# Characteristics of Thymine Molecule System Behave as Molecular Electronic Device

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## Abstract

The I-V characteristics of thymine are presented by using tightbinding model with steady state. The current as function of gate voltage which is varying between -4 to 4 eV is plotted. Also, the tunneling phenomena is appeared into the features of molecules. The appliance of gate voltage shows good ON/OFF keying of the two applied voltages- bias voltage and gate voltage. In our work the thymine molecule is proposed as a turn on and turn off key, MOSFET properties can be used in thymine molecular electronic devices. Further, the magnetic flux has been studied for transmission, current and conductance.

**Keywards**: Thymine, Gate, Molecule, Transmission, Tightbinding

## Introduction

Molecules give an attending choice for use as an molecule in nanoelectronic devices. Molecular electronics tilts to use the electronic attributes of finite molecules. Because of the molecule is too little, its functions may be controled. Growth of molecular and nanoelectronic devices byword diode, transistor, oscillator and switche [1,2]. Many attempts have been letting theoreticall interpreting for the I-V characteristics of the molecular systems [3, 4] There are various candidates for the molecular devices that have multiple types qualifications like organic polymers [5, 6] large bio-molecules [7, 8], nanotubes & fullerenes [9]. Molecular electronics is an interdisciplinary field that involves the use of molecules asf undamental electronic components

such as wires, transistors, memory units, and logic elements[10]. DNA is one of the outstanding candidates for molecular electronics. Self- assembly and self- distinction properties of DNA make it as most appropriate for generating of analogous molecular electronic devices. The bases style an attending motif for use in single molecule electronics. In this work, transmission, I-V characteristics ,conductance and magnetic flux are calculated for thymine and they have been analysed for use in molecular electronic devices.

**Theory and Treatment**

The electron straggles from one bridge that contains one molecule of DNA. The tight binding procedure of thymine 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 (that shown in Fig. (1)) the time-independent Hamiltonian (using Dirac's notations) is used. This electronic Hamiltonian takes into account all the sub-systems interactions. The different indexes D, A, L, R and Th denote the donor and acceptor, the left lead, right lead, and thymine. The model Hamiltonian is written as follows:

$$\tilde{H} = E_D|D\rangle\langle D| + E_A|A\rangle\langle A| + E_{Th}|Th\rangle\langle Th| + [(V_{ATh}|A\rangle\langle Th| + h.c) + (V_{DTh}|D\rangle\langle Th| + h.c)] + \sum_{k_R}(V_{Ak_R}|A\rangle\langle k_R| + h.c) + \sum_{k_L}(V_{Dk_L}|D\rangle\langle k_L| + h.c) \quad (1)$$

The index $k_i$ is the energy wave vector with i types the indexes D, A, L, R and Th. $E_i$ types the ith energy level position and $|i\rangle$ and $\langle i|$ types the ket and bra states respectively. $V_{ij}$ types the coupling interaction between the subsystems i and j. The system wave function can be written as,

$$\psi(t) = C_D(t)|D\rangle + C_A(t)|A\rangle + C_{Th}(t)|Th\rangle + \sum_{k_L} C_{k_L}(t)|k_L\rangle + \sum_{k_R} C_{k_R}(t)|k_R\rangle \quad (2)$$

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

$$\frac{\partial\psi(t)}{\partial t} = -i\bar{\bar{H}}\psi(t) \qquad (3)$$

So, we get the following set of related equations,

$$\dot{C}_D(t) = -iE_D C_D(t) - i\sum_{k_L} V_{Dk_L} C_{k_L}(t) - iV_{DTh} C_{Th}(t) \qquad (4)$$

$$\dot{C}_A(t) = -iE_A C_A(t) - i\sum_{k_R} V_{Ak_R} C_{k_R}(t) - iV_{ATh} C_{Th}(t) \qquad (5)$$

$$\dot{C}_{Th}(t) = -iE_{Th} C_{Th}(t) - iV_{ThD} C_D(t) - iV_{ThA} C_A(t) \qquad (6)$$

$$\dot{C}_{k_L}(t) = -iE_{k_L} C_{k_L}(t) - iV_{k_L D} C_D(t) \qquad (7)$$

$$\dot{C}_{k_R}(t) = -iE_{k_R} C_{k_R}(t) - iV_{k_R A} C_A(t) \qquad (8)$$

With, $V_{ij} = V_{ji}$ and $i, j = A, D, k_L, k_R$ and $Th$

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

$$V_{k_i\alpha} = v_{ki} V^{i\alpha} \qquad (9)$$

$$\bar{C}_{ki} = v_{ki}\bar{\bar{C}}_i \qquad (10)$$

With i=L, R and α=A, D and Th. By substituting these definitions in eqs.((4)-(8)) we get,

$$\bar{C}_A(E) = \frac{1}{E - E_A}\left\{V^{AR}\sum_{k_R}|v_{k_R}|^2\bar{\bar{C}}_R + V_{ATh}\bar{C}_{Th}(t)\right\} \qquad (11)$$

$$\bar{C}_D(E) = \frac{1}{E - E_D}\left\{V^{DL}\sum_{k_L}|v_{k_L}|^2\bar{\bar{C}}_L + V_{DTh}\bar{C}_{Th}(t)\right\} \qquad (12)$$

$$\bar{C}_{Th}(E) = \frac{1}{E - E_{Th}} (V_{ThD}\bar{C}_D + V_{ThA}\bar{C}_A) \quad (13)$$

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

$$\bar{\bar{C}}_R(E) = \frac{1}{E - E_R} V^{RA}\bar{C}_A \quad (15)$$

By subtuting (13) and (15) in (11) , we get

$$\bar{C}_A(E) = \frac{1}{E - E_A - \sum_{AR}(E) - \frac{V_{ATh}V_{ThA}}{E-E_{Th}}} \left\{ \frac{V_{ATh}V_{ThD}\bar{C}_D}{E - E_{Th}} \right\} \quad (16)$$

Thus, we obtain an obvious expression for

$$\frac{\bar{C}_A(E)}{\bar{C}_D(E)} = \frac{X_1(E)}{X_2(E)} \quad (17)$$

Where

$$X_1(E) = \frac{V_{ATh}V_{ThD}}{E-E_{Th}} \quad (18)$$

$$X_2(E) = E - E_A - \sum_{AR}(E) - \frac{V_{ATh}V_{ThA}}{E - E_{Th}} \quad (19)$$

Where,

$$\Sigma_{ij}(E) = |V^{ij}|^2 \Gamma_j(E) \quad (20)$$

is the interaction, self-energy, with: $\Gamma_j(E) = \sum_{k_j} \frac{|v_{k_j}|^2}{E - E_{k_j}}$ (21)

With $k_j=k_L$ and $k_R$.

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

$$t(E) = \frac{\bar{C}_A(E)}{\bar{C}_D(E)} \qquad (22)$$

and ,

$$T(E) = |t(E)|^2 \qquad (23)$$

The steady state electric current through the active region may be calculated by employing the Landauer formula [13]:

$$I = \frac{2e}{h}\int_{-\infty}^{\infty} T(E)[f_L(E) - f_R(E)]dE \qquad (24)$$

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

$$f_\alpha(E) = \left\{1 + \exp\left[\frac{E-\mu_\alpha}{K_B T_\alpha}\right]\right\}^{-1} \qquad (25)$$

h is planck constant, e is the electron charge, $\mu_\alpha$ is the chemical potential of the lead α, with $\mu_L = \frac{V}{2}$ and $\mu_R = -\frac{V}{2}$ , where V is the bias voltage, while $T_\alpha$ is the temperature of the lead α, with $T_L$=$T_R$=T, T is fixed at 300K, this means that both electrodes are in a thermal equilibrium situation.

The conductance for the thymine molecule will be accounted as a function of temperature, i.e. the lead temperature, in the thermal equilibrium state. Our results for the conductance will summarize, as long as the transmission probability is obtainable in our model computation, by using the next form [14]

$$G = \frac{2e^2}{h}\int_{-\infty}^{\infty} dE\, T(E)\frac{\partial f(E)}{\partial E} \qquad (26)$$

With f(E) is defined in eq(24). As the thermal equilibrium is considered in our calculation $T_R$=$T_L$=T with T= 300 K.

**Molecular Model**

The systematic structure of thymine is putting between two gold leads. The form metal-molecule-metal assembly is shown in Fig 1. A voltage bias V 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 fallen at an energy E cross a device beneath effect of a bias voltage V. The Landauer equation based on the tight binding model come back to the elastic conductance of a molecule to the probability that an electron with energy E syringed in one lead will be transported to other lead through an active region which in this work is thymine base. The capability to dominancy on the current cross a solo molecule is a prime target in molecular electronics. The making of three-ends devices, as the field effect transistor (FET), and the knowing of their fulfilling get very prime for the futurity evolution of molecular electronics. Lee et al. gauged many of FET set with phyenylen-based paired molecules and noted that just the set at[11] 1,3-benzenedithiol molecule appears a measurable gating influence. By using the up-said executing, we calculated I-V characteristics of thymine. The effect of gate voltage on the characteristics of thymine base was investigated by capasitating the gate and giving gate bias. Every contact requires to carry the canal into balance with itself. The trying to fulfilment balance causes the current to flow from left lead to right lead[12].

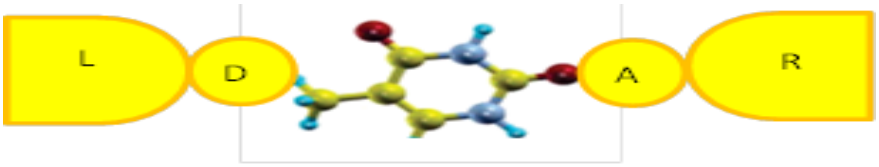



**Fig (1): A schematic illustration of the line model. The left and right ends of the DNA(Bases) are connected to the electrode L and R in addition to D(doner) and A(accepter).**

### Using Thymine Molecule as Molecular Gate

The base of digital electronics are logic gates. They may be used as memories, registers and counters. Thymine molecule behaves as switch, therefore it may be used to style logic gates

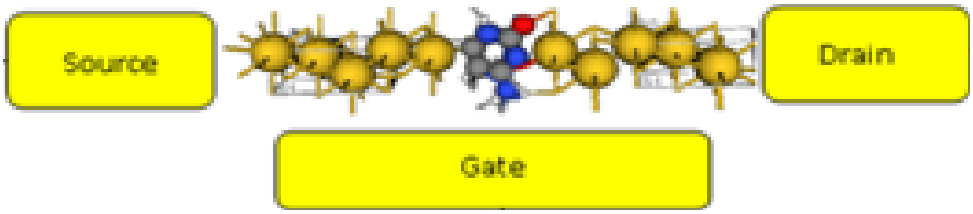



**Fig.(2): Schematic representation of gated Gold-Thymine-Gold structure**

## Results and Discussion

### The transmission probability

The transmission probability T(E) are plotted as a function of energy E in the case that belong to the active region, which consists of thymine. The gate act may be best known by viewing at the dispensation of the orbitals that unoccupied. In Fig.(3), the spectra of the transmission of the device up the Fermi level with three different gate voltages, +4, 0 and -4V are depicted. There are orbitals with large intensity in the spectral window (below 1.0eV). They rely variouslly on the voltages of the gate. The orbital at biggest value of T(E) submits the gating effect, means 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. Fig.(3) shows the result which obtained by assuming the molecular model with thymine molecule, employing the factors $V^{DTh}$= $V^{ATh}$=- 0.3 eV. Where, we note that the states close to the active region edges own a very low transmission probability. While high transmission probability will be at site close to energy of thymine. This is reasonable because of the coupling interactions of the active region with the donor and accepter are equal, also an energy of the site is rely on a type of a molecule. There are three different locations of the onsite energy due to the change of the gate voltages,

which applied on the molecule.There are groups work in this field as Wasielewski Research Group [15]. The calculations of the transmission spectrum are the most important step in studying the transport and dynamic properties of the electron transfers feasibility in molecule. Our transmission spectrum calculations will be employed to get the electric current, conductance and magnetic flux for thymine molecule.

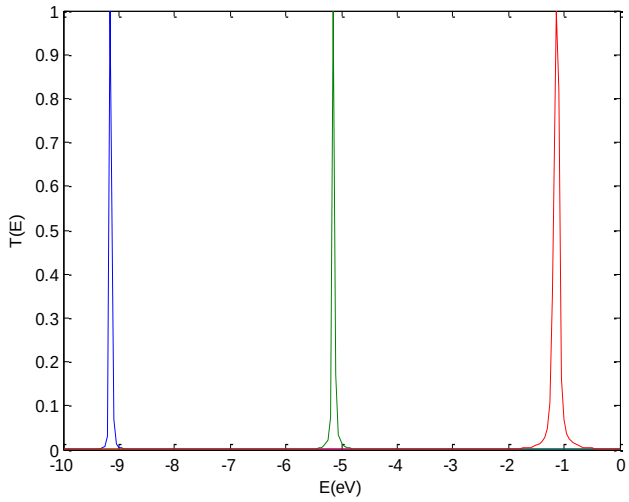



**Fig.(3): The transmission as a function of energy at gate voltage Vg=-4 eV (blue line), Vg=0 (green line) and Vg=4 eV (red line).**

**The tunneling current calculation**

The characteristics of I-V was plotted between current and gate voltage for zero source voltage. The resonant tunneling occurs via molecular orbitals of thymine which give an open lane for conduction when alined with the Fermi level. The tunneling current features are researched by vibrating the voltage from -4 eV to 4 eV. The I-V curves for the same over mentioned connections are shown over the extended bias window as shown in the Figs.((4)-(6)). The I-$V_g$ curves evidentially depict a nonlinear reliance. Interpenetration of electrons in solo molecule is an innovator act. Fig.(4) is shown two states, firstly the current is vanished for finite values (-4 to 2.7 eV) of a gate voltage. The current emerges just when the gate voltage is put up to 2.5 eV, while the computed current has values near zero at little voltage. It might be affined to the

sensitivity of the bonding between molecule and electrodes. The gate act may be best know by seeing the dispensation of the vacant orbitals. Fig.(5) and Fig.(6) illustrate the oscillations in the current as a function of magnetic flux($\Phi/\Phi_0$), where $\Phi$ measures the total flux through our system in units of the flux quantum, $\Phi_0$ ($h/e$) at defferent values of the gate voltage with different values of bias voltage, and those give the features of AND gate. In this work, designing is suggested for a switch that may be employed in AND gate by employing thymine as molecular transistor.

**The Conductance Calculations**

By the hopping transport mechanism amid the chemical potentials and active region energy levels (which inter fermi level and adjacent sites), the conductance is enhancing. Fig.(7) illustrate the conductance as a function of gate voltage. The conductance offers three behaviors with gate voltages. Firstly (from -4 to 2.6 eV), the conductance is independent on gate voltages. Secondly, the conductance has weak dependence on gate voltages at (-2.6 to 1.25 eV), and thirdly the conductance has strong dependence on the gate voltages at (1.25 to 4 eV). These behaviors come back to changes in onsite energy of the active region due to the change in gate voltages. The independent and strong behaviors give two satuations, which are OFF and ON state respectively. There are many papers include employing a molecules to fabricate logic gates as L. N. PAWAR et. Al[16].

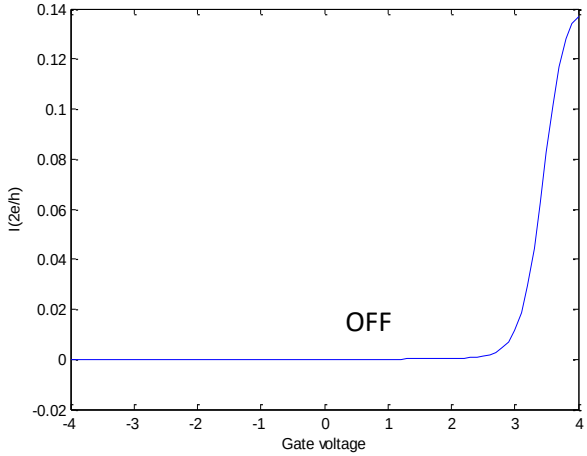



**Fig.(4): The current as a function of gate voltage.**

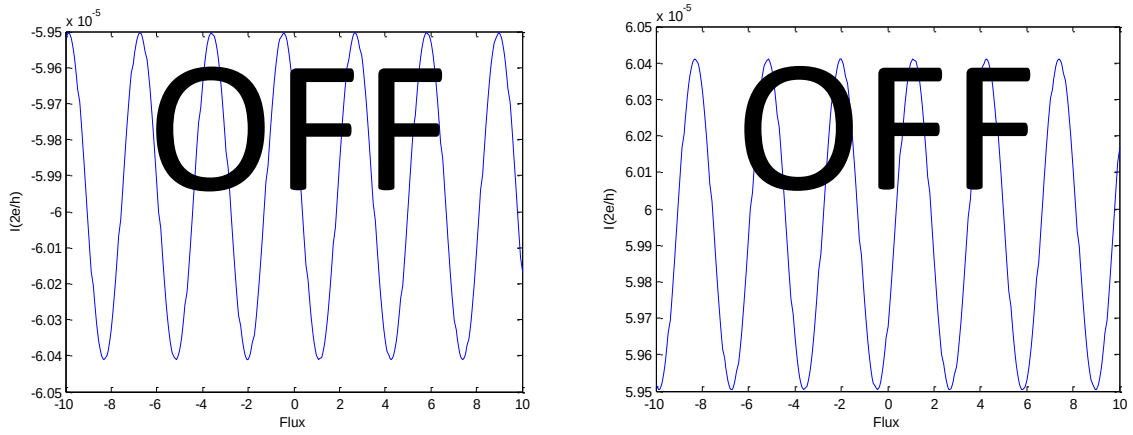
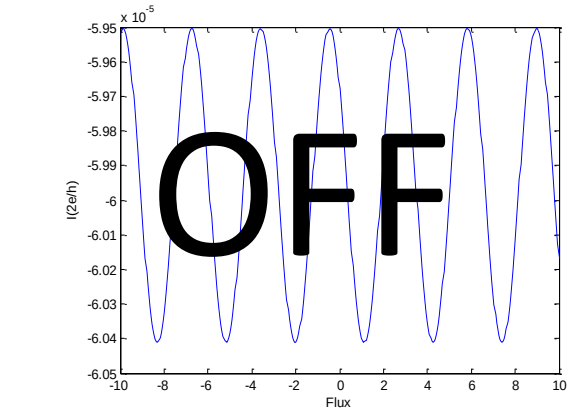



**Fig.(5): The current as a function of a magnetic flux, (a) at bias voltage V=-4eV(off) and Vg=4eV(on), (b) at V=4 eV(on) and Vg=-4eV(off).**



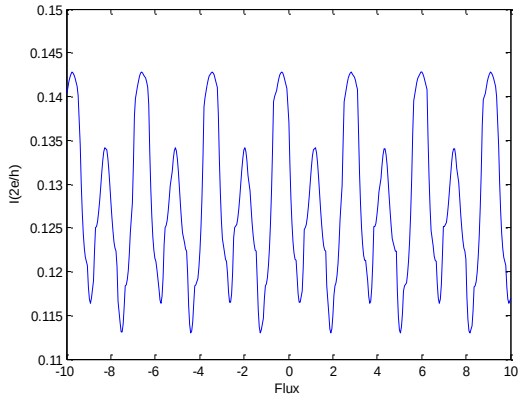




**Fig.(6): The current as a function of magnetic flux, (a) at V=-4eV(OFF) and Vg=-4eV(OFF), (b) V=4eV(ON) and Vg=4eV(ON).**

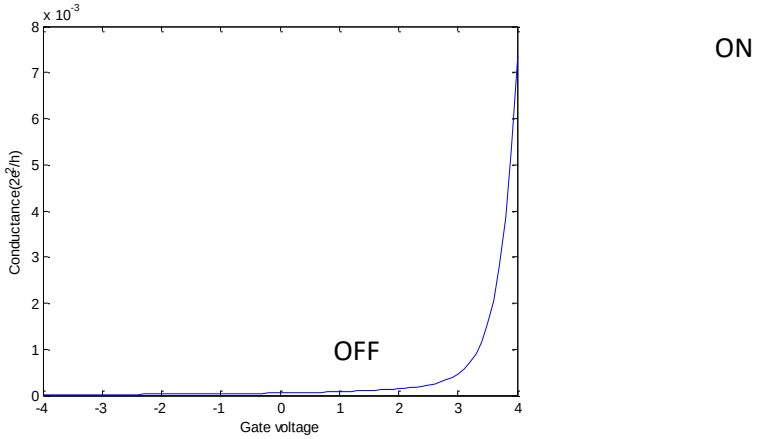



**Fig.(7): The conductance as a function of gate voltage.**

## Conclusion

Our results can be summerized in following points:

1) The states close to the active region edges own a very low transmission probability, while high transmission probability will be at site close to energy of thymine. Also, there are three different locations of the onsite energy because of the change of the gate voltages, which apply on the molecule. The calculations of the transmission spectrum are the most important step in studying the transport and dynamic properties of the electron transfers feasibility in molecule.

2) The I-$V_g$ curves evidentially depict a nonlinear reliance interpenetration of electrons in solo molecule is an innovator act. They are shown two states, firstly the current is vanished for finite values at (-4 to 2 eV) of a gate voltage, which give OFF state, secondly the current emerges when the gate voltage is put up 2 eV, until reach 4 eV, at this value get ON state. It is might be affined to the sensitivity of the bonding between molecule and electrodes. The current as a function of magnetic flux get vibrant. Further, the features of AND gate appear at different values of the gate voltage with defferent values of bias voltage.

3) The conductance as a function of gate voltage, offers three behaviors with gate voltages. They are independent, weak dependence and strong dependence on the gate. These three behaviors result from changes in the onsite energy of the active region due to change in the gate voltages. The independent and strong behaviors give OFF state and ON state.

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