

Tunable arsenene bandgap in Arsenene/Graphene Heterostructures

Zhen Luo¹, Dedong Han^{1*}, Junchen Dong¹, Huijin Li¹, Wen Yu², Shengdong Zhang^{1,2}, Xing Zhang¹ and Yi Wang^{1*}

¹Institute of Microelectronics, Peking University, Beijing 100871, China

²Shenzhen Graduate School, Peking University, Shenzhen 518055, China

Phone:+86-10-62766516 Fax:+86-10-62751789 *E-mail: handedong@pku.edu.cn, wangyi@ime.pku.edu.cn

Abstract

Using density functional theory calculations with van der Waals (vdW) corrections, we investigate how the interlayer orientation affects the electronic properties of arsenene/graphene heterostructures. It is demonstrated that the orientation of the heterostructures can induce different bandgap of arsenene, while not significantly altering the binding energy. We show that the physical origin of this tunable bandgap arises from different degree of electron transfer in heterostructures with different orientations.

1. Introduction

Two-dimensional (2D) materials have attracted tremendous attentions due to their unique properties and potential applications [1]. Most recently, a novel 2D material, arsenene was first identified by means of density functional theory (DFT) calculations [2]. Arsenene possesses high thermoelectric figure of merit, optical properties and tunable electronic properties, bringing great potential for nanodeivces and applications [3-4]. In order to take advantages of different 2D materials, efforts have been focused on integrate them into a multilayer stack via van der Waals (vdW) forces [5], opening a new route towards high-performance electronic devices.

In this paper, we perform studies on arsenene/graphene (As/G) heterostructure using DFT calculations, and investigate how the interlayer orientation affects the electronic properties of the heterostrucutres.

2. Computational Methods and Model

The DFT calculations are performed using CASTEP package with ultra-soft pseudo-potential (USPP). Exchange and correlation energy is approximately by generalized gradient approximation (GGA) with Perdew-Burke-Ernzerhofer (PBE) functional. To describe the interlayer vdW interactions, Grimme's DFT-D correction is added. The cut-off energy is set to be 500 eV for the plane wave expansion, and a $9 \times 9 \times 1$ k-mesh in the first Brillouin zone (FBZ) is employed. All of the structures are fully relaxed until the Hellmann-Feynman force is smaller than 0.03 eV/Å.

In this work, we adopt As/G heterostructures with two orientations, 0° and 10.9° , as shown in Fig. 1, and the supercell configurations will be represented as As(2)/G(3) and As($\sqrt{3}$)/G($\sqrt{7}$) in the text.

3. Results and Discussion

The results on interlayer binding energies and structural properties of As/G heterostructures are summarized in Table 1. To quantitatively characterize the interaction strength between arsenene and graphene, we define a binding energy (E_b , per As atom) in the As/G heterostructure as

$$E_b = (E_{As/G} - E_{As} - E_G)/N_{As} \quad (1)$$

Where $E_{As/G}$, E_{As} and E_G represent the total energies of the heterostructure, corresponding monolayer arsenene and monolayer graphene, respectively, and N_{As} is the number of As atom in this structure. As shown in Table 1, the binding energies and interlayer distance do not change significantly with the orientations, indicating that As/G heterostructures with different interlayer orientations could coexist at room temperature. However, the structural and electronic properties of the heterostructures with different orientations vary a lot. It can be seen that the bond length and angle of arsenene exhibit a small variations, while the distributions are relatively uniform in As($\sqrt{3}$)/G($\sqrt{7}$) as displayed in Fig. 2. It indicates that the lattice symmetry of arsenene layer is slightly broken in As(2)/G(3).

Then, we calculate the electronic structures of As(2)/G(3) and As($\sqrt{3}$)/G($\sqrt{7}$) heterostructures shown in Fig. 3. The Dirac point of graphene is well preserved and still retains its semi-metallic character in two structures, while the band structure of arsenene changes with the orientation. Specifically, arsenene has the bandgap of 1.728 eV and 1.377 eV in As(2)/G(3) and As($\sqrt{3}$)/G($\sqrt{7}$), respectively, indicating that different orientations can induce tunable bandgap of arsenene. The key information is the arsenene thickness, which has a great impact on the electronic properties of the buckled structure. As seen in Table 1, arsenene rotating different angle with respect to graphene shows different arsenene thickness, resulting in different band structures.

Last, we perform the electronic charge transfer calculations as displayed in Fig. 4. Focusing on Fig. 4(a), the triangle area and the rectangle area denote the downwards and upwards As atom directly above C atom, respectively. In triangle region, there is intense electron exchange between graphene and arsenene, indicating strong interlayer coupling. In the rectangle region, the interaction is weakened. Thus, the structure parameters of arsenene exhibit variations in As(2)/G(3). On the other hand, where the orientation is 10.9° , the special regions are not present because graphene has a different registry with respect to the As atoms in arsenene. Therefore, the arsenene thickness is larger in

As(2)/G(3) than that in As($\sqrt{3}$)/G($\sqrt{7}$), resulting in different bandgap in arsenene.

4. Conclusions

In conclusion, we have reported the orientation between graphene and arsenene in the heterostructure affects the bandgap of arsenene, and have investigated its physical origin. The results demonstrate that different orientations result in different degree of interfacial electronic transfer, which affects the arsenene thickness and hence the band-structure.

Acknowledgements

Table 1 Calculated properties of the As/G heterostructures: arsenene thickness, interlayer distance, mismatch, binding energy, local strain and arsenene bandgap

System	Orientation ($^{\circ}$)	Arsenene thickness Δ As ($\text{\AA}$)	Interlayer distance d ($\text{\AA}$)	Mismatch	Binding En-ergy (meV/atom)	Local strain	Bandgap_As (eV)
As(2)/G(3)	0	1.37	3.37	1.89%	-67.6	-2.29%	1.73
As($\sqrt{3}$)/G($\sqrt{7}$)	10.9	1.35	3.39	0.06%	-46.5	-0.72%	1.38

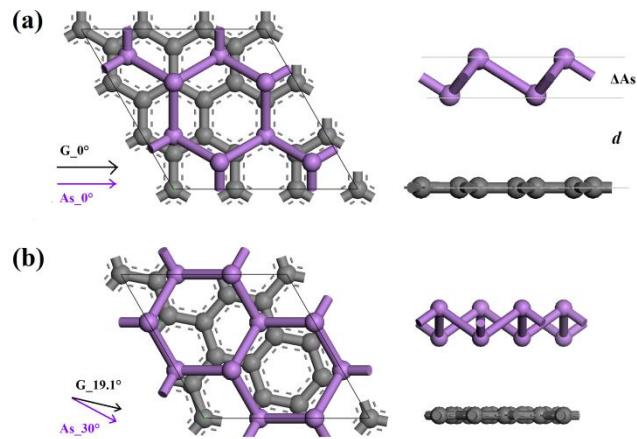


Fig. 1 Front view and side view of As/G heterostructures with the orientation of (a) 0° and (b) 10.9°

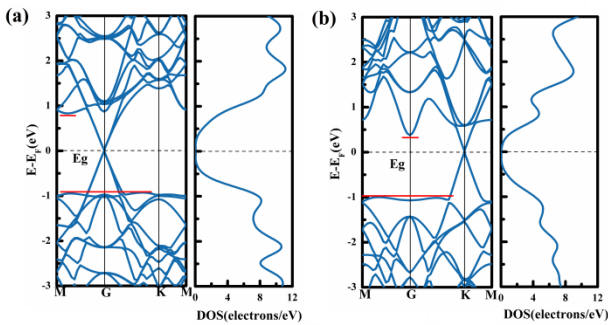


Fig. 3 The band structure and density of state of (a) As(2)/G(3) and (b) As($\sqrt{3}$)/G($\sqrt{7}$)

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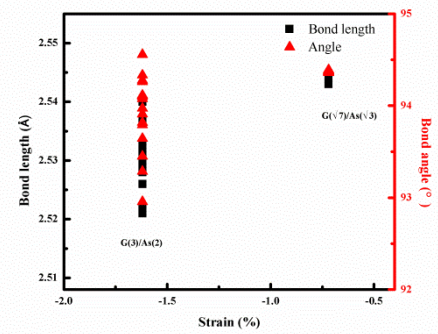


Fig. 2 The bond length and bond angle distribution of arsenene in As/G heterostructures as a function of local strain

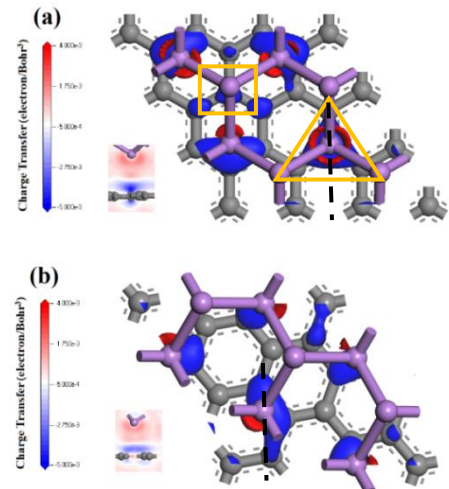


Fig. 4 Electronic charge transfer between arsenene and graphene layers for two different relative orientations present in (a) As(2)/G(3) and (b) As($\sqrt{3}$)/G($\sqrt{7}$). The insets are side views for the normal cross-sections shown as dashed lines in the main views