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First Principles Study of Interactions of Graphene Layer Adsorbed With Beryllium

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Abstract: *The interactions between graphene layer, graphene layer adsorbed with Beryllium are studied. Band gap energies at different positions are studied by means of DFT calculations and in all the cases the band gap has been increased .Negative differential resistance is observed for 0V and -1V applied at 900 k for graphene layer adsorbed with Beryllium at various temperatures due to non linear carrier transport under a strong electric field while studying the electrical characteristics. This NDR property enables a number of important applications, such as high frequency oscillators, ultra- fast logic devices and multi state memory devices. Graphene has received intense interest in fields such as physics, chemistry, biology and materials science due to its exceptional electrical, mechanical, thermal and optical properties as well as its unique two-dimensional (2D) structure and large surface area.*

Keywords: *Graphene layer, Adsorption, band gap, negative differential resistance, non linear carrier transport.*

1. INTRODUCTION

Graphene, a two-dimensional, single-layer sheet of sp^2 hybridized carbon atoms with zero band-gap has attracted remarkable attention and research interest, due to its exceptional physical properties, such as high electronic conductivity, good thermal stability, optical transparency, large surface area and excellent mechanical strength [1]. Graphene and its derivatives have been explored in a wide range of applications, such as electronic and photonic devices, clean energy systems and sensors. The lack of a band gap in graphene has stood as a challenge for graphene-based field effect devices [2, 4]. However, it has opened new opportunities in analogue and RF electronics. Resonant Tunneling Diodes (RTDs) are a family of diodes with unique capabilities, as they do not only act as rectifiers, but also exhibit Negative Differential Resistance (NDR). This NDR property enables a number of important applications, such as high frequency oscillators, ultra-fast logic devices and multi-state memory devices [5].

2. GRAPHENE DEVICE STRUCUTRE

The Graphene is constructed by using 32 carbon atoms with a bond length of $1.5A^0$.The device is constructed with left and right electrodes of 5 A^0, then optimized and the coordinates were relaxed using the Tersof potential until forces on individual atoms were smaller than 0.001 eV/A^{02}

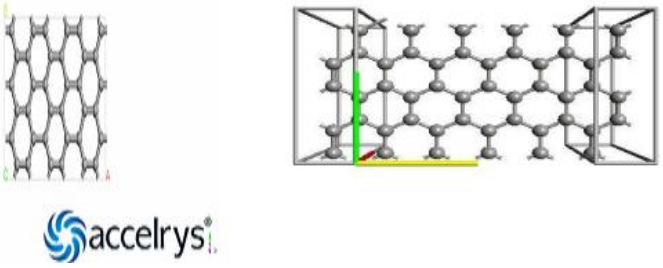


Fig1. *Graphene device structure*

The device structure is portioned as three regions. Semi-infinite left electrode(L),central scattering region(C) and semi-infinite right electrode(R), and the length of each electrode is $5A^0$ the mesh

points in real space calculation were defined as uniformly spaced K points of 1×20×50,with 50 sample points along the transport direction, and 20 points along the width.

2.1. Calculation Method

We studied the device's electronic properties and performance of Pure Graphene as well with Graphene adsorbed with one Beryllium atom[10] using Nonequilibrium Green's Function (NEGF) formalism and the Extended Huckel (EH) method. Transport calculations conducted on the device were based on the EH method and NEGF formalism as implemented in Atomistic Tool Kit (ATK 12) software package. I-V characteristics are analyzed using transmission spectrum [6, 7, 8].

2.2. Electronic Properties of Graphene

Pure graphene is a zero-gap semi conductor or semi metal. Semi metal is a material with a very small overlap between the bottom of Conduction Band and top of Valence Band, and has no band gap with negligible density of states at the Fermi level. The Fermi surface of graphene is situated at the connection points between conduction band and valence band (6 points) as shown in Fig 2. [9]. The Fermi level can be tuned by the application of an electric field. The energy momentum relation (dispersion relation) is linear for low energies near the six corners of a 2-D hexagonal Brillion Zone, leading to zero effective mass for electron and holes. Due to this linear or conical dispersion relation at low energies, electrons and holes near these six points behave like relativistic mass less particles travelling at a constant speed as described by the Dirac. Hence, the electrons and holes are called Dirac fermions, and the six corners of the Brillioun zone are called the Dirac points. Graphene is a zero-overlap semimetal in which the electronic properties are dictated by the bonding and anti-bonding (the valance and conduction bands) of the pi orbitals. At the Dirac point in graphene, electrons and holes have zero effective mass and the graphene electrons act very much like photons in their mobility. The prominent electronic properties of graphene are very sensitive to a change of external conditions. The electronic states near Dirac points are modulated easily by adsorption of some molecules structural corrugation and intraction with substrate surfaces. [11]

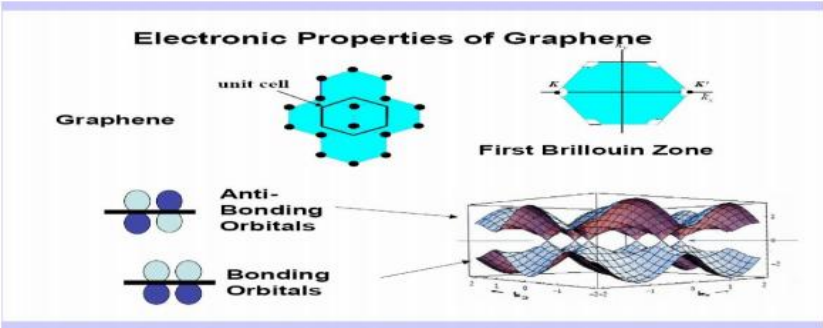


Fig2. *Electronic Properties of Graphene*

2.3. Temperature Dependence of Resistivity in Graphene

In a perfect crystal the electrons move as if they are free particles with effective mass m* moving in a vacuum. Otherwise, we say that the electrons undergo collisions and are scattered. It is due to these collisions the material is resistant to the flow of electric current. There are many scattering mechanisms which can affect the electrons, the major ones being defects in the crystal, phonons and impurities. The scattering is mainly due to Coulomb scattering by charged impurities from the environment. The Ohmic resistivity of the graphene electrons is calculated by the finite-temperature Drude-Boltzman theory.Materials are said to exhibit negative differential resistance in which an increase in voltage across the device's terminals results in a decrease in electric current through it. Negative resistance varies depending on the voltage or current applied to the device, and a device can have negative resistance over only a limited portion of its voltage or current range due to Ridley and Watkins mechanism of electron transfer into the satellite valley that occurs in the conduction bands. Due to this conduction electrons transfer from high mobility valley to lower mobility, high energy valleys. In a multivalve semiconductor, higher energy may push the carries into a higher energy state where they actually have higher effective mass and thus slow down [11].

2.4. Density of States of Pure Graphene

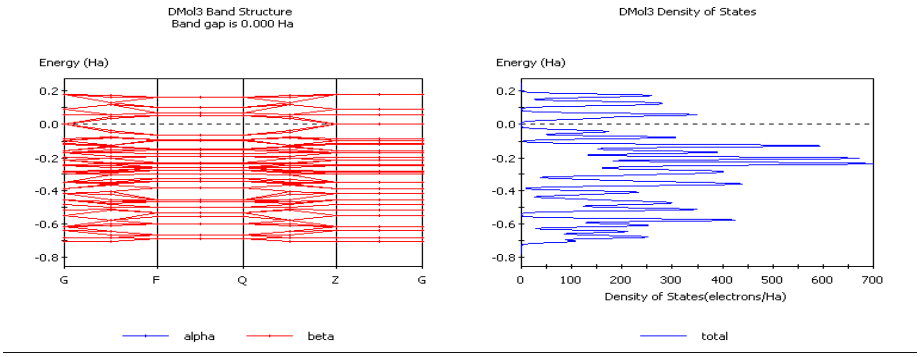


Fig3. *Band structure and Density of States of pure Graphene*

From Fig: 5, the maximum available density of states of pure graphene at 0.28 Ha are upto 700, and the band gap energy is 0 Ha. One Ha = 27.211eV.

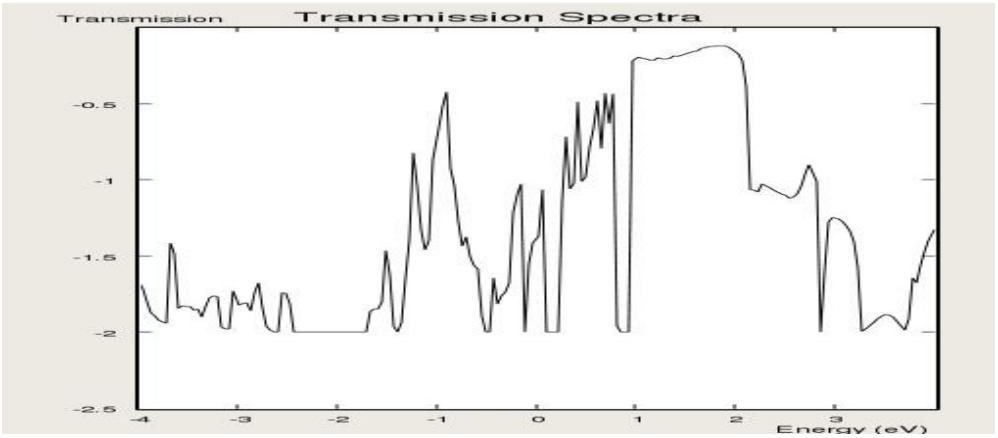


Fig4. *Pure Graphene transmission spectra with -2 bias Voltage*

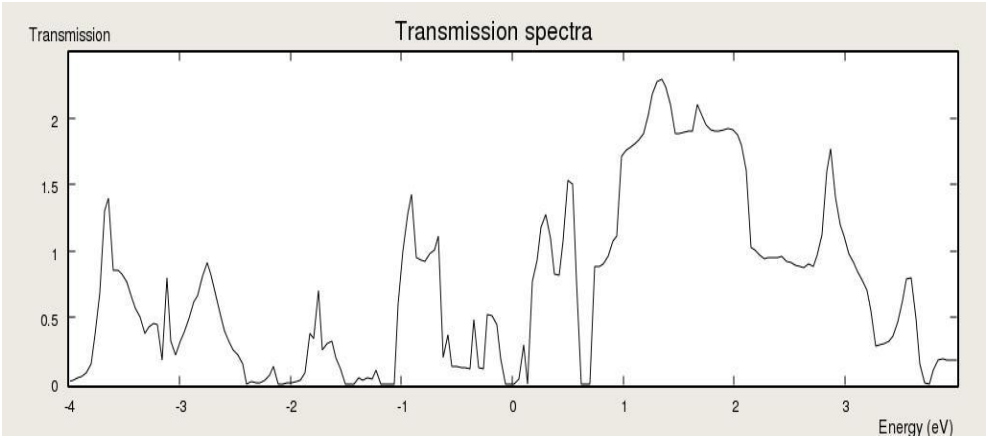
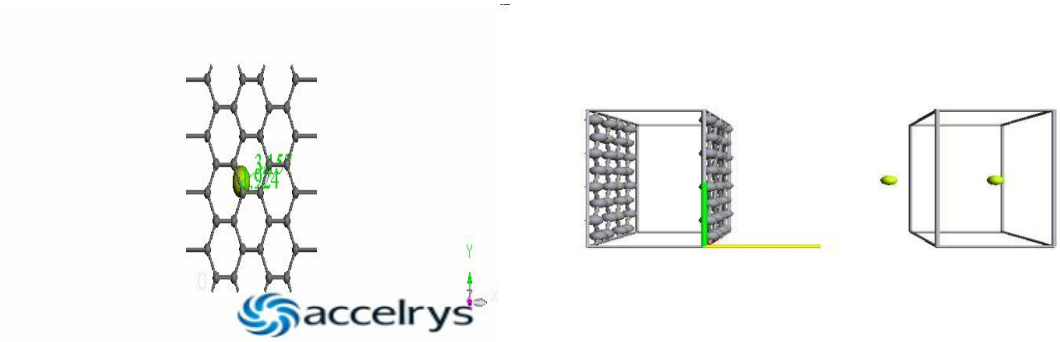


Fig5. *Transmission Spectrum of Pure graphene with 2 Bias Voltage*

3. GRAPHENE ADSORBED WITH ONE BERYLLIUM ATOM



3.1. Density of States of Graphene Adsorbed with Beryllium

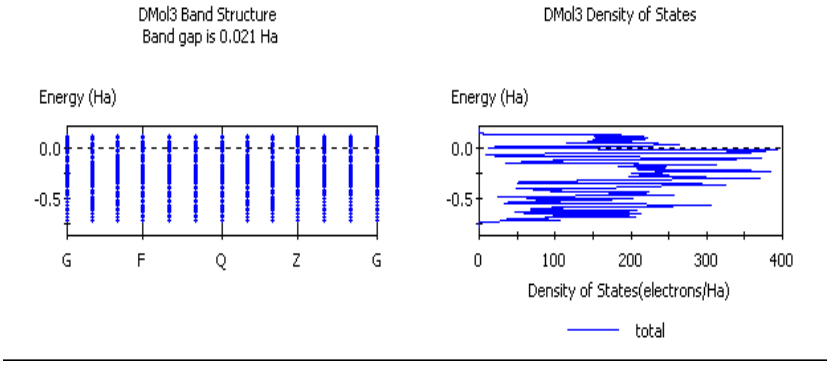


Fig6. *Band structure and Density of States of Graphene adsorbed with one Beryllium atom*

From Fig: 6, the maximum available density of states of graphene adsorbed with one Beryllium atom are 400 at 0.1Ha and the band gap has increased to 0.021Ha.

3.2. Transmission Spectrum of Graphene Adsorbed with One Beryllium

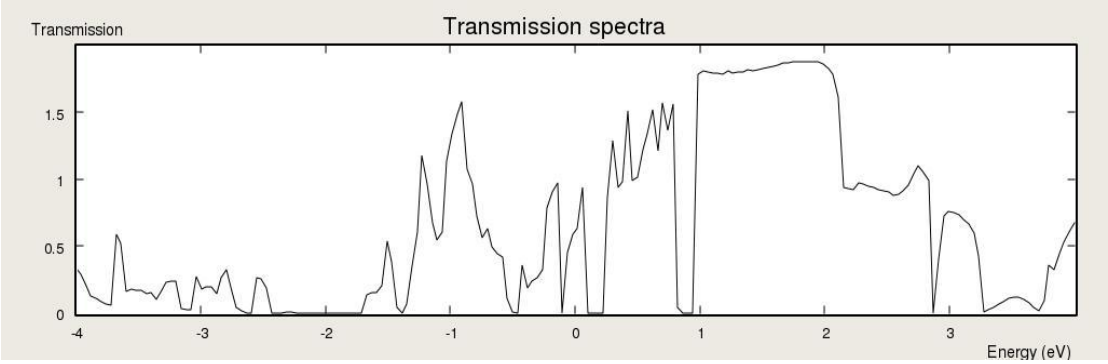


Fig7. *Transmission Spectrum of Graphene adsorbed with Beryllium at -2v*

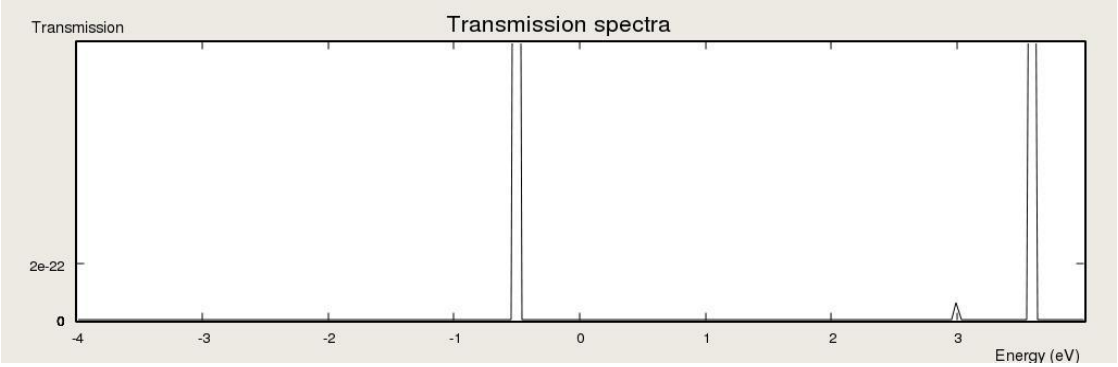


Fig8. *Transmission Spectra of Graphene adsorbed with Beryllium at 2V*

Very sharp transmission peak is observed between (0 and -1V)eV below Fermi level and at all other energies the transmission is almost zero. This may be due to extreme confinement within the graphene quantum well.

4. FABRICATION FEASIBILITY

Their fabrication can be achieved by the following steps. Once monolayer is transferred to an insulating substrate, it can be patterned into the planer DB-RTD structure using a single photolithography step. Metallic contacts such as platinum or gold are then formed. It is important to note that the process described above gives rise to GNRs with rough edges, and may not be able to define narrow trenches for the insulating barriers. Before performance of such devices would require a Monto Carlo simulation study, in order to investigate the effect of GNR edge roughness on the devices performance, especially its resonance behavior. Such a statistical reliability study is an important further step required before the mass production of such devices. [13].

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REFERENCES

[1] K.S. Novoselov, A.K. Geim, S.V. Morozov, D. Jiang, M.I. Katsnelson, I.V. Grigorieva, S.V.Dubonos, A.A. Firsov, Two-dimensional gas of massless Dirac fermions in graphene. *Nature **438**, 197–200 (2005).*

[2] M.Y.Han et al.; *Phys.Rev.Lett.98, 206805 (2007).*

[3] G.Giovannetti et al., *Phys.Rev.B 76.073103 (2007).*

[4] T.Palacios, A.Hsu, and H.Wang, ‘‘Applications of graphene devices in RF communications”.*IEEE Commun.Mag, Vol 48, no.6 pp.122-128, Jun 2010*

[5] B. K. Ri, dey and T. B. Watkins. “The possibility of negative resistance effects in semiconductors.” *Proc. Phys.Soc., vol. 78, PP. 293-304; 1961.*

[6] Kohn, W.; Sham, L. J. (1965). "Self-consistent equations including exchange and correlation effects". *Physical Review **140** (4A): A1133–A1138.*

[7] K.Stokbro et al., ‘‘Density-functional method for nonequilibrium electron transport,”*Phys.Rev.B, Condens.Matter .Phys. Vol.82, p.075420, Aug.2010.*

[8] QuantunWise.(2013,Sep.27).ATKSEPackage(12.8)Avaliable:http//www.quantumwise.com

[9] Novoselov,K.S.;Geim,A.K.;Morozov,S.V.;Jiang,D.;Zhang,Y.;Dubonos,S.V;Grigorieva,I.;Dubonos,S.V.;Firsov,A.A.(2005).Electrical Field Effect in Atomically Thin Carbon Films.*Science,Vol.306,No.5696,Page numbers (666-669),ISSN 0036-8075.*

[10] Adsorption of beryllium atoms and clusters both on graphene and in bilayer of graphite investigated by DFT. *J.Phys.:Condens.Matter 25(2013)015002*

[11] X.F.Fan, W. T. Zheng, ViorelChihaia, Z.X.Shen and Jer Lai Kuo, *J.Phys:Condens.Matter 24(2012) 305004 (10pp).*

[12] B. K. Ri, dey and T. B. Watkins. “The possibility of negative resistance effects in semiconductors.” *Proc. Phys. Soc., vol. 78, PP. 293-304; 1961.*

[13] M.Y.Han, B.Ozyilmaz, Y.Zhang and P.Kim, ‘‘Energy band gap engineering of graphene nanoribbons,*’’Phys.Rev.Lett, Vol.98, P.206805, May 2007.*

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K.Vagdevi working as an Asst Prof in physics department has 12 years of Teaching experience for under graduate B.Tech students in Gokaraju Rangaraju Institute of Engineering & Technology, Hyderabad and 5 yrs of research experience in condensed matter physics and has 4 papers in National/ international conferences. Attended various national and International workshops.

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