Simulation study on Stone wales defect in Si-Nanowire based Graphene-lithium ion batteries

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Abstract: In this paper we study of atomic scale properties of Si-Nanowire based graphene lithium ion batteries with stone-walves defect which is simulated by using Atomistix tool kit (ATK). The differences in the *transmission spectrum, Fermi level and defects are* discussed in detail. ATK is a research tool which provides proficient calculations of materials electron transport properties and atomic structures. The simulation results were obtained by using Extended Huckel approximation.

Index Terms— ATK, EXTENDED HUCKEL, Graphene,

I. INTRODUCTION

Nowadays, an increase of technology results in the increase of energy demands. High power batteries which can sustain the charge cycle for the long duration of time can be most prominently used. From last 5 years, Li-ions batteries are the most significantly used batteries in all electronics and electrical application [1]. These lithium ion batteries have many unique significant properties which can replace the conventional batteries. Advantages of these batteries are high energy density, no pollution, low self-discharging rate and long useful life span. Using of graphene as the anode material, increase the electronic property of battery which can further increase the efficiency of the battery. This honeycomb-like structure is one atom thick layer which has multiple properties in electronics,mechanical, chemical and many areas. It is used in solar cell, capacitors, biomedical, semiconductors and also used for high mechanical strengthen of materials [2]. This novel graphene material is chemically stable and due to the high electrical conductivity, this material is a most promising material which can be used as the alternative in the battery. In this paper we have, find the atomic property of graphene and lithium atom and also observe the transmission spectrum, conductance and Fermi energy of this material. Apart from this we also observe the atomic property when the material consists of some defect. Nanowires (NW) have shown great potential in low-cost high-performance solar cells[3-6]. Silicon (Si) NW solar cells are particularly promising due to the low cost, abundance in nature, nontoxicity, and long-term stability and have been widely reported in recent years [7–10]. However, due to its indirect bandgap, Si has a poor absorption of light at small thicknesses, particularly in the 600–1100-nm spectral range [11]. As the NW commonly has a short length of several microns, Si NW array solar cells typically have a low conversion Efficiency [7–9]. An efficient way of increasing the efficiency of Si NW solar cell is to enhance its absorption in the 600–1100-nm range via introducing new structures or materials. Recently, a family of methylammonium lead halide perovskites $CH_3NH_3PbX_3$ (X = I, Br, Cl) has attracted great attention for its breakthrough in low-cost high-efficiency solar cells [12–14]. The excellent properties including a direct bandgap, large absorption coefficient, long exciton diffusion length (100~1000 nm) and lifetime, and low cost processes make perovskite an ideal light absorber [12, 15, 16]. The perovskite materials typically have high and flat absorption efficiency in a wide spectrum.

II. DEVICE SIMULATION

Here we used Atomistix Tool Kit (ATK) for simulation and calculating the electrical transport property for graphene and lithium ion-atom. In ATK-DFT, semi-empirical tight bindings and classical function are used to simulate the device structure. In this, for simulating the nano scale device structure we use non – equilibrium greens function[17-19]. Here we used extended Hückel method which is the semi-empirical quantum chemistry method developed by the Roald Hoffmann. This method is used for determining the structural geometry of organic molecule
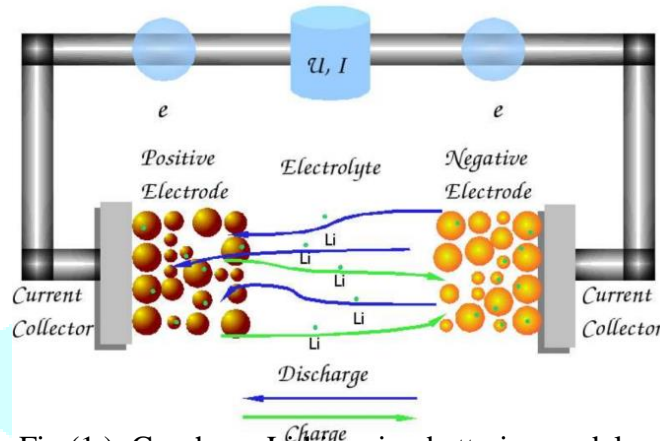

Fig (1): Graphene-Lithium ion batteries model

and for molecular orbital's. It can calculate the relative energy of different geometrical structure, calculation of electronic interactions [3].

For solving the electronic structure we use basis of Hamiltonian local atomic orbital (LCAO)

$$\emptyset_{nlm}(r) = R_{nl}(r)Y_{lm}(r) \qquad (1)$$

Where Y_{lm} is is a spherical harmonic, R_{nl} is a radial function.

$$S_{ij} = \int_v^{\partial ij} \emptyset i\,(r - Ri)\emptyset j(r - Rj)dr \qquad (2)$$

Where R is the position of orbital center, i is composite index of nlm. For

calculating the basic function of integral form,

$$R_{nl}(r) = \frac{r^{n-1}}{\sqrt{(2n)!}}\left[C_1(2n_1)^{n+\frac{1}{2}}e^{-n1r} + C_2(2n_2)^{n+\frac{1}{2}}e^{-n2r}\right] \qquad (3)$$

Where n_1, n2, C1 and C_2 are the adjustable parameters. These are used to defined angular shell of valence bond orbital's for each element [4].

Hamiltonian overlap matrix defines,

$$H_{ij} = \frac{1}{4}(\beta_i + \beta_j)(E_i + E_j)S_{ij} \qquad (4)$$

Where E_i is the onsite orbital energy and β_i is a Hückel fitting parameterDFT Calculation is used to

investigate the electronic property of atomic structure.nical modelling method.The DFT calculate the Interacting of electrons at different state. The red balls showed the interaction of electron[21]. In DFT the density matrix is calculated by non-equilibrium Green's functions (NEGF)
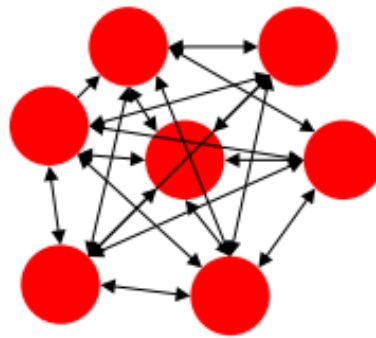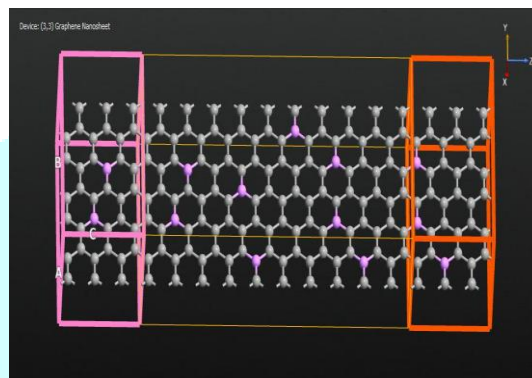
Fig (2): Interaction of electron

III. FIGURES
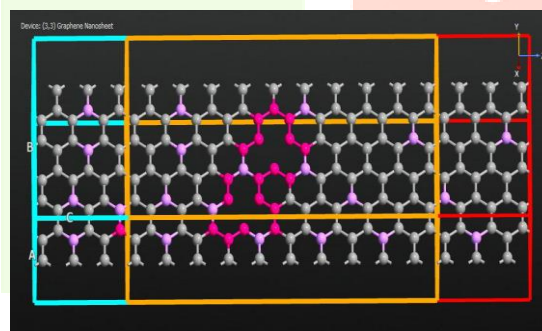
Fig (3):Si-Nanowire with no defect

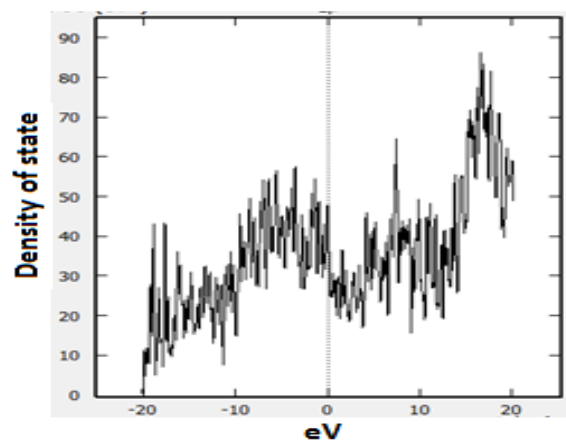Fig (4):Si-Nanowire with Stone-Wales defect
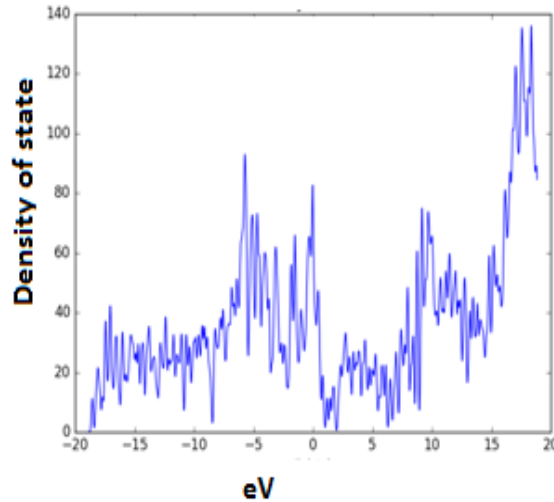

Fig (5): DOS VS eV with defect
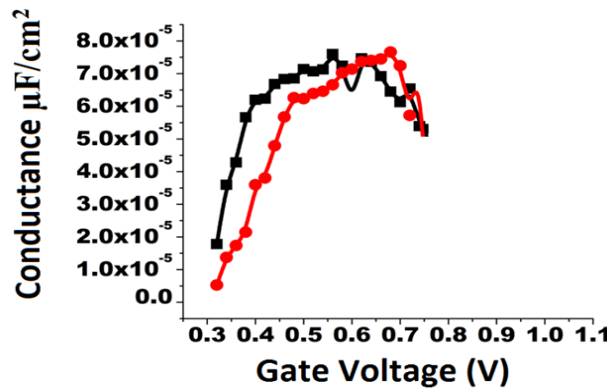
Fig (6): DOS VS eV with no defect

Fig (7): Conductance VS Gate Voltage

IV.   RESULTS AND DISCUSSION

By using the Hückel semi empherical method, we observe that when the graphene and lithium ion atom is mix without any defect in there atomic structure the Fermi level for Left electrode = -3.190716e+00 eV and for Right electrode Fermi level = 3.190716e+00 eV. Whereas in the presence of a defect, the Fermi level is increased to the 4.46 eV. The density of state in fig(7) show the number of electron occupies in per state. In no defect area the electron occupies maximum number of state whereas in defect area the electron occupancy is less.

In no defect area the transmission of electron is high and covers the whole part as it can be seen in fig (24). Where as in defect area the transmission is high in starting area where as it get decreased slowly [25]. In fig (5), we will get higher spikes region, these is due to the in proper flow of electron where as in fig (6) the spikes are less as it doesn't have any defect in

atomic level. Fig 9 shows the electron density where in first part shows the higher number of electron whereas in second part shows least dense area due to the distortion in the atomic structure[28-30].
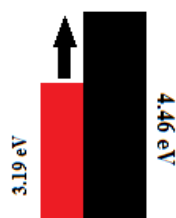

Fig (8): Increase in Fermi Level

(V) CONCLUSION

The extended Hückel method is the suitable for solving atomic scale structure and obtaining the electronic property of it. Here we observe that if there is no defect present in graphene then conductivity will be high whereas if there is any atomic defect present the there will change in the conductivity property. In fig (10), It is shown by using DFT and Extended Huckel calculation[31], the Fermi level of graphene – lithium ions increase upto 4.46 eV due to the structural defect.

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