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Effect of External Electric Field Applied to Bilayer Graphene Bandgap: Density Functional Theory Study

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Abstract: Graphene is a prominent material in a wide range of applications, however, the gapless nature of graphene limits its great performance in certain applications, such as in optoelectronic and photocatalytic applications field. Opening the bandgap has become one of the focused studies on graphene material today. Here, we used density functional theory (DFT) calculation to investigate the bandgap opening of bilayer graphene by external electric field applying. The calculation was performed on hexagonal stacked bilayer graphene structure using three different approximations and functional DFT; that is generalized gradient approximation (GGA) PBE and PW-91, as well as Local-density approximations (LDA) -CAPZ. The external electric field varied from 0.0 to 0.5 eV/Å/e in various electric field directions. The calculations results shows that the external E-F applied in perpendicular direction open the bandgap almost 4-times than non-determined the electric field direction. The bandgap opening by LDA functional calculation perform smaller bandgap opening compared to GGA calculation results, while the PBE and PW-91 of GGA produced similar values at low electric field applied. The larger bandgap of 0.80 eV obtained at 0.3 eV/Å/e electric field applied calculated with both GGA functional At 0.5 eV/Å/e electric field applied, bandgap with GGA-PBE almost zero, and the crystal structure changed from cubic to triclinic with layer position become apart.

Keywords: bilayer graphene, bandgap, electric field, DFT

1. Introduction

Graphene, a single-atom-thick layer of carbon atoms arranged in a hexagonal lattice, is the thinnest and lightest material notable. Graphene has remarkable properties like mechanical strong about 100 times higher than steel, high electronic and thermal conductivity, very low surface shear, etc [1]. Therefore, graphene potentially used in a wide range applications and industry, medicine, electronic, integrated circuit, transparent conducting electrode, water distillation, solar cell, coolant additive, etc [2,3]. However, in the optoelectronic devices application, the superiority of graphene still cannot overcome silicon material, because graphene has zero energy band gap [4]. The zero-bandgap of graphene is due to the symmetry between two kinds of nonequivalent carbon atoms. To open the band gap, it is necessary to break the symmetry [5].

Method to open the band gap become focus of graphene research today, it can be done by doping, nanoribbons, grown on certain substrate and by apply an external electric field. Some previous study reported that bilayer graphene bandgap can be adjusted by changing the applied external electric field voltage, which could lead to new types of electronic and optical devices [6]. Kanayama & Nagashio 2015 has investigated experimentally the effect of electric field to the bilayer graphene by measure the quantum capacitance (CQ) through the capacitance measurements (C-V).

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They reported that an energy gap of ~0.25 eV is obtained at the maximum displacement field of ~30.0 V/Å [7]. Furthermore, study of effect external electric potential applied theoretically for the first reported by Tian et al. 2010. They used LDA calculation has reported that 0.077 V/Å applied external electric field open the bandgap of bilayer graphene up to 0.253 eV and opening at the Dirac point (K) about 0.306 eV [8].

In this study, we investigated the effect of applied external electric field potential on the band gap opening of bilayer graphene theoretically using density functional theory (DFT) calculation. As known, most DFT software today has been equipped with a function to calculate various properties, including the effect of an external electric field applied on the electronic structure of a system molecule in various directions [9-11]. Here, we compare the three different level of DFT, that is GGA-PBE, GGA-PW91, and LDA-CAPZ on the hexagonal bilayer graphene stacking. The electric field will be varied and the bandgap, as well as interlayer distance of the bilayer, will be exposed.

2. Calculation Methods

All calculations in this work were performed based on DFT calculation method implemented within CASTEP module of Biovia material studio 2016 package code. Graphite structure downloaded from crystallography database (cif. No. 9000046) was used as initial structure of graphene and bilayer graphene (Fig.1). A 3x2 supercell of graphite consist of 28 carbon atoms at each layer was optimized produce an orthorhombic crystal structure with lattice constant of 7.37, 8.51 and 6.70 Å. The graphene monolayer then built by deleting the two symmetry layers of the graphite and optimized. The optimized graphene monolayer then used to build a hexagonal stacking (AA') of graphene bilayer. Build layered structured as a crystal used to form graphene bilayer with vacuum slab of 1.7 Å at both layers. All structures were optimized by first-principles calculations on three different functional, that is GGA- PBE, GGA- PW91 and LDA-CAPZ. The convergence tolerance of energy and force acting on each atom during structure relaxation is chosen as 2 x 10−5 eV/atom and 0.05 eV/Å, respectively. The OTFG ultrasoft pseudopotential method with fine quality k-point set were used for the electronic expansion treatment. External electric potential applied were varied from 0 – 0.6 eV/Å/e, with a non-direction and Z-direction of electric field.

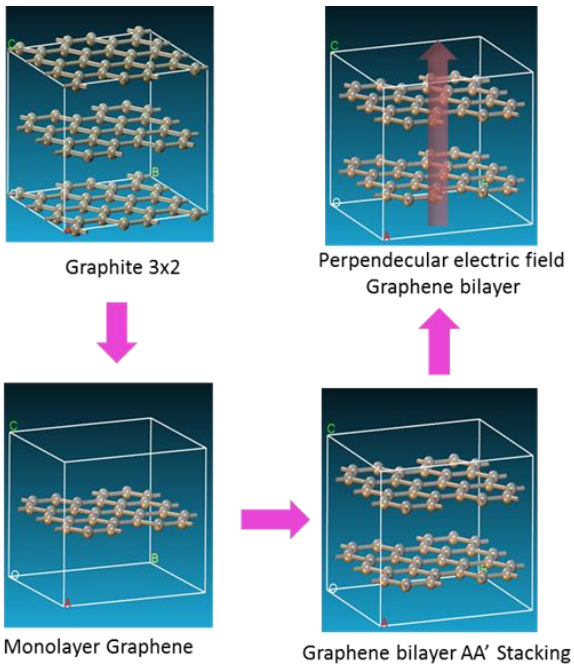

Fig. 1 - Mechanism to build of mono- and bilayer graphene structures

3. Results and Discussion

A 3x2 supercell of bilayer graphene were produced with lattice parameter of the optimized bilayer is 7.43, 8.58 and 6.80 Å, and the distance between layers is 3.3 Å. The lattice parameters slightly greater than the optimized graphite lattice. Fig. 2 is the electronic structure of monolayer, bilayer and bilayer graphene applied an external electric field calculated with GGA-PBE functional. Electronic structure of monolayer graphene shows overlapping the valence band and conduction band at G and Z points of Brillouin zone, which a metallic characteristic band structure material. Furthermore, the electronic structure of bilayer graphene slightly different to the monolayer, where the bandgap at G point already totally opened, meanwhile at Z point, a very small gap about 0.06 eV just created. And the gap was clearly shown when external electric field applied.

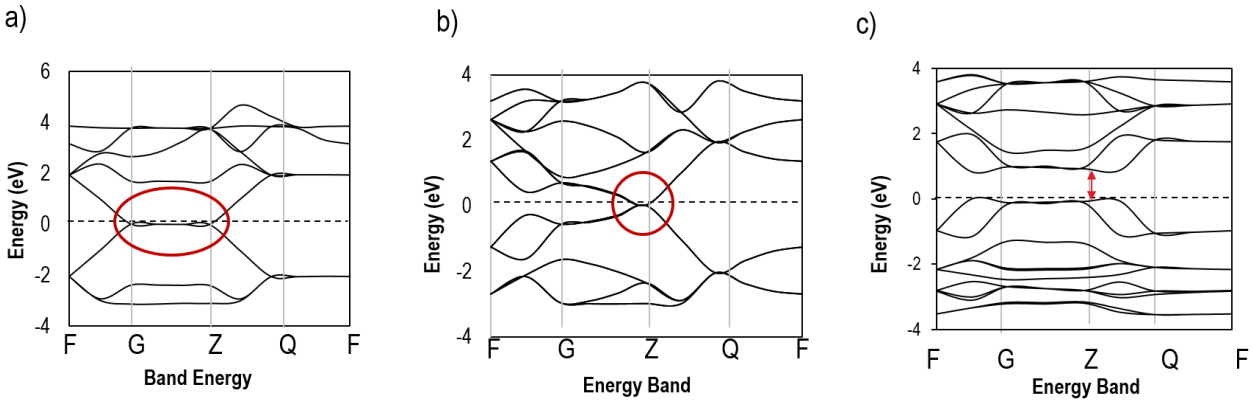

Fig. 2 - Electronic structure of a) monolayer; b) bilayer; c) an applied external electric field – bilayer graphene

The bandgap opening response to external electric applied is shown in Fig. 3. As many reported, the perpendicular direction of the applied electric field on the graphene bilayer is the most efficient to open the bandgap. Here, we compared the effect of the perpendicular direction and a non-direction of the electric field applied, in which the bandgap resulting by the perpendicular direction is ~ four times higher than the non-determined of the electric field applied (Fig. 3a). The two directions shown different patterns, in which by using perpendicular direction resulting a parabolic pattern with optimum bandgap opening 0.8 eV produced by 0.3 eV/Å/e electric field applied. And at higher potential the bandgap becomes smaller which is related to the crystal structure changes. Meanwhile, at a non-directed external electric field applied, the bandgap opening keep increasing. A higher applied potential might be needed to achieve the optimum bandgap opening.

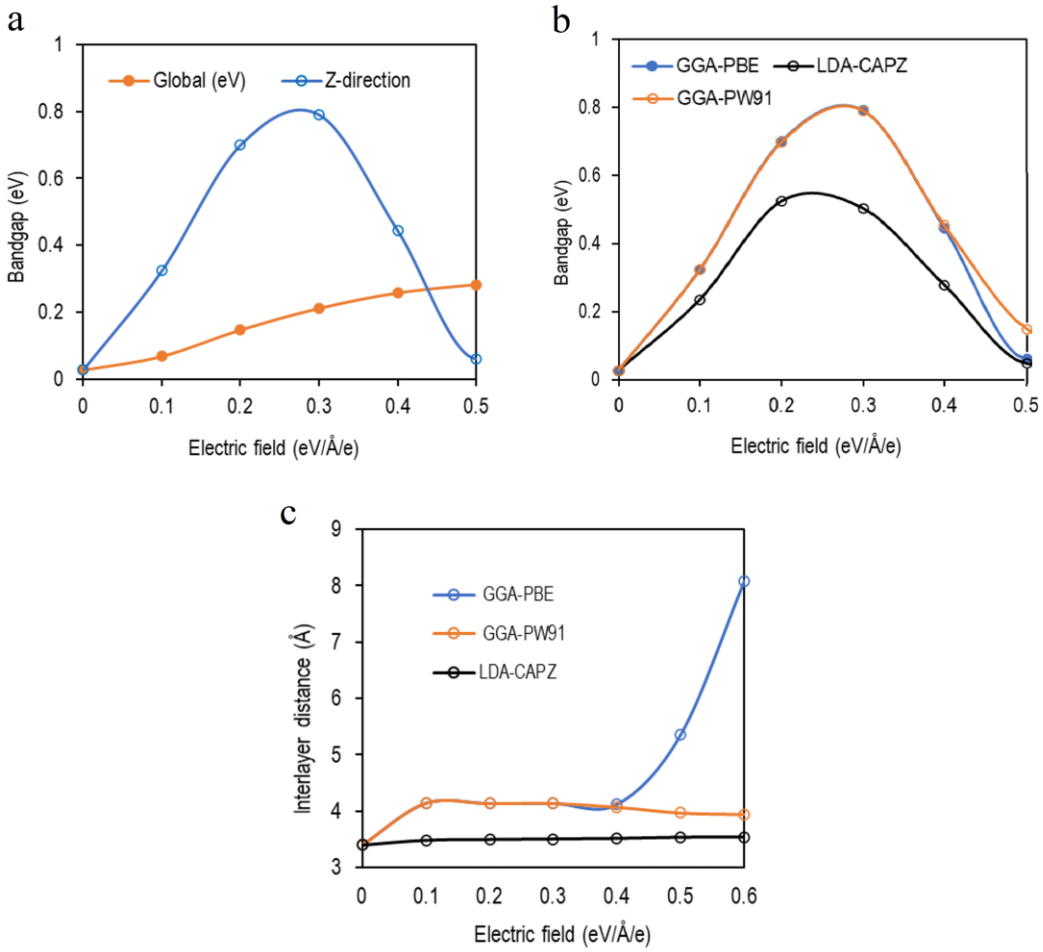

Fig. 3 - The bandgap opening response to external electric field applied

The calculation using perpendicular electric field also performed with two other functional that is GGA-PW91 and LDA-CAPZ (Fig. 3b), in order to know comparison of the three DFT approximations and functional calculation result on the electric field applied. The two GGA, PBE and PW91 were resulting similar value of bandgap on the low applied potential. The maximum bandgap 0.80 eV obtained at 0.3 eV/Å/e electric field, and becomes decrease at higher potential. However, at 0.5 eV/Å/e electric field applied, bandgap by GGA-PW91 slightly larger than PBE results. Furthermore, LDA-CAPZ calculation result bandgap opening is smaller than GGA calculation result. The higher bandgap opening by LDA is about 0.53 eV at 0.20 eV/Å/e electric field applied. The bandgap opening reported in this study were higher than calculation study reported by Tian et al. 2010, where the bilayer graphene bandgap ~ 0.25 eV at 0.3 V/Å applied external electric field [8].

Besides the bandgap opening, the electric field applied also effect to interlayer distance (Fig. 3c). The interlayer distance by the two GGA at low electric field applied (0 up to 0.4 eV/Å/e) shows similar value, meanwhile at 0.5 eV/Å/e and above, the distance is start different. The interlayer distance by GGA-PBE calculation result much larger (~8.2 eV), and the crystal structural has changes from cubic to triclinic (Fig.4). The large distance on PBE because of, and the bandgap causing bandgap opening near to zero, representative of monolayer characteristic. While the distance at GGA-PW91 and LDA relatively stable with cubic crystal structures.

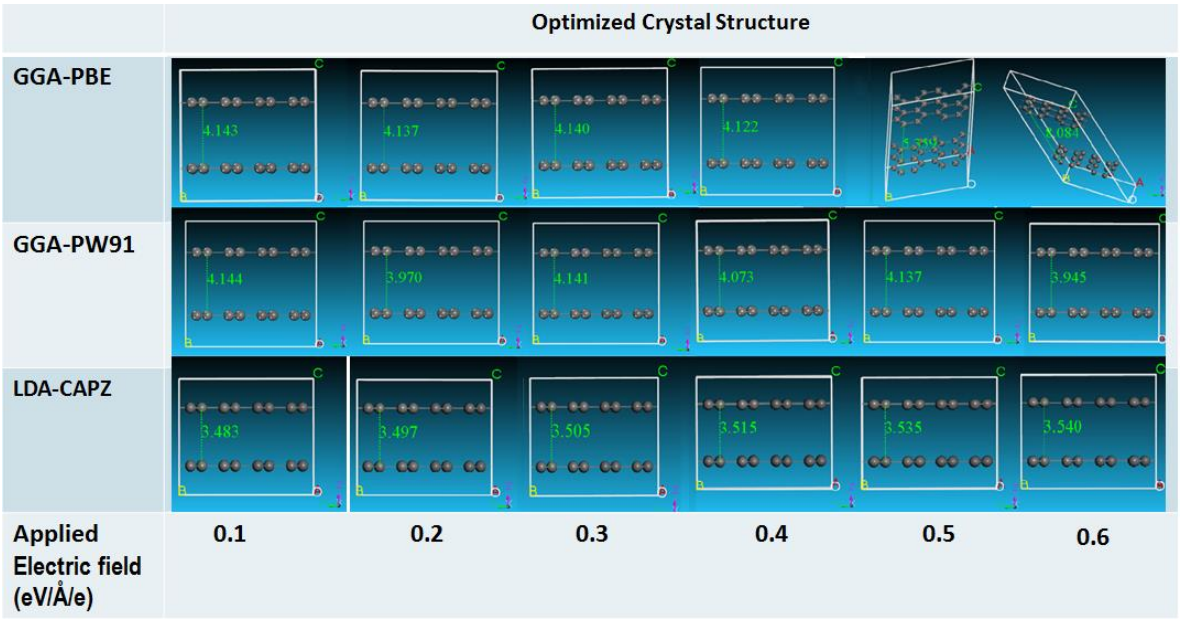

Fig. 4 - Bilayer graphene Optimized structure at different applied external electric field potential

4. Conclusion

In conclusion, calculation on effect of external electric field by using three different DFT approximation and functional have been done. The three DFT calculations showing different result, where the two GGA produce bandgap opening larger than LDA-CAPZ. The two GGA produce similar results on applied electric field potential below 0.4 eV/Å/e. At higher applied potential, the bilayer structure changes from cubic to triclinic and the distance of bilayer become larger and resulting monolayer graphene bandgap.

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