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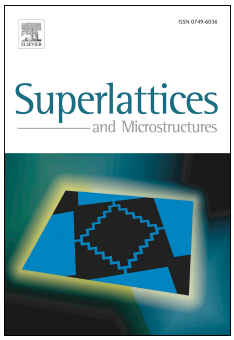

Out-of-plane strain and electric field tunable electronic properties and Schottky contact of graphene/antimonene heterostructure

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Out-of-plane strain and electric field tunable electronic properties and Schottky contact of graphene/antimonene heterostructure

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Abstract

In this paper, the electronic properties of graphene/monolayer antimonene (G/m-Sb) heterostructure have been studied using the density functional theory (DFT). The effects of out-of-plane strain (interlayer coupling) and electric field on the electronic properties and Schottky contact of the G/m-Sb heterostructure are also investigated. The results show that graphene is bound to m-Sb layer by a weak van-der-Waals interaction with the interlayer distance of 3.50 Å and the binding energy per carbon atom of -39.62 meV. We find that the n-type Schottky contact is formed at the G/m-Sb heterostructure with the Schottky barrier height (SBH) of 0.60 eV. By varying the interlayer distance between graphene and the m-Sb layer we can change the n-type and p-type SBH at the G/m-Sb heterostructure. Especially, we find the transformation from n-type to p-type Schottky contact with decreasing

the interlayer distance. Furthermore, the SBH and the Schottky contact could be controlled by applying the perpendicular electric field. With the positive electric field, electrons can easily transfer from m-Sb to graphene layer, leading to the transition from n-type to p-type Schottky contact.

Key words: Graphene; Antimonene; DFT calculations; Schottky contact.

1 Introduction

Two-dimensional (2D) materials, such as graphene [1–3], hexagonal boron nitride (h-BN) [4,5], molybdenum disulfide [6,7], phosphorene [8], and antimonene [9, 10] have attracted considerable interest recently due to their unique structural, electronic, optical and transport properties. In particular, graphene is well-known as a 2D material with one atom thickness, the high carrier mobility of 200 000 cm^2/Vs, and massless Dirac fermions [3]. These extraordinary properties make graphene a potential material for application in optoelectronic and nanoelectronic devices. However, the gapless of graphene limits its applications to large-off current and high on/off ratio electronic devices, such as field effect transistors (FETs). Recently, most stable monolayer antimonene (m-Sb) has been successfully realized on 3D topological insulators Bi_2Te_3 and Sb_2Te_3 [11]. In contrast to graphene, m-Sb is a semiconductor with a band gap of 1.43 eV at Γ point [12]. The structural, electronic, magnetic and transport properties of m-Sb have been investigated theoretically and experimentally [9, 12–14]. It can be seen that these properties of m-Sb could be controlled by applying uniaxial and biaxial strains. Thus, m-Sb can be considered as a potential 2D material for various electronic device applications including FETs, gas sensors, and solar cells.

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Currently, vertical heterostructures based on graphene and other 2D materials are being considered as a novel way to design the graphene-based electronic devices. For example, T. Roy *et al.* [15] presented FETs using stacked two-dimensional materials for all of the components, where MoS_2 was used as the active channel material, h-BN as the top-gate dielectric, and graphene as the source/drain and the top-gate contacts. C. Shih *et al.* [16] demonstrated a new type of FET device based on G/MoS_2 heterostructure. They showed that the high carrier mobility in graphene can be combined with the permanent band gap of MoS_2. On the theoretical aspect, heterostructures based on graphene and other 2D materials have been widely studied, such as graphene/MoS_2 [17–19], graphene/phosphorene [20, 21], graphene/h-BN [22, 23]. These vdW heterostructures show many more new properties far beyond their single components. Additionally, the electronic properties of these vdW heterostructures are well preserved due to the weak vdW interactions between graphene and the semiconducting layers.

It is well-known that the study of the electronic properties of the G/m-Sb heterostructure plays a crucial role in designing the graphene-based electronic devices such as FETs [1, 24]. In the present work, we study the structural and electronic properties of the G/m-Sb heterostructures using the density functional theory (DFT). The effects of the vertical electric field and interlayer coupling on the electronic structures and Schottky barrier of G/m-Sb heterostructure are also investigated. Our results show that due to the weak vdW interactions between graphene and m-Sb layer, the electronic properties of the G/m-Sb heterostructure are well preserved upon their contact. In addition, the electronic properties and the Schottky contacts of the G/m-Sb heterostructure could be controlled by out-of-plane strain and vertical electric field. Our results provide an useful information for applications of graphene in nanoelectronic and optoelectronic devices.

2 Theoretical methods and models

In the present work, we use the density functional theory (DFT) method, which was implemented in the simulated Quantum Espresso Package [25], to consider the structural and electronic properties of the G/m-Sb heterostructure. The general gradient approximation (GGA) in the Perdew-Burke-Ernzerhof (PBE) [26] form is used for the exchange-correlation energy of the interacting electrons with the frozen-core full-potential projector augmented wave (PAW) method. The kinetic cut-off energy of electron wave functions is 500 eV in the calculations. The $(9 \times 9 \times 1)$ k-point meshes are used for the Brillouin zone. All structures are relaxed with the atomic forces on each ion of less than 0.001 eV/Å. A vacuum layer of 18 Å is used in the direction normal to the heterostructure, representing the isolated slab boundary condition. It is clear that the traditional DFT method based on the GGA approximation is known to overestimate the binding in weakly bonded systems where interactions are mainly of van der Waals type [27, 28]. On the other hand, much research effort has been devoted to include vdW forces in the studies of graphene/substrate interfaces [23, 29, 30]. Therefore, to give a better description of the weak vdW interactions between graphene and m-Sb semiconductor, we choose the semi-empirical dispersion-corrected DFT-D2 method, which was proposed by Grimme [28]. This method has also been used successfully in our previous calculations [19, 31, 32].

The G/m-Sb heterostructure is calculated by using a supercell as shown in Fig. 1, which consists (1×1) supercell of m-Sb semiconductor and (3×3) supercell of graphene. The lattice mismatch for the G/m-Sb heterostructure is just less than 1%, which does not affect the main results. The out-of-plane strain is defined as $\Delta d = d_0 - d$ (Å), where d_0 is the interlayer distance after out-of-plane strain. The out-of-plane strain Δd varies from -1 Å to +1 Å. The electric field is applied

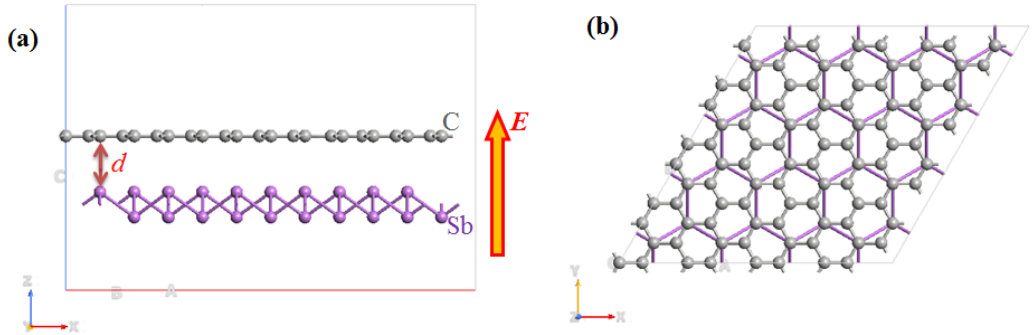

Fig. 1. Side (a) and top (b) view of the relaxed atomic structure of G/m-Sb heterostructure, with the carbon atoms in gray and the antimony atoms in purple. The interlayer distance between graphene and m-Sb layer after relaxation is denoted by d, Å.

perpendicularly to the G/m-Sb heterostructure with the magnitude varying from -1.5 V/Å to +1.5 V/Å.

3 Results and discussion

To study the electronic properties of the composing G/m-Sb heterostructure, we first recall the lattice constants of pristine graphene and m-Sb. Our calculations show that the equilibrium lattice parameters for pristine graphene and m-Sb are 2.461 Å and 4.125 Å, respectively, which are in good agreement with previous results [2, 33]. We also investigate the electronic properties of pristine graphene and m-Sb at the equilibrium state. In Fig. 2(a,b) we show the band structures and projected density of states (PDOS) of C and Sb atoms in pristine graphene and m-Sb, respectively. It is shown that graphene has a cone-like band structure with linear dispersion near the Dirac point making the gapless in pristine graphene, as shown in Fig. 2(a). In contrast, pristine m-Sb is an indirect band gap semiconductor with a band gap of 1.20 eV, which is in good agreement with previous theoretical calculations [12, 33].

We now study the electronic properties of G/m-Sb heterostructure. In Fig. 2(c)

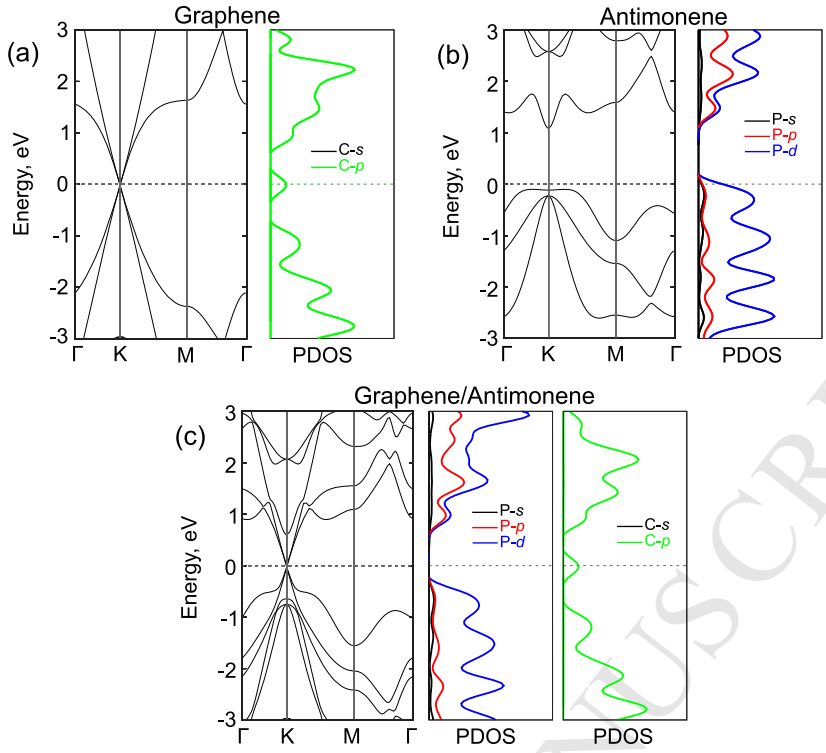

Fig. 2. Band structure and projected density of state of C, Sb atoms in (a) freestanding graphene, isolated monolayer antimonene (b), and the van der Waals graphene/antimonene heterostructure (c). The Fermi level is set to be 0 eV.

we show the band structure and PDOS of C and Sb atoms in the G/m-Sb heterostructure at the equilibrium state. It should be noted that the equilibrium interlayer distance after relaxation between graphene and Sb layers is 3.50 Å which is in consistent with previous calculations in 2D vdW heterostructures such as G/As [30], G/MoS_2 [17], G/P [21], and G/g-GaN [34]. This interlayer distance is much larger than the sum of the covalent radii of C and Sb atoms. Thus, the interaction between graphene and m-Sb layer is characterized by a weak vdW bond. To establish the stability of G/m-Sb heterostructure, we also calculate the binding energy per carbon atom in G/m-Sb system, E_b, which can be calculated as: $E_b = [E_{G/m-Sb} - (E_G + E_{m-Sb})]/N_C$, where $E_{G/m-Sb}$, E_G, and E_{m-Sb} are the total energy of the combined G/m-Sb heterostructure, pristine graphene, and pris-

tine m-Sb, respectively; and also N_C is the number of the carbon atoms in the heterostructure. The calculated value of $E_b = -39.62$ meV is in good agreement with the available results of 2D vdW heterostructures [17, 21, 30]. The negative binding energy also demonstrates a weak vdW interaction between graphene and m-Sb surface.

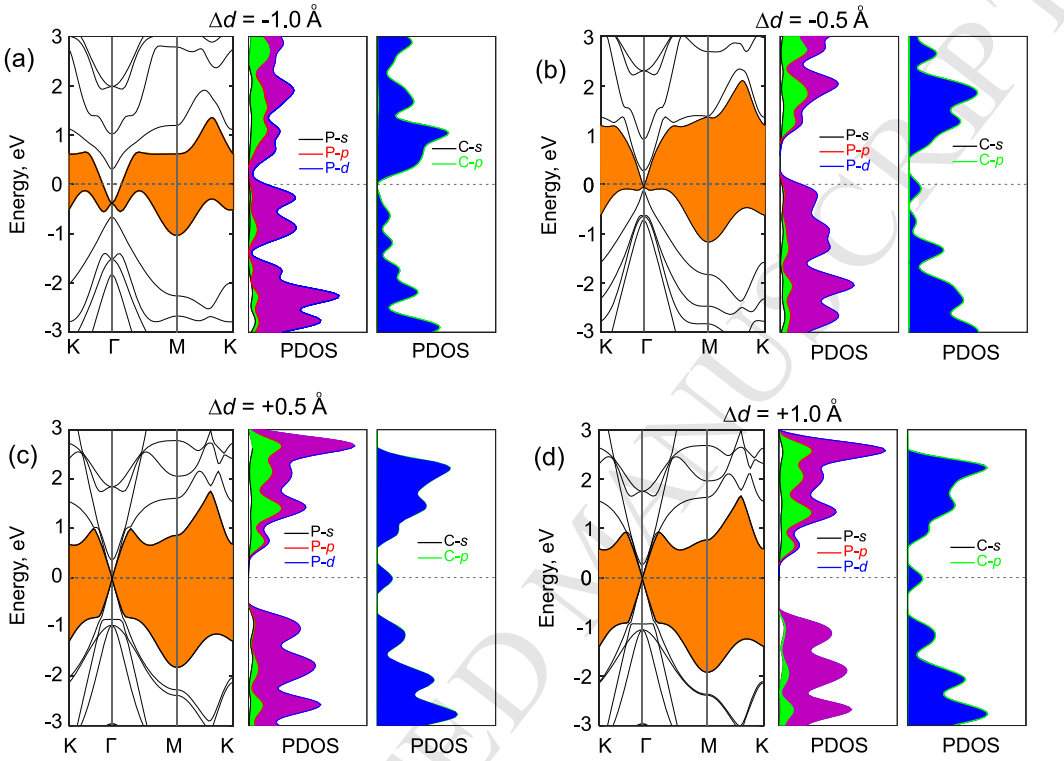

Fig. 3. Band structure and PDOS of C, Pb atoms in the G/m-Sb heterostructure at different interlayer distance (a) $\Delta d = -1.0$ Å, (b) $\Delta d = -0.5$ Å, (c) $\Delta d = +0.5$ Å, and (d) $\Delta d = +1.0$ Å. In all case of the interlayer distance the Fermi level is set to be 0 eV.

From Fig. 2(c) we can see that the composed band structure of the G/m-Sb heterostructure seems to be a simple sum of those of each component. The Fermi velocity at the Dirac point of graphene in the G/m-Sb heterostructure is preserved owing to a weak vdW interaction between graphene and m-Sb surface. It means that the weak vdW interaction gives a minor influence on the electronic band structure of graphene. Additionally, in comparison with the electronic band structure of

pristine m-Sb (Fig. 2(b)), we can see from Fig. 2(c) that the Fermi level of the m-Sb layer in the G/m-Sb heterostructure moves up to the conduction bands of semiconducting m-Sb. This shift can be explained by the presence of the charge transfer from graphene layer to the m-Sb layer upon the bonding, shifting up the Fermi level close to the conduction band of the semiconducting m-Sb.

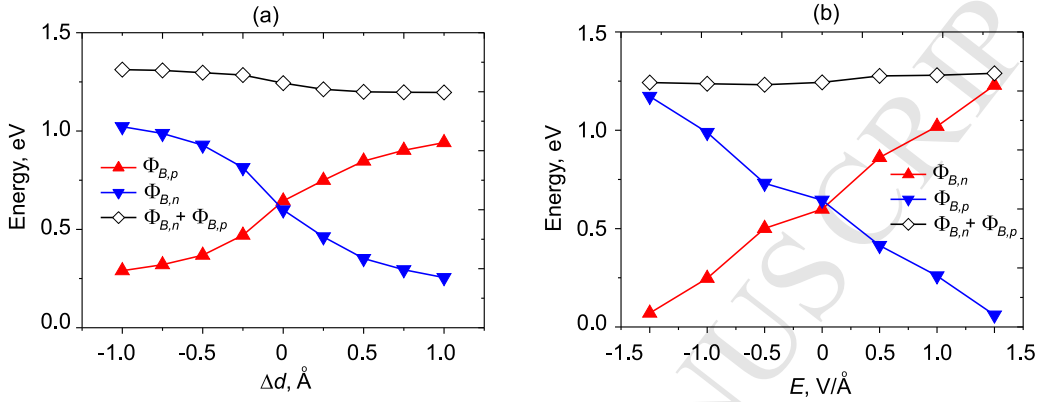

Fig. 4. The dependence of the n-type and p-type SBH on the interlayer distance (a) and vertical electric field (b).

Interestingly, it can be found that a Schottky contact could be formed between semi-metallic graphene and semiconducting m-Sb, which is similar to the cases of composing graphene with other semiconductors, such as G/SnS [35], G/As [30], and G/g-GaN [34]. The Schottky contact plays an important role in the device performance. The Schottky barrier height (SBH) is one of the most important measures of metal/semiconductor system. Thus, it is important to calculate the SBH of G/m-Sb heterostructure. Based on the Schottky-Mott model [36] for the metal/semiconductor heterostructure [37], the n-type Schottky barrier is defined by $\Phi_{B,n} = E_C - E_F$, where E_C is the conduction band minimum (CBM) and E_F is the Fermi energy level, respectively. The p-type Schottky barrier is defined by $\Phi_{B,p} = E_V - E_F$, where E_V is the valence band maximum (VBM). Note that the sum of the n-type and p-type Schottky barrier is approximately equal to the band

gap of the semiconductor, i.e., $\Phi_{B,n} + \Phi_{B,p} \approx E_g$(m-Sb). Our calculated work function (the energy difference between the vacuum level and the Fermi level) of graphene is W_G = 4.3 eV, that is very close to the electron affinity (the energy difference between the vacuum level and the CBM) of the m-Sb semiconductor ($\chi = 4.20$ eV). For the G/m-Sb heterostructure we find a n-type Schottky contact with the SBH of 0.60 eV.

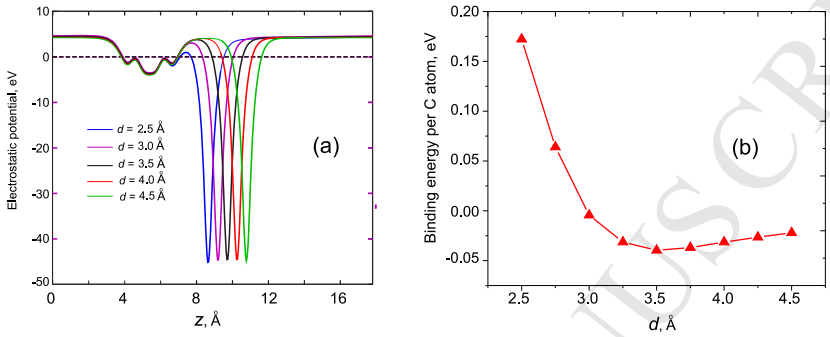

Fig. 5. (a) Plane-averaged electrostatic potentials and (b) the binding energy per carbon atom of G/m-Sb heterostructure at different values of interlayer coupling d.

We next investigate the effects of interlayer coupling and vertical electric field on the electronic properties and Schottky contact of the G/m-Sb heterostructure. Fig. 3 shows the electronic band structures and PDOS of C, and Sb atoms in the G/m-Sb heterostructure at the different interlayer distances. With the increasing interlayer distance d from 3.50 Å to 4.50 Å the Fermi level moves up to conduction bands from valence bands of semiconducting m-Sb, leading to the decrease of n-type SBH from 0.60 eV to 0.25 eV, and to the increase of the p-type SBH from 0.65 eV to 0.94 eV, respectively. On the contrary, with the decreasing interlayer distance from 3.5 eV to 2.5 Å, the Fermi level moves down to valence bands of the m-Sb semiconductor, leading to the increase/decrease of the n-type/p-type SBH from 0.60 eV/0.65 eV to 1.02 eV/0.38 eV, respectively. These results also indicate the transition from a n-type to a p-type Schottky contact with the decreasing in-

terlayer distance. The dependence of the n-type and p-type SBH on the interlayer distance is illustrated in Fig. 4(a). Our results also show that the interlayer coupling has different effects on the charge density. For example, the more interlayer distance decreases, the more electrons transfer from graphene to m-Sb layer, shifting down the Fermi level to the valence band at the G/m-Sb heterostructure. Whereas the more interlayer distance increases, the more electrons transfer from m-Sb layer to graphene layer, shifting up the Fermi level to the conduction band at the G/m-Sb heterostructure. In Fig. 5(a) we present the plane-averaged electrostatic potentials of the G/m-Sb heterostructure at different values of interlayer coupling d. As the interlayer distance decreases, the increased interaction between graphene and m-Sb layers enhances the charge transfer. The variation of the binding energy per carbon atom at the G/m-Sb heterostructure as a function of the interlayer distance d is shown in Fig. 5(b). The results show that the G/m-Sb heterostructure achieves the most stable state at the interlayer distance of 3.5 Å which presents the lowest binding energy.

The electronic band structures of the G/m-Sb heterostructure at different vertical electric fields are shown in Fig. 6. Compared with the band structure of the G/m-Sb at the equilibrium state $d = 3.5$ Å shown in Fig. 2(c), it can be seen that when the negative vertical electric field increases from 0 V/Å to -1 V/Å, the Fermi level moves up gradually from the valence band to the conduction band of the m-Sb semiconductor, leading to a decrease/increase in the n-type/p-type SBH at the G/m-Sb heterostructure from 0.60/0.64 eV to 0.25/0.99 eV, respectively. On the other hand, with the positive vertical electric field increases from 0 V/Å to +1 V/Å, the Fermi level moves down from the conduction band to the valence band of the m-Sb semiconductor, leading to a increase/decrease in the n-type/p-type SBH of the G/m-Sb semiconductor from 0.60/0.64 eV to 1.23/0.06 eV, respectively. This means that the positive electric field can be used to control the transformation from

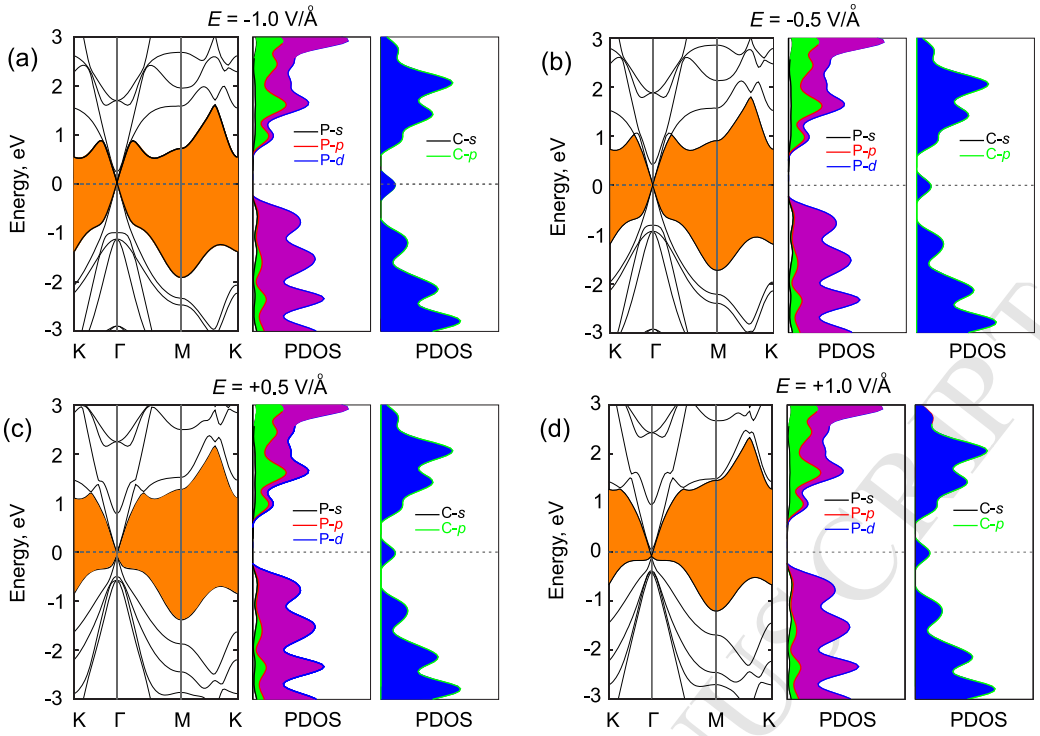

Fig. 6. Band structure and PDOS of C, Pb atoms in van der Waals graphene/antimonene heterostructure under different interlayer distance of -1.0 eV/Å (a), -0.5 eV/Å (b), respectively, and under positive electric field of +0.5 eV/Å (c), +1.0 eV/Å (d), respectively. The Fermi level is set to 0 eV.

a n-type to a p-type Schottky contact. The reason for this transformation can be explained by the fact that with the applied positive electric field, more electrons will transfer from m-Sb to graphene layer, shifting down the Fermi level close to the valence band of m-Sb semiconductor. The Fermi level shift can achieve the transition of Schottky contact from n-type to p-type Schottky contact in the G/m-Sb heterostructure under different out-of-plane strain and electric field.

4 Conclusion

In summary, using density functional theory (DFT) method we have studied the electronic properties of the G/m-Sb heterostructure at the equilibrium state under out-of-plane strain and electric field perpendicular to the surface. Our results

show that the electronic properties of the G/m-Sb are well preserved under bonding due to a weak vdW interaction between graphene and the m-Sb surface. We also find that a n-type Schottky contact is formed in the G/m-Sb heterostructure with the n-type SBH of 0.60 eV. Furthermore, the out-of-plane strain and vertical electric field could be used to control not only the SBH but also the Schottky contacts (n-type, p-type) at the G/m-Sb heterostructure. Especially, we have observed the transformation from n-type to p-type Schottky contact with the decreasing interlayer distance or by applying the positive electric field perpendicularly to the surface. Our results provide the promising potential applications of graphene-based vdW heterostructures in nanoelectronic and optoelectronic devices.

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References

[1] A. K. Geim, K. S. Novoselov, The rise of graphene, Nature Materials 6 (3) (2007) 183–191.

[2] A. C. Neto, F. Guinea, N. M. Peres, K. S. Novoselov, A. K. Geim, The electronic properties of graphene, Reviews of Modern Physics 81 (1) (2009) 109.

[3] K. Novoselov, A. Geim, S. Morozov, D. Jiang, M. Katsnelson, I. Grigorieva, S. Dubonos, A. Firsov, Two-dimensional gas of massless dirac fermions in graphene., Nature 438 (7065) (2005) 197–200.

[4] K. Watanabe, T. Taniguchi, H. Kanda, Direct-bandgap properties and evidence for ultraviolet lasing of hexagonal boron nitride single crystal, Nature Materials 3 (6) (2004) 404.

[5] L. Song, L. Ci, H. Lu, P. B. Sorokin, C. Jin, J. Ni, A. G. Kvashnin, D. G. Kvashnin, J. Lou, B. I. Yakobson, et al., Large scale growth and characterization of atomic hexagonal boron nitride layers, Nano Letters 10 (8) (2010) 3209–3215.

[6] K. F. Mak, C. Lee, J. Hone, J. Shan, T. F. Heinz, Atomically thin MoS_2: a new direct-gap semiconductor, Physical Review Letters 105 (13) (2010) 136805.

[7] Z. Yin, H. Li, H. Li, L. Jiang, Y. Shi, Y. Sun, G. Lu, Q. Zhang, X. Chen, H. Zhang, Single-layer MoS_2 phototransistors, ACS Nano 6 (1) (2011) 74–80.

[8] L. Li, Y. Yu, G. J. Ye, Q. Ge, X. Ou, H. Wu, D. Feng, X. H. Chen, Y. Zhang, Black phosphorus field-effect transistors, Nature Nanotechnology 9 (5) (2014) 372–377.

[9] S. Zhang, Z. Yan, Y. Li, Z. Chen, H. Zeng, Atomically thin arsenene and antimonene: semimetal–semiconductor and indirect–direct band-gap transitions, Angewandte Chemie 127 (10) (2015) 3155–3158.

[10] G. Wang, R. Pandey, S. P. Karna, Atomically thin group V elemental films: theoretical investigations of antimonene allotropes, ACS Applied Materials & Interfaces 7 (21) (2015) 11490–11496.

[11] T. Lei, C. Liu, J.-L. Zhao, J.-M. Li, Y.-P. Li, J.-O. Wang, R. Wu, H.-J. Qian, H.-Q. Wang, K. Ibrahim, Electronic structure of antimonene grown on Sb_2Te_3 (111) and Bi_2Te_3 substrates, Journal of Applied Physics 119 (1) (2016) 015302.

[12] S. Zhang, M. Xie, F. Li, Z. Yan, Y. Li, E. Kan, W. Liu, Z. Chen, H. Zeng, Semiconducting group 15 monolayers: a broad range of band gaps and high carrier mobilities, Angewandte Chemie International Edition 55 (5) (2016) 1666–1669.

[13] Y. Xu, B. Peng, H. Zhang, H. Shao, R. Zhang, H. Zhu, First-principle calculations of optical properties of monolayer arsenene and antimonene allotropes, Annalen der Physik 529 (4).

[14] J. Liang, L. Cheng, J. Zhang, H. Liu, Topological phase transition in antimonene induced by biaxial tensile strain, arXiv preprint arXiv:1502.01610.

[15] T. Roy, M. Tosun, J. S. Kang, A. B. Sachid, S. B. Desai, M. Hettick, C. C. Hu, A. Javey, Field-effect transistors built from all two-dimensional material components, ACS nano 8 (6) (2014) 6259–6264.

[16] C.-J. Shih, Q. H. Wang, Y. Son, Z. Jin, D. Blankschtein, M. S. Strano, Tuning on–off current ratio and field-effect mobility in a MoS_2–graphene heterostructure via schottky barrier modulation, ACS nano 8 (6) (2014) 5790–5798.

[17] Y. Ma, Y. Dai, M. Guo, C. Niu, B. Huang, Graphene adhesion on MoS_2 monolayer: An ab initio study, Nanoscale 3 (9) (2011) 3883–3887.

[18] M. Ghorbani-Asl, P. D. Bristowe, K. Koziol, T. Heine, A. Kuc, Effect of compression on the electronic, optical and transport properties of mos2/graphene-based junctions, 2D Materials 3 (2) (2016) 025018.

[19] N. Hieu, V. P. Huynh, V. Ilyasov, D. Chien, N. Poklonski, V. Hieu, V. N. Chuong, First-principles study of the structural and electronic properties of graphene/MoS_2 interfaces, Journal of Applied Physics 122 (11).

[20] B. Liu, L.-J. Wu, Y.-Q. Zhao, L.-Z. Wang, M.-Q. Caii, Tuning the schottky contacts in the phosphorene and graphene heterostructure by applying strain, Physical Chemistry Chemical Physics 18 (29) (2016) 19918–19925.

[21] J. Padilha, A. Fazzio, A. J. da Silva, van der waals heterostructure of phosphorene and graphene: tuning the schottky barrier and doping by electrostatic gating, Physical Review Letters 114 (6) (2015) 066803.

[22] G. Giovannetti, P. A. Khomyakov, G. Brocks, P. J. Kelly, J. Van Den Brink, Substrate-induced band gap in graphene on hexagonal boron nitride: Ab initio density functional calculations, Physical Review B 76 (7) (2007) 073103.

[23] W. Hu, J. Yang, First-principles study of two-dimensional van der waals heterojunctions, Computational Materials Science 112 (2016) 518–526.

[24] Q. Tang, Z. Zhou, Graphene-analogous low-dimensional materials, Progress in Materials Science 58 (8) (2013) 1244–1315.

[25] P. Giannozzi, S. Baroni, N. Bonini, M. Calandra, R. Car, C. Cavazzoni, D. Ceresoli, G. L. Chiarotti, M. Cococcioni, I. Dabo, A. D. Corso, S. de Gironcoli, S. Fabris, G. Fratesi, R. Gebauer, U. Gerstmann, C. Gougoussis, A. Kokalj, M. Lazzeri, L. Martin-Samos, N. Marzari, F. Mauri, R. Mazzarello, S. Paolini, A. Pasquarello, L. Paulatto, C. Sbraccia, S. Scandolo, G. Sclauzero, A. P. Seitsonen, A. Smogunov, P. Umari, R. M. Wentzcovitch, Quantum espresso: a modular and open-source software project for quantum simulations of materials, J. Phys.: Conden. Matter 21 (39) (2009) 395502.
URL http://stacks.iop.org/0953-8984/21/i=39/a=395502

[26] J. P. Perdew, K. Burke, M. Ernzerhof, Generalized gradient approximation made simple, Phys. Rev. Lett. 77 (18) (1996) 3865.
URL https://doi.org/10.1103/PhysRevLett.77.3865

[27] S. Grimme, Accurate description of van der waals complexes by density functional theory including empirical corrections, Journal of computational chemistry 25 (12) (2004) 1463–1473.

[28] S. Grimme, Semiempirical GGA-type density functional constructed with a long-range dispersion correction, J. Comput. Chem. 27 (15) (2006) 1787–1799.
URL http://onlinelibrary.wiley.com/doi/10.1002/jcc.20495/full

[29] P. Xu, Q. Tang, Z. Zhou, Structural and electronic properties of graphene–zno interfaces: dispersion-corrected density functional theory investigations, Nanotechnology 24 (30) (2013) 305401.

[30] W. Li, T.-X. Wang, X.-Q. Dai, X.-L. Wang, Y.-Q. Ma, S.-S. Chang, Y.-N. Tang, Tuning the schottky barrier in the arsenene/graphene van der waals heterostructures by electric field, Physica E: Low-dimensional Systems and Nanostructures 88 (2017) 6–10.

[31] V. Ilyasov, B. Meshi, V. Nguyen, I. Ershov, D. Nguyen, Magnetism and transport properties of zigzag graphene nanoribbons/hexagonal boron nitride heterostructures, Journal of Applied Physics 115 (5) (2014) 053708.

[32] V. V. Ilyasov, C. V. Nguyen, I. V. Ershov, N. N. Hieu, Effect of electric field on the electronic and magnetic properties of a graphene nanoribbon/aluminium nitride bilayer system, RSC Advances 5 (61) (2015) 49308–49316.

[33] A. Rudenko, M. Katsnelson, R. Roldán, Electronic properties of single-layer antimony: Tight-binding model, spin-orbit coupling, and the strength of effective coulomb interactions, Physical Review B 95 (8) (2017) 081407.

[34] M. Sun, J.-P. Chou, Q. Ren, Y. Zhao, J. Yu, W. Tang, Tunable schottky barrier in van der waals heterostructures of graphene and g-GaN, Applied Physics Letters 110 (17) (2017) 173105.

[35] W. Xiong, C. Xia, X. Zhao, T. Wang, Y. Jia, Effects of strain and electric field on electronic structures and schottky barrier in graphene and SnS hybrid heterostructures, Carbon 109 (2016) 737–746.

[36] J. Bardeen, Surface states and rectification at a metal semi-conductor contact, Physical Review 71 (1947) 717–727.

[37] W. Chen, E. J. Santos, W. Zhu, E. Kaxiras, Z. Zhang, Tuning the electronic and chemical properties of monolayer MoS_2 adsorbed on transition metal substrates, Nano Letters 13 (2) (2013) 509–514.

HIGHLIGHTS

- Electronic properties of the G/m-Sb heterostructure without and with out-of-plane strain and vertical electric field have been studied using DFT calculations.
- The electronic properties of the G/m-Sb are well preserved under bonding due to a weak vdW interaction between graphene and the m-Sb surface.
- We also found that a n-type Schottky contact is formed at the G/m-Sb heterostructure with the n-type SBH of 0.60 eV.
- Furthermore, the out-of-plane strain and vertical electric field could be used to control not only the SBH but also the Schottky contacts at the G/m-Sb heterostructure.
- The results provide the promising potential applications of graphene-based vdW heterostructures in nanoelectronic devices.