*Study of Electronic Structure of Boron-Nitride /Graphene Bilayer by Using DFT

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Abstract:

In this work, we study the electronic structure (number of open channels (NOC), band structur(BS), density of states (DOS), and I-V curve) of boron nitride/ graphene sheet using SIESTA and GOLLUM codes. Ab initio structural optimization performs for all structures using the local density approximation (LDA) with norm-conserving pseudopotentials, double zeta polarized (DZP) basis sets of pseudoatomic orbitals, and the Ceperley-Alder exchange correlation functional with the atomic forces relaxed to 0.02 eV/°A. Three types of simulated heterostructures sheets have been studied: 1- One graphene strip and one boron nitride strip sheet. 2- Two graphene strip and one boron nitride strip sheet. 3- Three graphene strip and one boron nitride strip sheet. We show that there is a dramatic reduction in energy gap 'E_g' of heterostructures comparing with the insulator boron nitride ($E_g \approx 4.6$ eV) and increasing in energy gap comparing with semimetallic graphene (zero gap).

Keywords: graphene, energy gap, band structure.

mathematical Classification QC 170-197

* The researches is apart of an Ph.D. dissertation in the case of the third researcher.

1.Introduction

Graphene is a two-dimensional allotrope of carbon and made up from carbon atoms which are arranged on a honeycomb structure to form hexagonal rings, in 2004 another interesting carbon allotrope which no wadays called graphene was discovered by a group of physicists from Manchester University,led by Andre Geim and Kostya Novoselov[1]. This discovery produced a revolution in the field of nanotechnology. Graphene can be defined as amonolayer of carbon atoms packed into a dense honeycomb crystal structure that can be viewed as an individual atomic plane an extracted from graphite[2-5], as an unrolled single walled carbon nanotube [6]. This discovery produced a revolution in the field of nanotechnology. Since its fabrication in 2004, it has attracted researchers interest as it is promise of large area electronics [7]. Clean graphene is a semimetal contains a vanishing density of states at the Fermi energy with remarkably high carrier mobility at room temperature and therefore a single-layer graphene can be considered as a semiconductor with zero energy gap or behave as semimetallic material [2, 5-7].

Boron nitride is one of the candidates in this material family considered as sister material of graphene due to its structural similarities , another interesting material has received intensive interest which is boron

nitride (BN). Boron nitride (BN) is a two dimensional materials[8-10] and commonly fabricated by mechanical peeling and chemical vapor deposition (CVD), single-layer h-BN has a wide band gap of up to 4.6 eV[11] .As well as, h-BN has the same atomic structure as graphene[7]. It has two allotropes hexagonal boron nitride (hBN) and cubic boron nitride(cBN) similar to graphite (hexagonal) and diamond (cubic)[12].

Recently, a heterostructures of graphene and hexagonal boron nitride has been synthesised by a scientific group [7], they show that domains of graphene in single hexagonal layer of boron nitride ‘h-BN’ can be synthesized. This new interesting heterostructure has received much attention from many scientists and groups to study it and understand their properties. The electronic properties of armchair graphene nanoribbons confined by boron nitride nanoribbons has been studied, a published paper reported that the armchair graphene nanoribbon which terminated by hydrogen and confined by boron nitride nanoribbons led to open the energy gap remarkably [13]. Graphene confined by boron nitride strips exhibited as semiconductors with direct energy gap, this lead to manipulate the size energy gap of graphene [14], another study reported that the electronic states change from semi-metallic to insulating depending on the number of boron and nitrogen atoms of hybrid boron nitride (BN) and graphene hetrostructures [15]. On the hand the electronic properties of hetro nanotubes and sheets has been investigated by many groups, they showed the importance of the interface between graphene and BN. For such impurities, a characteristic peak near the Fermi energy is found, with the peak associated with boron below the Fermi

energy and the peak associated with nitrogen above the Fermi energy [16-19].

2.Computational Method

Our calculations are performed by using the SIESTA implementation of DFT [20]. In this work, an ab initio structural optimization was performed for all structures using the local density approximation (LDA) with norm-conserving pseudopotentials, double zeta polarized (DZP) basis sets of pseudoatomic orbitals, and the Ceperley-Alder exchange correlation functional with the atomic forces relaxed to 0.02 eV/°A. Using SIESTA, the density of states 'DOS' was calculated using one k-point in X direction, 200 k-points in Y direction and 200 k-points in Z direction. Next, we calculate the band structures. The transmission coefficients T(E) have investigated, they can be obtained using the non-equilibrium Green's function code Gollum [21], which utilises the DFT-based hamiltonian from SIESTA. The number of open channels, for ideal periodic structure is equivalent to the transmission coefficients T(E) . current (I) and voltage (V) characteristics are widely measured experimentally, so a routine to calculate I-V curve is useful for characterizing the structures. The current (I), with respect to voltage (V), can be calculated from the transmission probability [22]:

$$I(V) = \frac{2e}{h} \int_{E_f - \frac{eV}{2}}^{E_f + \frac{eV}{2}} T(E,V)dE \qquad (1)$$

Where:(e)electronic charge,(h)blank constant , (E_f) fermi energy and T(E) transmission coefficient in this equation, the transmission depends on the bias voltage.

Within a Landauer description of electron transport, since the sheets investigated are periodic, the transmission coefficient T(E) for electrons of energy E travelling from left to right is identical to the number of open channels and therefore the maximum current I(V) carried by the sheets shown in figure 1 at a finite voltage V, is given by[22]:

$$I(V) = \frac{2e}{h} \int_{E_f - \frac{eV}{2}}^{E_f + \frac{eV}{2}} T(E)dE \qquad (2)$$

For a perfectly periodic system, the transmission probability $T(E)$ is equal to the number of open channels at energy E.

3. Electronic structure of boron nitride/ graphene sheet

In this study, we focus on the electronic structure of boron nitride/ graphene sheet. We simulated three types of boron nitride- graphene sheets. The first structure is contain one strip of boron nitride and one strip of graphene (figure 1a). The second sheet is contain one strip of boron nitride and two strips of graphene (figure 1b) while the third one composed of one strip of boron nitride and three strips of graphene (figure 1c). All hetrostructures under study are periodic in YZ plane. Figure (1) shows the relaxed structures and their number of openchannels.

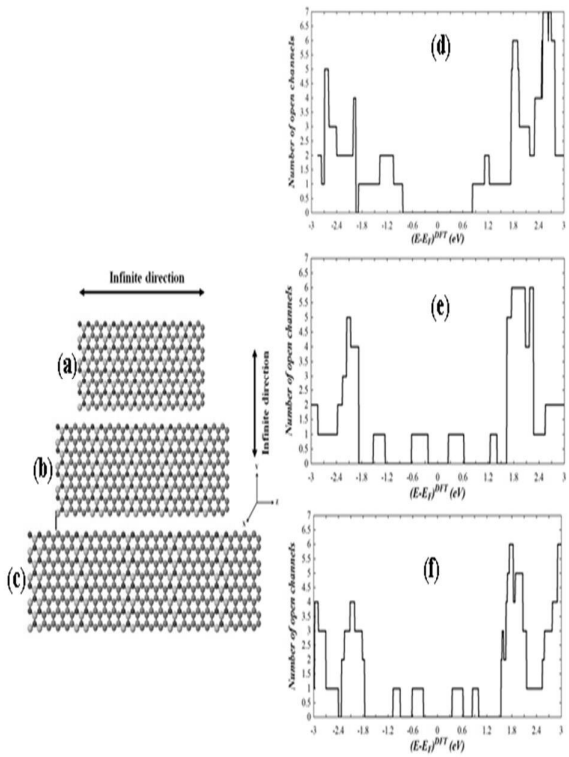
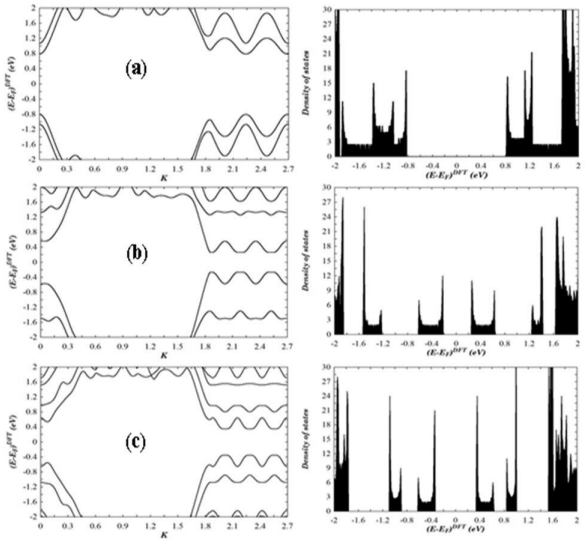


Figure (1) : Shows the relaxed supercell of hetero boron nitride/ graphene sheet, (a) with one

graphene strip, the supercell contains 240 carbon, boron and nitrogen atoms, (b) with two graphene strips, the supercell contains 320 carbon, boron and nitrogen atoms, and (c) with three graphene strips, the supercell contains 400 carbon, boron and nitrogen atoms. (d-f) show the number of open channels of the structures in (a-c) respectively. All structures are in infinite direction in Y-axis and Z-axis.

Figure(1) shows that there is huge change in the size of the energy gap for both graphene and boron nitride sheets due to the hybridisation . that's simplest reduction obtained in the energy gap is clear in figure(1a), in contrast we can see that pure boron nitride sheet is insulator with 4.6 eV, on the other hand it became smaller when we simulated the structure the sheet shown in figure (1a), the obtained energy gap is about 1.75 eV which is close to the energy gap of silicon which is equals to 1.2 eV [23]. This is a remarkable change lead us to say that the new material in figure (1a) is a semiconductor. Similarly, we can see similar outcome with the structures in figures (1b) and (1c) which their energy gaps are about 0.45 eV and 0.65 eV respectively. As well as, looking at the figures 1b and 1c and comparing with the heterostructures in figure (1a), there are extra energy gaps appears around Fermi energy which reduce the possibility of electron to travel comfortably through the simulated sheets, the band structure and density of states are calculated of the sheets in figure(1) and they are shown in figure (2)



Figure(2): The density of states and band structure for the boron nitride/ graphene sheet with (a) one graphene strip, (b) two graphene strips and (c) three graphene strips. The density of states carried out with 1x200x200 k-points.

Figure 2 shows band structure and density of states for the heterostructures which are shown in figure 1(a-c). The size of energy gaps around Fermi energy are agreed with what we obtained from the calculated number of channels shown in figure (1),to clarify the results in figure(1) and figure(2), we used the equation 2 to calculate the I-V curves of the heterostructures as shown in figure (3).

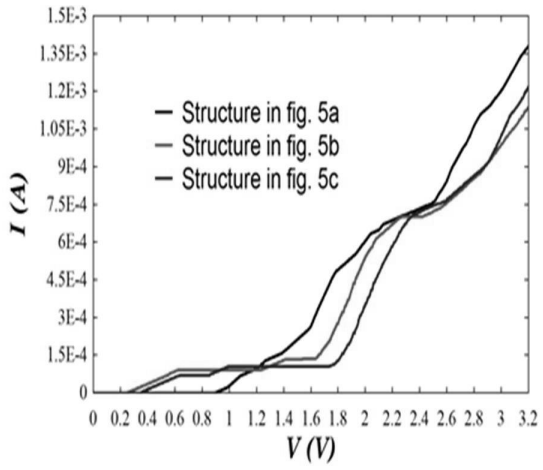


Figure (3): The current for the systems

shown in fig. 1a, 1b, 1c.

Having a look at figure(3) and at selected voltage value, for example 3.2 V, we can see that the structure in figure(1a) has the lowest current, while the highest current is related to the heterostructures with one boron nitride strip and two graphene strips (figure 1b).

4. Summary

The electronic structure of the hetero structures composed of boron nitrid /graphene with various graphene strips have been investigated. A huge reduction in energy gap of the heterostructures material (figure 1) compares with the pure single layer of boron nitride and this reduction compares with ideal graphene sheet, we found there is a remarkable increasing in energy gap. For example the heterostructures shown in figure(1a)has energy gap of about (1.75 eV) which is smaller than the energy gap of boron class of semiconductor material to be used in design nano-electronic devices.

nitride (≅4.6 eV)[18] which means the energy gap of boron nitride reduced by more than (2.85 eV), and as a comparison with ideal graphene (zero energy gap), its energy gap increased remarkably. Furthermore, we could decrease the energy gap around Fermi energy much more by increase the graphene strips from one strips to two and three strips in between the boron nitride strips as shown in figures(1b) and(1c). Our theoretical results led us to predict that confining the hetero structures by different strips of graphene led to change the size of the energy gap of the hetero structures. This fabrication of adding various graphene strips in between boron nitride to form hetero structures could be a good methodology to manipulating or control the energy gap around Fermi energy. The studied hetero structures might be a new

References

1. Novoselov, K., et al,(2005)," Two-dimensional gas of massless Dirac fermions in graphene. "Nature, Vol. 438(7065), pp. 197-200.
2. Algharagholy, L.A,(2013)," quantum transport through nanoscale sculpturenes," in Physics, Lancaster University, UK. pp. 190-196.
3 Partoens, B. and F. Peeters,(2006)," From graphene to graphite: Electronic structure around the K point". Physical Review B,Vol. 74(7), pp. 075404-075408.
4. Neto, A.C., et al,(2009), "The electronic properties of graphene." Reviews of modern physics, Vol. 81(1), pp. 109-114
5. Novoselov, K.S, et al,(2004)," Electric field effect in atomically thin carbon films." science, Vol. 306(5696), pp. 666-669.
6. Eda, G., et al,(2009), "Insulator to semimetal transition in graphene oxide." The Journal of Physical Chemistry C, Vol. 113(35), pp. 15768-15771.
7. Zunger, A,(1972), "Iterative extended Huckel calculation on hexagonal boron nitride." Solid State Communications, Vol. 11(12), pp. 1727-1730.

8 Liu, Z., et al,(2013), "In-plane heterostructures of graphene and hexagonal boron nitride with controlled domain sizes."Nature nanotechnology, Vol. 8(2),pp. 119-124.

9. Zhang, Z. and W. Guo,(2008), "Energy-gap modulation of BN ribbons by transverse electric fields: First-principlescalculations". Physical Review B, Vol. **77**(7), pp. 075403-075408.

10. Widany, J., T. Frauenheim, and W.R. Lambrecht,(1996)," Investigation of the stability of the hexagonal–cubic born nitride prism interface." Journal of Materials Chemistry, Vol. 6(5), pp. 899-901.

11. Kester, D.J. and R. Messier,(1992), "Phase control of cubic boron nitride thin films." Journal of Applied Physics, Vol. 72(2),pp. 504-513.

12. Seol, G. and J. Guo,(2011), "Bandgap opening in boron nitride confined armchair graphene nanoribbon". Applied Physics Letters, Vol. 98(14) pp. 143107-143107-3.

13. Sławińska, J., I. Zasada, and Z. Klusek,(2010), "Energy gap tuning in graphene on hexagonal boron nitride bilayer system." Physical Review B, Vol. 81(15),pp. 155433.

14. Sun, J.-T., A.T.S. Wee, and Y.P. Feng,(2012),"Theoreticalinvestigation of the electronic structures and carrier transport of hybrid graphene and boron nitride nanostructure."AIP Advances, Vol. 2(3), p. 2133-2138.

15. Zhao, M., et al,(2013), "Electronic states in hybrid boron nitride and graphene structures."Journal of Applied Physics, Vol. 114(6): p. 063707-063712.

16. Charlier, J.C,(2002)," Defects in carbon nanotubes." Accounts of chemical research, Vol. 35(12), p. 1063-1069.

17. Algharagholy,L.,etal,(2014)," Electronic properties of sculpturene." New Journal of Physics, Vol. 16(1),p. 013060-013010.

18. Wiggins-Camacho, J.D. and K.J. Stevenson,(2009)," Effect of nitrogen concentration on capacitance, density of states, electronic conductivity, and morphology of N-doped carbon nanotube electrodes." The Journal of Physical Chemistry C, Vol. 113(44) pp. 19082-19090.

19. Xu, Y.-N. and W. Ching,(1991)," Calculation of ground-state and optical properties of boron nitrides in the hexagonal, cubic, and wurtzite structures." Physical Review B, Vol. 44(15), pp. 7787-7792.

20. Soler,J.M.,et al,(2002), "The SIESTA method for ab initio order-N materials simulation." Journal of Physics: Condensed Matter, Vol. 14(11), pp. 2745-2749.

21. Ferrer, J., et al,(2014)," GOLLUM: a next-generation simulation tool for electron, thermal and spin transport."New Journal of Physics, Vol. 16(9), pp. 093029-093034.

22. Shen,L.,etal,(2010),"Electron transport properties of atomic carbon nanowires between graphene electrodes." Journal of the American Chemical Society, Vol. 132(33), pp. 11481-11486.

23. Barone, V. and J.E. Peralta,(2008), *Magnetic boron nitride nanoribbons with tunable electronic properties.* Nano letters, Vol. **8**(8), pp. 2210-2214.

دراسة التركيب الالكتروني لطبقة من بورون نيترايد- كرافين

باستخدام نظرية دالة الكثافة*

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الخلاصة:

في هذا العمل تم دراسة التركيب الالكتروني (عدد القنوات المفتوحة، التركيب الالكتروني لحزم الطاقة ،كثافة الحالة، و منحني التيار- الفولتية) لطبقة من البورون نترايد - الكرافين باستعمال برنامجي الـ GOLLUM و SIESTA وبالطريقة التامة (ab initio) تم الوصول إلى أفضل تركيب لجميع المركبات تحت الدراسة بالاعتماد على تقريب الكثافة الموضعية (LDA) والجهد الكاذب والدالة (DZP) تم خفض القوة بين الذرات إلى 0.02 eV/A^o . درست ثلاث تراكيب من المواد في اعلاه وهي: 1- شريحة كرافين واحدة مع شريحة بورون نترايد. 2- شريحتين من الكرافين مع شريحة بورون نترايد. 3- ثلاث شرائح من الكرافين مع شريحة بورون نترايد. من خلال هذه الدراسة تم ايجاد بأنه هناك انخفاض كبير في عرض فجوة الطاقة للتراكيب المدروسة مقارنة مع المادة العازلة بورون نترايد ذات الفجوة 4.6 eV مع زيادة في عرض فجوة الطاقة مقارنة مع المادة شبه المعدنية الكرافين ذو فجوة طاقة صفرالكترون-فولت.

الكلمات المفتاحية: الكرافين،فجوة الطاقة،التركيب الالكتروني

mathematical Classification QC 170-197

*البحث مستل من اطروحة دكتوراه للباحث الثالث