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Calculation of Current-Voltage Characteristics for Small DNA Chains

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ABSTRACT

This study explores the electronic transport characteristics of short deoxyribonucleic acid (DNA) chains, which have emerged as promising nanostructures for future bioelectronic applications. DNA, a molecule essential to the storage and transmission of genetic information in all known living organisms and many viruses, has attracted increasing interest in the field of molecular electronics due to its unique structural and conductive properties. In this research, the current–voltage (I–V) behavior of homogeneous nucleotide chains are analyzed using the Non-Equilibrium Green's Function (NEGF) formalism, a powerful quantum mechanical approach for studying charge transport in nanoscale systems under non-equilibrium conditions. The chains are modeled as linear sequences composed of identical nucleotides to isolate the intrinsic transport features. The applied bias voltage is systematically varied in the range of 0 to 4 volts to assess the electrical response of the system across both sub-gap and above-gap energy regimes. The simulation results reveal key insights into the conduction mechanisms within such molecular structures, which are highly sensitive to the applied voltage and molecular configuration. These findings contribute to a better understanding of DNA-based conductive behavior and may inform the design of future molecular-scale components in nanoelectronic circuits.

1. INTRODUCTION

Investigating the conductivity of the Deoxyribonucleic Acid (DNA) molecules attracted lots of attentions due to its wide applications in molecular bioelectronics [1-6]. It is already proposed that DNAs can be applied as semiconducting, metallic and isolating material in the nano-structures [1-6]. This DNA is a long molecule in the range of nanometer having a thickness of around 2nm. The interesting property of such a molecule is the feasibility of tuning its length according to the desired application. Therefore, DNAs can be considered as a fascinating candidate for the length-adjustable one-dimensional nanowires in the quantum devices. In addition, since the DNAs are fairly stable molecules consist of four basic fragments named Guanine, Cytosine, Adenine and Thymine, they provide the exciting capability of montaging the desired nanostructures in the field of molecular engineering [1].

In the past years, a wide range of empirical works has been done to address the electronic transport properties of the DNA molecules. For instance, the current-voltage characteristics of linear DNA in the range of micrometer is

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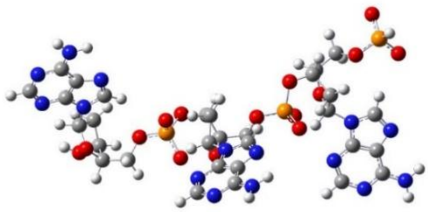
measured [1]. Furthermore, the current-voltage characteristics of a single DNA molecule having the energy gap of 2eV are observed previously [4]. Interestingly, based on these two studies, the DNAs can show both conducting and semiconducting behaviors on different geometrical conditions. Temperature-dependence of the DNA chains attached to the Platine electrodes with the spacing of 100nm is also investigated and shown to have metallic conductance [3].

Despite the wide range of the empirical works and IV measurements, the exact electronic transport mechanism of DNA molecules is debating. In this regard, the energy gap is proposed to be the underlying electron transmission mechanism. For instance, between two structures of poly-G and poly-C 20nm-separated were analyzed and their corresponding IV-characteristics obtained. This work has obtained similar bandgap of previous studies [1]. Based on many works, a semiconducting region around 0V is expecting. In addition, the energy gap of 1.5eV to 3eV in the dried condition observed for the DNA molecules [6]. On the other hand, in the humid environment, the G-C content would be the determining factor of the DNA conductivity. Therefore, the chamber humidity and the DNA composition would be the main factors in the transport properties [5].



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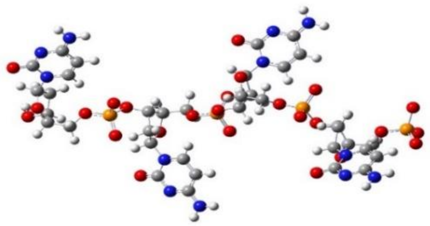

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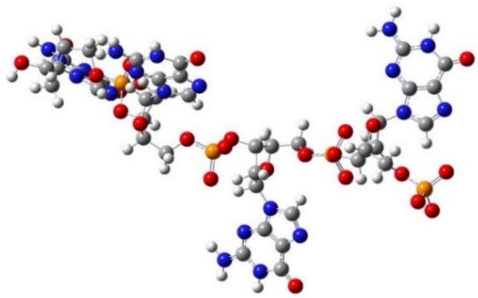

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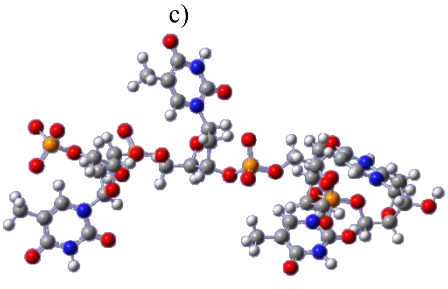

d)

Fig. 1. The considered nucleotide chains consist of identical monomers of a) Adenosine, b) Cytosine, c) Guanosine and d) Thymine

Here, we investigate the transport properties of the DNA molecules by the mean of Density Functional Theory (DFT) in uniform linear chains. In this regard, some small DNA molecules are modeled in GGA pseudo potentials and the transport properties are obtained using Non-Equilibrium Green's Function (NEGF) method. The current-voltage characteristics are calculated by applying a voltage sweep over the molecule through two contactless electrodes. The effect of the perpendicular electric field (Electronic Gate) on the passing current is also investigated using a metallic gate structure.

2. RESULTS AND ANALYSES

The considered chains having three monomers of Adenosine, Cytosine, Guanosine and Thymine are shown Fig.1. These chains are linear ones and one Phosphate fragment remains for each nucleotide.

In each chain, there exist three similar nucleotides conforming a small linear DNA structure. The choice of similar nucleotides make is easier to investigate the effect of each nucleotide in the considered chains. The electric contact is also shown in figure 2. This contact is consisting of two opposing Graphene Nanoribbon (GNR) with zigzag edge cut (ZGNR). This type of nanoribbons shows better conducting characteristics. Either of the nanoribbons has a protruding raw of three carbon atoms to minimize the coupling between their edge and the DNA chain.

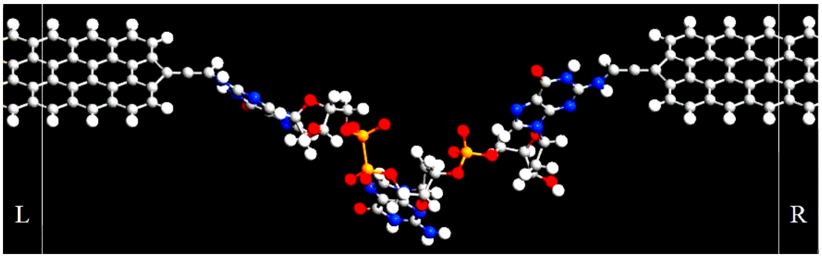

Fig. 2. Complete device structure with Guanosine molecule at the center. Left and right electrodes are shown by L and R letters

The complete structure was then subjected to the geometry optimization to relax the interatomic forces down to 6^{-10}eV/Å or less. This step is necessary for taking the structure to the minimized energy level. A three-step molecular dynamic analysis has been used to obtain the relaxed structure of the device at the desired spacing between the conducting electrodes and the central DNA molecule considering the fixed axis orientation for this molecule. In this regard, the density mesh cut off energy of 150 Rydberg are used. The convergence coefficients for Hamiltonian and the electron density are 10^{-4}. The structure can mainly be divided into the three parts: right and left electrodes, two graphene nanoribbons conforming the central region and the chain of the nucleotides. The central region contains two similar ZGNRs opposite to each other. Assuming a hypothetical axis along the molecule chain, the device is formed to be parallel to this chain and also thirty degrees tilted with respect to the graphene plate. Nearest neighbor atoms across the tunneling junctions are set to be 2.5Å apart. The central region is selected to be three-unit-vector long to obtain a fast convergence condition. The complete structure for Guanosine chain is depicted in Figure 2.

Table 1. Average bond lengths and angles after geometry optimization

a) Average bond lengths after geometry optimization (nm)				
N-C	C-C (Methyl)	C-C (Carboxyl)	C-O	**C=O**
1.38	1.60	1.48	1.34	**1.20**

b) Average bond angle after geometry optimization (degree)		
N-C-C (Methyl)	N-C-C (Carboxyl)	**C-C=O**
107.8	**120.7**	**122.6**

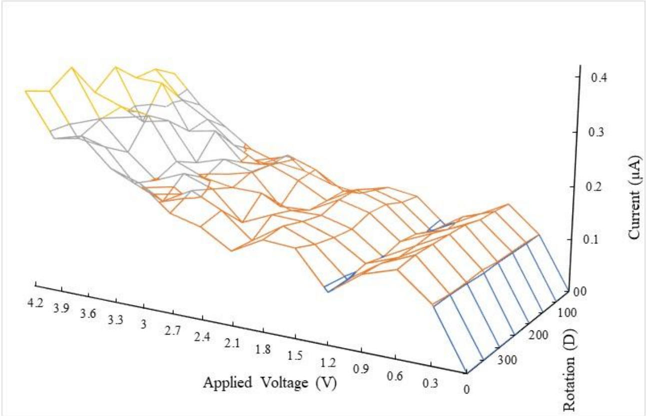

Fig. 3. The current-voltage characteristics of the Adenosine chain with respect to rotation angle

The external voltage is applied to the left (positive contact) and right (negative contact) conducting ZGNR electrodes and the current passing from the central molecule is obtained from the NEGF calculations performed at different voltages. The dangling bonds in the boundary outermost atoms are passivated using the hydrogen atoms to avoid numerical errors.

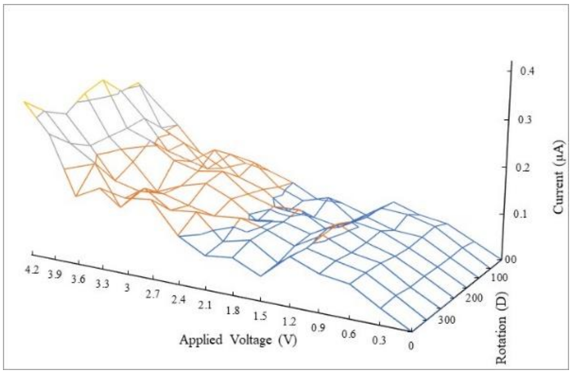

Fig. 4. The current-voltage characteristics of the Cytosine chain with respect to rotation angle

The average bond lengths and angles after geometrical optimization are presented in Table 1.

Figure 3. shows the current-voltage characteristics of the Adenosine chain at several different rotation angles of the molecule around the central axis. The rotation of the molecule around this axis can better demonstrate whether the conductance is isotropic or not. The current peaks around their corresponding maximum transmissions as it is expected. The rotation around the central axis seems to have minor effect on the transport properties as small perturbations are found in the 3D plot along the rotation axis. Interestingly, current decay after some peaks which demonstrate the negative differential resistance for the DNA chain. As it is obvious from the Figure 3., the current shows several swinging behaviors with respect to the increasing voltage. This behavior leads to negative differential resistance (NDR) in the different ranges of the considered voltage sweep. The behavior is more dominant at lower and higher voltages for the structure having non-deviated central molecule and tilted central molecule, respectively. The DC resistively is trivially affected by the swinging current.

Figure 4 shows the current-voltage characteristics of the Cytosine chain at several different rotation angles of the molecule around the central axis. Similarly, the current peaks are observed around their corresponding maximum transmissions. As it was shown for the Adenosine chain, the rotation around the central axis can fairly affect the transport properties. It should also be mentioned that the negative differential resistance is again observed for the guanosine although such effect basically occurs at lower voltages. This makes the Guanosine a better choice for applications which needs NDR around 1V.

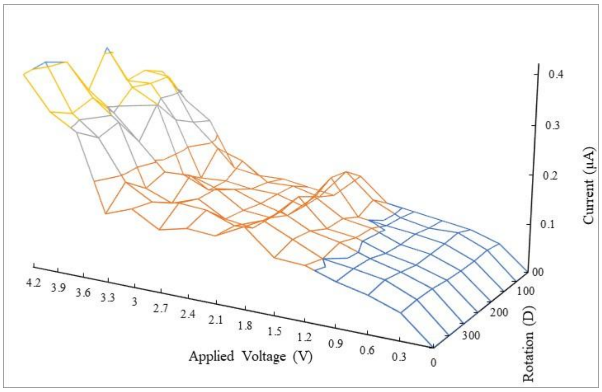

Fig. 5. The current-voltage characteristics of the Guanosine chain with respect to rotation angle

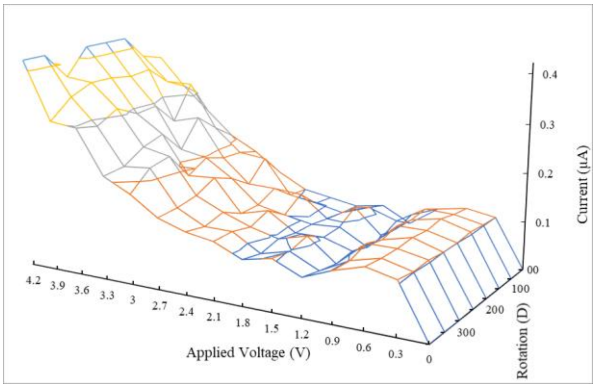

Fig. 6. The current-voltage characteristics of the Thymine chain with respect to rotation angle

The variation of the current-voltage characteristics for the chain of the Guanosine with respect to different rotation angles of the molecule around the central axis is depicted in Figure 5. Here, the position of the current peaks is mostly similar to that of Cytosine. The rotation of the chain molecule around the central axis has also negligible effect at lower voltages while this effect is much bolded at higher ones.

Finally, we investigate the transport properties of the Thymine chain in Figure 6. In contrast to previous chains, that of Thymine has higher conductivity around 4V. The main current peak spreads over a wider range of voltages while the second one is narrower and less dominant.

3. RESULTS AND ANALYSES

The transport properties in small chains of identical nucleotides are investigated here using the NEGF method. In the considered analysis, the central part of the conducting electrode is a ZCNR and the small DNA chain is fixed between two ZGNRs as conducting electrodes. The obtained current-voltage characteristics shows more than one region of Negative Differential Resistance below the considered maximum voltage of 4V. It is also shown that the rotation of the considered DNA molecule around the central axis of the conducting electrodes has no major effect on the obtained current.

CONFLICTS OF INTEREST

The authors declare no conflict of interest.

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