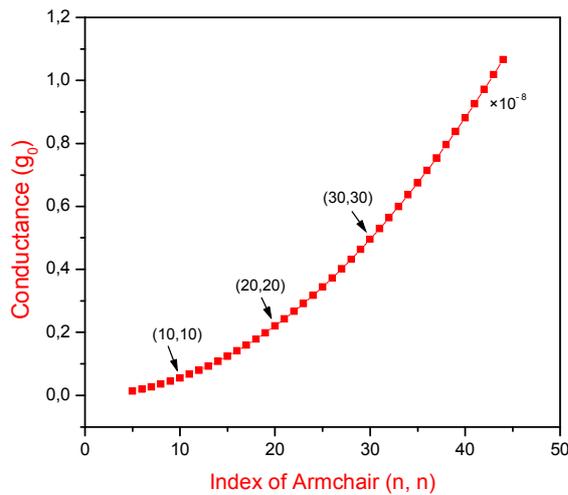
with the Fermi function  $f(E) = \left( e^{\beta E} + 1 \right)^{-1}$  and  $\beta = (k_B T)^{-1}$ . The Fermi function is the difference between charge distributions before and after transport [31, 32]. The driving force here is the electric potential bias. Figure 3 shows the I-V characteristics at the temperatures of 3 K and 300 K in a step-like curve and in smoothed curve, respectively. The I-V curves show clearly a nonlinear dependence. Our results show a good qualitative agreement with the energy gap of DNA (see figure 2) along the zero current part of the I-V curves. On the other hand, the low-voltage part of the I-V curves arises from the semiconducting behaviour of poly(dG)-poly(dC) DNA molecule. Also steps in the I-V curve, at low temperature, may be explained as the result of the transmission structure (figure 2(b)) caused by the interaction of DNA molecule with the nano-electrodes. However, as the temperature increased, this feature modified and at the higher



**Figure 3.** (Color online) The current-voltage characteristics of DNA molecule for low temperature ( $T=3$  K, step-like blue curve) and room temperature ( $T=300$  K, smoothed red curve) in the SWNT/DNA/SWNT system. Here, for armchair (5, 5) nanotubes as the nano-electrodes,  $t_{SWNT} = -3$  eV,  $t_C = 0.3$  eV and 30 bps for DNA molecule are set.



**Figure 4.** (Color online) The differential conductance (in units of  $g_0$ ) versus the applied bias between DNA molecule ends in the SWNT/DNA/SWNT system. Here, for armchair (5, 5) nanotubes as the nano-electrodes,  $t_{SWNT} = -3$  eV,  $t_C = 0.3$  eV and 30 bps for DNA molecule are set.



**Figure 5.** (Color online) The differential conductance (in units of  $g_0$ ) versus the tube diameter of electrodes with  $t_{SWNT} = -3$  eV,  $t_C = 0.3$  eV and 30 bps for DNA molecule in the model structure.

temperatures the step-like part of the I-V curve smoothed, as expected.

To study the effect of the varying of electric potential between DNA molecule ends on the conductance of the system, the differential conductance  $\left(\frac{dI}{dV}\right)$  of the system versus applied bias displayed in figure 4. Our results suggest that any increase in the value of the electric

potential across the molecule give rise to an increase in the conductance of the system. This is due to the fact that increasing the applied voltage makes the molecular orbitals wider, and thus electron tunneling will be easier.

Figure 5 illustrates the differential conductance of the system for some selected armchair nanotubes with different tube diameters as the electrode. We find that, as the tube radius ( $R$ ) increases, the conductance of the system considerably increases too. From the most experimentally observed carbon nanotube sizes, there is a tiny gap in the armchair nanotube types which arises from curvature effects [33]. Thus the increasing of the tube diameter give rise to decrease of the resistance [34] and also decreasing in the gap as  $\frac{1}{R^2}$  [35] and causes a large enhancement in the conductance of the system.

#### 4. Conclusion

To conclude, based on the presented methodology and our model in section 2 we have focused on investigating some of the significant electronic conduction properties of poly(dG)-poly(dC) DNA molecule in the SWNT/DNA/SWNT system. In the framework of Fishbone model, we consider DNA molecule with 30 base pairs as a planar molecule includes M cells and 3 further sites in each cell sandwiched between two semi-infinite armchair single-walled carbon nanotubes as the nano-electrode. Calculating of I-V characterizations, our results suggest a good agreement with the semiconducting behaviour of DNA, which the Porath et al experimental work emphasized on it. In addition, we

find that the increasing of (i) the applied bias between the molecule ends and (ii) the tube diameter of the

electrodes give rise to a large enhancement in the conductance of the system, respectively.

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