



Tuning the Schottky barrier in the arsenene/graphene van der Waals heterostructures by electric field



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ABSTRACT

Using density functional theory calculations, we investigate the electronic properties of arsenene/graphene van der Waals (vdW) heterostructures by applying external electric field perpendicular to the layers. It is demonstrated that weak vdW interactions dominate between arsenene and graphene with their intrinsic electronic properties preserved. We find that an n-type Schottky contact is formed at the arsenene/graphene interface with a Schottky barrier of 0.54 eV. Moreover, the vertical electric field can not only control the Schottky barrier height but also the Schottky contacts (n-type and p-type) and Ohmic contacts (n-type) at the interface. Tunable p-type doping in graphene is achieved under the negative electric field because electrons can transfer from the Dirac point of graphene to the conduction band of arsenene. The present study would open a new avenue for application of ultrathin arsenene/graphene heterostructures in future nano- and optoelectronics.

1. Introduction

Since the successful invention of isolated graphene in experiments [1], two-dimensional (2D) materials [2–6], such as graphene [7,8], silicene [9–11], hexagonal boron nitride [12–14], Molybdenum disulphide [15–17] and phosphorene [18–22] have received considerable interest recently owing to their fascinating optical, mechanical, electrochemical, electronic and thermal properties. In particular, graphene, a hexagonal lattice of carbon monolayer, has a high carrier mobility of up to $10^6 \text{ cm}^2 \text{ V}^{-1} \text{ s}^{-1}$ [8], but the absence of a bandgap limits its applications of large-off current and high on-off ratio for graphene-based electronic devices.

Very recently, arsenene, which is single-atom-thick layer of gray arsenic, has been proposed as a new member of group-V nanosheets [23–27]. Gray arsenic adopts a stacking structure of warped graphene-like layers and the layers are bonded together through vdW force. Due to weak bonding between the layers, gray arsenic is so brittle that layered arsenic can be isolated from the bulk gray arsenic structure as in the case of graphene and phosphorene. Arsenene was predicted to be an indirect bandgap semiconductor, and an indirect-to-direct bandgap transition occurs by applying suitable strain [23,28]. Wang et al. [29] found that for arsenene, the armchair nanoribbons are indirect

semiconductors while the zigzag nanoribbons are direct ones regardless of the ribbon width. Moreover, studies show the electronic structures of arsenic nanosheets depend sensitively on interlayer spacing, layer number and layer stacking [25]. In addition, the bandgap of arsenene is larger than that of phosphorene and monolayer MoS_2 , which will further facilitate the development of 2D materials based optoelectronic devices with response to photons with wave lengths of less than 620 nm, such as photodetectors and blue light-emitting diodes [30]. Meanwhile, by solving the Boltzmann transport equation for phonons, a highly anisotropic thermal conductivity along the zigzag and armchair directions at room temperature has been predicted in arsenene [31]. All these properties make arsenene important for applications in optoelectronics and nanoelectronics.

Currently, vertical heterostructures based on 2D vdW materials, especially heterobilayers made layer by layer from 2D monolayers, are being considered as a novel way to construct devices that combine the properties of their individual components [32–34] with ideal properties to be applied in optoelectronics and nanoelectronics. These hybrid vdW heterobilayers show many more new properties far beyond their single components. Furthermore, due to the weak electron coupling and the lack of dangling bonds at the interface of vdW heterobilayers, their intrinsic electronic properties are preserved without any degrada-

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tion. In particular, among these vdW heterobilayers, graphene-based vdW heterobilayers have received intensive attention. For example, Many 2D ultrathin graphene-based vdW heterobilayers, have been widely studied theoretically and experimentally, such as graphene/silicene [35–37], graphene/h-BN [38–42], graphene/MoS₂ [43–48] and graphene/phosphorene [49–51]. McDonnell et al. [52] demonstrated that the defects in MoS₂ dominate the Schottky barrier and the variations in defect density strongly impact the measured currents. Consequently, the deliberate formation of low hole and low electron Schottky barriers with predictable junction currents could be achieved via the sufficient control of the defect density. Giannazzo et al. [53] showed that a local increase in the density of sulfur vacancies can lead to a reduction of the Schottky barrier height and to an increase of the carrier concentration, i.e., to a reduction of the local resistivity. Shih et al. [54] reported that a new field-effect transistor device composed of a graphene/MoS₂ heterobilayer has been constructed, where graphene acts as both source or drain and gate electrodes and MoS₂ as the channel, researchers start to use graphene as the contact in a device rather than the channel. Recent works have demonstrated good electrical contacts between graphene and MoS₂ [55,56]. Moreover, the modulation of the graphene work function, e.g., by an electric field, can be exploited to adjust the graphene Fermi level to the MoS₂ conduction band minimum to completely remove the Schottky barrier at the interface [56]. Therefore, an interesting question arise: whether arsenene and graphene can form a 2D arsenene/graphene vdW heterostructure to obtain some new properties beyond pristine arsenene and graphene? If so, whether electric field for Schottky barrier tuning can also be employed in arsenene/graphene vdW heterostructure? We address this question in the context of arsenene/graphene vdW heterostructure in this paper.

In the present work, we study the effects of the electric field on the electronic structures of arsenene/graphene vdW heterostructure by first-principles calculations. We show that both the properties of arsenene and graphene are preserved upon their contact. Moreover, the electric field can be used to effectively control the Schottky barriers (n-type and p-type) and contact formation (Schottky and Ohmic contacts) at the arsenene/graphene interface.

2. Models and computational methods

All the calculations performed in this work are based on density functional theory as implemented in the VASP package [57,58]. The generalized gradient approximation of Perdew, Burke, and Ernzerhof (GGA-PBE) [59] with vdW correction proposed by Grimme (DFT-D2) [60] is chosen due to its good description of long-range vdW interactions [61–64]. The projected augmented wave (PAW) potential [65] is employed to describe the electron-ion potential and a kinetic energy cutoff is set to 500 eV. The 2D Brillouin zone integration using the Γ -center scheme is sampled with a $9 \times 9 \times 1$ grid for geometry optimization and a $15 \times 15 \times 1$ grid for static electronic structure calculations. All the geometric structures are fully relaxed until energy and forces are converged to 10^{-5} eV and 0.01 eV/Å, respectively. The vacuum size is larger than 20 Å between two adjacent images to prevent spurious interactions between periodic images of the slabs. Electric fields were applied normal to the slabs, the uniform electric field is handled in VASP by adding an artificial dipole sheet in the supercell [66]. The calculated lattice parameters of the arsenene and graphene unit cells are 2.459 Å and 3.752 Å, respectively, which agrees well with previous studies [67–71]. In order to simulate the arsenene/graphene vdW heterostructure, a 3×3 supercell of graphene (18 carbon atoms) is obtained as shown in Fig. 1. to match a 2×2 supercell of arsenene (8 arsenic atoms) with a negligible lattice mismatch less than 2%.

3. Results and discussion

To quantitatively characterize the interface mechanical properties,

the binding energy (E_b) per carbon atom between arsenene and graphene is calculated as $E_b = (E_{\text{arsenene/graphene}} - E_{\text{arsenene}} - E_{\text{graphene}}) / N_c$, where $E_{\text{arsenene/graphene}}$ is the total energy of the arsenene/graphene vdW heterostructure, E_{arsenene} is the total energy of the isolated single layer arsenene, E_{graphene} is the total energy of the isolated graphene layer and $N_c = 18$ is the number of carbon atoms in the unit cell. For the arsenene/graphene system, the calculated binding energy per carbon atom is -29.7 meV with an equilibrium interlayer distance of 3.61 Å. According to the negligible binding energy and the large interlayer distance (much larger than the sum of the covalent radii of the C and As atoms), the graphene is found to interact very weakly with arsenene. The results suggest the graphene is bound to arsenene via vdW interaction.

Electronic properties of pristine arsenene and graphene monolayers are calculated and their band structures are plotted in Fig. 2b and c, respectively. Fig. 2c indicates that pristine graphene has a zero bandgap, indicating a linear Dirac-like dispersion relation $E(k) = \pm \hbar v_F |k|$ around the Fermi level, where v_F is the Fermi velocity, and the calculated Fermi velocity is 8.07×10^5 m/s at the Dirac point of graphene. Compared with the band structures of pristine graphene primitive cell, the Dirac cone of the 3×3 graphene supercell is mapped to the Γ point due to the K and K' points are folded to Γ point. Fig. 2b shows that arsenene is an indirect bandgap semiconductor with a value of 1.51 eV, which is in agreement with previous theoretical studies [29]. We then study the electronic structures of arsenene/graphene vdW heterostructure. In Fig. 2a, we plot the projected band structures of arsenene/graphene vdW heterostructure. The linear Dirac-like dispersion relationship around the Fermi level of graphene is still preserved in the arsenene/graphene vdW heterobilayer, though a tiny bandgap of 11 meV is opened at the Dirac point of arsenene, which is lower than thermal fluctuation (about 25 meV) at room temperature and tends to vanish in experiments. The part of arsenene retains the indirect bandgap semiconductor with the bandgap of 1.49 eV. Compared with the band structures of pristine antimonene and graphene shown in Fig. 2b and c, respectively, the band structure of the arsenene/graphene heterostructure seems to be a simple sum of those of each component. The Fermi velocity at the Dirac point is almost unchanged in the arsenene/graphene vdW heterobilayer compared to pristine graphene. These results show that the electronic structure of both the graphene and the arsenene layers are quite well preserved upon binding. The above characteristics are an important behavior for the 2D vdW heterostructures.

In practice, it is difficult to fabricate 2D vdW heterostructures without defects. Similar to the modification of properties for MoS₂ and metal/MoS₂ contact [52,53], vacancy defect will affect the electronic properties of arsenene/graphene heterojunction greatly. In Fig. 3, we plot the projected band structures and partial density of states of arsenene/graphene heterobilayer with single arsenic vacancy. Comparing Fig. 3(a) with 2(a), we find that the presence arsenic mono-vacancy introduces gap states in the bandgap. The gap state is a donor state close to the conduction band edge (~ 0.29 eV below CBM), arising from the dangling bonds of arsenic atoms due to their unsaturated charges. The gap state is dominated by As 4p orbitals, showing a strong degree of delocalization due to the interactions between sulfur vacancies in adjacent supercells.

From a device point of view, when using graphene as the metal contact and monolayer arsenene as the channel, it is very important to know its Schottky barrier. For these systems, we can define the Schottky barrier via the Schottky–Mott model [72] at the metal/semiconductor interface [73]. an n-type Schottky barrier (Φ_{Bn}) is defined as: $\Phi_{Bn} = E_C - E_F$, where E_C and E_F are the conduction band minimum (CBM) and the Fermi level, respectively. Similarly, a p-type Schottky barrier (Φ_{Bp}) is defined as: $\Phi_{Bp} = E_F - E_V$, where E_F and E_V are the Fermi level and the valence bandmaximum (VBM), respectively. Note that the sum of both Schottky barriers are approximately equal to the bandgap (E_g) of the semiconductor, namely, $\Phi_{Bn} + \Phi_{Bp} \approx E_g$.

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