

## Quantum Simulation Study of DNA nucleotide Thymine for use in Molecular Devices

ISHA SHARMA<sup>1</sup>, ER. DEEP KAMAL KAUR RANDHAWA<sup>2</sup>,  
DR. KANCHAN L.SINGH<sup>3</sup>

<sup>1</sup>Nanoscience & Technology  
D.A.V.I.E.T, Jalandhar  
Punjab, PTU, India

<sup>2</sup>Electronics & Communication Engg,  
GNDU Regional Campus, Jalandhar

<sup>3</sup>Applied Science Department  
D.A.V.I.E.T, Jalandhar

**Abstract:** *The soft-computing techniques provide us with tools that can be used to calculate the various parameters that cannot be measured easily. In this paper computational study of DNA base Thymine has been carried out using two probe set up. The metal-molecule-metal assembly was realized by inserting Thymine molecule between two gold terminals and analyzed for current-voltage characteristics. The current-voltage characteristics are obtained using Density Functional theory within Non-equilibrium Green's function formalism (NEGF-DFT). Negative differential resistance is exhibited in the characteristics of Thymine. In two probe set-up without using gate, oscillating behavior of current through thymine is observed rendering its use to drive electronic circuits. It is also observed that the current-voltage characteristics of Thymine can be modulated by gating the two probe setup. The analysis shows that Thymine is suitable for use in two and three terminal Nanoelectronic devices.*

**Keywords:** *computation, DNA base Thymine, negative differential resistance, resonant tunneling.*

### I. INTRODUCTION

The development of electronic industry in terms of size and speed is pushing electronic devices into the realm of molecular electronics. Molecular electronics attempts to find the use of single molecule or group of molecules to function as basic element of electronic devices. Molecular electronic uses material having dimensions below 100 nm, such as organic molecules, carbon nanotubes, and nanowire as substitute for the solid-state layers of traditional semiconductor devices. To accumulate knowledge of molecules and to investigate the electronic properties of molecules interdisciplinary approach is used. Chemistry tools synthesize various molecular architectures. Electrochemical and spectroscopic tools are used to characterize the molecules. Nanofabrication tools are used to fabricate functional single molecule devices for measurement at cryogenic temperature, which help to understand precisely the quantum mechanical nature of current flowing through individual molecules. Similarly computational design tools are contributing for understanding the theoretical model for such devices.

Simulation techniques provide us with an excellent solution to probe the various parameters of a system. Simulation helps in predicting the behavior of a system before realizing the actual system. So, to analyze the electronic properties of molecules also we take aid of simulation and computational methods. In this paper we are analyzing the current-voltage characteristics of thymine for use in electronic circuits.

DNA a natural nanowire is proving itself the leading candidate for molecular electronics. Due to its two important features self assembly and self replication it could produce structures in the nano range that does not seem possible with classical technologies. For DNA molecule to work as single electronic devices, it is necessary for it to be workable at room temperature. For operations like quantum tunneling and coulomb blockade (CB) the HOMO-LUMO gaps should be larger than thermal energy at room temperature (300K) which is equivalent to 0.026eV. Researchers have observed that HOMO-LUMO gap for all DNA Bases is larger than the thermal energy at room temperature [1].

## II. CURRENT-VOLTAGE CHARACTERISTICS OF THYMINE

### 2.1 METHODOLOGY

New modeling tools and techniques incorporating quantum effects that can describe the atomic scale details of device are introduced. Virtual Nanolab software is the simulation and modelling software that combines both Non-Equilibrium Green functional and Density Functional Theory [2].

In this paper Green's function (NEGF) incorporating various electronic structure methods that will model the electronic properties of nanoscale devices has been used. To avoid large Schrödinger equations. Kohn and coworkers invented one such mean field approaches i.e Density functional theory(DFT)[3]. DNA base thymine is created using HYPERCHEM 7 software. We are using Local density approximation [4], one of the important and improved exchange correlation potential.

Each electron in Density functional theory is influenced by exchange correlation potential and Hartree potential. LDA(Local Density Approximation) and GGA(Generalized Gradient Approximation)[5] are the two important and improved exchange –correlation potential. We have used local density approximation potential for this paper.

In this paper two probe techniques is being used to calculate the current-voltage characteristics of DNA base thymine as shown in figure Left and right electrodes are taken of gold material and central region is a thymine base.

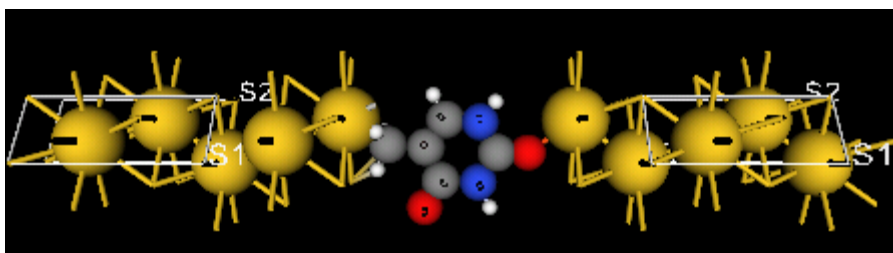


Fig 1. Two probe system showing left and right electrode incorporating DNA Base Thymine.

Gold is used to construct thin electrodes as it is a promising monoatomic nanowire. Double Zeta Polarization test is used to calculate electronic structure computation. Landauer's formula is used to calculate current-voltage calculations [6]. Under a bias  $V$ , the total tunneling current through the two probe system can be written as

$$I = \frac{2e}{h} \int_{-\infty}^{\infty} dE T(E, V) [f(E - \mu_1) - f(E - \mu_2)] \quad (1)$$

Where  $\mu_1$  and  $\mu_2$  are electrochemical potential of two gold electrodes under an external bias  $V$ .  $f(E)$  is Fermi- dirac distribution function.  $T(E, V)$  is the electron transmission function which can be calculated by molecular energy levels and their coupling to metallic contacts[7].

### 2.2 RESONANT TUNNELING DIODE

Resonant tunneling diode technology is now becoming one of the most promising candidates for digital circuit application. Due to its features like Negative differential characteristics, simple structure, versatile functionality etc it could be the next possible device for practical applications. RTD's ability to work at room temperature distinguishes it from other quantum device concepts [8].

### 2.3 CURRENT-VOLTAGE CHARACTERISTICS

Organic molecules are, in general, poor conductors of electrons, and “conduct” by tunneling. However, when molecules have low-lying orbitals (usually the HOMO or LUMO), applying a potential across the electrodes of a metal–molecule–metal junction can cause the energy of the molecular orbital to fall between the Fermi levels of the electrodes [9].

Two probe system consists of three regions left electrode (gold), central region (thymine) and right electrode (gold). The two gold electrodes are taken as source and drain. Figure 2 is representing the gated two-probe set-up.

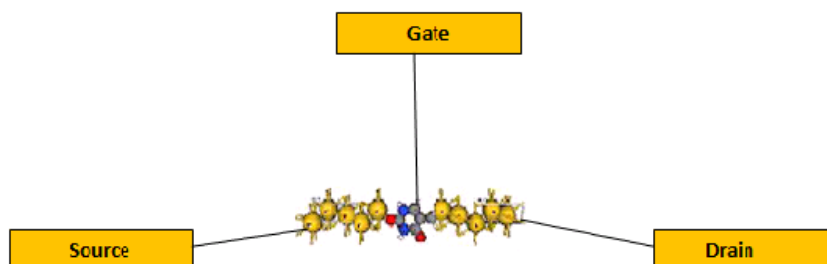


Fig 2. Gated Gold-Thymine-Gold Structure [6]

On applying positive source voltage from 1V to 5V in the step difference of 0.1V and without applying gate to two-probe system it is observed that the current oscillates between peaks and valleys thus showing the small magnitude of current passing through molecule rendering its use for electronic circuits as shown in figure 3. The variation in magnitude of current passing through metal-electrode-metal junction also depends on metal-electrode coupling and applying bias voltage [10].

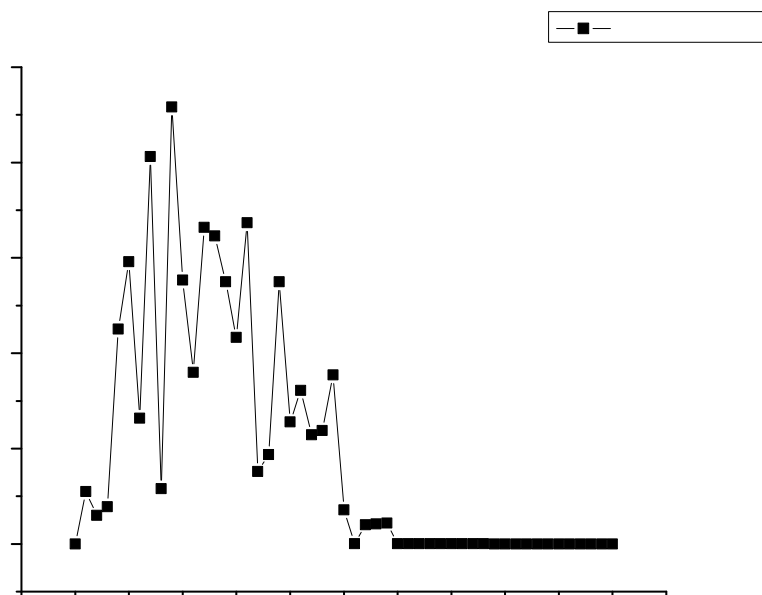
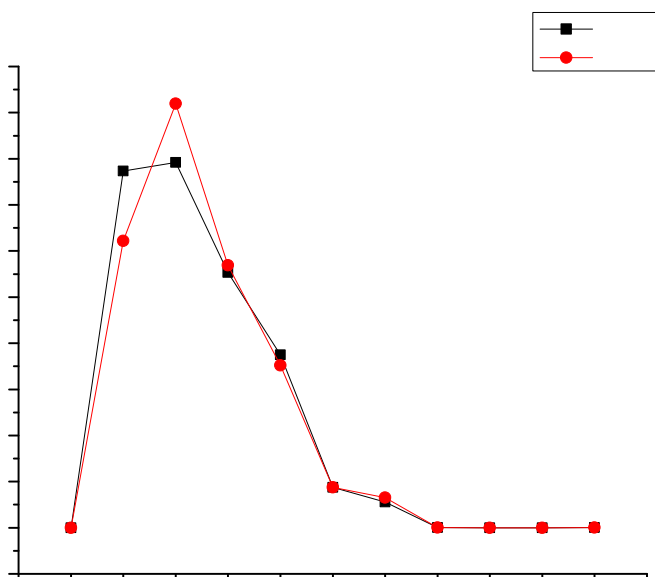


Fig 3. Current-Voltage Plot for Thymine without applying Gate Voltage.

## 2.4 NEGATIVE DIFFERENTIAL REGION-

### 2.4.1 CURRENT VERSUS SOURCE VOLTAGE AT CONSTANT GATE VOLTAGE



**Fig 4.** I-V Characteristics of thymine at gate voltage 0.1V and 0.2V

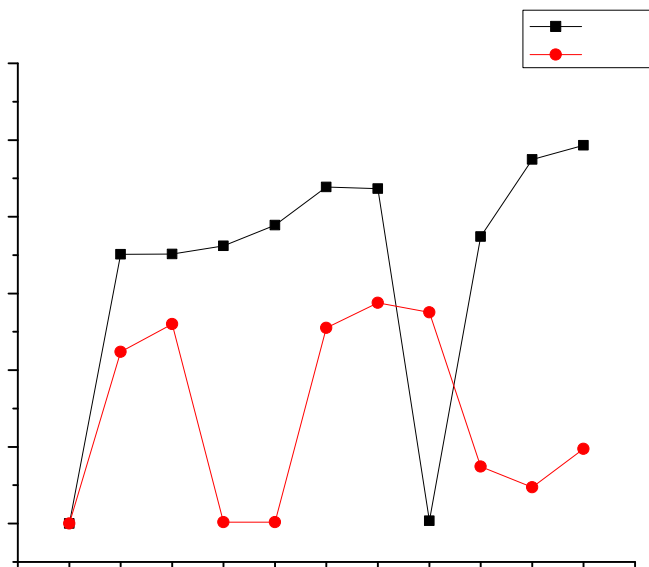
Positive source voltage from 1V to 5V is applied with the step difference of 0.5V while applying fixed drain potential  $V_d$  to 0V. This would cause different potential at left and right electrode which leads to different Fermi functions that will try to achieve equilibrium in channel causing current to flow from source to drain. We have evaluated the current-voltage characteristics at two different Gate voltages 0.1Vg and 0.2Vg. The curve for both the gate voltages is showing negative differential region for Source voltage (Vs) from 1V to 2.5V thus making thymine suitable for tunneling applications.

At zero applied voltage electrochemical potential of both left and right electrodes are equal i.e.  $\mu_L = \mu_R$  because the Fermi energy level of electrodes lies in the middle of HLG gap (13.68) for thymine molecule. This shows none of the molecular orbital is in resonance with Fermi energy level of electrodes. Equation (1) depicts that left and right electrodes are at different electrochemical potential. The difference between the electrochemical potential of the two terminals causes the current to flow. After increasing source voltage an electron-transfer process is induced in which the Fermi level of electrodes comes in resonance with the HOMO-LUMO of molecular bridge (thymine) and which will change non-resonant to resonant tunneling resulting in an abrupt increase of current in I-V curve shown as above in Fig 2. confirming the negative differential resistance region. Change in Peak current from 1.58e-006A to 1.83e-006A is observed for an applied source of 1V by fixing gate to 0.1Vg and 0.2Vg. It means the peak current increases with the increase in gate voltage from 0.1Vg to 0.2Vg. This ability of controlling the current is the most interesting feature of molecular devices.

The peak to valley current ratio increases from 9.02 to 10.47 for constant gate voltages 0.1Vg and 0.2Vg rendering the use of thymine in different devices like switches, logic gates and memory devices.

### 2.4.2 CURRENT VERSUS GATE VOLTAGE AT CONSTANT SOURCE VOLTAGE

Current–voltage curve in Figure 4 shows a very little change in current values after source voltage 3V for both gate voltages 0.1Vg and 0.2 Vg. Therefore we evaluated the graph by fixing source voltages to 2.5Vs and 3.0Vs and varying gate voltage from 0 to 5V with a step difference of 0.1V to examine whether thymine for different gate voltages shows tunneling behavior, as seen in fig 4:



**Fig 5.** The Current-voltage graph for variable Gate voltage from 0 to 5V with a step voltage of 0.1V.

The above figure 4 shows that with increase in gate voltage in fixed step of 0.1V for fixed source voltage to 2.5Vs and 3.0Vs the negative differential peaks increases and shows coulomb oscillations. Thus the Fig 4 goes consistent with the research that has shown in its previous results that the characteristics of Thymine display an oscillating behavior where the current shuffles between peaks and valleys [6]. The NDR features can be shifted by tuning the gate voltages as shown in above figure 4 is also concluded in this reference [11]. This is due to resonant tunneling via molecular orbitals of thymine that provides an open path for conduction whenever they get aligned with the Fermi level. The above study on thymine proves this molecule another promising candidate for various applications like molecular switching and tunneling devices.

### III. CONCLUSION

In this paper for modeling electron transport in nanoscale systems quantum mechanical approach based on NEGF-DFT is used. Current-voltage characteristics have been plotted for thymine using virtual nanolab. Increasing value of current with applying different gate values assures the presence of single electron effects in molecule. Thymine not only showed the Negative differential region but also the resonant tunneling effect which is useful in device modeling for nanoelectronic applications in various switching and tunneling devices.

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