Quantum Molecular Effects in Nano scale Devices

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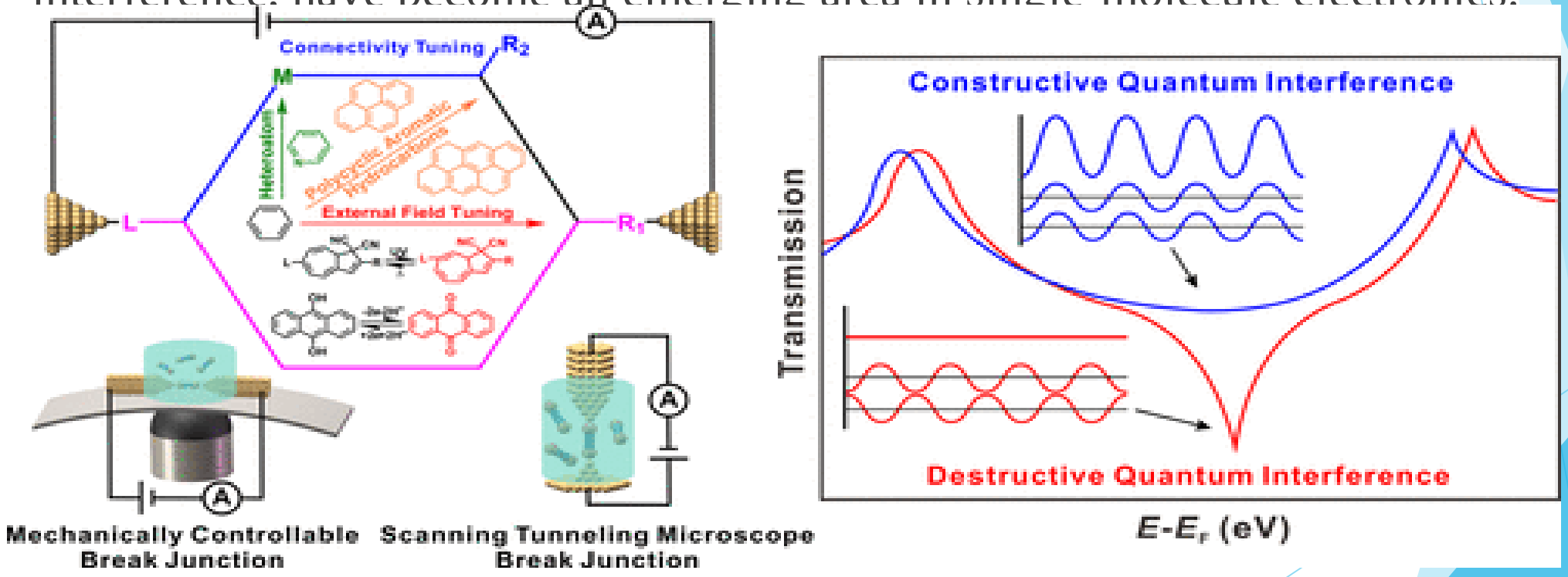
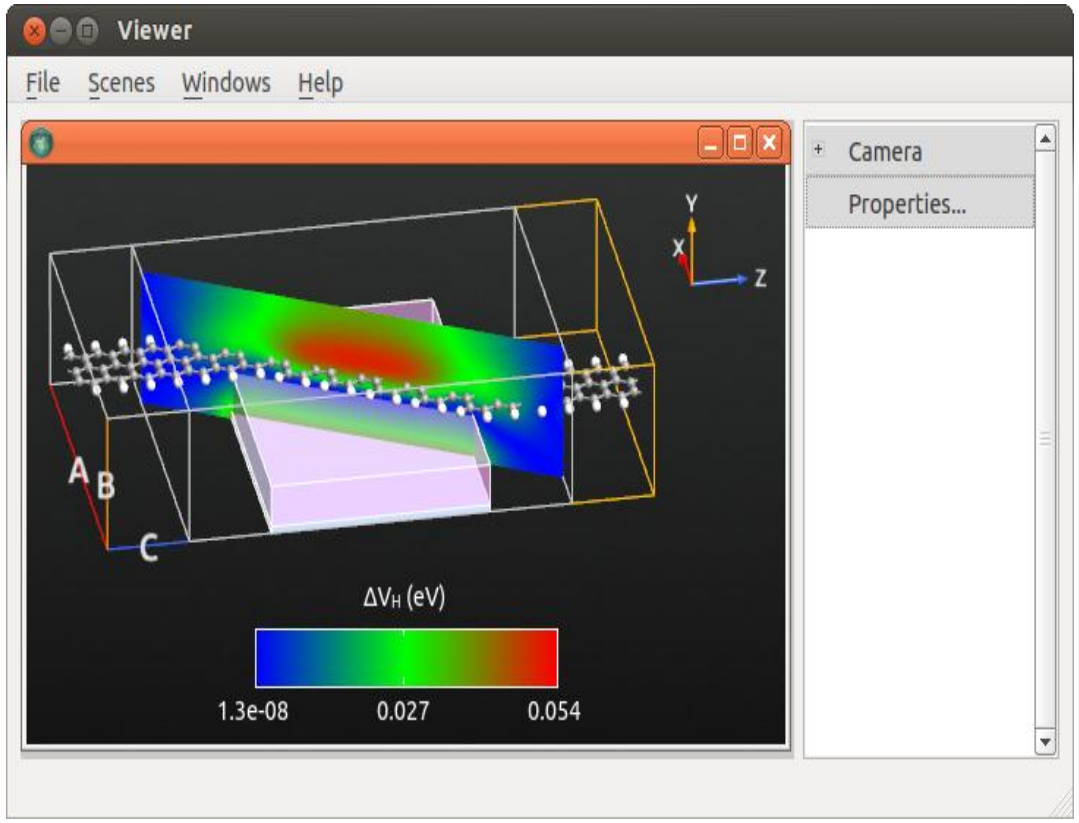
Quantum interference effects (QIEs)

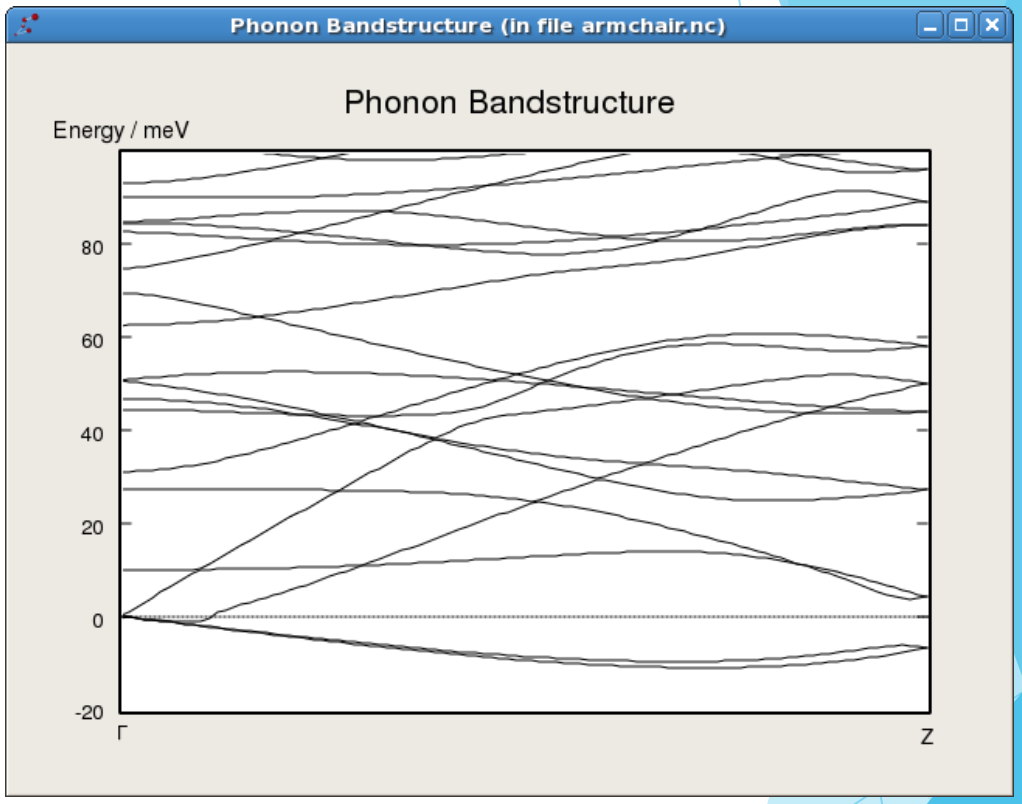
- Quantum interference is a hallmark of quantum mechanics.
- applications in optics, quantum computing, super conductivity.
- QIEs offer unique opportunities for the fine-tuning of charge transport through molecular building blocks by constructive or destructive quantum interference, have become an emerging area in single-molecule electronics.



Source: Liu, Junyang, et al. "Quantum interference effects in charge transport through single-molecule junctions: detection, manipulation, and application." *Accounts of chemical research* 52.1 (2018): 151-160.

Quantum effect in graphene nano ribbon

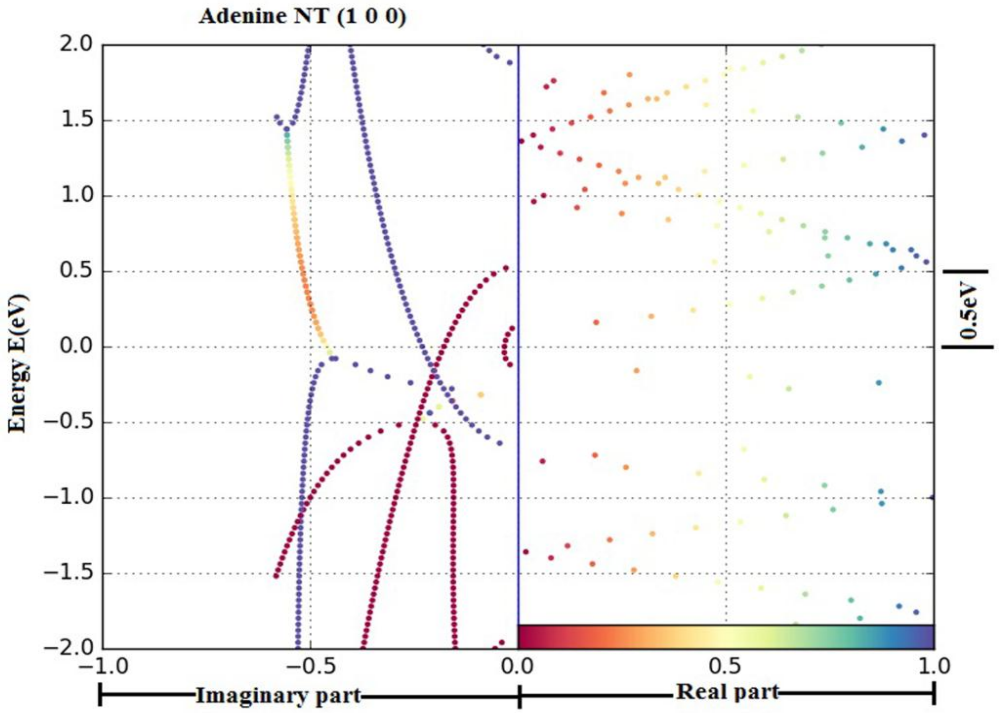


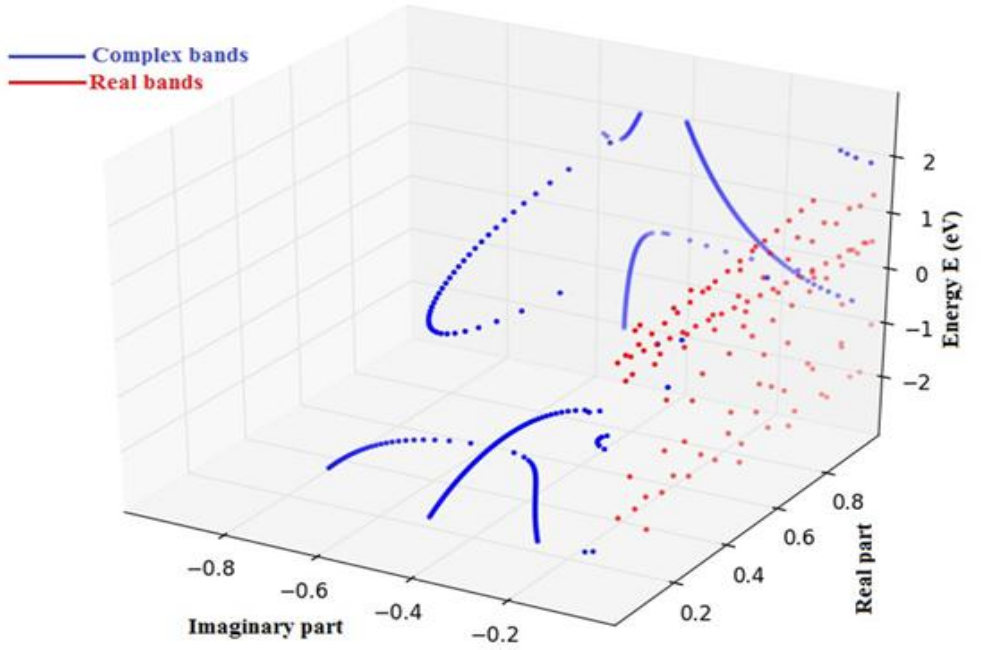


contour plot illustrates the electrostatic potential and phonon bandstructure through the system

Source: https://docs.quantumatk.com/tutorials/phonon_calcs/phonon_calcs.html

Quantum band structure for bio-molecular FET

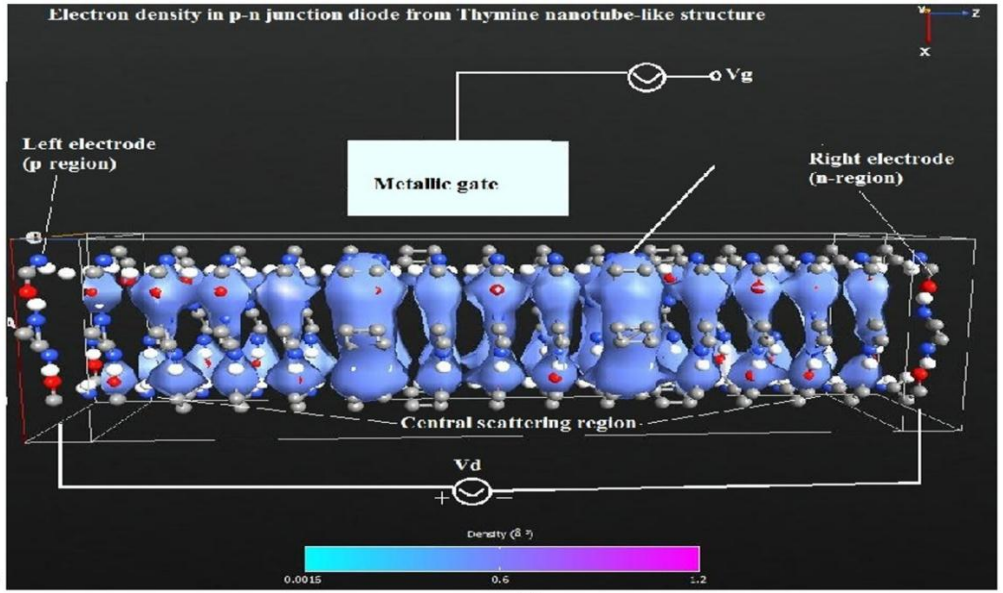


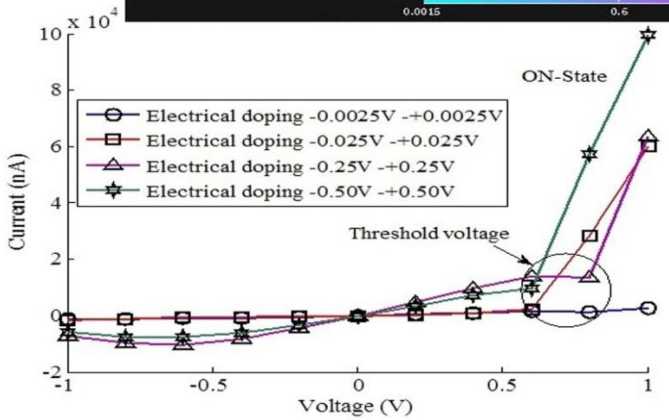


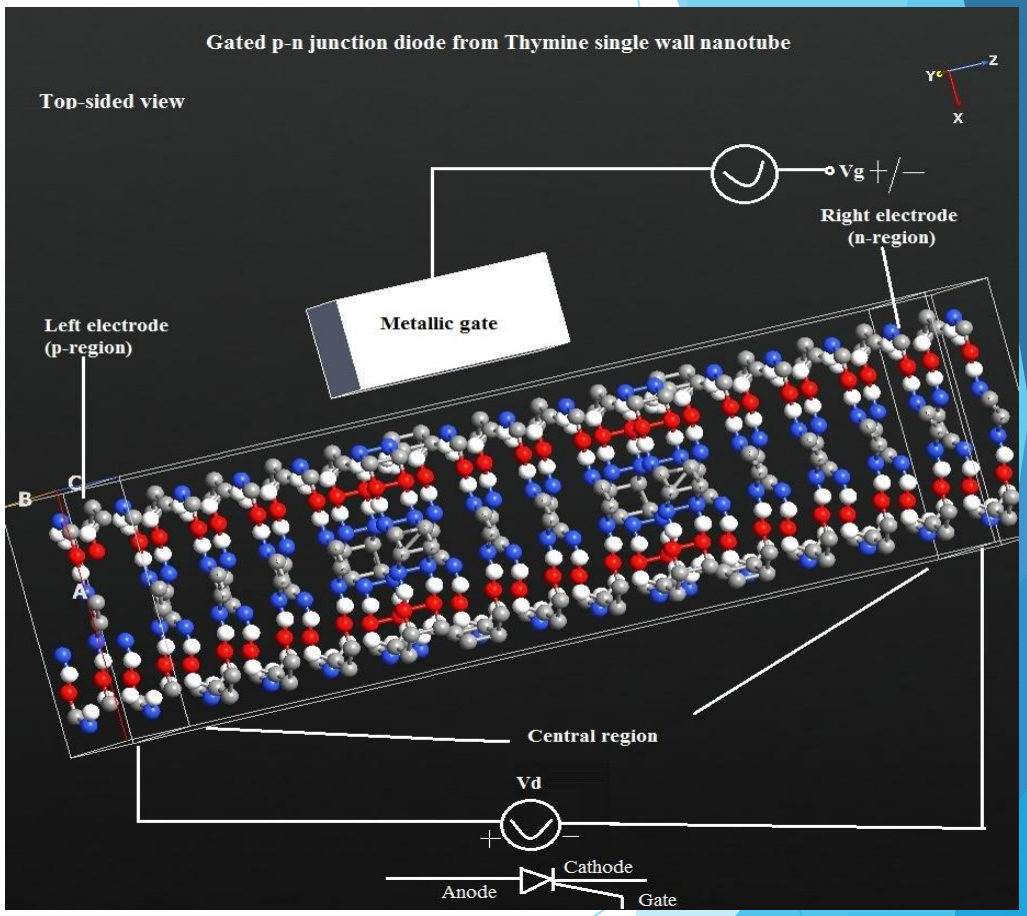
Complex band structure of the bio-molecular nanotube FET.
(a) 2D view, the left-hand part shows the complex bands plotted against the imaginary part, the right-hand part shows the real part,
(b) 3D view, the real bands are plotted with red dots and the complex bands are plotted with blue dots

Source: Dey, D., Roy, P., & De, D. (2017). Atomic scale modeling of electrically doped pin FET from adenine based single wall nanotube. Journal of Molecular Graphics and Modelling, 76, 118-127.

Quantum Molecular Devices

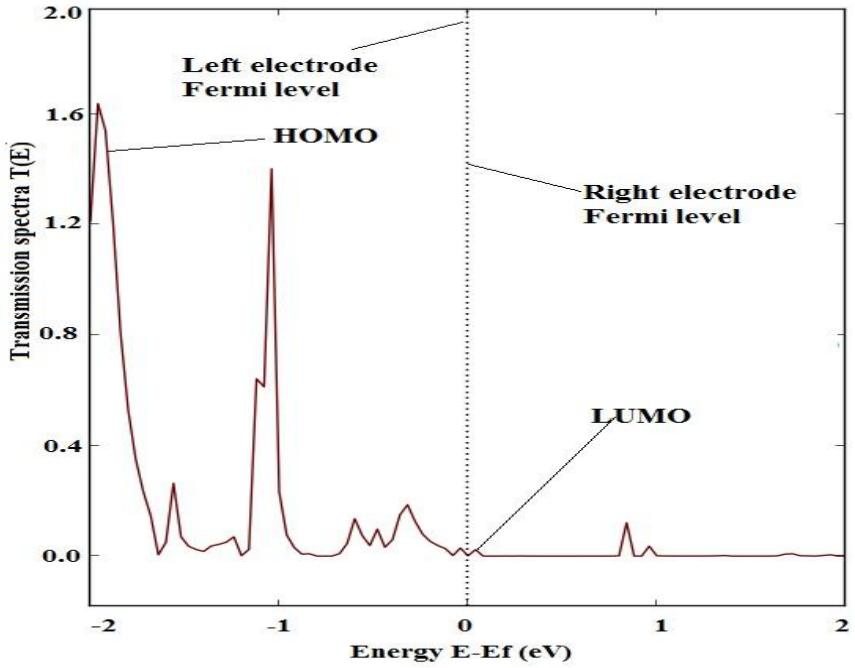


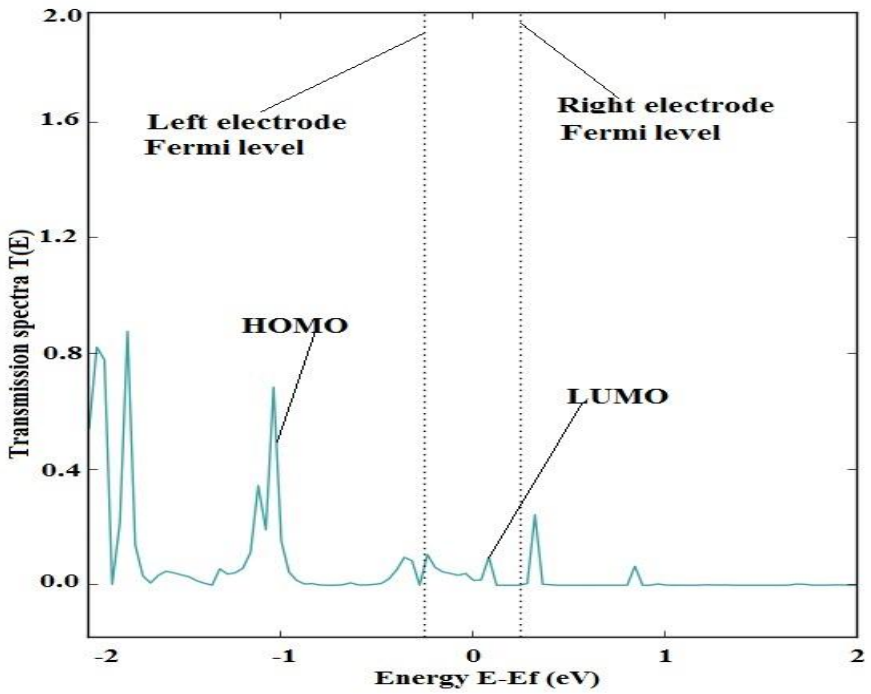




Source: Dey, D., & De, D. (2018). A first principle approach toward circuit level modeling of electrically doped gated diode from single wall thymine nanotube-like structure. Microsystem Technologies, 24(7), 3107-3121.

Quantum-Ballistic Transmission Effects

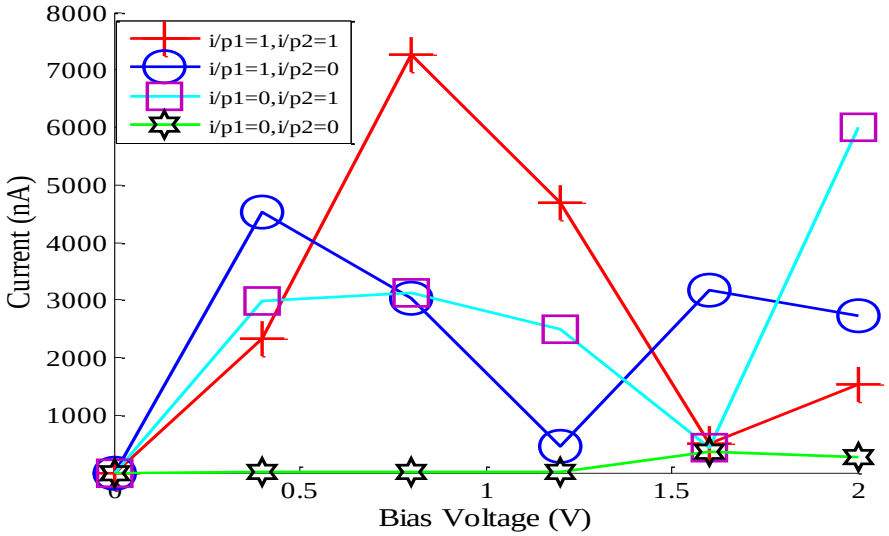


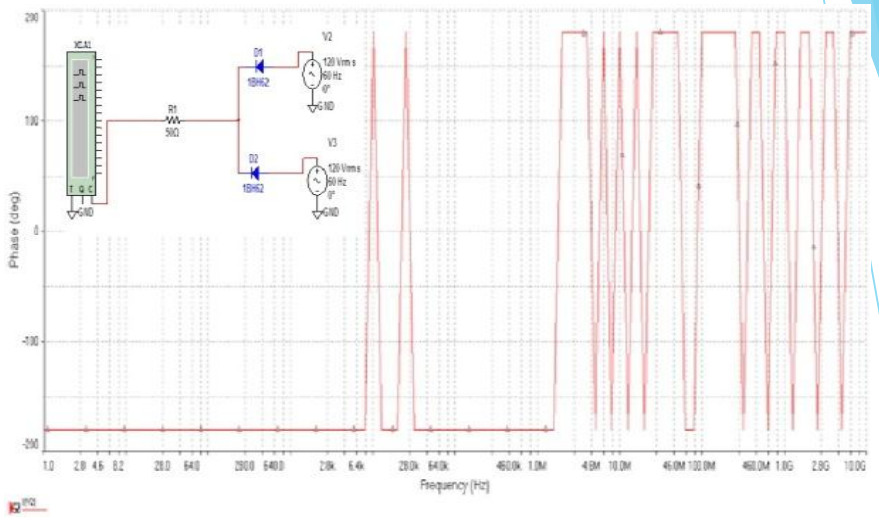


*Transmission spectra.**(a)** Electrical doping ±0.0025V, **(b)** Electrical doping ±0.025V.*

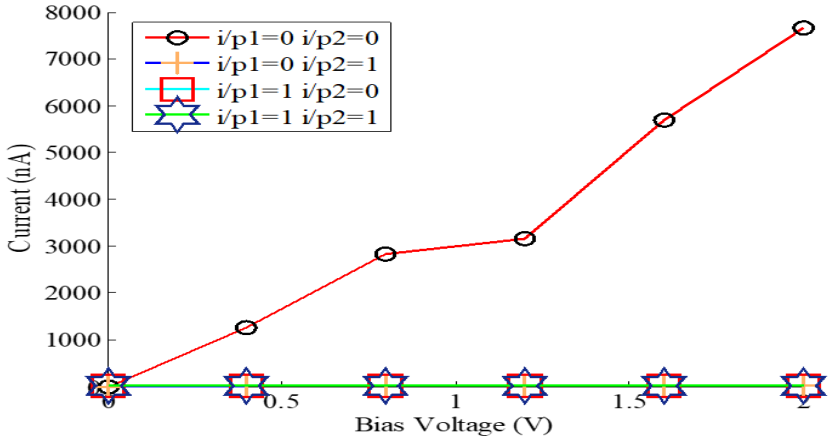
Source: Dey, D., & De, D. (2018). A first principle approach toward circuit level modeling of electrically doped gated diode from single wall thymine nanotube-like structure. Microsystem Technologies, 24(7), 3107-3121.

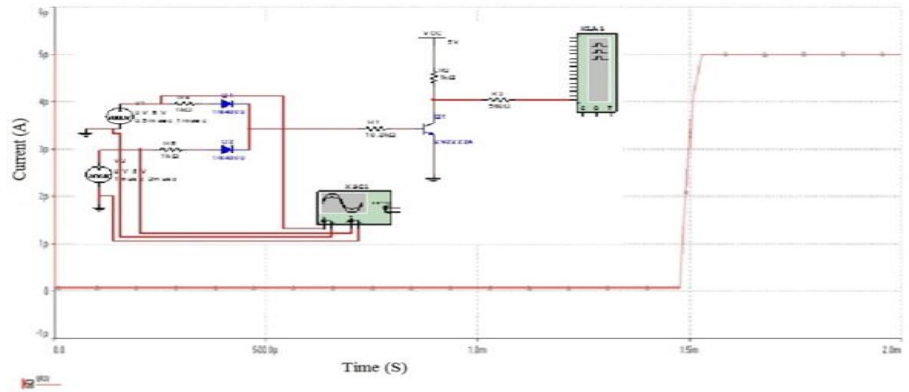
Quantum-Ballistic Transmission Effects





*Circuit level implementation of logic gates with I-V response and validating the result with Multi-sim simulator of **OR** gate and **NOR** gate*





Source: Dey, D., & De, D. (2018). A first principle approach toward circuit level modeling of electrically doped gated diode from single wall thymine nanotube-like structure. Microsystem Technologies, 24(7), 3107-3121.

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TECHNICAL PAPER

A first principle approach toward circuit level modeling of electrically doped gated diode from single wall thymine nanotube-like structure

Debarati Dey[1] · Debashis De[1,2]

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Abstract
This article presents a circuit level representation from gated diode which is developed from Thymine single wall nanotube-like structure using density functional theory and non-equilibrium Green's function. Electrical doping process has been introduced to form the p and n region of this gated diode. This p–n junction diode is originated from the single wall Thymine bio-molecular nanotube-like structure. The atomically thin three-dimensional diode that can be realized from a single wall Thymine nanotube-like structure with optimum process step in 300 K. The operating frequency of this device is 1000 THz. The quantum-ballistic carrier transmission is analyzed using molecular projected self-consistent Hamiltonian and Hilbert space spanned basis functions quantum simulation process which ensures that this device acts as a diode and also shows strong non-linear current–voltage characteristics. Due to electrical doping process, no impurity or dopants are added externally to form p and n junction of the gated diode. A metallic gate has been incorporated to this theoretical model to vary the channel current of the diode. By varying the potential at the p and n side of the gated diode, the doping concentration can be varied. The 3.75 nm long and 1.42 nm wide Thymine single wall nanotube-like structure gated diode shows maximum 99.3 μA current at + 1 V applied bias voltage. This diode is used to implement the basic logic gates like AND, OR and NOR gate. First principle results and the available experimental results are therefore validated using atomistic simulation of the test bed molecules. These results suggested that this bio-molecular nano diode is capable for circuit level realization like implementation of logic gates and logic circuits, in high operating frequency oscillator, switches, memory devices etc. This theoretical study is an approach to implement circuit level modeling of molecules.

1 Introduction

Gated diode has potential application in the field of semi conductor industry. This type of diode generally used to design memory cells (Luk and Dennard 2014). In case of semi-conductor industry one can also vary the gate bias voltage and tune the current–voltage (I–V) response of the gated diode. GaAs p–i–n gated nano diode can be designed using electrical doping process also (Dey et al. 2016) Electrical doping procedure has been introduced for this theoretical experiment. Electrical doping process is totally different from the conventional doping procedure. In conventional doping process, external dopants are added to the electronic devices to enhance its electrical properties. But this insertion of impurity leads to the generation of various faults like electro chemical property of the material changes, heat produced due to the insertion of dopants etc. The conventional doping process also reported with huge heat generation. In case of nano scale device modeling these types of faults are not acceptable. To overcome this kind of problems electrical doping process has been introduced.

Electrical doping is very interesting way to provide carrier injection to the molecular thin films. Electrical doping is used to control and modify the thin molecular film interfaces. Though it has been found that the electrical doping for the organic molecular film is less when compared with the doping in inorganic molecular film. In this electrical doping procedure traditional p and n dopants are not required. The attractive characteristic of electrical doping is that by enhancing carrier injection and lowering drive voltage it can improve device efficiency. So literally,

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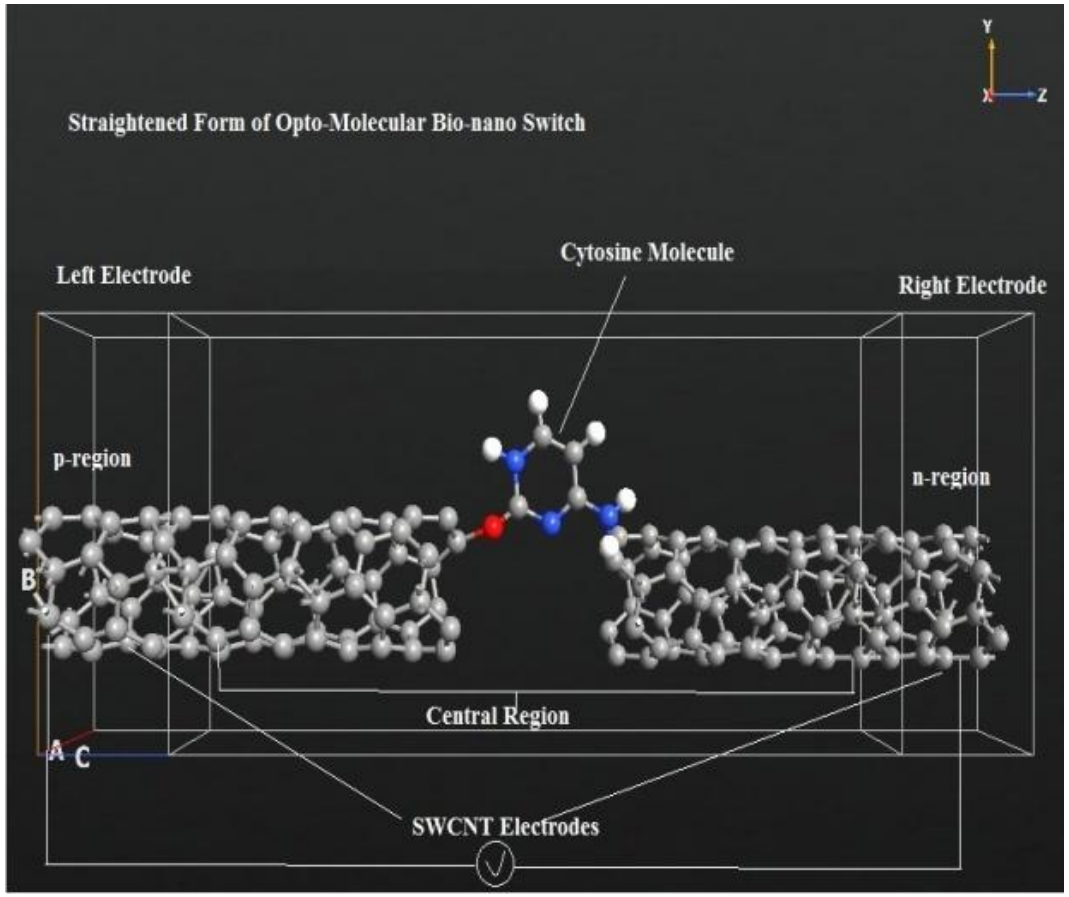
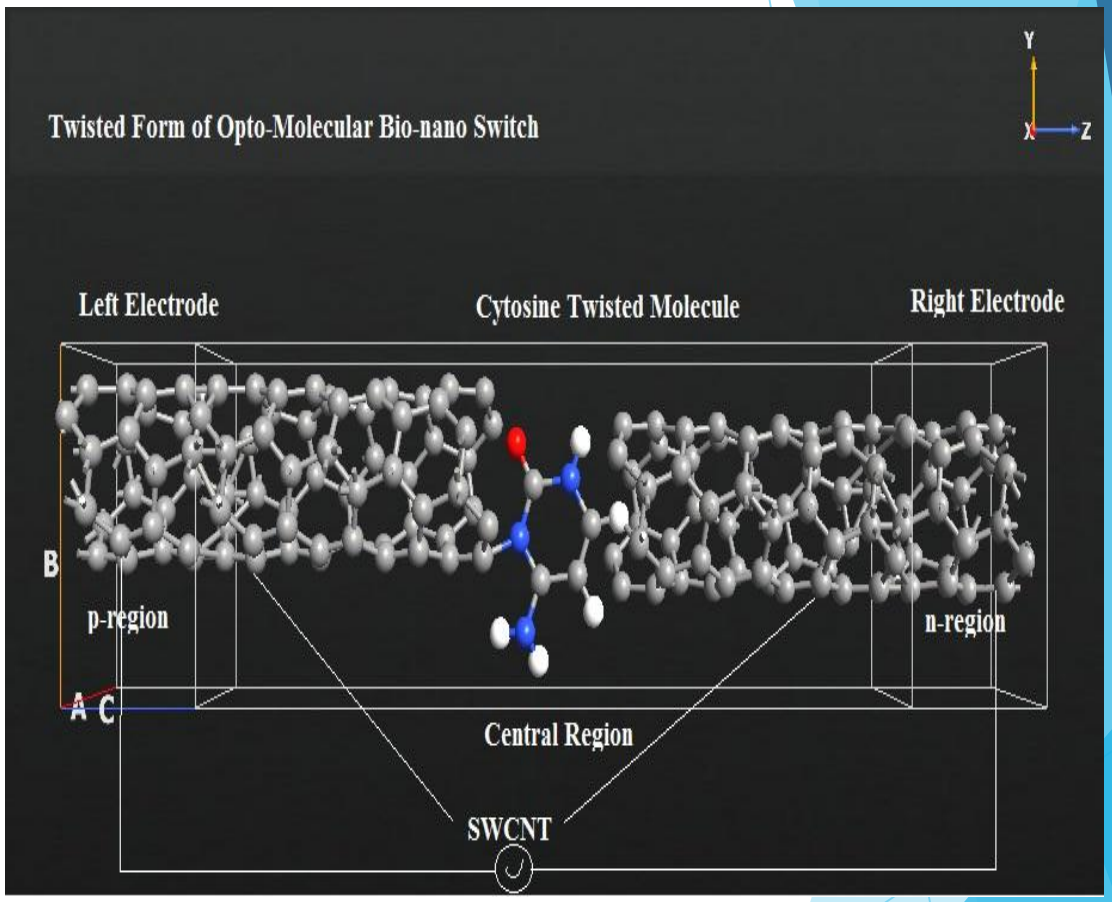
Quantum Molecular Switch





Two different structural forms of the optical bio-molecular switch
***(a)** Straightened, **(b)** 90° Twisted form*

Source: Dey, D., Roy, P., & De, D. (2019). Electronic transport properties of electrically doped cytosine-based optical molecular switch with single-wall carbon nanotube electrodes. *IET Nanobiotechnology*, *13*(5), 484-492.

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Electronic transport properties of electrically doped cytosine-based optical molecular switch with single-wall carbon nanotube electrodes

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Abstract: This study represents an empirical model of cytosine-based optical molecular switch. This possible biomolecular switch has been designed using the first principle approach which is based on density functional theory and non-equilibrium Green's function. The quantum-ballistic transport property and current–voltage (I–V) characteristics of cytosine-based optomolecular switch have been investigated at 25 THz operating frequency. The influence of highest occupied molecular orbital–lowest unoccupied molecular orbital (HOMO–LUMO) gaps on the electronic transmission and I–V characteristics has been discussed in detail. The aim of this study is to highlight the minimum conformational change during a single ON–OFF switching cycle. The biomolecule comprises switching behaviour when converts from straightened to twisted form during photo-excitement. The straightened and twisted forms of the molecule are represented as logic '0' and logic '1', respectively. This p and n regions of this switch has been made using electrical doping process. The current through the twisted form of the cytosine biomolecule is ~1000 times higher than the straightened form. The maximum switching ratio 62.1 is obtained at 1 V bias. The origin of the switching behaviour of the biomolecule can be interpreted by quantum–ballistic transport model along with HOMO–LUMO gaps.

1 Introduction

Cytosine is an important key molecule of DNA and RNA. It is one of the nitrogen bases which carry genetic information from one biological cell to another. It has a unique property to modify itself into different bases to carry epigenetic information [1]. Researchers thus take interest in the application of biomolecular devices. The nanodevice fabrication has already been merged with molecular especially nano-biomolecular device fabrication [2, 3]. The typical molecular switches have been illustrated using different organic and inorganic molecules. These optical molecular switches exhibit their switching property during their various isomeric forms. These molecular switches have been designed using density functional theory (DFT) conjugated with non-equilibrium Green's function (NEGF)-based first principle approach [4–12]. Comparing to these molecules, cytosine provides highly satisfactory switching property at 300 K operation. In this paper, the opto-molecular switching property of this biomolecule using single-walled carbon nanotube (SWCNT) electrodes has been investigated. CNT has great potential in the field of nanotechnology. This can be used as an electro-mechanical sensor, transistor, spin filter, spin valve etc [13–17]. SWCNT has several advantages as an electrode. This SWCNT can be used as a nanoelectrode. This nanoelectrodes based on CNT can be fabricated efficiently in an atomic level. These SWCNT-based nanoelectrodes have very low site density. This CNT electrode can be easily grown on the conductive surface to provide good electrical conductivity [18]. SWCNT electrodes are chemically stable with high quantum transmission and thermal properties [11, 19, 20]. The various quantum-mechanical features of the proposed biomolecular switch have compared with the existing optical molecular switch in Table 1.

In this paper, the electrical doping process has been introduced to create p and n regions at the end of the SWCNT. This doping process is different from the conventional doping process. Electrical doping injects electrons by donating an electron and thus n-dopant has been created. Electron acceptation creates the formation of p-dopants for this nanoscale switch. The central molecular region that means single cytosine molecule along with the extended molecular part of SWCNT has been demonstrated as an intrinsic region (i-region). In this paper, the potential difference has been created between two electrodes which lead to the shift of Fermi levels. This generated potential drop drives the current flows through the channel. There are several advantages existing for electrical doping process.

Conventional doping process can be avoided; thus, the possibility of fault arising due to ionic bombardment in molecular films can be restricted.

No external impurities or dopants required.

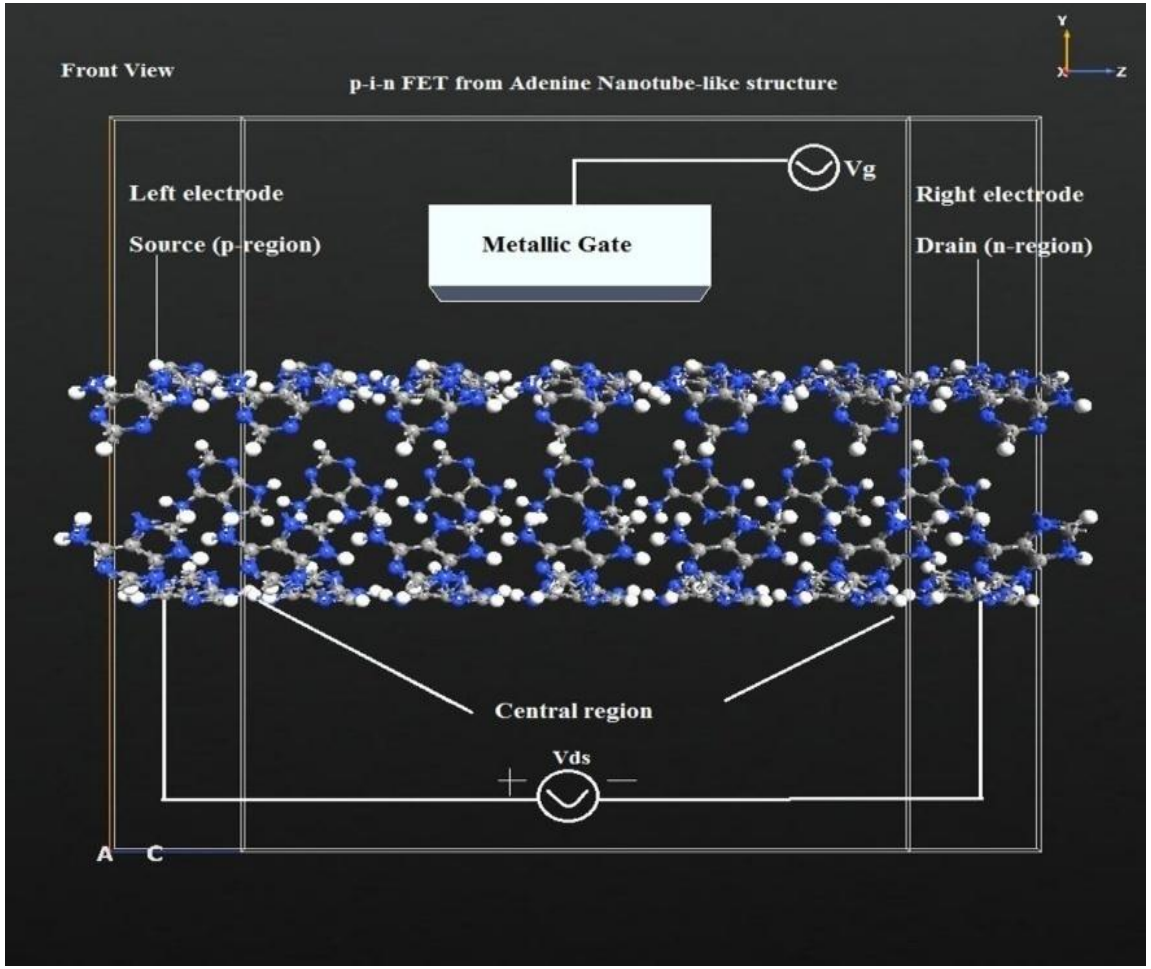
High doping concentration can be achieved for molecular thin films.

Tuning of energy level in the molecular level of a photovoltaic cell can be possible [21–24].

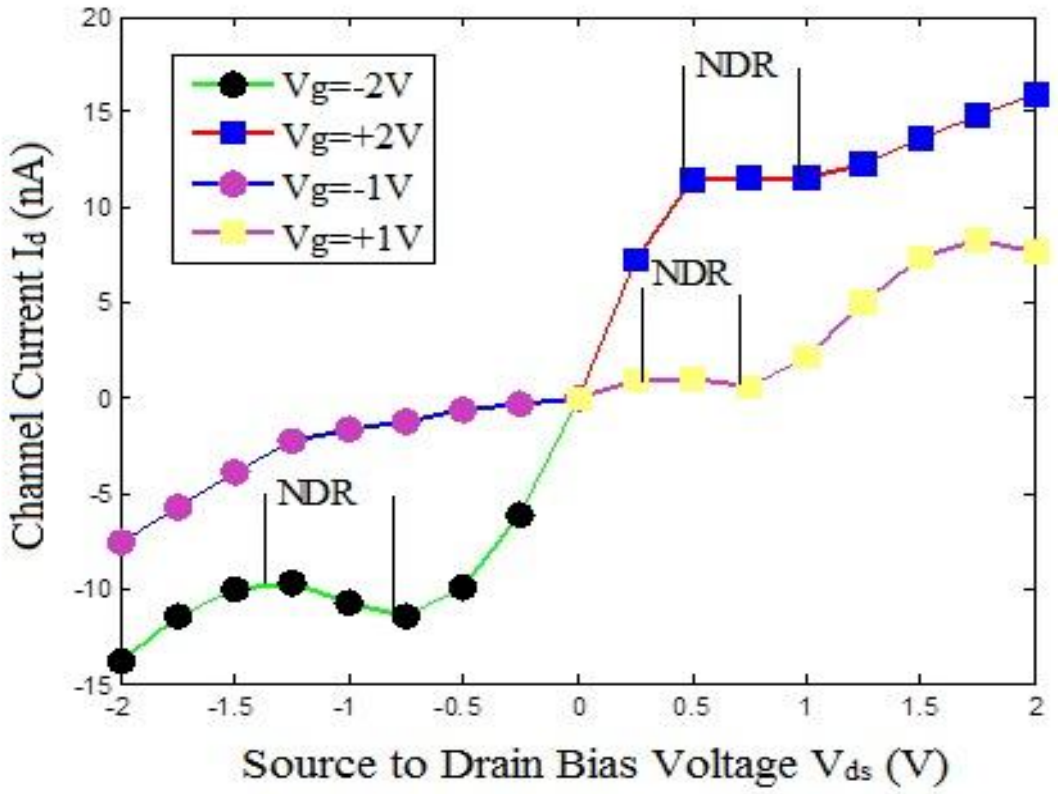
An ideal switch operates either in 'OFF' (cut off) or 'ON' (saturation) conditions. However, the operating characteristics differ significantly of a molecular switch from an ideal controlled switch. The switching mechanisms of this molecular device are stated as follows:

- It can conduct only a finite amount of current in one direction when 'ON'.
- It can block only a finite amount of current in one direction.
- It has a voltage drop during 'ON' condition.
- It may carry a small leakage current during OFF condition.

Quantum Molecular Transistor



Front View of the p-i-n FET based on Adenine nanotube structure.



I_d-V_{ds} characteristics of the bio-molecular nanotube p-i-n FET both in forward and reverse bias for different gate bias voltages

Source: Dey, D., Roy, P., & De, D. (2017). Atomic scale modeling of electrically doped pin FET from adenine based single wall nanotube. *Journal of Molecular Graphics and Modelling, 76*, 118-127.

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Atomic scale modeling of electrically doped p–i–n FET from adenine based single wall nanotube

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ABSTRACT

The Field Effect Transistor (FET) characteristics has been observed from a single-walled Adenine nanotube device using Density Functional Theory associated with Non Equilibrium Green's Function based First Principle approach. This device is electrically doped which shows both n and p channel characteristics of a p-i-n FET. This device is designed and originated from a single-walled biomolecular nanotube structure. The p and n regions have been induced at the two ends of the device using electrical doping process. Thus both n and p channel current-voltage response can be obtained within a single nano-scale device at room temperature operation. The device is 3.35 nm long and 1.4 nm wide. The quasi-ballistic quantum transmission property reveals impressive and almost ideal current-voltage characteristics of the FET. Highest Occupied Molecular Orbital (HOMO) and Lowest Unoccupied Molecular Orbital (LUMO) gap reveals the possibility of quasi-ballistic coherent transmission of the device. The electronic properties based on Molecular Projected Self-consistent Hamiltonian are analyzed using Hilbert space spanned basis functions. The maximum tunneling current observed for the bio-molecular FET is 15.9 μA for n-channel and 13.8 μA for p-channel. The device is operated in atomic scale regime with 1000 THz frequency. The present results reveal the role of quantum-ballistic tunneling phenomenon in the current-voltage characteristics and channel conductance properties of the bio nanotube structure, which is useful in future generation nano-electronics.

1. Introduction

Electrical doping process is one of the promising areas in the field of nano-scale fabrication. This fault free doping procedure is acceptable for both the organic and in-organic molecular device designing in atomic scale region. Electrical doping procedure is also introduced in the investigations of nano devices to obtain fabrication-fault free output [1–3]. The discovery of Single Wall Carbon Nanotube (SWCNT) makes explosion in the era of nanotechnology. The applications of SWCNT are tremendous in the field of nano-electronics due to their versatile properties. Various types of inorganic nanotubes are also being introduced with their metallic properties. This nanotube can be used as transistor, diode, switch, sensor and many more [4–6]. Though various in-organic powerful electro-chemical materials are present, but DNA proofs itself as a most promising candidate in the field of conventional nano bio electronics due to their self-assemble property and versatility. DNA detection can be possible through single electron transistor, graphene nanopore and also the recognition of its four nucleobases can be made using gold electrodes [7–10]. Conductivity enhancement, double proton transfer, current-distance response of the single strand DNA (ss-DNA) can also be possible using Density Functional Theory (DFT) along with Non-Equilibrium Green's Function (NEGF) based First principle approach [11–15].

In this paper, Adenine based nanotube structure has been designed and investigated using Atomistix Tool Kit-Virtual Nano Lab (ATK-VNL) software simulation package. Adenine is one of the nucleobases of DNA and it also takes part in human metabolism

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A First Principle Approach to Design Gated p-i-n Nanodiode

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Keywords: DFT, GaAs nano wire, Negative Differential Resistance, NEGF, p-i-n diode.

Abstract. Thanks to the world of nano technology; it is possible to build molecular nano devices. In this paper, GaAs single nano wire molecular p-i-n diode is designed and its electronic transmission properties, Local Device Density of States, Highest Occupied Molecular Orbital-Lowest Unoccupied Molecular Orbital plot and Negative Differential Resistance property are investigated from the atomic perspective using first principle Density Functional Theory-Non Equilibrium Green's Function approach. This molecular structure is built and simulated in Virtual Nano Lab atmosphere. The Negative Differential Resistance of the device is revealed through the current-voltage characteristics of the nano wire. The band-to-band tunneling current is observed for this p-i-n junction nano diode. Thermal co-efficient, Peltier co-efficient, and Seebeck co-efficients at different gate bias are obtained. This nano wire GaAs molecular diode is attractive for the next generation low power nano device design. Electrical doping effect has been introduced in the wire without adding unambiguous dopants to the molecular wire.

Introduction

Gallium Arsenide (GaAs) is a direct band gap semi conductor with huge applications in the field of applied physics. Due to its direct band gap property, this material is commonly used in the Optoelectronics. In this paper, the gated diode characteristics and tunneling effect of the GaAs single molecular nano wire has been investigated. The Band-to-Band tunneling (BTBT) effect of this device is clearly highlighted through its current-voltage (I-V) characteristics. In this paper, electrical doping process has been introduced to this molecular wire without using explicit dopants.

Electrical doping is the process of insertion of electronic donation or electron acceptation to the molecular films. This process has been used to modify interfaces. The main attraction of this process is that, conventional n and p doping has not been a constraint to accomplish bipolar carrier transmission. W. Gao and A. Kahn have highlighted the demonstration of electrical doping into molecular films [1]. Furthermore, In an United States Patent by Serge L. Rudaz, (Patent No.: 5,729,029 dated Mar. 17, 1998) it is stated that, electrical doping in III-V inorganic compounds have been successfully fabricated N-type compound device layer, which consists of several sub-layers [2]. Electrical doping at molecular level has been used in Organic PhotoVoltaic Cell (OPVC) for the tuning of energy level alignment [3].

Improvement of device efficiency by enhancing carrier injection and lowering drive voltage can be achieved by electrical doping [1, 4]. Electrical doping both p-type and n-type has shown to increase film conductivity to a large extent [1]. Electrical doping is extensively used to form Ohmic contacts on inorganic semi-conductors [4]. Optimization of n-type electrical doping in III-V Nitride inorganic compounds [2] results in improvement of Contact resistance, Biasing voltages, Minority carrier injection and Recombination characteristics.

Relative density of molecular dopant required for electrical doping in organic molecules is much larger than that required for inorganic molecular doping [5].

This wire acts as a gate bias controlled p-i-n diode with significant tunneling current at room temperature. This single molecular wire exhibits Negative Differential Resistance (NDR) property which is prominent from its tunneling effect. The metallic cylindrical gate is used to control the

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ARTICLE

Nanoscale Modeling of Molecular Nano Bio *p–i–n* Tunnel FET with Catalytic Effect of Iron Nanofiber

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ABSTRACT

In this paper Density Functional Theory and Non-Equilibrium Green's Function based First Principle approach is used to design an analytical model of DNA based *p–i–n* Tunnel FET. The quantum mechanical properties of the FET are investigated from the device level analysis using Extended Hückel Theory. Significant current is achieved due to iron catalyst for the device in both the *p* and *n*-channel FET using electrical doping. Electrical doping helps to induce both *p* and *n* type doping at the two ends of the FET without ionic bombardment process. The strong coupling held between the biomolecules and electrodes in naoscale regime which results in coherent transmission. Catalytic behavior of iron nanofiber increases the channel transmission probability. Transmission spectra of the device show that due to the catalytic effect of iron nanofiber, transmission co-efficient is sufficiently high for the *p–i–n* FET. Iron nanofiber increase channel conductivity to obtain better current transmission as well as it provides mechanical strength to the molecular device. HOMO-LUMO gaps also satisfy that lower barrier height is obtained when the device is supported with nanofiber. This lower transmission barrier height helps to conduct satisfactory current for both *n* and *p* channel FET during room temperature operation.

KEYWORDS

1

1. INTRODUCTION

Bio *p–i–n* Tunnel FET (TFET) is one of the challenging aspects in the field of nano bio technology. This is strong and fundamental building block in bio technology due to its amplification and switching characteristics. In this paper an ultra short conducting channel TFET has been designed to transmit current from source to drain terminal and this current has been controlled with a metallic gate or base. The electrical doping has been introduced to make this TFET as both *n*-channel and *p*-channel TFET.

DNA has ideal property of charge transport so that the DNA detection can be possible through Single Electron Transistor (SET) based grapheme nanopore.[1,2] Adenine, Thymine, Guanine and Cytosine are four nucleobases of DNA sequence. Recognition of these nucleobases along with sugar groups can be possible via gold electrodes along ⟨100⟩ direction.[3] Conductivity enhancement can also be done using copper modification of the DNA molecules.[4] Double Proton Transfer (DPT) effect on charge transfer technique can be realized on conductivity of DNA using Density Functional Theory (DFT) along with Non-Equilibrium Green's Function (NEGF) based First Principle approach.[5] Electronic transport property and current distance property can be investigated for the DNA sequence and separate nucleotides by the changing of tunneling current.[6,7] Conductance of the short DNA sequence has been investigated due to the self assembled property of DNA using gold electrodes.[8,9] Reverse DNA translocation can also be possible using optical or magnetic tweezers.[6,10,11] Computational study has been done in GaAs nanoribbon can be used as *p–i–n* diode at atomic scale. This nanoribbon also exhibits its *p–i–n* diode characteristics.[12]

In this paper electrical doping procedure has been introduced for the formation of *p* and *n* region of the TFET, which leads to the formation of DNA based *p–i–n* TFET. This way both *n* and *p*-channel characteristics are available in a single FET. Electrical doping provides improvement in carrier injection into molecular films. Though the electrical doping found literally less for organic molecules compared to inorganic but using this process the interfaces can be modified.[13] Experimentally this process has been illustrated in doping of III–V compounds in the year

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Design and Electronic Characterization of Bio-Molecular QCA: A First Principle Approach

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Keywords: BMQCA, DFT, HOMO-LUMO, NEGF, Nucleotide.

Abstract. Molecular Quantum-dot Cellular Automata is the most promising and challenging technology nowadays for its high operating frequency, extremely high device density and non-cryogenic working temperature. In this paper, we report a First Principle approach based on analytical model of 3-dot Bio Molecular Quantum-dot Cellular Automata. The device is 19.62Å long and this bio molecular Quantum dot Cell has been made with two Adenine Nucleotide bio-molecules along with one Carbazole and one Thiol group. This whole molecular structure is supported onto Gold substrate. In this paper, two Adenine Nucleotides act as two quantum dots and Carbazole acts as another dot. These 3-Quantum-dots are mounted in a tree like structure supported with Thiol group. This model has been demonstrated with Extended Hückel Theory based semi-empirical method. The quantum ballistic transmission and HOMO-LUMO plot support the polarization state change. This state changing ability has been observed for this molecular device. Therefore, this property has been investigated and reported in this paper. HOMO-LUMO plot shows the two logic states along with null state for this 3-dots system. This phenomenon illustrates how the charge transfers take place. Two polarization states along with one additional null state have been obtained for this bio molecular nano device. This molecular device has been operated with 1000THz frequency. This nanoscale design approach will initiate one step towards the modeling of high frequency bio molecular Quantum dot Cell at room temperature.

Introduction

The study of Molecular Quantum-dot Cellular Automata (MQCA) can be the successful and fruitful substitute of CMOS technology as the information passes through with polarization states changing ability at ultra high speed. DNA is a versatile molecule due to its self-assembled property. In this paper, two Adenine molecules have been taken to build the nano Bio Molecular Quantum-dot Cellular automata (BMQCA). Adenine is the basic building block of DNA and RNA. Adenine when added with Deoxyribose sugar group, converts itself to Nucleoside which is essential for cancerous cell detection. The chemical synthesis of Nucleoside with Phosphate forms Nucleotide. When this Adenine is attached with three phosphate groups then it transforms itself into Adenosine-tri-phosphate (ATP) which is very essential for metabolism. DNA can be used as the natural sensor through nano-pore single electron transistor [1]. Quantum Transport property through nucleotides has been studied when the four nucleobases are kept between two pairs of electrodes [2]. Nano-pore based DNA analysis is made possible through graphene electrodes [3]. Replacement of Hydrogen (H) atom with Copper (Cu) enhances the conductivity of DNA [4]. Double proton transfer effect on DNA conductivity enhances the transverse electronic communication between the base pairs [5]. DNA sequence shows its cross-tunneling currents when attached with Gold (Au) electrodes [6]. A nano-pore based graphene nano ribbon helps to carry micro ampere current through the DNA base [7]. Making use of the First Principle, the study of a grapheme nano ribbon based nano sensor has

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Electronic characterisation of atomistic modelling based electrically doped nano bio p-i-n FET

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Abstract: In this study, electrically doped bio-molecular p-i-n field-effect transistor (FET) is designed and its electronic properties are investigated. Density functional theory along with non-equilibrium Green's function based first principle approach is used to design the bio-molecular FET at sub-atomic region. Three Adenine and two Thymine molecules are attached together to form 6.24 nm long and 1.40 nm wide bio p-i-n FET. This device is attached with two platinum electrodes and wrapped with a metallic cylindrical gate at high vacuum. Intrinsic n and p regions can be made possible within a bio-molecular device at room temperature by electrical doping without explicit dopants, which leads to conduct current by the device both in forward and reverse bias. The various quantum mechanical properties have been calculated using Poisson's equations and self-consistent function for the bio-molecular FET. Among these various quantum mechanical properties, the authors obtain high quantum transmission along with satisfactory current for the proposed device during the room temperature operation. The goal of this study is to highlight the design of a bio-molecular p-i-n FET with satisfactory large current using ultra low power dissipation.

1 Introduction

The successful realisation of bio-molecules leads to evolve a new era in bio-nanotechnology. Bio-molecules integrated with inorganic materials provide great response towards the emerging bio-nanotechnology. In this paper, electrical doping procedure has been introduced which restrict the possibility of fault arising during the ion-bombardment. This technique presents enhancement to the carrier injection into the thin films. Electrical doping procedure introduces electron insertion by donating electron which creates n-dopants and electron acceptation leads to the formation of p-dopants to the molecular films. Traditional n and p doping cannot be a constrained to achieve bi-polarity. Electrical doping has been successfully implemented in inorganic semiconductor rather than organic molecules [1–3]. Tuning of energy level alignment is carried out in organic photo voltaic cell using electrical doping at molecular level [4]. Rudar [5] has successfully fabricated N-type compound, which consists of several sub-layers in III–V inorganic materials using electrical doping in his patent.

Inclusion of electronic contribution or electron acceptation is the basis of electrical doping to the molecular films. Interfaces can be modified by electrical doping. According to Gao and Kahn [1], bipolar carrier transmission into molecular films can be accomplished without conventional n and p doping. In this analytical study electrical doping process has been used to set up the system as a p-i-n junction, by adding a certain amount of charge at the two electrodes. This will lead to the shift of Fermi levels of the two electrodes relative to each other. Thus a potential drop is generated into the system. The electrodes have different Fermi levels; so their difference of charge represents an applied bias voltage to the system [6–8]. Thus the platinum (Pt) metal electrodes have not doped explicitly. This is a theoretical approach to shift the Fermi level and generation of potential drop into the system without introducing conventional doping procedure. Explicit dopants are not being used for the electrical doping method, because this will give very high doping concentration [6–8]. Therefore, traditional doping is not being used for the Pt metal. The advantages of electrical doping are:

(i) Device efficiency can be improved by applying enhancement in carrier injection and drive voltage reduction [2, 4].
(ii) Both p-type and n-type electrical doping leads to increment in film conductivity to great extent [2].
(iii) Ohmic contacts on inorganic semiconductors can be achieved by electrical doping [4].
(iv) N-type electrical doping optimisation [3] results the following improvement in III–V nitride inorganic compounds.
  (a) Contact resistance
  (b) Biasing voltages
  (c) Minority carrier injection
  (d) Recombination characteristics.

In this doping process the left and right electrodes are modelled with their respective Fermi levels $F_L(E)$ and $F_R(E)$. When the voltage is applied between the two electrodes then V_{ds} is defined in (1) [7].

$$q \cdot V_{ds} = F_L(E) - F_R(E) \quad (1)$$

The p-i-n photodiodes show its natural optical properties along with its transistor nature [9, 10]. Adenine and Thymine are one of the most powerful and primary nucleobases for DNA and RNA. DNA molecules can be used as natural sensor due to its powerful self-assembled property [11]. Four nucleobases, i.e. adenine, thymine, guanine and cytosine shows inhabit electronic properties when they are kept between two pair of electrodes [12]. The electrical field driven neurotransmitter bio-device has also been made using molecular adrenaline bio-liquid on insulator [13]. Nanoporous silicon membrane based bio-molecular devices has also been used in drug delivery system [14]. Using the similar concept of silicon on insulator, lipophylic and hydrophylic bio-liquids have been used as test bio-device using the

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Electrically Doped Adenine based Optical Bio Molecular p-i-n Switch with Single Walled Carbon Nanotube Electrodes

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The photo excited electronic transmission properties of Adenine based bio molecular switch is investigated at room temperature. Landauer formalism combined with both Density Functional Theory and Non- Equilibrium Green's Function has used to determine electronic transport characteristics of this quasi one-dimensional optical switch. Two metallic single walled carbon nanotube (4, 2) electrodes have been used to provide favorable channel for charge transfer. The charge migration from the molecular junction governs considerable difference in conducting current. This tunneling current is relatively small due to the weak coupling between the molecule and the electrodes. This bio molecular switch has operated in Coulomb-blockade regime. The bio molecule comprises its switching property between straightened ('OFF') to 90° twisted ('ON') form upon photo excitation. HOMO-LUMO gaps and the spatial distribution of the molecule are discussed in detail using Hilbert space spanned based basis functions of the bio molecule. The theoretical results show that this molecule conducts upto 23mA current when it has been twisted at 90° than the straighten form. This property suggests this system has attractive prospective application in future generation optical bio molecular switch technology. Electrical doping process has been introduced for this analytical model of p-i-n switch. This process enhanced the quantum -ballistic current transmission through the scattering region of the molecule.

Keywords: Adenine, DFT, Electrical doping, NEGF, p-i-n Switch, SWCNT

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Electronic enhancement effect of doped ferromagnetic material in biomolecular heterojunction switch

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Abstract: Density functional theory conjugated with non-equilibrium Green's function-based first principle approach is used to determine the ferromagnetic-doping effect in the current–voltage characteristics for the heterojunction biomolecular analytical structure. The quantum-mechanical transport phenomenon and multiple switching activities associated with sequential negative differential resistance properties have been observed for this adenine-thymine chain. The authors investigate the quantum-transport properties of conventional doping effect for ferromagnetic atoms in this bimolecular chain. The results show an electronic enhancement effect in quantum-ballistic conductivity for this chain along with sequential switching property. Among these ferromagnetic metals, Nickel shows significant transmission spectrum, sharp and prominent highest occupied molecular orbital (MO) and lowest un-occupied MO peak along with maximum quantum-ballistic current at room temperature. It is observed from the device density of states that large numbers of conducting channels are available for Nickel doping. This ensures high quantum-transmission current flow within the central molecular region for these ferromagnetic dopants. Compared to Iron and Cobalt, the current has been enhanced up to 4.05 times for Nickel dopant. High doping concentration (13.3%) has been introduced for this ab-initio model. It has found that the number of total switching process is increased during ferromagnetic doping mainly for Cobalt and Nickel dopants.

1 Introduction

This paper presents the enhancement effect in quantum-electronic properties for nitrogen base molecules of single strand DNA (ssDNA), i.e. adenine and thymine. In this analytical model, two adenine and thymine molecules are paired up and connected with platinum (Pt) electrodes. Pt is inert toward any type of chemical reaction with nitrogen bases. Therefore, Pt has been chosen as an ideal material for electrodes. The adenine and thymine molecular chain is, therefore, hydrogenated to make the device improved toward current conductivity and more efficient for quantum-ballistic transmission process in nanoscale. A single electron transistor (SET)-based nanopore switch has been designed to investigate DNA sequencing [1]. Transverse electronic transport property has been investigated due to the tunnelling effect between DNA and electrodes. The transverse electronic transport has been considered for the nucleotides when they are placed between gold (Au) electrodes [2]. Researchers establish DNA analysis through nanopore graphene electrodes [3]. Electronic enhancement with copper (Cu) modification in DNA chain was introduced using first principle approach. Within these base pairs, hydrogen atoms (H) have been replaced by Cu which leads to the conductivity enhancement in the nitrogen base pair [4]. Double proton transfer effect in the conductivity of DNA base pairs has also been investigated. This technique improves transverse communication through base pairs [5]. Nucleotides through the cross-tunnelling effect of DNA sequencing has also been recognised [6]. Transverse edge current of DNA sequence is analysed using graphene nanoribbon [7]. Conductivity of short DNA sequence has been demonstrated using density functional theory (DFT) and non-equilibrium Green's function (NEGF), where they found 20 pA current for 1.5 V applied bias voltage to the DNA sequence [8]. Current distance response of ssDNA sequence has been investigated using first principle formalisms [9]. Important structural factors which control conductivity of DNA sequence has also been demonstrated [10]. Gradual power supply switching technology is helpful in low-power complementary metal–oxide–semiconductor design technology with class-G audio amplifier [11]. The switchable charge pump has also been used to eliminate the need for multiple (both positive and negative voltages) charge pump. Hence, the available silicon area is utilised more efficiently [12]. DC–DC switching converter can also be introduced to generate both positive and negative voltages for active-matrix liquid-crystal display [13]. The zero-voltage switching technique has also been used for induction cookers nowadays. This type of soft switching activity has been carried out by reverse conducting – insulated gate bipolar transistor [14].

Theoretical study of quantum-electronic properties of DNA sequences has been already turning to emerge technology in the field of nano-biotechnology. This sub-atomic molecular theoretical investigation has been carried out with Atomistic Tool Kit–Virtual Nano Laboratory (ATK–VNL) version 13.8.0 software simulation package.

The design of graphene metal-insulator-semiconductor field-effect diode MISFED's based on extended Hückel theory and NEGF has a high operating frequency with optimum atomic force [15]. Gated graphene self-switching diode shows prominent negative differential resistance (NDR) property when designed using NEGF formalisms [16]. Authors have shown a heterostructure of Cu/amorphous-tantalum pentoxide (a-Ta_2O_5)/Pt atomic switch using molecular dynamics simulation technique in room temperature. The amorphous switch which is made with Cu, also simulated using molecular dynamics shows minimal stress while operating at 300 K [17]. The reduced atomic force with a low amount of power dissipation is applicable for the smooth functionality of the nano-device.

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First principle study of the self-switching characteristics of the guanine based single optical molecular switch using carbon nanotube electrodes

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Abstract: The switching property of an optical single molecular switch based on a single DNA molecule guanine with a single walled carbon nanotube electrode has been investigated using density functional theory along with non-equilibrium Green's function based first principle approach. The semi-empirical model of this single bio-molecular switch has been operated at an ultra-high 25 THz frequency in mid-UV range. This single bio-molecule comprises switching activity upon UV photo-excitation. The influence of the highest occupied molecular orbital and lowest unoccupied molecular orbital gap and the quantum ballistic transmission into the switching activity are discussed in detail in this study. It has been observed that the maximum ON–OFF ratio, i.e. 327 is obtained at +0.8 V bias voltage. Theoretical results show that current through the twisted form is sufficiently larger than the straightened form, which recommends that this structure has smart prospective application in the future generation switching nanotechnology.

1 Introduction

Nano-bioelectronic devices based on single molecule have the attractive potential to opt the challenges to be an alternative of semiconductors. These nano-biomolecular devices have a significant impact on the nanotechnology. The elementary functions in nano-bioelectronic devices have been explored both experimentally as well as theoretically. The basic electronic properties like negative differential resistance, diode, transistor, molecular rectification, sensing properties of this single molecular system have been well explored [1–11]. During the past decades, it has been observed that the characterisation and manipulation of molecular devices made it possible to design the nanodevices with different elementary functionalities like switches, nanotubes, nanowires and so on [12–15]. The optical nano-biomolecular switch demonstrates its bi-stability nature with high conductivity, i.e. "ON" state and low conductivity, i.e. "OFF" state [16–18]. The comparison between the proposed nano-bioswitch with the various existing nano-molecular switches has been made in Table 1, which shows the various comparative parameters among the existing opto-molecular switches with the proposed nano bio-molecular switch.

This bio-molecular optical switch is activated under UV-B photo-excitation. The wavelength of the light is ~300 nm. The

Table 1 Comparison between existing approach and proposed model

Features	Various molecular switches			
	Existing approach			Proposed approach
	1,3-Diphenyltriazene opto-molecular switch [19]	Phenoxynaphthacenequinone opto-molecular switch [20]	Pyridine-substituted dithienylethene optical molecular switch [21]	Proposed bio-inspired molecular switch
design based on	DFT + NEGF	DFT + NEGF	DFT + NEGF	DFT + NEGF + EHT + first principle approach
applied bias vol.	−2 to +2 V	−2 to +2 V	−2 to +2 V	−0.01 to +0.01 V
max. transmission peak	0.89 (approx.)	0.9 (approx.)	0.87 (approx.)	1.04
electrode	gold	gold	gold	SWCNT
operating frequency	—	—	—	25 THz
distance between two electrodes	16.92 Å	—	optimised distance	3.4 nm
photo-excitation range	—	UV	UV	mid-UV (UV-B)
wavelength of light	—	313–546 nm	—	300 nm
HOMO–LUMO gap for two forms	—	—	—	1.4 eV (twisted form)
2.25 eV (straight form)	—	—	—	—
atomic force	0.05 eV/Å	—	—	0.02 eV/Å

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Circuit Level Modeling of Electrically Doped Adenine–Thymine Nanotube Based Field Effect Transistor

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ABSTRACT We investigate the gate-controlled, electrically doped tunnelling current in Adenine-Thymine heterojunction nanotube-based Field Effect Transistor (FET). This analytical model FET is designed by Density Functional Theory (DFT) and Non-Equilibrium Green's Function (NEGF) based First principle formalisms. It is demonstrated that Band to Band Tunnelling (BTBT) is possible in relaxed Adenine-Thymine heterostructure nanotube. The evaluation of BTBT tunnelling probability to estimate tunnelling current for only ±0.01V applied bias voltage is calculated using Wentzel-Kramers-Brillouin approximation. Electrical doping is introduced to eliminate the probability of fault generation. By keen observation on the shift of energy levels in the band structure, the availability of high transmission co-efficient peaks and current-voltage response we demonstrate the Schottky barrier nature for this geometrically pre-optimized bio-molecular FET. The doping concentration is varied from 0.0001V to 0.1V to achieve a substantially large amount of tunnelling current when the electronic temperature is kept at 300K. The E-k diagram or complex band structure of this heterostructure nanotube ensures its bi-direct semi-conducting nature. This is a first attempt to present a circuit-level demonstration using this Adenine-Thymine nanotube-based bio-molecular FET and validate the obtained results with the existing approaches.

INDEX TERMS Adenine-thymine, DFT, nanotube, NEGF, TFET.

I. INTRODUCTION

The tunnel FET (TFET) has been proved as a strong candidate for future generation low power application due to its low sub-threshold slope. Though Silicon does not achieve low sub-threshold slope and sufficiently high "ON"-state current due to its indirect energy bandgap, therefore alternative channel materials for FET are being investigated [1], [2]. In the field of organic electronics, recently Carbon Nano Tube (CNT), Graphene nano-ribbon based FETs draw the attraction of the researchers [1], [3]–[5]. Due to high carrier mobility and zero-band gap, graphene nano-ribbon FET fails to prove itself in the field of transistor application [1], [6]. Researchers are also trying to find an alternative TFET due to the presence of leakage current in the MOSFET which uses SiO_2 as gate dielectric [7], [8].

In this study, BTBT probability through the bio-molecular channel has been investigated using DFT conjugated with NEGF based First principle approach with the help of Atomistix Tool Kit-Virtual Nano Laboratory (ATK-VNL) software simulator package version 12.8.0. Considering Poisson's solution the drain current of this bio-molecular TFET is being investigated at 300K electronic temperature. To avoid the probability of fault arising, electrical doping is introduced to design the analytical model TFET. In case of electrical doping, a potential drop is to be created between the two terminals of a system or in this case the two terminals of electrodes by inducing two different and opposite potentials

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Electrically Doped Nanoscale Devices Using First-Principle Approach: A Comprehensive Survey

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Abstract

Doping is the key feature in semiconductor device fabrication. Many strategies have been discovered for controlling doping in the area of semiconductor physics during the past few decades. Electrical doping is a promising strategy that is used for effective tuning of the charge populations, electronic properties, and transmission properties. This doping process reduces the risk of high temperature, contamination of foreign particles. Significant experimental and theoretical efforts are demonstrated to study the characteristics of electrical doping during the past few decades. In this article, we first briefly review the historical roadmap of electrical doping. Secondly, we will discuss electrical doping at the molecular level. Thus, we will review some experimental works at the molecular level along with we review a variety of research works that are performed based on electrical doping. Then we figure out importance of electrical doping and its importance. Furthermore, we describe the methods of electrical doping. Finally, we conclude with a brief comparative study between electrical and conventional doping methods.

Keywords: Electrical doping, DFT, NEGF, First principle, Molecular modeling

Introduction

Doping plays a crucial role in determining physical characteristics and their applications of various organic or inorganic materials, especially for semiconductors. This method has been successfully proved for the semiconductor physics industry. A small amount of addition of impurities determines the dopant concentration and electrical conductivities of the materials. It is observed that an ideal dopant should exhibit an ideal solubility in its host material, and it also exhibits a low defect level. However, some basic problems are related to this type of conventional doping process, for example, doping bottleneck which powerfully affects the device performance. This type of performance degradation has been observed severely for wide bandgap materials.

For example, in the case of the minima of high conduction band device, n-type doping is challenging, whereas for maxima of the low valence band device is also complicated [1, 2]. Therefore, some problems arise for the bipolar doping process in wideband semiconductors. It is observed that either p-type or n-type dopants can be inserted but not together [3]. Therefore, to compensate for this type of problem, a feasible solution has been incorporated into the domain of doping. This type of proposed approach is known as electrical doping, which does not depend on this type of bipolar doping. Electrical doping has been introduced to solve the problems of bipolar doping. In the late 1980s' and 1990s', researchers observed that III–V compounds like a single crystal of GaN are difficult to grow. Even more, for commercial use of GaN substrates were also unavailable at the era of the late 1990s'. The reason behind it was explained in such a manner that the difference between lattice constants and coefficients of thermal expansion of the sapphire substrate and the GaN semiconductor made it difficult to grow a high-quality GaN-based epitaxial layer on the

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ORIGINAL PAPER

Implementation of biomolecular logic gate using DNA and electrically doped GaAs nano-pore: a *first principle* paradigm

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Abstract

One of the emerging areas of today's research arena is molecular modeling and molecular computing. The molecular logic gate can be theoretically implemented from single-strand DNA which consists of four basic nucleobases. In this study, the electronic transmission characteristics of DNA chain are investigated to form the logic gate. This biomolecular single-strand DNA chain is passed through an electrically doped gallium-arsenide nano-pore to achieve reasonably improved transmission along <1 1 1> direction. Current-voltage characteristic and device density of states with HOMO-LUMO plot of the device are explained along with the conductivity of the device to confirm the characteristics of some important logic gates like a universal gate. Ultimately the property of resistivity proves the law of Boolean logic of AND gate and universal logic gate, viz., NAND and NOR gate. All the electronic properties of the Boolean logic gate are explored based on the first principle approach by non-equilibrium Green's function coupled with density functional theory in room temperature.

Keywords DFT · NEGF · Oligonucleotide · ssDNA · Universal DNA logic gate

Introduction

A handful of research on the molecular circuit is going on over the last few decades after Adleman's experimental finding of DNA can be used as a computing tool [1]. In recent times, the researchers give emphasis on field effect transistor (FET) to build logic circuitry instead of applying macro-molecule as material [2–5]. Nowadays, biomolecules are used to build logic devices. Single biomolecules, as well as the complex structure of a biomolecule, are used to form different logic circuitry [2, 6]. An artificial nucleobase was developed to set up a steady bond between cytosine and thymine by exploited whole transport property efficiently [7]. Hairpin-like DNA has tremendous application in molecular computing [8–11].

DNA and other biomolecule were used to construct molecular automaton [12, 13]. The simple molecular level autonomous computer was described which was capable to take input and provide output in the molecular form [14]. Deoxyribozyme-based DNA logic ware also proposed where substrate and oligonucleotides are mixed together to form the solution, and the output is obtained from the cleaved product after annealing [15, 16]. Some complex logic circuit was also suggested where the researchers gave an idea of how DNA is used to build different multiplexers and demultiplexers [17, 18]. DNAzyme-based molecular logic gate was also proposed [19].

The basic DNA logic gates were designed by managing DNA origami structure with the assistance of aptamer-substrate strategy [20]. In another experiment, the researchers show that the fluorescent signal has been activated while the DNAzyme-based logic gate is trying to manage DNA tile self-assembly to form DNA origami [21]. The DNA origami was used in basic logic gate designing along with majority gate by using strand displacement strategy [22]. The operation of various logic gates and their algorithmic representation was described and molecular beacon input was provided to the DNA

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ORIGINAL RESEARCH ARTICLE

Algorithmic Approach of Electrically Doped Single-walled Cytosine Nanotube-based Biomolecular Logic Gate: A First Principle Paradigm

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Biomolecular modeling and its associated analytical software simulation tools have a significant role in the rapid progress of bio-inspired semiconductor technologies. This paper presents the implementation of logic gates using molecular modeling of a cytosine-based single-walled nanotube. Density functional theory in and the nonequilibrium Green's function-based first-principles approach are used to perform the quantum mechanical calculations for the electronic transmission within the nanotube. The gated cytosine single-walled nanotube shows high current-voltage response during room-temperature operation where the electrode voltage is kept at ± 0.02 V. This is a first attempt towards the circuit-level modeling of logic gates using a cytosine nanotube. The quantum transport phenomenon of this analytical model is investigated using an atomistic software simulation technique. The basic logic gates and XNOR gate are implemented with the study of the current-voltage characteristics. The maximum current observed during the simulation process is 52.6 μA. Moreover, the local device density at different energy levels proves the candidature of cytosine nanotubes as logic gates. The transmission spectrum analysis also confirms the high channel conductivity at the central scattering region of the nanotube.

Key words: Cytosine, DFT, logic gates, nanotube, NEGF

INTRODUCTION

Nowadays, the world is moving towards bio-stimulated systems, and scientists are working to construct circuits from biomolecules. Several logic devices have been created with the help of a biomolecules. Single biomolecules or sometimes complex biomolecular structures have been used to investigate different logic devices.[1] Currently, researchers are considering field effect transistors (FETs) built with biomolecules instead of macro-molecules as logic devices.[1–4] The charge transport characteristics are proficiently explored to fabricate a single-molecular bio-device. An artificial nucle-obase was designed for competent hole transport through deoxyribonucleic acid (DNA) to form a steady base pair with a biomolecule.[5] Benenson et al. designed biomolecular circuits with the help of supplementary limited enzymes.[6,7] A hydrogen-doped single-strand DNA-based molecular approach was proposed to design different types of logic gates.[8] A DNA hairpin-like configuration was used

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ORIGINAL ARTICLE

First principle study of structural and electronic transport properties for electrically doped zigzag single wall GaAs nanotubes

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Abstract

Emerging trend in semiconductor nanotechnology motivates to design various crystalline nanotubes. The structural and electronic transport properties of single walled zigzag Gallium Arsenide nanotubes have been investigated using Density Functional Theory (DFT) and Non-Equilibrium Green's Function (NEGF) based First Principle formalisms. Structural stability and enhanced electronic transmission property of Gallium Arsenide nanotubes (NT's) have been analyzed for the chiral vector $3 \leq n \leq 7$. This analysis based on the Perdew Burke Ernzerhoff type of parameterization along with Generalized Gradient Approximation (GGA) procedure. Several structural properties like dependency of diameter along with bond length, buckling and band gap have been analyzed. The investigation confirms that buckling property and bond length of these nanotubes decreases as the diameter of the tubes are increasing. It has been observed that (7, 0) nanotube is being considered as most stable nanotube among all. Binding energy also increases with the increasing diameter of the tubes. This two probe experiment is being carried out at room temperature when two opposite bias voltages have given at the end of these nanotubes using electrical doping procedure. Introducing this procedure a potential drop has been created between the two electrodes' chemical potential level. Due to this potential drop, the device performance has been enhanced and results in the flow of high conducting current through the central part of the NTs.

Keywords: Chiral Vector; DFT; GaAs; Nanotube; NEGF.

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INTRODUCTION

Gallium Arsenide (GaAs) is one of the most challenging and direct band gap semiconductor, which plays an important role in semiconductor nanotechnology. Due to the direct band gap property, GaAs plays the crucial role in the optical domain. Since the evolution of Carbon Nano Tube (CNT), tremendous theoretical and experimental research works have been demonstrated all over the world. Quantum transport properties, spin-filtration property and spin transport of CNT have been investigated when CNT formed composites with Copper, Chromium, and Iron [1-3]. CNT has also been proved as high sensing device when it senses NO_2 molecules or any foreign molecules [4-6]. Researchers have also investigated several types of nanotubes (NTs) and their quantum-mechanical properties [7-14]. Several properties like structural and quantum-transport phenomenon, voltage and spin dependent transportation features, effect of moister and defect and absorption effects have been demonstrated for these NTs using Density Functional Theory (DFT) and Non-Equilibrium Green's Function (NEGF) based First Principle approach.

In this paper, the structural stability and quantum-ballistic properties of electrically doped GaAs NTs have been investigated at room

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