ABSTRACT

The present thesis involves the investigation of electronic transmission through graphene and allied forms (graphene nanoribbon (GNR) and carbon nanotube (CNT)) at room temperature. As electrons propagates between the two electrodes (left electrode (LE) and right electrode (RE)) via a transmission channel in a streamline manner, it shows negligible interactions with the ions and thus experience no scattering during its movement from one end to other. This imparts ballistic nature to electron transport at nano scale, since at nano scale quantum mechanical effects comes into effect. The occurrence of ballistic transport give rise to unique characteristics in nano devices. The transmission spectrum is the first step towards the analyzation of possible electron transport through the nano devices. It may be calculated at desired specific applied bias voltages, starting at 0 V and going upto 2.0 V. However, it has been shown for 0.0, 0.5, 1.0, 1.5 and 2.0 V only to manifest a lucent transmission spectrum. In molecular systems, the aim is to achieve successful coupling of channel material with that of electrode. Its often desired for the occurrence of ballistic transport. This in turn avoid heat generation arising out of interface mismatch at the joints, which in turn effect the systematic motion of electrons as well as the proper device functioning. Non equilibrium Greens function formalism (NEGF) is an effective tool to compute the electron transmission spectrum. It is essential in solving the differential equation in context of many body wave function. The corresponding eigen values and eigen functions are obtained on employing Schrodinger equation. This forms the basis for calculating the

transmission coefficient of electrons traveling from source (LE) to drain (RE) respectively. Instead NEGF formalism in coordination with density functional theory (DFT) incorporated into phyton based programming software termed as ATK-VNL tend to be more efficient and precise despite time consuming computation. However, prior to calculating transmission coefficient of electrons, the geometry of the device needs to be optimized (i.e. attainment of maximum force acting between the atoms). The maximum attained force desired to be small for obtaining accurate results. Moreover, selection of suitable Monkhorst sampling points (K_x, K_y, K_z) and exchange correlation potential too accounts to more accuracy. In this regard, LDA as exchange correlation potential and Monkhorst k-point grid $(1, 1, 100)$ are used to achieve the same. Similarly, effective basis set selection (i. e single zeta polarized) is important too as it accounts to more accuracy in lesser computational time. Since more precise and accurate results proceeds at a slow pace.

The devices through which electron transport mechanism has been analyzed are categorized below:

Graphene and allied forms

a) Graphene nanoribbons

In order to obtain graphene nanoribbons, precise cutting of a graphene sheet along a specific direction (n, m) at a specific angle is required. The structure so obtained is classified into zigzag and armchair nanoribbon based on the edge design.

Zigzag nanoribbon (ZGNR) are so far found to metallic as compared to its counterpart armchair nanoribbons (AGNR) that are semi metallic or metallic depending upon the no of atoms present along its width.

Electron transport mechanism through AGNR based devices was evaluated by selectively setting the transport parameters to achieve accurate results. The current-voltage curve depicts the semiconducting behavior of two diodes (i.e. normal diode and tunnel diode). Consequently, the occurrence of negative differential resistance (NDR), a phenomenon that involves decrease in current magnitude on increasing the applied bias is also observed. This enhances the applicability of selected device for various electronic application such as logic and memory related operations.

Investigation of electron transport through ZGNR based devices reveals much more enhanced features like amplification, rectification, switching and memory related operations.

b) Carbon nanotube (CNT)

This allotrope of carbon results on rolling the graphene sheet in a specified manner. They are of two type single and multi-walled. In addition to these forms of CNT, analysis of transport properties is carried out in bamboo shaped CNT (BCNT). The investigation reveals similar interesting feature as in the case of planar device discussed above. BCNT is either used with both side open or partially covered. Coronene ($C_{24}H_{12}$) has been used as a cap to cover the face of BCNT. Further BCNT is equally partitioned and its two modeled version (BCNT 1 and BCNT 3) has been utilized for computing the transmission spectrum.