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REVIEW ARTICLE

Bio-molecular nano scale devices using *first principle* paradigm: A comprehensive survey

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Abstract

Computational study plays an important role to discover the potential of the bio-inspired nano scale molecular devices. Density Functional Theory (DFT) is one of the popular methods to calculate the properties of the molecules which can not be possible with ab initio process, preferably for transition metals. This method is important for electronic structure calculation along with structure of molecules, atoms and solids can also be calculated using this DFT method. It is the quantitative method to understand the material properties using the laws of fundamental quantum mechanics. The key benefit of Non Equilibrium Greens' Function (NEGF) is that it preserves the wave character of the electrons, which leads to a extremely precise description of nanoscale. Combining theses DFT and NEGF calculation first principle approach reveal the quantum-ballistic properties of atomic scale electronic structures which is therefore attracts the researchers for their innovative calculations for nano scale device modelling. In this paper, we briefly discuss the review on various bio-molecular devices and their significances. Now-a-days bio inspired devices show more attractions due to their versatility compared to the conventional electronic devices. These nano scale devices are popular due to their performance, speed and high charge transmission properties compared to other conventional semi-conductor devices. This review work presents some experimental works at the molecular level along with a variety of research works that are performed based on first principle approach. Several case studies prevails the importance of DFT and NEGF based first principle approach for nano scale device modelling.

Keywords: *Bio-Molecular Device; DFT; First Principle; Nano Scale Device; NEGF.*

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INTRODUCTION

In the year 1964, Hohenberg and Kohn established that there survived a universal functional for the density function which is independent of the external potential [1]. In the year 1965, Kohn and Sham reported their work in the advancement of Density Functional Theory (DFT). They replaced the many-body variation problem with the independent-particle calculation, including all the many-body systems using a potential which is called the exchange correlation term. By providing a set of auxiliary equations, they use a self-consistent procedure to solve the ground state of the system. DFT can elaborately describe the ground state of electronic systems. However, lots of physical phenomena like photo-emission, electron transmission, quantum-

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ballistic transportation, etc. are related to the excited states of electrons. For loosely coupled electronic systems, most of these phenomenons are related to the electrons which are close to the Fermi level. [1, 2]. This theoretical research work is also based on Non-Equilibrium Greens' Function (NEGF) formalisms. However, Greens' function formalisms provide a strong path to solve strongly interacting electronic systems. This theory emphasizes the self-energy of quasi particles which incorporate all the exchange and co-relation functions in terms of the interaction between particles [3]. DFT and NEGF formalisms are used in first principle calculation to solve many body systems, perturbation theory, un-bounded particle based systems and many more. This formalisms are not only provide information for the electronic properties of the conventional nano scale devices but also provide information for bio-inspired molecular devices. A computational investigation is proposed that is based on thymine bio molecule which is one of the major protein component of DNA. The <111> electrode crystallographic orientation of thiol and thymine molecules are considered for the two-probe experimental study. Therefore, the electrical transport phenomenon of this bio-molecular system is analyzed based on extended Hückel theory with two-dimensional (2D) Fast Fourier Transform (FFT) at 300K [4]. In case of molecular device designing, electrodes play a crucial role. The properties of electrodes are also important to investigate as they have influences in the charge transport characteristics. The molecular devices which are embracing of methylthiol-terminated permethyloligosilanes and face-centered crystal Au/Ag electrodes with crystallographic [111] and [100] orientations are observed for bio-inspired molecular junctions [5]. In case of in-organic materials Pentacene polycyclic aromatic hydrocarbons play an important role to develop new high-performance organic molecular devices using DFT and NEGF based first principle formalisms. The electron transport properties of this in-organic molecules are also investigated at room temperature through theoretical simulation process [6]. In case of charge transmission phenomenon through a molecular junction is complex. Electron donation by hydroxyl groups in the aromatic linker promotes electron transfer for various molecular devices [7, 8]. It is also much complex to design the circuitry using this molecular devices. An asymmetric bipyridine-biborinine and oligo-phenylene vinylene (OPV) molecular diode are proposed by the researchers using atomic simulation process [9]. Even more, optical molecular switches can be designed using DFT and NEGF based first principle paradigm [10-13]. Researchers are motivated after getting overwhelming responses from the bio-inspired molecular devices. These bio molecular electronic devices show similar response when comparing with conventional semi-conductor devices. For example bio-inspired diodes, transistors, logic gates are designed using first principle approach at room temperature [14-18]. Quantum-ballistic charge tunneling phenomenon is an important parameter for molecular junction. In this transport phenomenon, σ-system and π-system play crucial role. The conductivity of the molecular junction depends on this charge transmission factor [19-21].

Materials and methods for molecular device designing using first principle approach

Charge carrier transmission property is the key factor behind the molecular device designing using DFT and NEGF calculations. In this approach, choosing of electrodes also plays an important role. In case of first principle molecular device designing approach, two probe experimental set up is used. There are several electrical parameters are to be chosen to get accurate and fast simulation when the device is to be geometrically optimized. Various simulation parameters are chosen by the researchers to get accurate and feasible out puts from the first principle design. The few simulations parameters are shown in Table 1.

In many papers, these simulation parameters hold various values according to the experimental needs. In many cases, electron temperature is to be kept at 300K. The choice of electrodes' material also an important and essential part of this device modelling. The characterization of the nano scale devices mainly based on the charge transport phenomenon through the central molecular region. The nano scale molecular devices are generally divided into three parts, left electrode, right electrode and central molecular region. The layers of electrodes, their width, length and attachment with the central molecular region also important for nano scale simulation process [22-30]. It is possible to assign several bias voltages to the electrodes. Chemical potential of the electrodes are to be changed accordingly. Density

Table 1. Simulation parameters and their probable values.

Parameter	Value
Device Configuration	(A,B,C) direction
Poisson solver	FFT2D
Electron Temperature	300K
Right Electrode Voltage	–0.01 V
Left Electrode Voltage	0.01 V
Fermi Level (Left Electrode)	4.15 eV
Fermi Level(Right Electrode)	3.29 eV
Fermi Level (Bulk)	–1.29 eV
Fermi Level (Left Electrode for DOS)	4.11 eV
Fermi Level(Right Electrode for DOS)	4.09 eV
Fermi Level (Left Electrode for Transmission spectra)	4.11 eV
Fermi Level(Right Electrode for Transmission spectra)	4.09 eV
Fermi Level (Left Electrode for Transmission paths)	4.11 eV
Fermi Level(Right Electrode for Transmission paths)	4.09 eV
Conductance of the device	$5.743e^{-08}$ S
Total number of atoms in device	107
Density mesh cut-off	150 Ry
K-points for sampling	(1×1 ×100)
Left electrode chemical potential	4.11 eV
Right electrode chemical potential	4.09 eV
Real axis point density	0.01 Hartree
Infinitesimal point density	0.001 Hartree

mesh cut-off is one of the important parameter which increase the simulation accuracy. K-points sampling is generally taken along the length of the 2-D molecular nano scale devices. Maximum number of sampling is to be considered through the length of the molecular device. Different device algorithms are chosen so that more accuracy and faster simulation result can be obtained. Real axis point and infinitesimal point density are the two important parameter which determined the device density both for real and complex device structure. Generalized Gradient Approximation (GGA) along with various zeta polarized basis sets is the approximation parameter which determine the device simulation results. In case of nano scale device design, spin transport phenomenon also plays an important part which signifies the spin polarization effect for the molecular device [31-41]. The flow charts are showing the various steps to determine the molecular scale device designing procedure using Quantum- ATK software in Fig. 1.

Density Functional Theory

Since the last 30 years of downscaling in the semiconductor industry, DFT plays an important and obvious role to observe quantum-ballistic transport phenomenon. These formalisms are widely adopted by the researchers to discover the energies in molecules. The main associated theorem with this formalism is Hohenburg-Kohn Theorems demonstrated in 1964. The first theorem states that "*The electron density establishes the exterior potential (to within an additive constant)*". If this declaration is accurate then it follows the rule of "*electron density uniquely determines the Hamiltonian operator*". Hohenburg and Kohn directly prove this theorem and give a generalized solution for the inclusion of systems along with de-generate states [42]. There are several steps associated with DFT formalisms. These steps are as follows:

- By solving and finding the solutions for the Schrödinger Equation.
- The Hohenburg-Kohn Theorems.
- By finding Functional Energy.
- The Local Density Approximation.
- The Generalized Gradient Approximation
- Meta-GGA functional.
- Hybrid Exchange Functional.
- The Performance of Various Functional [42].

DFT is an extremely useful tool to design nanoscale electronic devices. For the last 50 years, DFT dominates the quantum-mechanical and quantum-ballistic simulation of the periodic systems. It is also used to calculate the surface energy of the nanoscale molecular devices.

Non-Equilibrium Greens' Function

Investigation and design of the mesoscopic and nano-scale system are some of the interesting

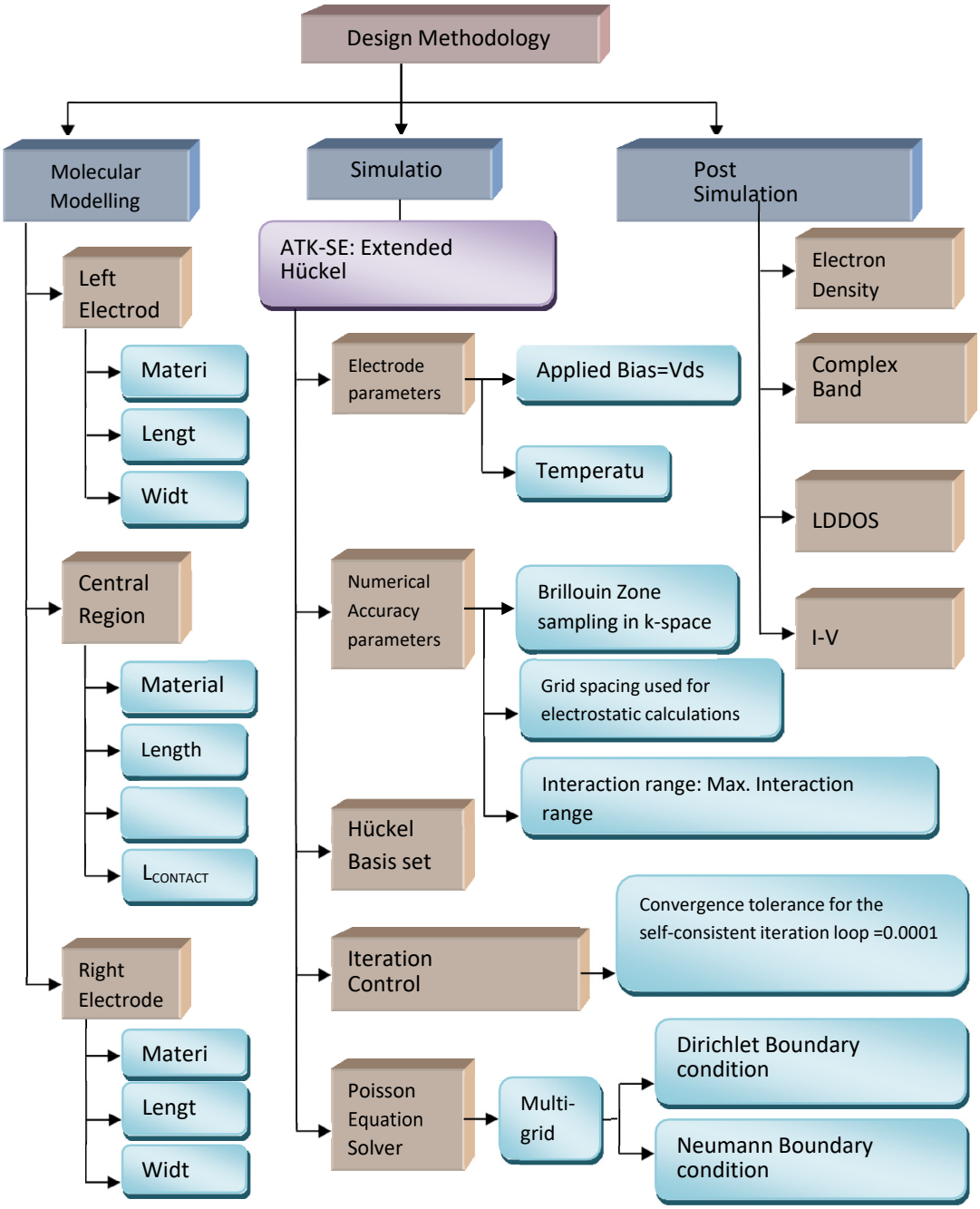

Fig. 1. Working flow diagram of Quantum-ATK software simulation process flow [14].

as well as challenging topics nowadays for researchers. The quantum-ballistic transport phenomenon is the key feature for molecular modeling. NEGF formalism is extensively used to demonstrate quantum transmission. This formalism again used to solve the time-dependent Schrödinger Equation. This is used to study static and time-dependent transport phenomena for nanoscale devices. This theory is also known as Keldysh formalism. The other equilibrium theory is different from the NEGF formalism. In the case of NEGF, all the time- dependent functions are

described for time arguments as a contour plot, which is called as Keldysh contour. In this formalism perturbation theory also plays an important role. There are several parts which are associated to form NEGF formalism is mentioned below:

- Contour-ordered Greens function
- Keldysh contour
- Analytic continuation: Langreth theorem
- Keldysh formulation
- Application to Steady-state transport
- Time-dependent transport [43]

The quantum-ballistic transport phenomenon can be satisfactorily explained with the help of NEGF. It is well described for the meso-scopic and nano scale systems. These nano scale and meso-scopic systems are the thrust area for the researchers nowadays. This low dimension quantum-ballistic transmission phenomenon is to be divided into two parts such as stationary and time-dependent occurrence. NEGF is also known as Keldysh formalism which is extensively used to describe the quantum transport phenomenon in the nano scale regime. NEGF helps to investigate and predict the interaction of particles within a time-dependent many-body system. Time-dependent current-voltage (I-V) characteristics can be eventually solved by using NEGF formalisms which is divided into two basic phases like (a) static and time-dependent electronic transport in meso-scopic systems. The main difference between ordinary Equilibrium theory and NEGF formalisms is that all time-dependent functions are determined for time-arguments on a contour which is called the Keldysh contour.

First principle calculations

In recent trends in nanotechnology, the investigation of quantum transport through mesoscopic and molecular-scale systems is one of the challenging and interesting aspects for scientists. This quantum transport through the molecular level is generally divided into two approaches. One is stationary and another is a time-dependent phenomenon. For the last few decades, DFT and NEGF formalisms are the dominant approaches for the quantum mechanical simulation process. The quantum chemical scientists adopt these approaches to simulate the energy surfaces in molecules. This paper introduces the basic concept of DFT and NEGF theory and outlines the basic mathematical concepts of DFT and NEGF formalisms. A short overview will be given for the electrical doping process and the various analytical design approaches of molecular level nanodevices. Electrical oping is one of the most fabulous approaches where no external impurity is provided to the main molecular nanosheet or wire. This doping method can be adopted for low dimension nanoscale device designing at ultra-low temperature. DFT is one of the major tools to calculate molecular structure efficiently. DFT and NEGF based first principle approach is used to calculate analytical model representation of the nanodevices at the molecular level. In-organic crystalline and amorphous structure of the materials as well as bio-molecular structure can be analyzed with the help of the first principle approach. The quantum-ballistic transport phenomenon by the active electrical carriers has been illustrated using the first principle method. Real-space, NEGF formalisms, and spin-polarization method based DFT method canbe illustrated using the ATK-VNL software simulation package. By introducing these formalisms a molecular device has been divided into three main portions such as left and right electrodes and central molecular region. The analytical calculations for two electrodes are performed using the sampling of the Brillouin zone integration method along with Monkhorst-pack parameters with regular k-point sampling, i.e., 1×1×100. Double zeta or single zeta polarization methods have been taken into account. Self-consistent calculations play an important role in DFT. High mesh cut-off density gives more accurate results for this first principle approach [44-46].

Simulation methods of molecular device designing process

The nano devices are analytically designed and simulated using Quantum wise software simulator version 13.8.0. The various quantum-electronic properties are therefore investigated. The device has been investigated using two probe experiments. The two electrodes are used to find out the results. The simulation parameters have been chosen according to the desired outcome. The geometrically optimized nano scale devices are generally designed using Adenine, Guanine, Cytosine, Thymine bio-molecules, and their combination. Another important crystallographic atomic device has been made using GaAs crystal at the molecular level. To design this analytical design, the combination of DFT and NEGF formalisms

have been implemented. The quantum-ballistic transmission properties have been investigated for the devices depending upon the nature of this transmission various electronic properties have beenstudied.

This Atomistix tool kit is a powerful software simulation tool that is used to implement various nano scale devices analytically. The calculations for DFT have been performing using Generalized Gradient Approximation (GGA) along with Perdew-Burke-Emzerhof single or double zeta polarization approaches. The mesh cut–off density has been chosen 150Ry (maximum). The k-point sampling is taken as 1×1×100. That means the maximum sampling point has been taken along the z-direction. The Brillouin zone integration is performed using Monkhorst–Pack k-point grid. The quantum-ballistic transmission has occurred along z-direction for these 2-D analytical devices, so maximum numbers of samples have been taken along the z-direction. The flow chart with different modules that are used to design these nano scale devices are shown in Fig. 2, 3 and 4 respectively [47-50].

Device Modelling and Case Studies

In this paper some of the important device modelling and their electronic characterizations are discussed. These electronic characterizations of these devices signify the importance of DFT and NEGF boundary conditions. These formalisms are important to investigate the electronic device structures even for unbounded molecular system. The device parameters are chosen precisely so that more accurate calculations can be obtained. For example, in GaAs nanowire is proved to be a p-i-n diode with high efficiency. The molecular level efficiency of this GaAs nanowire p-i-n diode is comparable with conventional diodes. The current-voltage characteristics at atomic

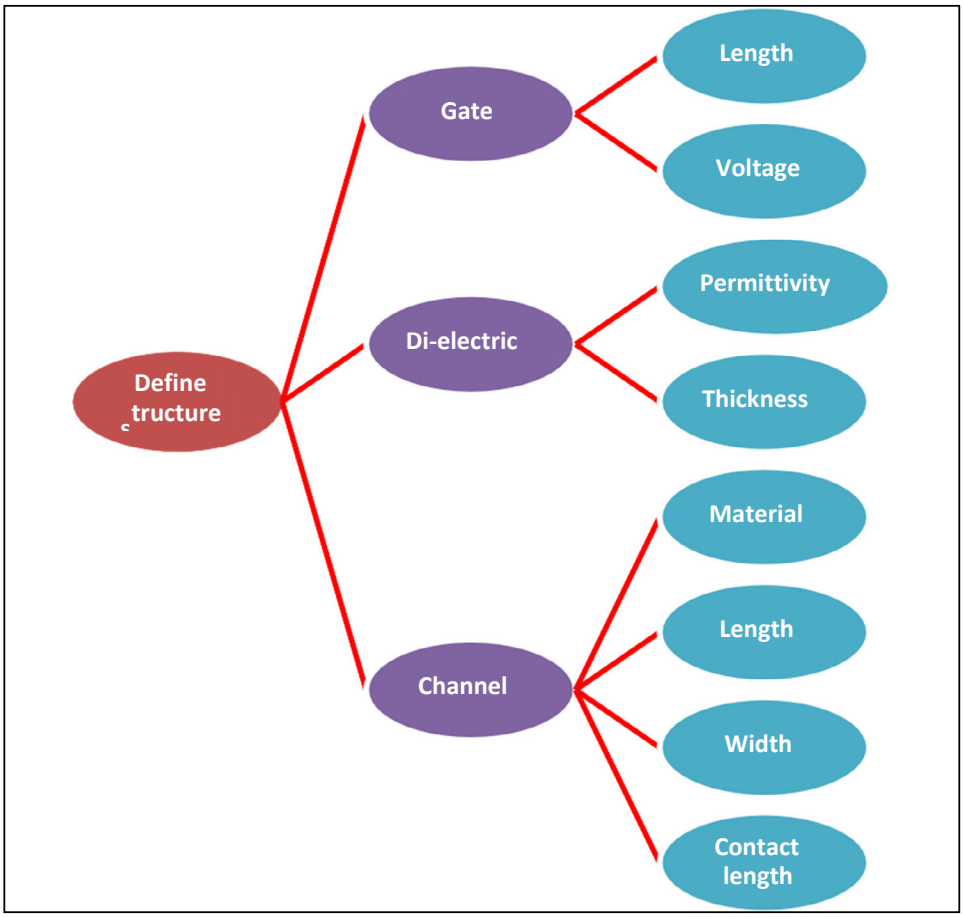

Fig. 2. Working flow chart diagram of molecular device simulation step-1 (pre-simulation) for Quantum-ATK software simulation.

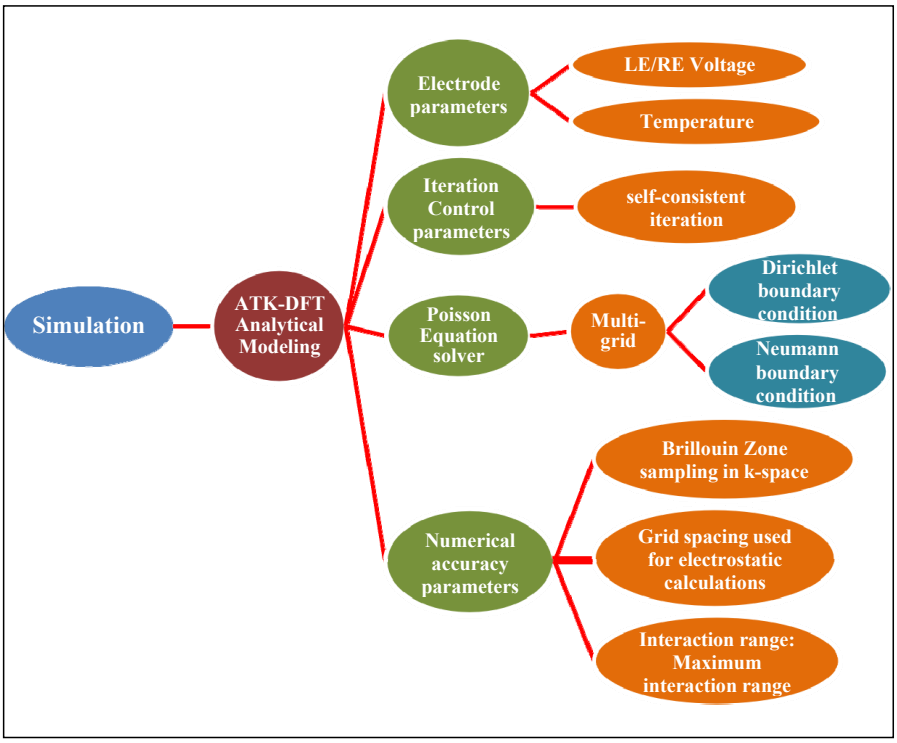

Fig. 3. Working flow chart diagram of molecular device simulation step-2 (simulation) for Quantum-ATK software simulation.

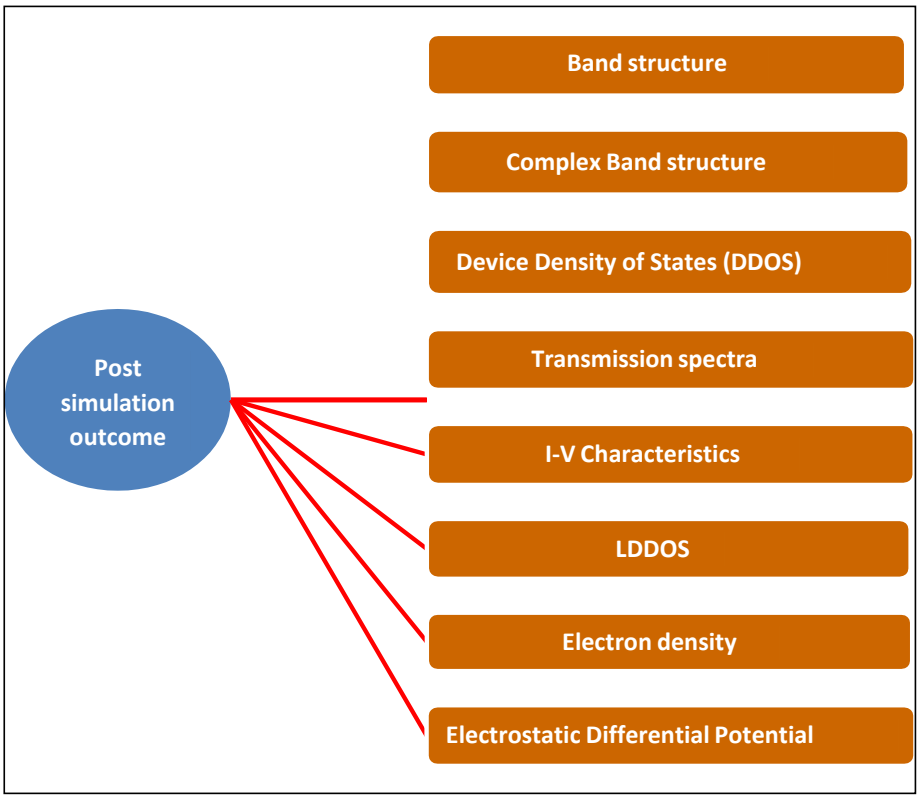

Fig. 4. Working flow chart diagram of molecular device simulation step-3 (post-simulation) for Quantum-ATK software simulation.

scale is similar with conventional p-i-n diode for semiconductor devices [51]. Not only inorganic materials but also bio-inspired nano scale devices show significant performance when simulated using DFT and NEGF formalisms based first principle approach. For example, Cytosine based optical molecular switch shows accurate switching activity which is comparable with conventional switching activity of semiconductor switching devices. The transmission spectra, current voltage characteristics are alike with the semiconductor switching devices. Carbon nano Tube (CNT) are used as the electrodes for this bio-molecular switch [11]. Bio inspired diode, transistors are also designed using DFT and NEGF based formalisms at room temperature simulation process. This bio inspired molecular diode, transistor showcase their electronic characteristics for example current-voltage properties, quantum-ballistic transmission properties, device density of states which are comparable with existing semi conductor diodes and transistors. Even more, logic gates can be implemented using this bio inspired transistors [14, 17]. Some of the proposed models are shown in Fig. 5, Fig.6 and in Fig. 7 where DFT and NEGF based molecular devices are designed

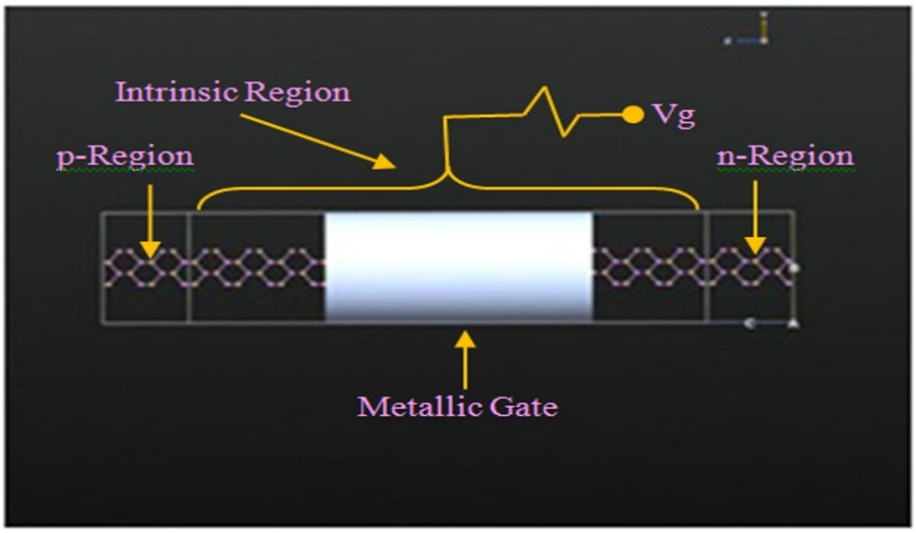

Fig. 5. GaAs Nano wire p-i-n diode [51].

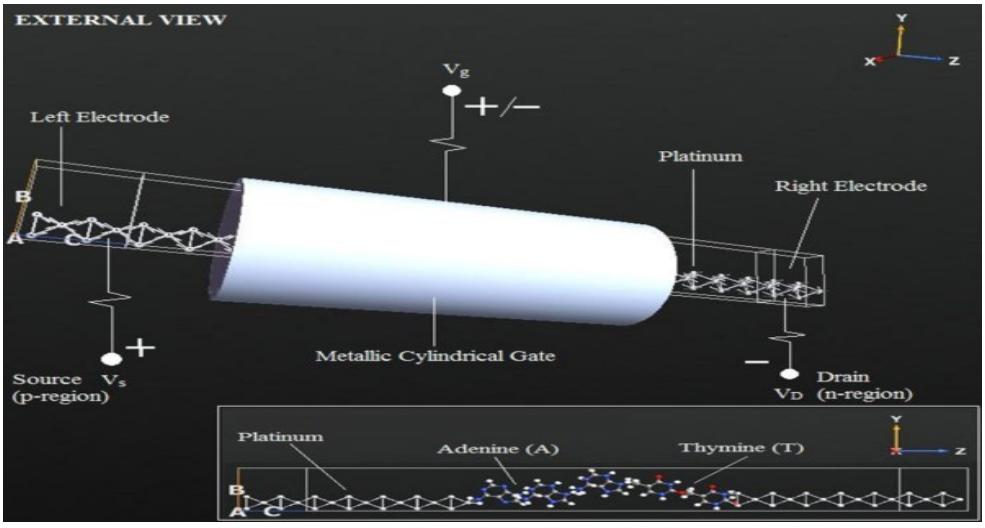

Fig. 6. Adenine-Thymine based p-i-n FET [17].

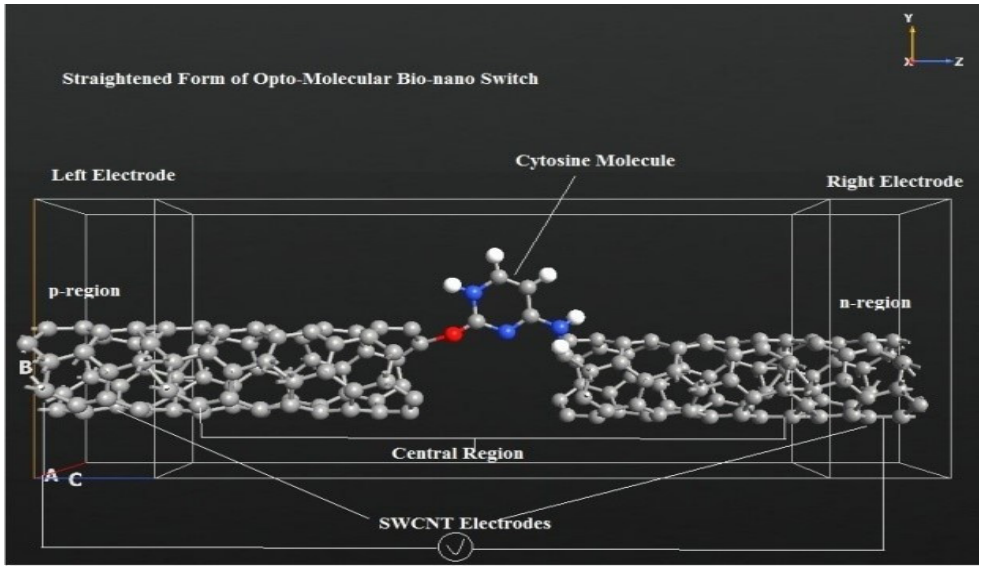

Fig. 7 . Cytosine based optical switch with CNT electrodes [11].

and their electronic properties are investigated and studied. Highest Occupied Molecular Orbital (HOMO) and Lowest Unoccupied Molecular Orbital (LUMO) plot of this molecular devices show the thermo dynamic stability and good charge carrier transmission capability of these bio molecular devices. These devices are geometrically optimized and minimum stress is applicable to the molecular device. The device parameters are chosen to get more accuracy in minimum simulation time. The device characteristics are always comparable with the existing devices. It is proved that the DFT and NEGF based theoretical models show satisfactory performance while comparing with others.

CONCLUSION

The major plus point of theoretical nano scale device designing is that it works based on the computational methodology. DFT and NEGF based theoretical nano scale devices are easy to design and their electronic characteristics are therefore investigated and studied at room temperature. HOMO-LUMO plot signifies the molecular device stability and the charge carrier transmission. Channel conductivity, current-voltage properties characterize the device and also provide significant similarities with the existing semi-conductor conventional electronic devices. Furthermore, the quantum-ballistic transport phenomenon helps to characterize the devices. Besides this depending upon the characterization of these nano scale devices, a comparative study can be made which is important to implement further modification of these devices. Moreover, geometrically stable devices can be modeled at a minimum stress level, which signifies further the stability of the devices. The atomistic design tools make it happened that various properties of these devices can be observed using different design rule platforms. For example, using DFT, Extended Hückel Theory, FFT one can design the nano scale devices. Even more, various properties of these nano scale devices, for example, band structure, complex band structure; DDOS, transmission spectra, I-V characteristics, etc. can be investigated, and also modification can be imposed where it is necessary. The key feature of these molecular structures can also be extracted with the help of post-simulation features. For example, like CNT, bio-molecular nanotubes can also be analytically designed and their key features are extracted for further studies. Moreover, an approach is taken to design hetero junction bio-molecular nanotube and its characteristics are also investigated. Lastly, the future aspect of this nano scale device designing is to implement these molecular devices to its corresponding circuit-level simulation approach.

CONFLICTS OF INTEREST

The authors do not have any conflicts of interest.

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