

STUDY OF AN ASYMMETRIC STRUCTURE OF (G/C) AND (A/T) MOLECULES AS A RECTIFIER AT NANOSCALEShakir A. A. AL-Saidi¹, Mohammed H. Mokhilif², Ali Natheer Tuaimah³^{1,2} Department of Physics, College of Education of Pure Sciences University of Thi-Qar, Nassiriyha, Iraq³ College of Science University of Thi-Qar, Nassiriyha, Iraq***Corresponding Author**Shakir¹ A. A. AL-SaidiShakir.hussain@sci.utq.edu.iqDOI: <https://doi.org/10.47957/ijciar.v6i2.154>*Received: 29 Feb 2023 Revised: 15 March 2023 Accepted: 30 April 2023***Abstract**

In this study, Nano-diode is proposed using an asymmetric structure of two different molecules attached to metal electrodes. The asymmetric molecular structure acts as a molecular diode (MD) in uniformity circuits at the Nano scale. A tight-binding model is adopted to describe MD, and the results are based on the steady-state formula to illustrate charge transfer. Theoretical calculations of the conductivity and current as a function of time, the study of the effect of heat on it, as well as the study of the rectification current ratio as a function of bias voltage, all these calculations were made using two types of molecules of DNA, they are (G/C) and (A/T). The results were encouraging because they gave the common features of the rectification. The analysis may be useful in the fabrication of electronic devices with Nanotechnology.

Keyword: Nanoscale diode, molecular rectifier, tight-binding model, conductance, current.

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**Introduction**

Nanotechnology is the treatment of matters on the atomic, molecular, and super-molecular scale. Nanotechnology is attracting increasing investment from both government and industries around the world, providing significant opportunities for the exploration of new emerging Nano devices such as carbon Nanotubes and DNA at the Nano scale [1, 2,3]. Molecules and Nano electronics using molecules are monostructures and nanoparticles as the active ingredients produce promising technology concepts that are receiving exponentially increasing interest. The science and technology of designing and manufacturing electronic devices based on nanostructures. Molecular electronics [4]. Is a new technology, but it is in its early stages as it holds hope for the future of atomic electronic systems. Molecular electronics uses molecules as basic components such as wires, switches, and transistors in building electronic circuits. Molecular electronics describes the field of use of molecules as an active or passive components in electronic devices [5]. Electron transfer through molecules sandwiched between metal electrodes has increased. It has attracted increasing interest for fundamental reasons and future applications. For Molecular Electronic Technology [6-8]. Experimental, No Precision Processing nor is the measurement of the atomic structure of the bonding of the molecule with the electrodes an easy task. Therefore, it is difficult to determine the effect of atomic structure on transport through hardware or to find a path to improve device performance. Subsequently, the ability to calculate atomic and electronic structures and transport properties with metallic molecular junctions is important and useful in this field. The wide use of the strategy of binding molecules to electrodes, such as bonding molecules with two suitable end groups, such as thiols, which can be covalently attached to the metallic electrodes. [9-15] two types of dithiol molecules have been extensively studied. One of these chains is alkane dithiol. These molecules are considered to be highly insulating due to the large energy gap between the highest occupied molecular orbital (HOMO) and Lowest Unoccupied Molecular Orbital (LUMO), but are relatively simple and chemically inert, making them a nice model system for testing experimental technologies or Theoretical methods [16, 17]. Dithiol II is based on conjugated aryl oligomers, such as Oligovinyl-dithiols and oligophenylene-ethylene-dithiols. [18, 19] conjugations, smaller HOMO-LUMO gap, and the operability of these molecules make them more Attractive potential for molecular electronic applications. These pioneering works have stimulated a great theoretical scope to investigate the Electron transfer properties of these molecules [20-22]. Other functional devices are dependent on Molecular junctions, such as molecular wires [9, 12, 15]. The asymmetric double quantum dot structure contains two sequentially asymmetric-sized quantum dots that are modeled as a rectifier. [23]. The probability of an electron traveling through an asymmetric molecular

structure as a molecular diode (MD) can be efficiently controlled by changing the direction of the current or the polarity of the voltage. The advantage of using MD as a diode is due to its Nanoscale size, and perfect operation. In addition, this nanostructure is a ballistic conductor, because electrons diffuse freely, which leads to reduced resistance [24]. The straightening process occurs in the asymmetric state, but it disappears in the symmetric state. The designed molecular diode (MD) will be millions of times smaller than the diodes found in the corresponding digital logic circuits manufactured on conventional integrated electronic chips.

In this paper, A theoretical model has been proposed for molecular diode (MD) design to check the functioning of the MD structure as a molecular diode, by using it in the rectifying process. All of our numerical calculations were performed based on the tight-binding model and the steady state formalism. The numerical results of conductance and current, which clearly show the electronic properties of the rectification process, this work may be useful for fabricating a rectifier at the Nanoscale using (MD) design.

2. Model and Theoretical Formulation

2.1. Rectification process

By relating the MD structure to the AC signal, see Fig.(1). It is found that the MD structure acts as a molecular diode effectively because it can straighten the AC signal well. The AC input signal can be described as [24],

$$V(t) = V_0 \sin(\omega t) \quad (1)$$

Where V_0 is the peak voltage, ω and t are the angular frequency and time, respectively. The fluctuation of the AC input signal as a function of ωt is shown in Fig.(2).

In Fig.(3) and Fig.(4), it is clear that the positive half-wave of the input signal can pass through the circuit. This behavior occurs when the MD structure of the diode is aligned as follows: the small molecule, which has a large ionization energy, is the first, and the second is the large molecule, which has a small ionization energy. While the negative half-wave of the AC input signal is suppressed by the reversal of the locations of the MD structure, which acts as a rectifier.

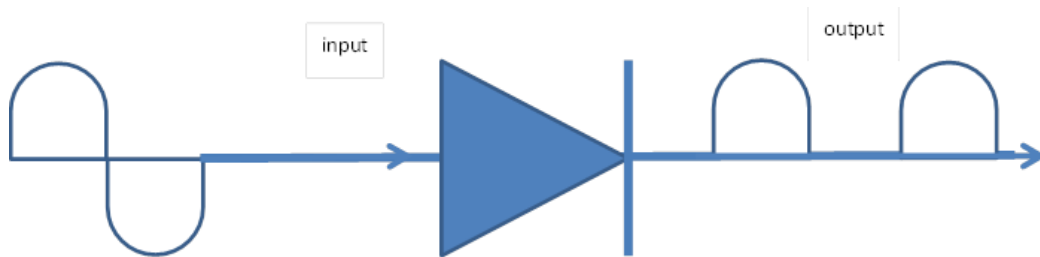


Fig. (1) The rectification process by using MD structure that acts as a diode. The diode attached to the source and drain.

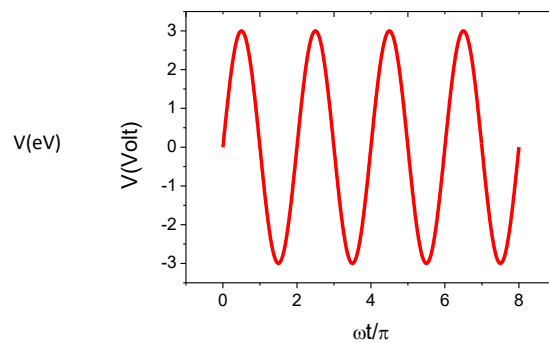


Fig. (2) Variations of AC input voltage signal as a function of the time.

In a rectifier connected to a single quantum wire, current flows in one direction through each half-wave of AC input voltage.

2.3. Theoretical formulation

In tight binding processing, the system can be converted into a sequential model, which takes into account the energy level of each molecule and the coupling interaction between two molecules. The eigenvalues of MD are calculated using a tight binding model such as [25],

$$E_j = E_Q - 2V_{mn} \cos\left(\frac{\pi j}{N+1}\right), \quad (2)$$

where E_Q is the energy level of the molecule. V_{mn} is the conjugation interaction between nearest neighboring molecules. N stands for the total number of molecules. The simplest MD tight-binding manipulation can be prepared as a one-dimensional string, every connection between the sites means that there is a coupling interaction. The description of MD as a single site is a simplification of the wiring model, and a description of the system under consideration (which is shown in Fig. 1) using the following time-independent Hamiltonian (using Dirac's notations). This Hamiltonian describes all the sub-systems interactions, is as follows,

$$H = E_D |D\rangle\langle D| + E_A |A\rangle\langle A| + \sum_{k_b} E_{k_b} |k_b\rangle\langle k_b| + \sum_{k_b} [(V_{Ak_b} |A\rangle\langle k_b| + \text{h.c.}) + (V_{Dk_b} |D\rangle\langle k_b| + \text{h.c.}) + \text{h.c.}] \\ + \sum_{k_L} (V_{Dk_L} |D\rangle\langle k_L| + \text{h.c.}) + \sum_{k_R} (V_{Ak_L} |A\rangle\langle k_L| + \text{h.c.}) \quad (3)$$

where the different indexes D , A , $L1$, $L2$, and b denote the donor, acceptor, first lead, second lead, and the molecules with total number N . The index k_i is the energy wave vector with i which represents the indexes D , A , $L1$, $L2$, and b . E_i represents the energy level position and $|i\rangle$ and $\langle i|$ represent 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,

$$\psi(t) = C_D(t) |D\rangle + C_A(t) |A\rangle + \sum_{k_b} C_{k_b}(t) |k_b\rangle + \sum_{k_{L1}} C_{k_{L1}}(t) |k_{L1}\rangle + \sum_{k_{L2}} C_{k_{L2}}(t) |k_{L2}\rangle, \quad (4)$$

where $C_i(t)$ represents the linear expansion coefficients. The equations of motion for $C_i(t)$ can be obtained by using the time-dependent Schrodinger equation,

$$\frac{\partial \psi(t)}{\partial t} = -iH\psi(t). \quad (5)$$

Then by substituting equations (3) and (4) in (5) we obtain,

$$\frac{\bar{C}_A(E)}{\bar{C}_D(E)} = \frac{X(E)}{Y(E)}, \quad (6)$$

where,

$$X(E) = V^{Ab} \Gamma_b(E) V^{bD}, \quad (7)$$

$$Y(E) = E - E_A - \sum_{AL1} \Sigma(E) - \sum_{Ab} \Sigma(E), \quad (8)$$

$$\text{here } \Sigma_{Ai}(E) = -i\Delta_{Ai}(E) + \Lambda_{Ai}(E),$$

where $\Delta_{Ai}(E)$ is the broadening function, while $\Lambda_{Ai}(E)$ is the quantum shift function, where $i = L1, b$. Thus, the transmission amplitude and the transmission probability are respectively defined by [26],

$$t(E) = \frac{\bar{C}_A(E)}{\bar{C}_D(E)}, \quad (9)$$

and,

$$T(E) = |t(E)|^2. \quad (10)$$

The current through the active region can be calculated using the Landauer transfer formula [27],

$$I = \frac{2e}{h} \int_{-\infty}^{\infty} T(E) [f_{L1}(E) - f_{L2}(E)] dE, \quad (11)$$

The conductivity can be calculated, as long as the transmission probability can be obtained in the calculations of this model under study, using the following formula [28],

$$G = \frac{2e^2}{h} \int_{-\infty}^{\infty} dE T(E) \frac{\partial f_{\alpha}(E)}{\partial E}, \quad (12)$$

where $f_{\alpha}(E) = \{1 + \exp[(E - \mu_{\alpha})/k_B T e_{\alpha}]\}^{-1}$ is Fermi distribution function of electrons in the lead $\alpha = L1, L2$. The chemical potential of the lead α is μ_{α} with $\mu_{L1} = -V/2$ and $\mu_{L2} = +V/2$ where V is the bias voltage. The temperature $T e_{\alpha}$ of the lead α . Here we use $T e_{L1} = T e_{L2} = T e$ is fixed at 300 K, which means that the leads are in thermal equilibrium.

3. Results and Discussion

In beginning, we referred to the magnitude of factors used for our numerical computations. The amplitude V_0 of the AC input signal is set at 2 eV. Closest-neighboring hopping strength V_{nm} is set to 0.01 eV. The coupling interaction of donor-bridge and acceptor-bridge are 0.1 eV. The coupling interaction of donor and acceptor with right and left lead is 1 eV. The balance Fermi energy E_F is at zero. The energy levels of the small molecules (Cytosine (C) and Thymine (T) are 3.75 eV and 4.15 eV respectively), and big molecules Guanine (G) and Adenine (A) are 2.63 eV and 3.25 eV respectively. To clearly describe the evaluation process, we draw the current as a function of time for both molecular groups (A/T) and (G/C) as shown in Fig. (3 and 4) are measured in units ($\frac{2e}{h}$). The current passes through the diode through the integrator on transmission function, see

Eq.(10) and Eq.(11). Non-fading current valueOnly checks at the positive half-wave of the alternating input signal of $n\pi < \omega t < (n+1)\pi$, where n is zero or an even number. The value of the current fadesat the negative half-wave input signal which is set at $n\pi < \omega t < (n+1)\pi$, where n is odd. It is clear that each of these properties shows that the molecular rectifier model is working effectively.The rectification process was performed, as shown in Fig.(5)for the conductivity as a function of time, measured in units ($\frac{2e^2}{h}$), which appears clearly from the drawing the conductivity has certain values only in the positive half-cycles of the AC input signal. On the other hand, the conductivity specifically disappears forthe half-wave negative of the same AC input signal,also observed that each peak in the conductivity spectrum is splitinto two secondary peaks. This split is clearly shown in Fig.(6)in the case of molecules (A/T) and more deeply than in the case of two molecules (G/C)due to the difference between the positional energies of those molecules.The results for the (G/C) and (A/T) molecules are shown in the two Figs. (7 and 8) illustrated that the current and voltage curves around the zero bias values are asymmetric,whilethe current under the influence of positive voltage is greater than the values of current under the influence of negative voltage wherethe higher values of electric current are pushed with an increase in the positive bias voltage much greater than the drag that occurs downwards for values for negative voltage with increasing reverse bias voltage. Moreover, the current output from the two molecules (A/T) is three times higher than the current from the two molecules (G/C) due to the difference between the positional energies of both molecules.Charge transfer due to the structure of the system back tothe interaction of (A/T) and (G/C) molecules with the Nanoelectrodes,any increase in the temperature leads to an increase in the absolute value of current with swing voltage values of bias between negative and positive of I-V curves.When the energy of electrons increasesat molecular levels, the chance of their transfer from one molecular level to another molecular level increases too, and thus the values of electric current increase as expected.When molecules are manufactured in a way that allows them to accept electrons from one terminal without the other, this type of molecule is called a molecular rectifier. These molecular ingredients mimic their bulk counterparts,these molecules should form an electron acceptor on one end and an electron donor on the other. The electron is expected to pass only from the donor part of the molecule towards the acceptor part of the molecule.Fig.(7) and Fig.(8) also show the properties of I-V at temperatures (100, 200, and 300 K), which are represented by the blue, green, and red lines, respectively,the I-V curves clearly show a smooth and non-linear dependence. Our results show a good qualitative agreement with the voltage gap of the (A/T) and (G/C) molecules along the zero electric current portion of the I-V curves, which gives the semiconducting behavior of the (A/T) and (G/C) molecules. Accordingly, the (A/T) and (G/C) particles clearly act as a rectifier (see Fig.(7) and Fig.(8), as they showed very high resistance in the case of reverse bias and good conductivity in the case of forwarding bias. Fig.(9) describes the rectification process, by drawing the relationship between the current rectification ratio($\frac{I_{forward}}{I_{reverse}}$) and the bias voltage.Where observed that the current rectification ratio for the two molecules (G/C) and (A/T) is not much affected by the change in the bias voltage, and this gives more stability to the molecular device.Also, noted a slight decrease in the rectifier ratio with the increase in the bias voltage, and this is very logical due to themolecules do not bear high voltages, and here stands outthe importance of knowing the determinants of the work of molecules as molecular devices. On the other hand, the current rectification ratio in the case of two (A/T) molecules is three times greater than the current rectification ratio of the two (G/C) molecules, due to the difference in the positional energies of each of these molecules. Based on our promising results, we believe that this asymmetric system of molecules is ideal for pushing the boundaries of orthodontics closer to achieving the goal of functional molecular devices.To study the effect of voltage variationConnection between the two ends of the molecules in the system, as a function of the applied bias voltage and as shown in Figs.(10 and 11) From the results obtained, it has been suggested that any increase in the value of the electric potential across the moleculeslead to an increase in system connectivity. This is because of the fact that increasing the applied voltage makes the molecular orbitals expand, so electron tunneling will be easier.It is also observed from Fig. (10) and Fig. (11) that the conductivity is zero at values of positive bias voltage near zero, as well as negative bias voltage values, therefore, molecules behave as insulators at these values, after that, the conductivity begins to increase with the increase of bias voltage until it reaches specific values, then the conductivity takes the greatest value and then begins to decline whenever the bias voltage values increase from this specific value. It has been observed that the increase in temperature increases the conductivity values. It is also noted that the conductivity begins to appear after a specific threshold voltage when the value of the positive bias voltage increases, as the positive bias voltage overcomes the molecular voltage barrier, allowing the passage of electrons through the molecule, and when the value of the positive bias voltage increases more, It is noticed that the conductivity value increases more until it reaches at maximum conductivity value after that, the conductivity value begins to decrease due to the consumption of the molecular electrons as a result of the effect of the increasing bias voltage on the molecules little by little, and this is also one of the determinants of the work of molecules as molecular electronic devices. It is also noticed a slight difference between the value of the threshold voltage and the greatest conductivity in the case of (G/C) and (A/T) molecules, due to the difference between the ionization energies of these molecules, also noted that the effect of temperature on conductivity contributes to narrowing the shape of the curve of the peak on both sides and increasing the value of the peak from the top as the temperature increases (100, 200 and 300K), and it is likely that the reason for this is due to the change in the molecular levels.

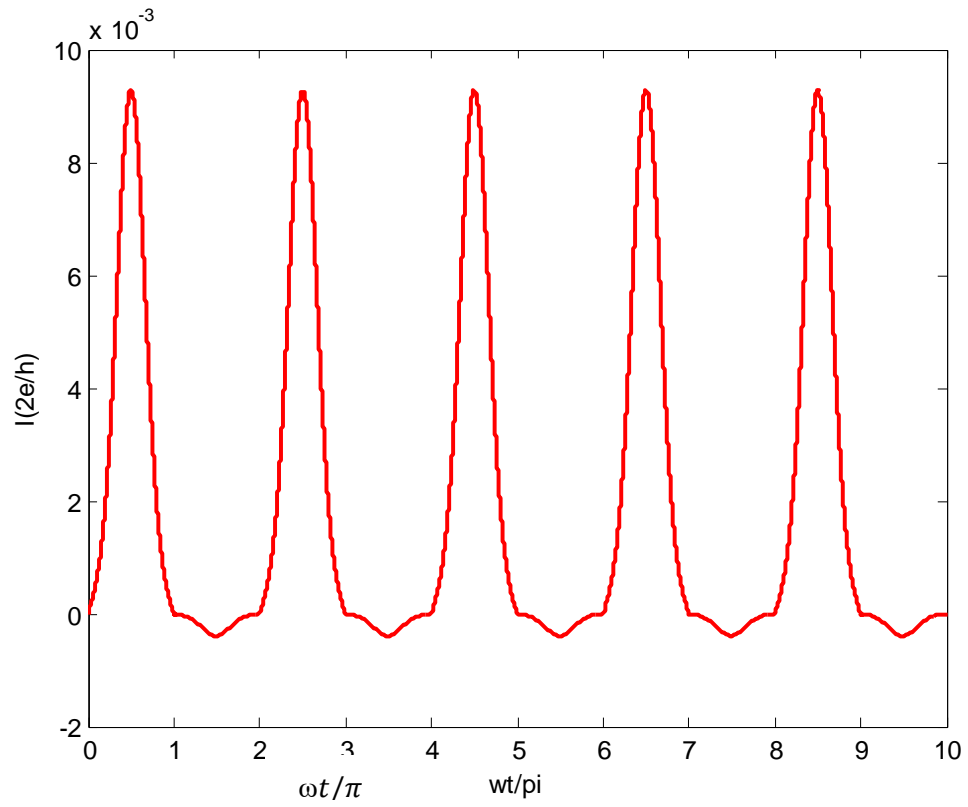


Fig.(3) The output current signal as functions of the time after half-wave rectification action of (G/C) molecule.

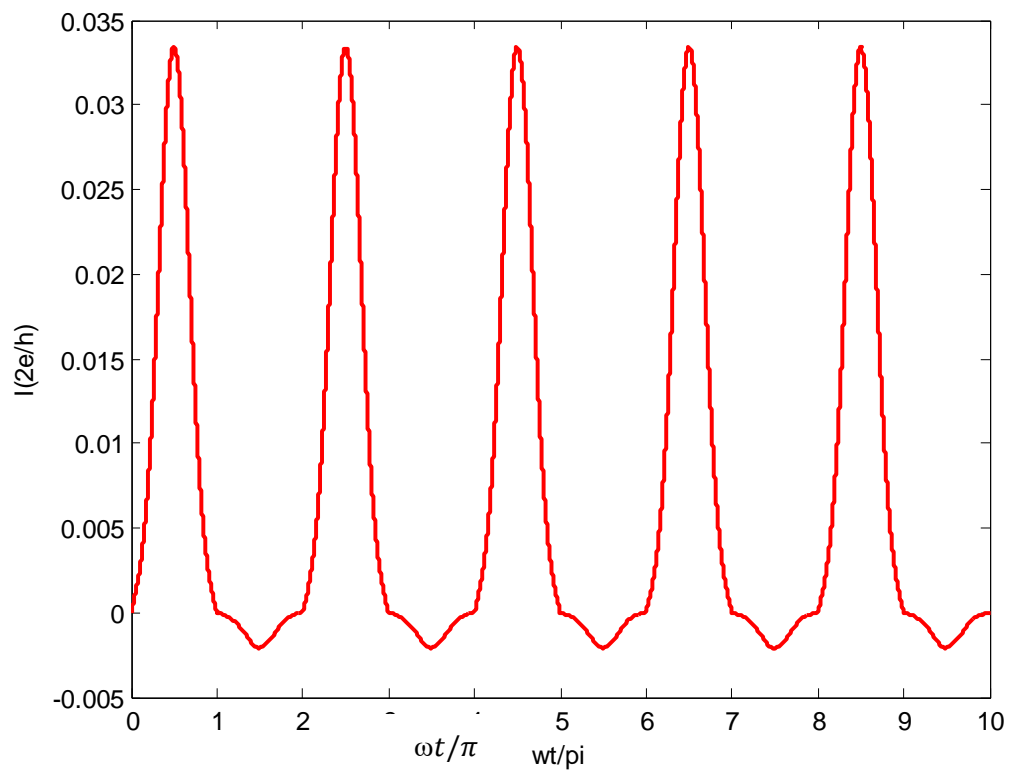


Fig.(4) The output current signal as functions of the time after half-wave rectification action of (A/T) molecule.

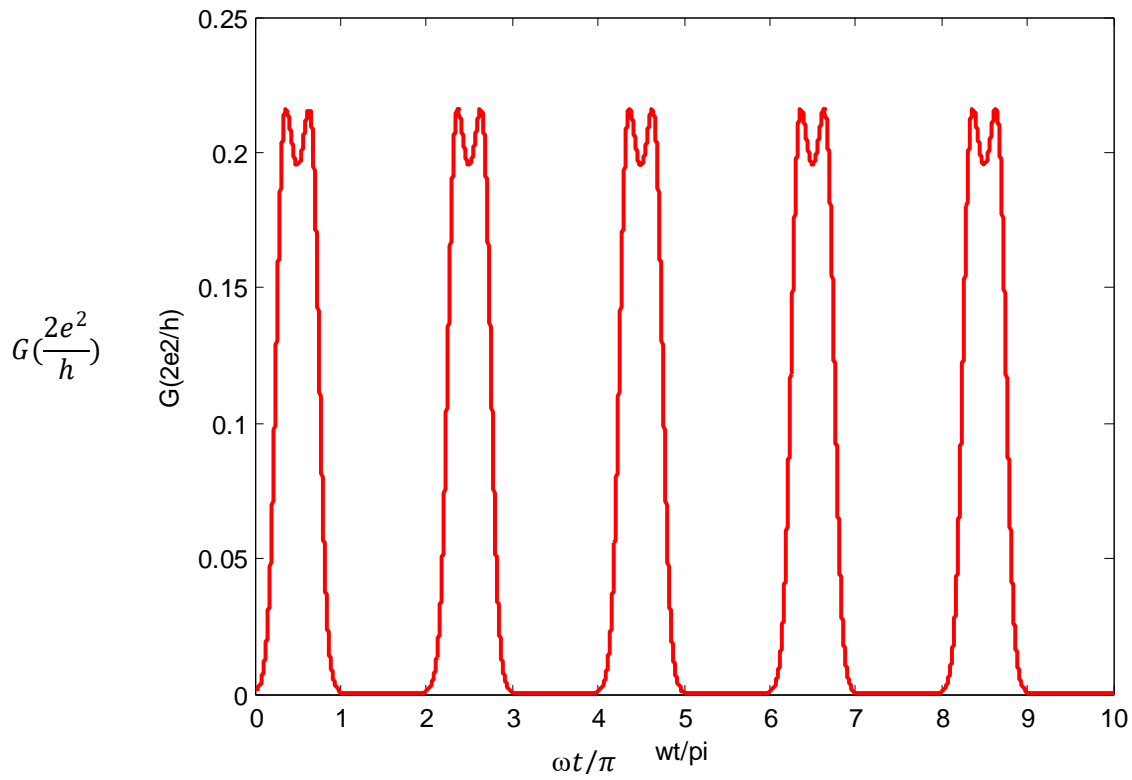


Fig. (5) The conductance signal as functions of the time after half-wave rectification action of (G/C) molecule.

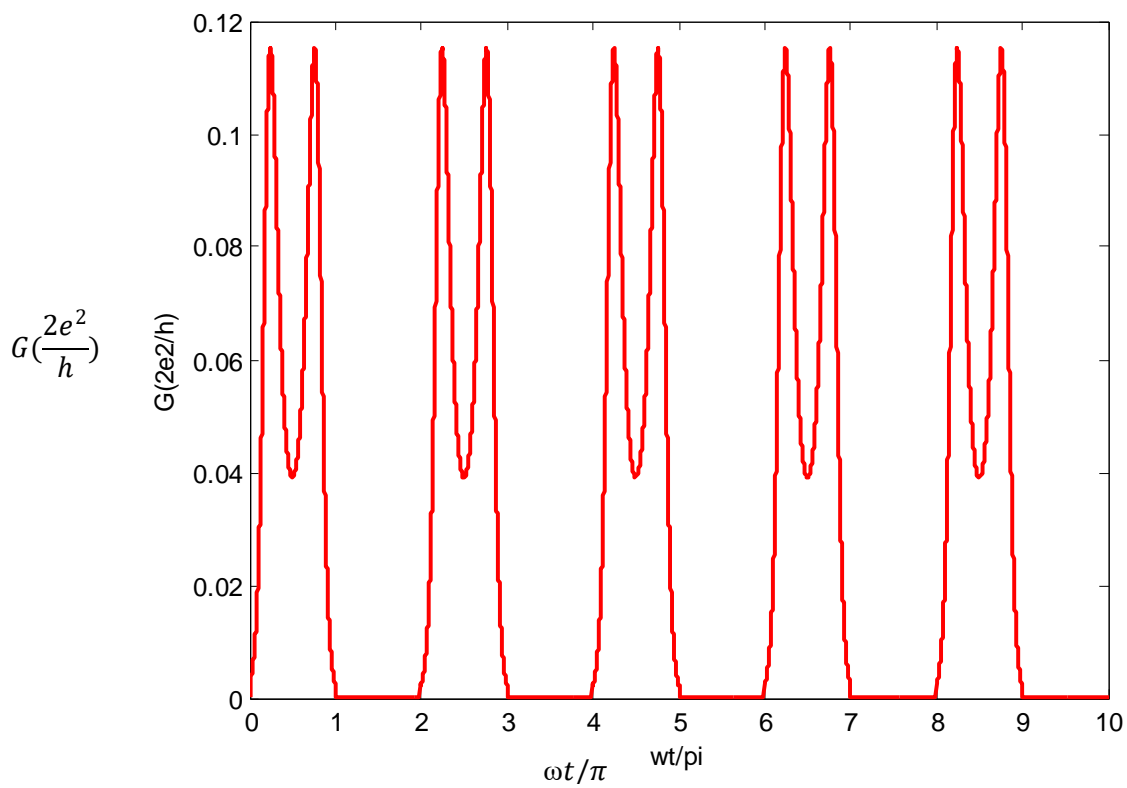


Fig. (6) The conductance signal as functions of the time after half-wave rectification action of (A/T) molecule.

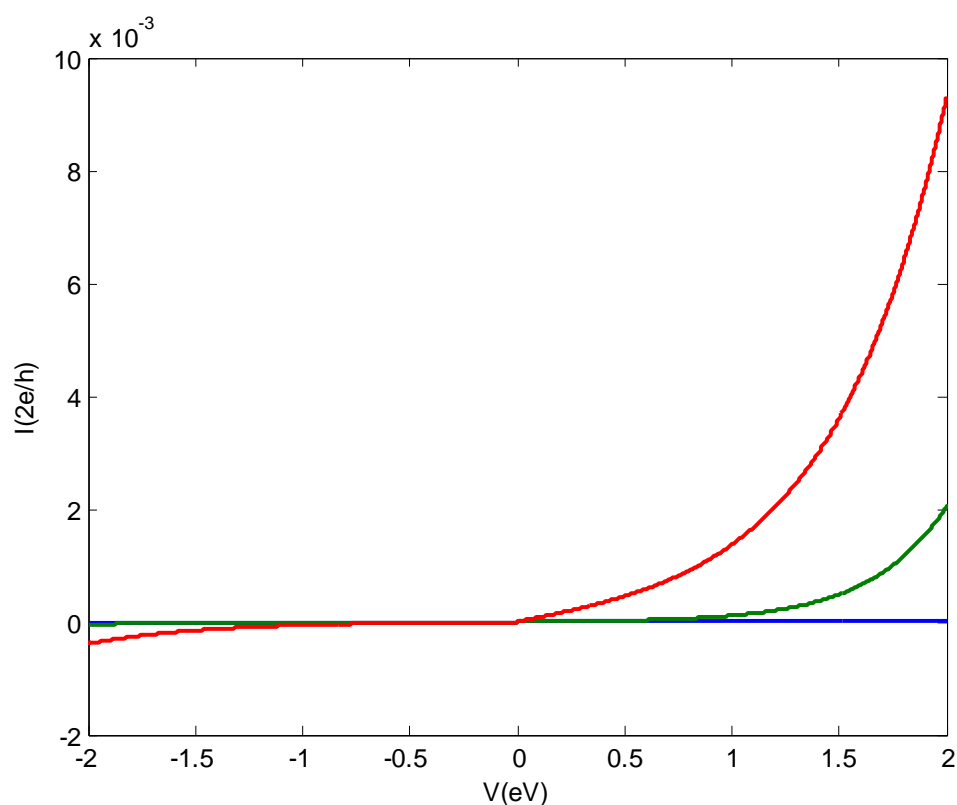


Fig. (7) The relationship between I - V characteristic of (G/C) molecule as molecular diode for three temperature (100, 200 and 300K).

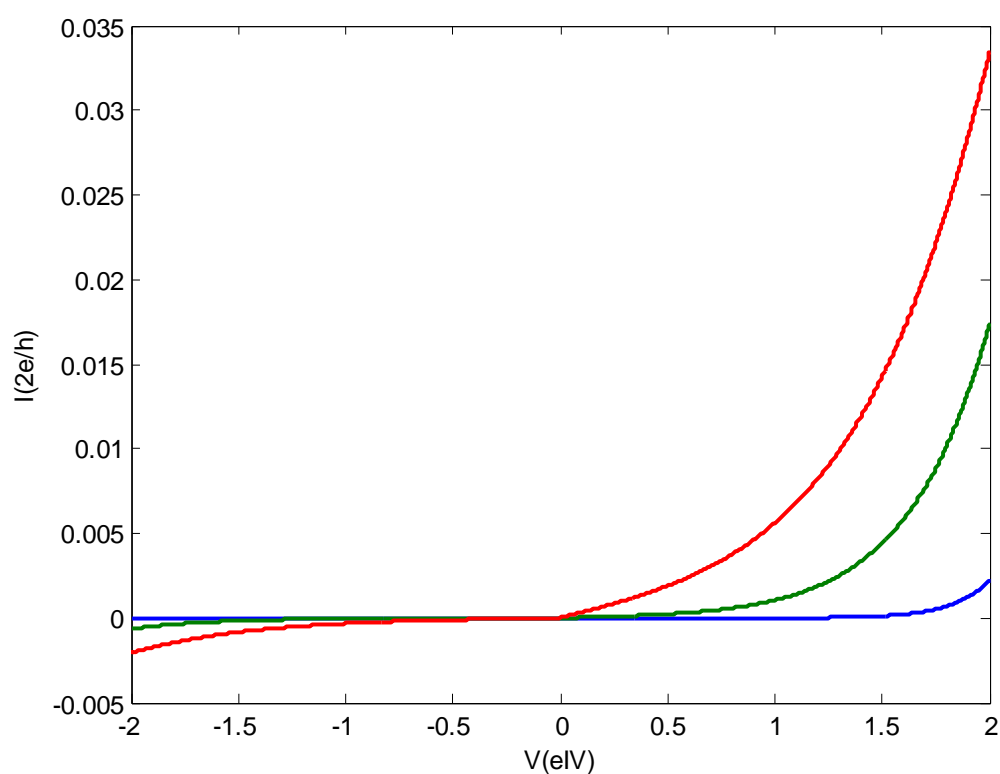


Fig. (8) The relationship between I - V characteristic of (A/T) molecule as molecular diode for three temperature (100, 200 and 300K).

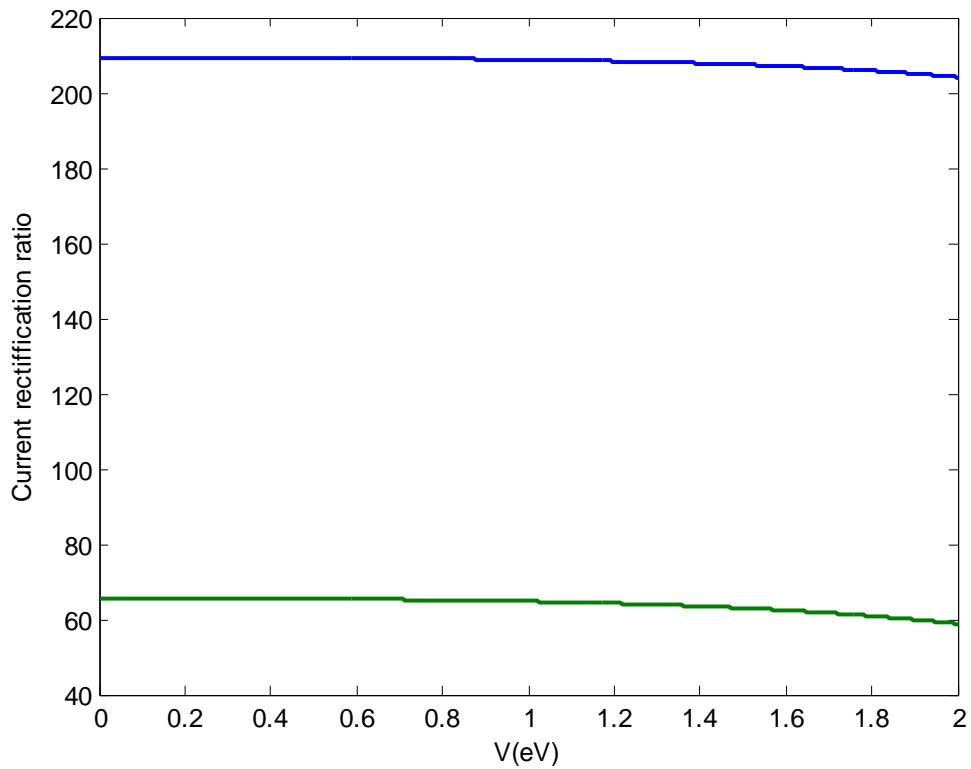


Fig. (9) The Rectification ratio as functions of the bias voltage for ((A/T)-blue line) and ((G/C)-red line) as molecular structures as molecular diode (MD).

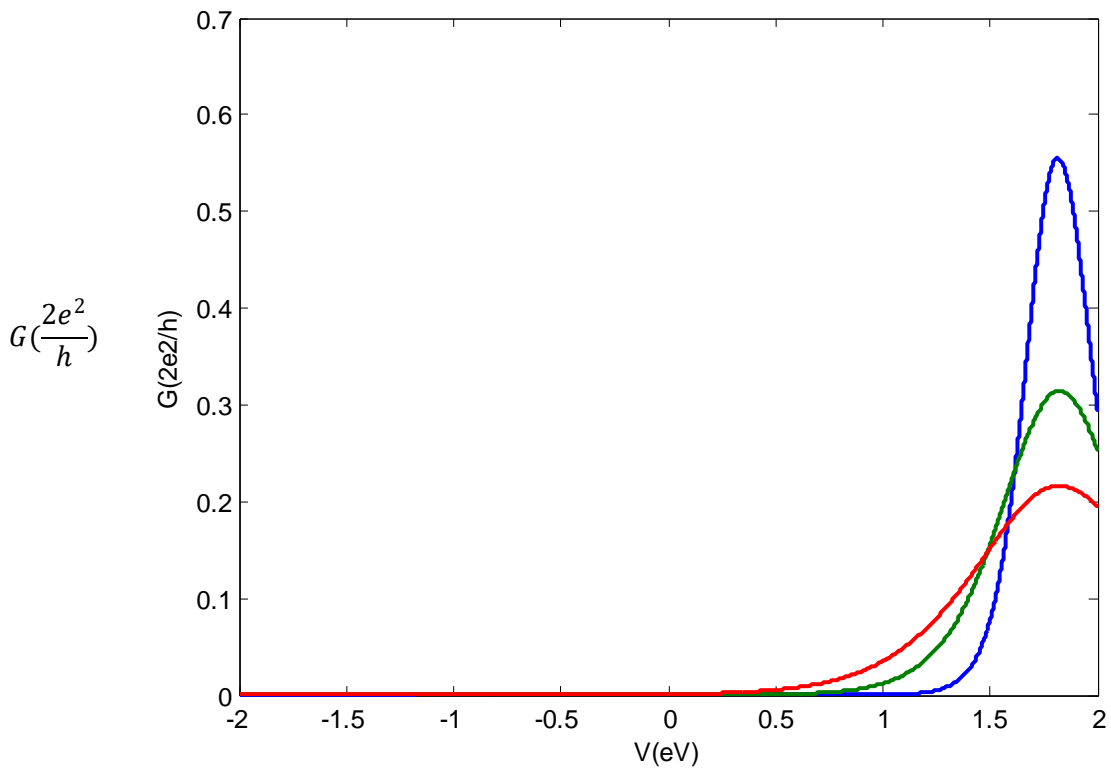


Fig. (10) The conductance as function bias voltage of (G/C) molecule as molecular diode for three temperature (100, 200 and 300K).

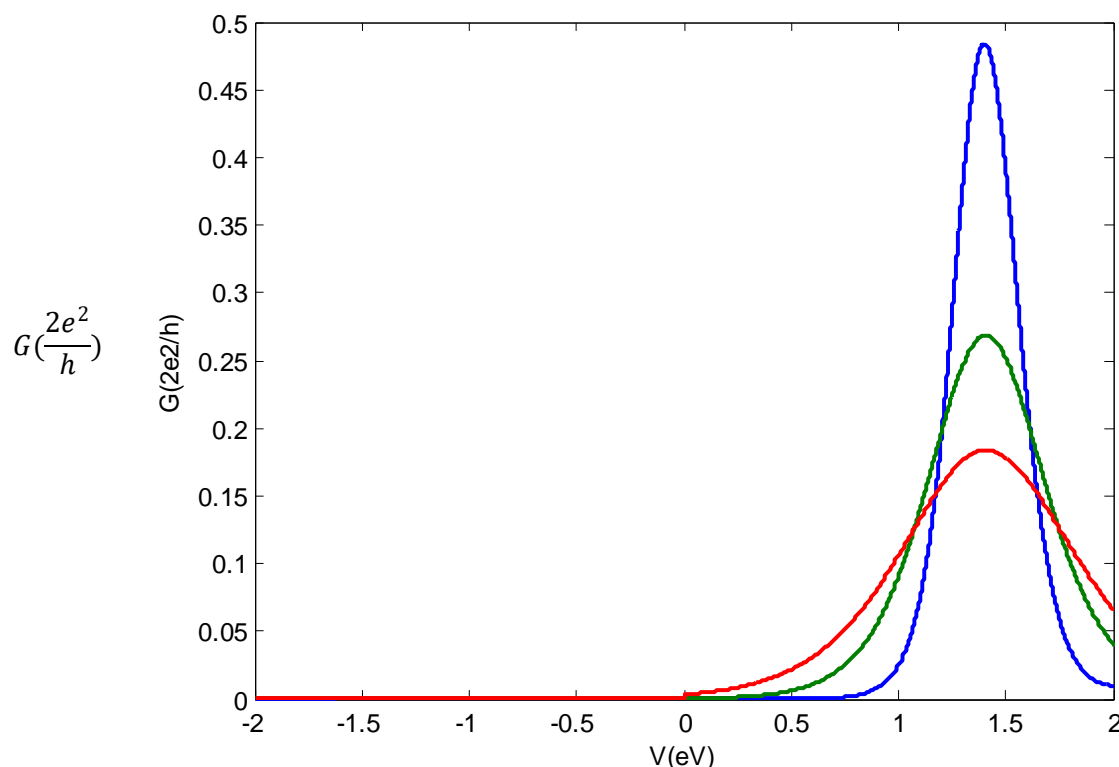


Fig. (11) The conductance as function bias voltage of (A/T) molecule as molecular diode for three temperature (100, 200 and 300K).

4. Conclusion

The permeability probability was exploited to calculate and investigate the I-V characteristic. I-V curves are realized to model the asymmetric molecular structure. The effect of the rectification process using guanine and cytosine molecules (G/C) or adenine and thymine (A/T) molecules as a molecular rectifier on the current and conductivity passing through this molecular system has been studied and already obtained an amazing value. The effective rate of the input signal. The relationship between bias current and voltage for this molecular model of (G/C) and (A/T) molecules, the two biased states, was also studied. The permeability potential is so greatly reduced that it is almost negligible, so the current passing through the molecular system is greatly affected by the permeability values. This behavior is very similar to that of the electronic rectifier of the AC input signal. It has also been observed that the conductivity of the asymmetric molecular system is very low for values close to zero in the positive direction and similarly for negative values of the bias voltage. For an increase in the bias voltage after a certain threshold value, the conductivity increases exponentially until it reaches the largest value after which the conductivity value begins to decrease, thus giving a behavior somewhat similar to that of a tunneling diode, or it could indicate the necessity to establish the determinants of the operation of similar molecular systems, for hardware limitations in large volume. The rectifier current ratio was also studied, and it was noted that this ratio was stable with increasing absolute value of the bias voltage, which means that this molecular system acts as a rectifier in a stable manner within a certain range of bias voltage. In addition, it was found that the rectification ratio of adenine / thymine is three times greater than the rectification ratio of guanine / cytosine, due to the difference in molecular levels or the so-called energy gap between (HOMO-LUMO) levels of these molecules. Bias It has been found that it pushes the curve up more with positive values of bias voltage and pulls it down with negative values of bias voltage and less and also temperature affects the conduction and bias voltage curves in the same way. The effect of temperature on the curves of the relationship between current and voltage was also studied. These thermal effects on the current and conductivity curves come as a result of the energy gained by the electrons within the molecular orbitals, which leads to a change in the electronic properties of the molecules under study accordingly. And it is these amazing results that have been achieved, which effectively push to say that the molecular component will become a reality in the foreseeable future if the technology is available to do so.

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