A Study Based Research Paper on Charge Transport Through Moletronics (Graphene Nano Tube) Concept Using Different types of Electrodes: A Review

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Abstract
In this paper, a study based or review section will be discussed the topic about GNT through pursue with the help of different electrodes & influence of changing the material of electrodes on the transport properties of single or multi junction comprising GNT (Graphene Nano Tube) stringed to two semi-infinite electrodes using semi empirical model. The investigation of electron transport through GNT was accomplished by linking it to different metallic electrodes like platinum, silver under different bias voltages within Keldysh's non- equilibrium Green Function formulism using Extended Huckel Theory (EHT) .By comparing the V-I curves obtained using different metallic electrodes, we perceived that platinum showed maximum conductance and silver showed transmission of current amidst strongest coupling and thus affirmed to be the most effective material for electrodes for nanometer scale molecular junctions, when compared with other metallic electrodes.

Keywords
GNT, Non equilibrium Green's Function, Extended Huckel Theory, Density Functional Theory.

I. Introduction

DFT has been very popular for calculations in solid-state physics since the 1970s. However, DFT was not considered accurate enough for calculations in quantum chemistry until the 1990s, when the approximations used in the theory were greatly refined to better model the exchange and correlation interactions. In many cases the results of DFT calculations for solid-state systems agree quite satisfactorily with experimental data. Computational costs are relatively low when compared to traditional methods, such as Hartree–Fock theory and its descendants based on the complex many-electron wave function. Since the report of the preparation of graphene by Novoselov et al. [1] in 2004, there has been an enormous and rapid growth in interest to the semiconductor industry because this material is compatible with planar technology. Graphene has attracted intensive interest due to its fundamental properties and potential applications in future electronic devices. The advancements in the semiconductor fabrication techniques led to the study of electron transport through hetero junctions comprising of single organic molecule stringed to side electrodes, which alleviated into an important area of research called molecular electronics. Molecular electronics, or Moletronics established itself as a key area of research for many physicists, engineers, quantum chemists and many more researchers due to following reasons [2]. The size of the molecule is inherently in the range of 1nm to 100nm, so the nanostructures of all dimensions can be implemented with these molecules, which would have the advantage of low cost, low power dissipation and technological superiority. Certain molecules have several isomers and thus having different geometries. These variations in geometry cause significant variations in electrical properties of molecules which has been the field of interest for many researchers. The self-assembled mono layers (SAM) will be the active components in electronic circuits as intermolecular interactions can be studied, thus providing varying transmission behavior leading to both switching and sensing capability. Moreover molecular electronics finds applications in processing and storage of information and biological applications as well. The molecular devices can interact directly with the molecules within the cell, and thus can be used for studying various processes within the cell [3]. The instability at high temperatures and the lack of robustness associated with the organic molecule based electronic devices are the two biggest causes of concern for implementation in real time applications.

II. Theory

Density Functional Theory: Density functional theory (DFT) is a computational quantum mechanical modelling method used in physics, chemistry and materials science to investigate the electronic structure (principally the ground state) of many-body systems, in particular atoms, molecules, and the condensed phases. With this theory, the properties of a many-electron system can be determined by using functionals, i.e. functions of another function, which in this case is the spatially dependent electron density. Hence the name density functional theory comes from the use of functionals of the electron density. DFT is among the most popular and versatile methods available in condensed-matter physics, computational physics, and computational chemistry.

III. Review and Compare with DFT & EHT

Both theories Density Functional Theory (DFT) and Extended Huckel Theory (EHT) had been worked upon by the various researchers for elucidating the electronic transport through single molecule junctions. Our computational approach has been based upon Hartree & Fock (HF) method approximation for the determination of the ground-state wave function and ground-state energy of a quantum many-body system along with Keldysh's Non Equilibrium Green's Function (NEGF).

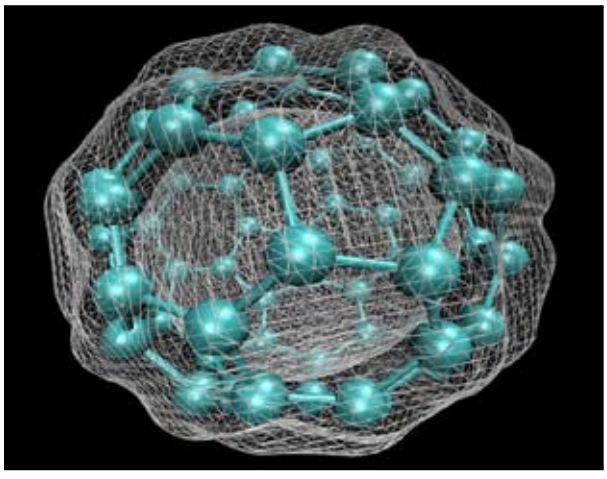

Fig. 1: Moletronics of GNT Silver and Platinum

Formalism combined with Ronald Hoffmann's tight binding approach Extended Huckel Theory (EHT). No doubt Density functional theory had been comprehensively used by researchers in the past, but EHT due to its simplicity and speed has gained much attention. EHT has been effectively employed to determine the molecular orbital's and relative energy of different geometrical configurations neglecting certain non-elastic scattering like electron-electron repulsions and expressing energy just as the sum of terms for each electron in the molecule. The results produced using semi-empirical EHT were accurate enough to explain the electron transport phenomenon through single molecular junction. The NEGF [4-8] combined with EHT forms the basis for our model in this research work. In our suggested model based on two probe method, a Graphene Nano Tube (GNT) is stringed to two semi-infinite electrodes. A GNT will studied with platinum and Silver. The Curve between them, then transmission spectrum and I-V curves can be assimilated.

IV. Conclusion

The electron charge transport of GNT was studied, when the GNT is sandwiched between two metallic electrodes like Silver and platinum. The material of the electrodes was varied and reviewed.

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