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Electronic properties of graphene-based heterostructures

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Abstract. Heterostructures based on graphene were investigated by using density function theory (DFT). It is found that energy gap appear in ZnS-graphene heterostructure. Heterostructures graphene-ZnO and graphene-phosphorene have almost zero-band gap. Binding energy between heterostructure layers was determined.

1. Introduction

It is known that graphene has zero-band gap that makes difficult using of this perspective material for micro- and nanoelectronic applications [1]. There are numerous different approaches to increase graphene band gap [2]. One of these approaches lies in formation of heterostructures based on graphene and graphene-like materials. This paper presents DFT-investigation of graphene-based heterostructures with zinc oxide (ZnO), zinc sulfide (ZnS) and phosphorene monolayers. The main criterion for choosing these materials is presence non-zero band gap in it and suitable lattice parameters.

ZnO and ZnS have semiconducting properties. Zinc refers to class of transition metals with completely filled 3d-shell. Heterostructures consisting of graphene and zinc-containing materials open new possibilities for their applications, because these structures are observed to have energetic gap and high charge carrier mobility via electronic interactions [3, 4]. Phosphorene, black-phosphorus monolayer, is also semiconductor with direct band gap of 2.0 eV. Phosphorene has high carrier mobility of $(10^3 \text{ cm}^2\text{V}^{-1}\text{s}^{-1})$[5, 6] and it may be prepared by scotching method [5, 7] like graphene.

The feature of layered materials is presence van-der-Waals interactions between layers. So it becomes very important to take into account this interactions when simulate properties of layered heterostructures to get an adequate results. To define which of the functional would be more suitable for layered heterostructure simulations, the investigation of interlayer distance in black phosphorus was carried out.

Thus, theoretical investigations of the graphene-based heterostructures have a great importance to learning and understanding their new properties and capabilities for application in micro- and nanoelectronic devices.

2. Description of method

Simulation of heterostructure electronic properties was performed using density function theory (DFT) which is realized in program VASP [8]. Calculations were carried out using different approaches to description of electronic density functionals, such as local density approximation (LDA) and generalized gradient approximation (GGA), using Perdew-Burke-Ernzernhof functional (PBE),

DFT-D2 method of Grimme and vdW-DF functional of Dion. The last two take into account the dispersion interactions (van-der-Waals forces), which play important role in layered systems.

The dependence of system full energy vs. interlayer distance for different functional is presented on figure 1. LDA functional shows interlayer distance to be of 2.92 Å. PBE, DFT-D2 and vdW-DF show interlayer distance of 3.54, 3.1 and 3.57 Å, respectively. The better conformity to the experimental value, which is 3,11 Å [9], gives DFT-D2 method. Therefore DFT-D2 functional was chosen for further simulations.
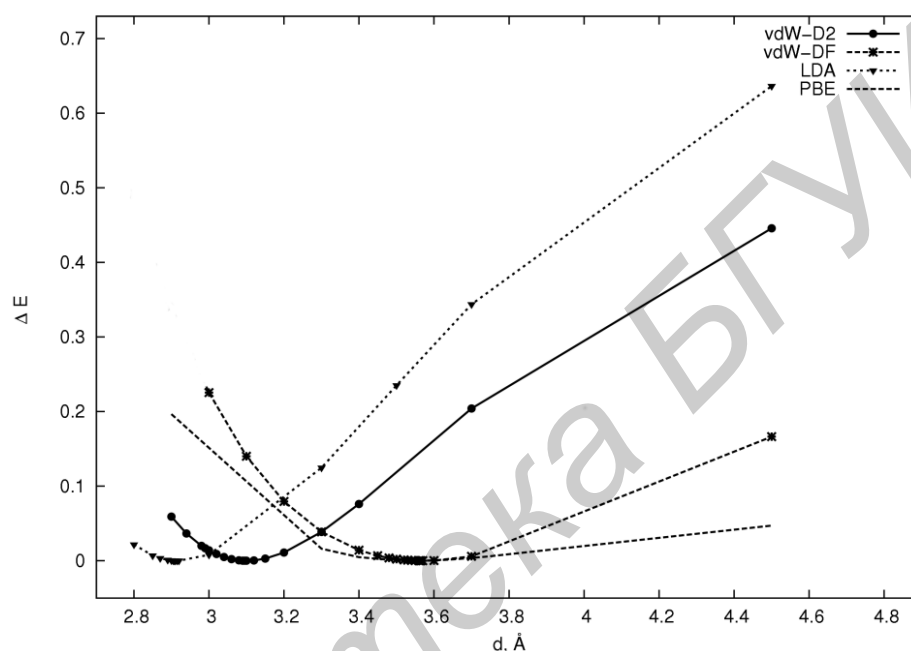

Figure 1. Dependence system full energy vs. interlayer distance in black phosphorus for different functional.

Interaction between atomic core and valence electrons was described by augmented plane wave method (PAW). Structure optimization converged when difference of full energy between the last two steps was equal to $1 \cdot 10^{-6}$ eV. Since VASP translates specified cell in all directions, vacuum layer was set to exclude energetic influence of two-layered structures on each other. Vacuum layer was added along the normal to layer surface. K-point mesh of reciprocal space was chosen $2 \times 4 \times 1$, $3 \times 3 \times 1$ and $8 \times 8 \times 1$ for graphene-phosphorene (G-P), graphene-ZnO (G-ZnO) and graphene-ZnS (G-ZnS) heterostructures respectively. Supercells of these heterostructures are shown on figures 2, (a), (b) and (c), respectively. Cutoff energy was 400 eV for G-P and 500 eV for G-ZnO and G-ZnS heterostructures.

Results

2.1. Graphene-phosphorene heterostructure electronic properties
Model of G-P heterostructure was created from 3×1 phosphorene unit cells and 4×1 graphene unit cells. Lattice mismatch is equal to 1.35 and 5.86% along to "zigzag" and "armchair" directions respectively. Vacuum layer is of 15 Å. Because phosphorene electronic properties highly depend on strain, it was preserved unchanged while graphene lattice was stretched up to phosphorene lattice constants. Investigation of G-P interaction using PBE and DFT-D2 functionals is shown that PBE functional slightly take into account this interaction (full energy minimum is observed when interlayer distance is 4.3 Å). DFT-D2 gives interlayer distance equal to 3.4 Å, that is corresponding to results

showed in [10]. Investigation of band structure revealed that energy gap in G-P system is equal to 0.01 eV that is too small for micro- and nanoelectronic applications (figure 3 (a)). Binding energy between graphene and phosphorene layers is -0.57 eV.
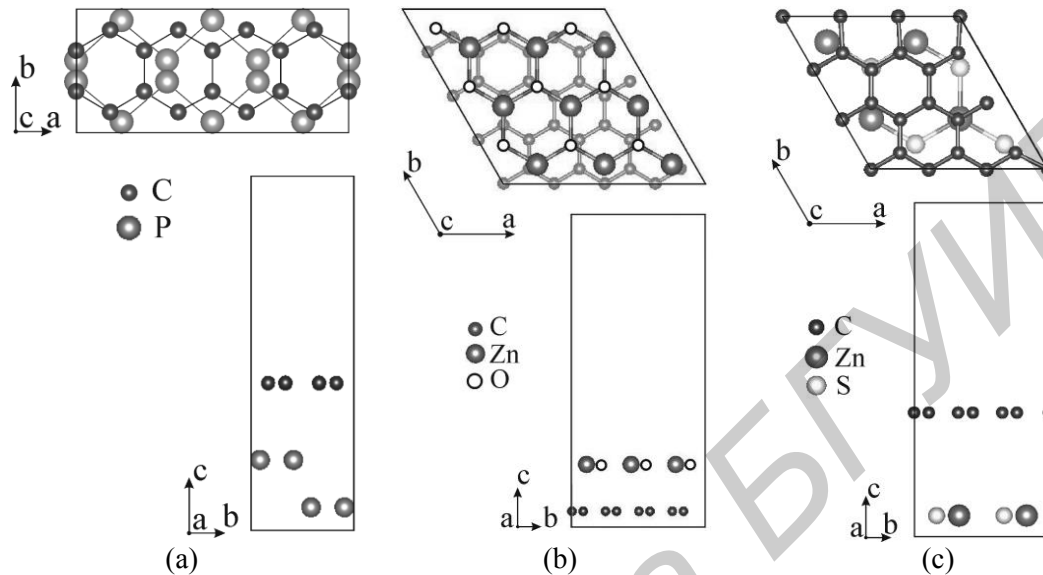

Figure 2. Supercells of (a) G-P, (b) G-ZnO and (c) G-ZnS heterostructures.

2.2. Graphene-ZnO heterostructure electronic properties
Model of G-ZnO heterostructure was created from 4×4 graphene unit cell and 3×3 ZnO unit cells. Lattice mismatch was less than 2%. Vacuum layer is of 20 Å. After atomic structure optimization was performed, ZnO lattice constant decreased on 1.85% and graphene lattice constant stayed unchanged. DFT-D2 functional shows energy minimum when distance between layers equals to 3.16 Å, while LDA functional doesn't show adhesion of graphene on ZnO. Band structure investigation reveals that energy gap in G-ZnO heterostructure becomes equal to $1 \cdot 10^{-4}$ eV, that is also too small to be used for micro- and nanoelectronic devices (figure 3(b)). Binding energy between graphene and ZnO layers is -0.5 eV.

2.3. Graphene-ZnS heterostructure electronic properties
Model of G-ZnS heterostructure was created from 3×3 graphene unit cell and 2×2 ZnS unit cells. Lattice mismatch is 1.72%. Vacuum layer is of 20 Å. Using DFT-D2 functional it was found that equilibrium interlayer distance is equal to 3.45 Å. Band structure investigation reveals that energy gap of G-ZnS structure is equal to 0.35 eV (figure 3 (c)). Zones have parabolic character, but curvature near the Dirac point is preserved that tells about slight losses of charge carrier mobility. This may be explained by energetic influence of wafer (ZnS). Binding energy between graphene and ZnS layers is 0.45 eV.

3. Conclusion
Electronic properties of heterostructures based on graphene (G-P, G-ZnO, G-ZnS) were investigated. It was shown that the best description of van-der-Waals forces which hold heterostructure layers together gives DFT-D2 functional. Also it was found that only ZnS opens considerable energy gap in graphene (0.35 eV), while in cases of G-ZnO and G-P energy gap equals to $1 \cdot 10^{-4}$ and 0.01 eV respectively, that is too small for micro- and nanoelectronic applications.
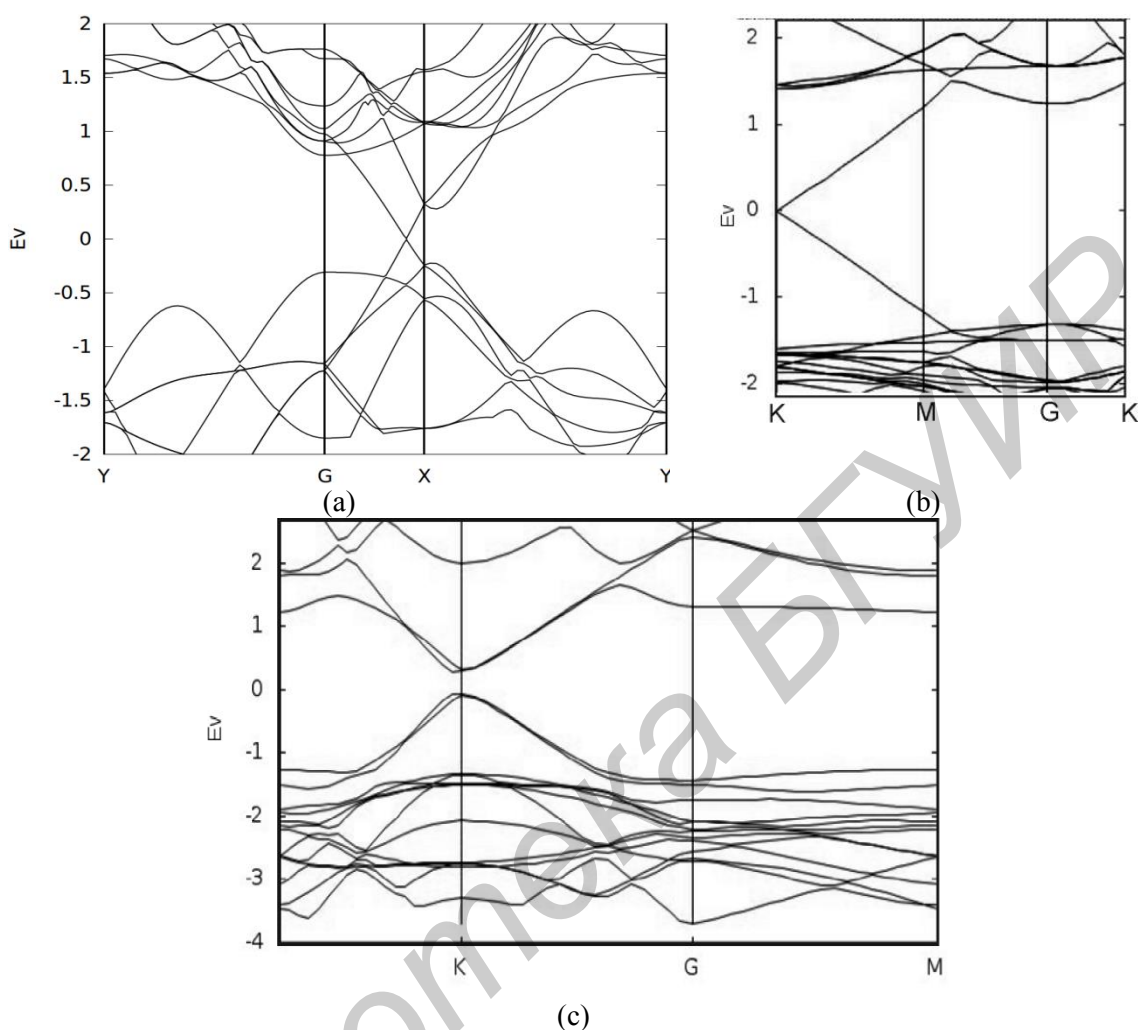
Figure 3. Band structure of (a) G-P, (b) G-ZnO and (c) G-ZnS heterostructures.

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