Electronic Properties Simulation of Guanine Molecule

Shakir A. A. AL-Saidi*, and Alaa Ayad K. Al-mebir**

Department of Physics, College of Education of Pure Sciences, University of Thi-Qar, Nasiriyah, Iraq

**alaa_ash28@yahoo.com, *Shakir.hussain@sci.utq.edu.iq

Abstract. This work studies, theoretically, electronic properties of DNA-based guanine molecule. General formula for the transmission probability for electron transfer through Guanine Molecule is derived. Guanine molecule is assumed to be as one active region connected between two leads. In the transmission calculation, three different locations of the onsite energy were noticed due to the change of the gate voltages applied on the molecule. Also, the (I-V) curve characteristics of Guanine was obtained by using tight binding model and steady state. The current as a function of gate voltage, that is varying between -4 to 4 eV, is also investigated. It is found that the current arises and vanishes at different gate voltage values to show gate switching states. Further, the relationship between different gate voltage values and different bias voltage values was presented to show the logic gate behavior. Moreover, conductance as a function of temperature study was stated. It shows two current behaviors, independent and strong dependence on temperature value, that changes the leads energy. These properties can be effectively used for molecular electronic devices.

Keywords; Electronic properties, DNA-based molecule, Guanine molecule, logic Gate

1. Introduction

Molecules have been used as remarkable choice for developing in nanoelectronics devices. Molecular electronics rely on using the electronic characteristics of finite molecules [1, 2]. Many molecular and nanoelectronics studies have been used to develop molecular and nanoelectronics devices for applications such as prototype diode, transistor, oscillator and switches [3, 4]. Other molecular devices designed for chemical and nonbiological applications like organic polymers [5, 6], large bio-molecules [7, 8], nanotubes and fullerenes [9, 10]. Many tests have been investigated theoretically including the (I-V) characteristics of the molecular model [11-13]. DNA-based molecules are one of the distinguished candidates for molecular electronics [14]. Self-assembly and self-distinction characteristics of DNA makes it among the most appropriate options for creating analogous molecular electronic devices. The designing and modification of three-ends devices such as the field effect transistor (FET) is well known to be a critical factor for evolution of molecular electronics [15]. Also, the capability to control the current flow through a single molecule is an essential goal in molecular electronics.

In this work, transmission, (I-V) characteristics and conductance are calculated for DNA-based Guanine molecule, and it has been analyzed for applications in molecular electronic devices. The structure metal-molecule-metal assembly can be shown in Fig (1). The Guanine molecule located between two gold leads. A voltage bias (V) range varying from -4 to 4 (eV) was applied to the four respective bases, and the corresponding current values were obtained. T(E) is the transmission probability for electrons located at an energy E through a device under the effect of the bias voltage (V). The Landauer equation based on the tight binding model. In which it is assumed that the elastic conductance of a molecule goes back to the probability that an electron with energy E injected in one lead will be transported to other lead through a active region. The active region in this work is Guanine base. By using theoretical MATLAB modeling, we calculated (I-V) characteristics of
Guanine. The effect of gate voltage on the characteristics of Guanine base was investigated by capacitating the gate and applying gate bias voltage. Every contact requires to carry the canal into balance with itself. The current flows from left lead to right lead to achieve the balance and equilibrium status [16].

Fig (1). A schematic illustration of the molecular model. The left and right ends of Guanine are connected to the electrode L and R in addition to D(donor) and A(accepter)

2. Theory and Treatment

The fundamental of digital electronics is logic gates. They may be using as memories, registers and counters. Guanine molecule acts as switch, thus it may be used to produce logic gates. In this paper, switch design suggested may be employed in logic gate by employing Guanine as molecular transistor as shown in Fig (2).

Fig (2). Schematic representation of gated Gold-Guanine-Gold structure

The electron straggles from one bridge that contains one Guanine molecule. The tight binding procedure of Guanine may be built as a molecular system. There is a single conduction channel in which site represent base. The depicting of DNA base as single location acts as molecular model. The system was depicted under assumption shown in Fig (1) in which the time-independent Hamiltonian (using Dirac’s notations) is used. This electronic Hamiltonian considers all the sub-systems interactions. The different indexes D, A, L, R and B denote the donor, acceptor, left lead, right lead, and bridge. The model, that you can also review in our previous paper [17], is begun with Hamiltonian as follows:

$$
\hat{H} = E_D|D⟩⟨D| + E_A|A⟩⟨A| + E_{k_b}|k_B⟩⟨k_B| + \sum_{k_R} [(V_{A k_R}|A⟩⟨k_R| + h.c) + (V_{D k_R}|D⟩⟨k_R| + h.c)]
+ \sum_{k_L} (V_{A k_L}|A⟩⟨k_L| + h.c) + \sum_{k_L} (V_{D k_L}|D⟩⟨k_L| + h.c)
$$

(1)

The index \(k_i\) is the energy wave vector, where \(i\) refers to the indexes D, A, L, R and b. \(E_i\) types the \(i\)th energy level position and \(|i⟩\) and \(⟨i|\) denote the ket and bra states respectively. \(V_{ij}\) represents the coupling interaction between the subsystems \(i\) and \(j\). The system wave function can be written as:
\[ \psi(t) = C_D(t)|D\rangle + C_A(t)|A\rangle + \sum_{k_B} C_{k_B}(t)|k_B\rangle + \sum_{k_L} C_{k_L}(t)|k_L\rangle + \sum_{k_R} C_{k_R}(t)|k_R\rangle \quad (2) \]

where \( C_i(t) \) represents the linear expansion coefficients. The equations of motion for \( C_i(t) \) can be obtained by using time dependent Schrödinger equation:

\[ \frac{\partial \psi(t)}{\partial t} = -iH\psi(t) \quad (3) \]

So, we get the following set of related equations:

\[ \dot{C}_D(t) = -iE_D C_D(t) - i \sum_{k_L} V_{Dkl} C_{k_L}(t) - i \sum_{k_B} V_{Dk_B} C_{k_B}(t) \quad (4) \]

\[ \dot{C}_A(t) = -iE_A C_A(t) - i \sum_{k_R} V_{Akr} C_{k_R}(t) - i \sum_{k_B} V_{Ak_B} C_{k_B}(t) \quad (5) \]

\[ \dot{C}_{k_B}(t) = -iE_{k_B} C_{k_B}(t) - iV_{k_B D} C_D(t) - iV_{k_B A} C_A(t) \quad (6) \]

\[ \dot{C}_{k_L}(t) = -iE_{k_L} C_{k_L}(t) - iV_{k_L D} C_D(t) \quad (7) \]

\[ \dot{C}_{k_R}(t) = -iE_{k_R} C_{k_R}(t) - iV_{k_R A} C_A(t) \quad (8) \]

where \( V_{ij} = V_{ji} \) and \( i,j = A \), \( D \), \( k_L \), \( k_R \) and \( k_B \)

By using condition stationary states, we define \( C_i(t) \) as \( \bar{C}_i(t) = \bar{C}_i e^{-iEt} \) with \( E \) denotes the system eigen values. So, we put \( \dot{C}_i = 0 \). Then follow separation procedure:

\[ V_{k_i \alpha} = v_{k_i} V^{\alpha} \quad (9) \]

\[ \bar{C}_{kl} = v_{k_i} \bar{C}_i \quad (10) \]

where \( i = L, R \) and \( B \) and \( \alpha = A \) and \( D \)

By substituting these definitions in eqs (4)-(8), we get:

\[ \bar{C}_A(E) = \frac{1}{E - E_A} \left( V^{AR} \sum_{k_B} |v_{k_B}|^2 \bar{C}_R(t) + V^{AB} \sum_{k_B} |v_{k_B}|^2 \bar{C}_B(t) \right) \quad (11) \]

\[ \bar{C}_D(E) = \frac{1}{E - E_D} \left( V^{DL} \sum_{k_L} |v_{k_L}|^2 \bar{C}_L(t) + V^{DB} \sum_{k_B} |v_{k_B}|^2 \bar{C}_B(t) \right) \quad (12) \]

\[ \bar{C}_B(E) = \frac{1}{E - E_B} \{ V^{BD} \bar{C}_D + V^{BA} \bar{C}_A \} \quad (13) \]

\[ \bar{C}_L(E) = \frac{1}{E - E_L} V^{LD} \bar{C}_D \quad (14) \]

\[ \bar{C}_R(E) = \frac{1}{E - E_R} V^{RA} \bar{C}_A \quad (15) \]
By substituting (13) and (15) in (11), we get:

\[
\bar{c}_A(E) = \frac{1}{E - E_A - \Sigma_{AR}(E) - \Sigma_{AB}(E)} \left\{ \frac{V^{AB}V^{BD}}{E - E_B} \right\}
\]  

(16)

Thus, we obtain an obvious expression for:

\[
\frac{c_{A}(E)}{c_{D}(E)} = \frac{X_{1}(E)}{X_{2}(E)} = \frac{1}{E - E_A - \Sigma_{AR}(E) - \Sigma_{AB}(E)} \left\{ \frac{V^{AB}V^{BD}}{E - E_B} \right\}
\]

(17)

Where

\[
X_{1}(E) = \frac{V^{AB}V^{BD}}{E - E_B}
\]  

(18)

\[
X_{2}(E) = E - E_A - \Sigma_{AR}(E) - \Sigma_{AB}(E)
\]  

(19)

Where,

\[
\Sigma_{ij}(E) = |V_{ij}|^2 \Gamma_{j}(E)
\]  

(20)

is the interaction, self-energy, where:

\[
\Gamma_{j}(E) = \sum_{k_j} \frac{|V_{kj}|^2}{E - E_k}
\]  

(21)

With \(k_k = k_L, k_R\) and \(k_{B}\)

The transmission amplitude and the transmission probability are respectively defined as:

\[
t(E) = \frac{\bar{c}_A(E)}{\bar{c}_D(E)}
\]  

(22)

and,

\[
T(E) = |t(E)|^2
\]  

(23)

The steady state electric current through the active region may be calculated by employing the Landauer formula [18]:

\[
I = \frac{2e}{h} \int_{-\infty}^{\infty} T(E) [f_L(E) - f_R(E)] dE
\]  

(24)

\(f_{\alpha}(E)\) is a Fermi distribution function of electrons in the lead \(\alpha\), with \(\alpha=L, R\),

\[
f_{\alpha}(E) = \left\{ 1 + \exp \left[ \frac{E - \mu_{\alpha}}{k_B T_{\alpha}} \right] \right\}^{-1}
\]  

(25)

\(\mu_{\alpha}\) is the chemical potential of the lead \(\alpha\), with \(\mu_L = \frac{V}{2}\) and \(\mu_R = -\frac{V}{2}\), where \(V\) is the bias voltage. \(T_{\alpha}\) is the temperature of the lead \(\alpha\), with \(T_{L}=T_{R}=T_{e}\), \(T_{e}\) is fixed at 300K, which mean that both electrodes are in a thermal equilibrium situation.

The conductance for the system will be calculated as a function of temperature, i.e. the lead temperature, in the thermal equilibrium state. After calculating the transmission probability using our model computation, the results for the conductance can be obtained by using the following equation [19]:
5

\[ G = \frac{2e^2}{h} \int_{-\infty}^{\infty} dE \frac{d^2 \langle E \rangle}{dE} \]  

(26)

where \( f(E) \) is defined in eq (25), and since the thermal equilibrium is considered in our calculation, we can write: \( T_eR_e = T_eL_e = T_e \) with \( T_e = 300 \) K.

3. Results and Discussion

3.1. Transmission probability

The calculations of the transmission spectrum are the most important step in investigating the mobility and dynamic properties of the electron transfers feasibility in molecule. The resulted transmission spectrum calculations will be used to get the electric current and conductance for Guanine molecule. The transmission probability \( T(E) \) is plotted as a function of energy \( E \) for the active region, which consists of Guanine. The gate performance can be checked by looking at the dispensation of the unoccupied orbitals. In Fig (3), the spectra of the transmission of the device up to the Fermi level with three different gate voltages, (+4, 0 and -4) eV, are shown. Large intensity orbitals in the spectral window (below 1.0 eV) rely variously on the voltages of the gate. The orbital at biggest value of \( T(E) \) refers to the gating effect. It is flogging up by positive voltage and repealing down by negative voltage. Hence, at low energy the current is often limited by the empennage of peaks of the highest transmission. They are got at zero source-drain voltage. Three different locations of the onsite energy were noticed due to the change of the gate voltages applied on the molecule.
Thus, from the transmission probability for the case of molecular model for three possibilities of gate voltage presented in Fig (3), we can conclude the following. First, the transmission spectrum contains three types of structures that are the resonance one (with narrow width), the anti-resonance one (i.e. Fano resonances) and the Breit-Wigner line shape. Second, the peak of the Breit-Wigner line shape lies on the energy of $E_A (=0.0)$ with certain shift in energy due to level self-energy. Also, the spectrum shows the interference effects manifested by one Fano resonance for (4 and 0) eV gate voltage lying above the Breit-Wigner line towards the positive energies, and this is because there are many channels for the electron to be transported. The number of the Fano resonances is determined according to the strength of coupling. Further, the interaction between the accepter and the lead
controls the height and width of the Breit-Wigner line shape as well as the type and height of resonance.

3.2. Tunneling current calculation
The characteristics of \((I-V)\) was characterized between the current and gate voltage for zero source voltage. The resonant tunneling occurs via molecular orbitals of Guanine which give an open lane for conduction when aligned with the Fermi level. The tunneling current features were obtained by vibrating the voltage from \(-4\) (eV) to \(4\) (eV) and are shown in the Fig (4).
Fig 4. Current as a function of bias voltage at gate voltage $V_g = -4 \text{ eV}$ (a), $V_g = 0 \text{ eV}$ (b) and $V_g = 4 \text{ eV}$ (c)

Fig (5). The current as a function of gate voltage (eV)

In Fig (5), the current as a function of gate voltage ($I-V_g$) curve is shown. It obviously represents a nonlinear reliance, and it can reflect two states. Firstly, the vanishing of current at finite values (-4 to 2) eV of a gate voltage. Second, the current appears just when the gate voltage is set at 2 (eV), while
the computed current has values near zero at little voltage. This can be due to the bonding sensitivity between molecule and electrodes. This phenomenon gives switching case for molecular model.

3.3. Conductance calculations
The conductance is enhanced due to the hopping transport mechanism between the chemical potentials and active region energy levels (which inter fermi level and adjacent sites). Fig (6) illustrates the conductance as a function of temperature, when gate voltage $V_g$ = -4 eV (a), $V_g$=0 eV (b) and $V_g$=4 eV (c). The conductance-temperature curve shows two behaviors. Firstly, from 0 to 300 K, the conductance is fixed, and it is independent on temperature. However, the conductance shows strong dependence on the temperature at T from 300 to 400 K. These two behaviors go back to the changes in the energy of the two leads due to the change in the temperature. This leads to concentration increment of charge carriers. Further, it can be noticed, from the difference between curves in a, b, and c figures, that the conductance increases with the increment of gate voltages.
4. Conclusion

In this study, transmission, ($I-V$) characteristics and conductance are theoretically calculated for DNA-based Guanine molecule to use in molecular electronic devices. The structure metal-molecule-metal assemble is used, and the Guanine molecule located between two gold leads. A voltage bias ($V$) range varying from -4 to 4 (eV) was applied. It was found that the states located close to the active region edges have a very low transmission probability. While high transmission probability was noticed close to energy of Guanine. Three different locations of the onsite energy were measured due to the change of the gate voltages that were applied on the molecule. Also, the measured $(I-V_g)$ curves shows a nonlinear dependence. The current is vanished at gate voltage values between (-4 to 2) eV, those give switching state, while is arises when the gate voltage is set at 2 (eV). This might be due to bonding sensitivity between molecule and electrodes. The resulted relation between different gate voltage values and different bias voltage values reflect the logic gate operation. Further, the study of conductance as a function of temperature offers two behaviors, independent and strong dependence, depending on temperature value that changes the leads energy.

Acknowledgments

We thank Prof. Jenan Majeed AL-Mukh and Prof. Shakier Ibraheem Easa from Basrah University for useful discussions. We also thank Iraqi Ministry of Higher Education and Scientific Research for its support of scientific researches through the Iraqi Virtual Science Library.

References

1. Jortner, J., et al., Molecular electronics. 1997: Blackwell Science Oxford.
2. Elke, S. and C.J. Carlos, Molecular electronics: an introduction to theory and experiment. Vol. 15. 2017: World Scientific.
3. Heath, J.R. and M.A. Ratner, Molecular electronics. 2003.
4. Datta, S., *Electronic transport in mesoscopic systems*. 1997: Cambridge university press.
5. Gómez-Herrero, J. and F. Zamora, *Coordination polymers for nanoelectronics*. Advanced Materials, 2011. 23(44): p. 5311-5317.
6. MacDiarmid, A.G., “Synthetic metals”: a novel role for organic polymers. Current Applied Physics, 2001. 1(4-5): p. 269-279.
7. Keren, K., et al., *Sequence-specific molecular lithography on single DNA molecules*. Science, 2002. 297(5578): p. 72-75.
8. Patil, S.R., et al. *Charge transport through DNA based electronic barriers*. in *AIP Conference Proceedings*. 2018. AIP Publishing LLC.
9. Tamersit, K. and F. Djeffal, *Carbon nanotube field-effect transistor with vacuum gate dielectric for label-free detection of DNA molecules*: a computational investigation. IEEE Sensors Journal, 2019. 19(20): p. 9263-9270.
10. Vittala, S.K., S.K. Saraswathi, and J. Joseph, *Self-Assembled Functional Fullerenes and DNA Hybrid Nanomaterials for Various Applications*. Tempted DNA Nanotechnology: Functional DNA Nanoarchitectonics, 2019: p. 271.
11. Zhou, Y.-h., et al., *Current rectification by asymmetric molecules*: An ab initio study. The Journal of chemical physics, 2006. 125(24): p. 244701.
12. Di Ventra, M., S. Pantelides, and N. Lang, *First-principles calculation of transport properties of a molecular device*. Physical review letters, 2000. 84(5): p. 979.
13. Bauschlicher, C.W. and J.W. Lawson, *Current–voltage curves for molecular junctions: the issue of the basis set for the metal contacts*. Theoretical Chemistry Accounts, 2008. 119(5-6): p. 429-435.
14. Wang, K., *DNA-based single-molecule electronics*: From concept to function. Journal of functional biomaterials, 2018. 9(1): p. 8.
15. Liu, J., et al., *Ultrsensitive Monolayer MoS2 Field-Effect Transistor Based DNA Sensors for Screening of Down Syndrome*. Nano letters, 2019. 19(3): p. 1437-1444.
16. Datta, S., *Quantum transport*: atom to transistor. 2005: Cambridge university press.
17. AL-Saidi, S.A., A.A.K. Al-mebir, and M. Hallool, *Characteristics of Thymine Molecule System Behave as Molecular Electronic Device*. Misan Journal of Academic Studies, 2019. 18(35): p. 130-143.
18. Brisker-Klaiman, D. and U. Peskin, *Coherent elastic transport contribution to currents through ordered DNA molecular junctions*. The Journal of Physical Chemistry C, 2010. 114(44): p. 19077-19082.
19. Gutiérrez, R., S. Mandal, and G. Cuniberti, *Dissipative effects in the electronic transport through DNA molecular wires*. Physical Review B, 2005. 71(23): p. 235116.