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Tuning the electronic properties and Schottky barrier height of the vertical graphene/MoS_2 heterostructure by an electric gating

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ABSTRACT

In this paper, the electronic properties and Schottky contact in graphene/MoS_2 (G/MoS_2) heterostructure under an applied electric field are investigated by means of the density functional theory. It can be seen that the electronic properties of the G/MoS_2 heterostructure are preserved upon contacting owing to the weak van der Waals interaction. We found that the *n*-type Schottky contact is formed in the G/MoS_2 heterostructure with the Schottky barrier height of 0.49 eV. Furthermore, both Schottky contact and Schottky barrier height in the G/MoS_2 heterostructure could be controlled by the applied electric field. If a positive electric field of 4 V/nm is applied to the system, a transformation from the *n*-type Schottky contact to the *p*-type one was observed, whereas the system keeps an *n*-type Schottky contact when a negative electric field is applied. Our results may provide helpful information to design, fabricate, and understand the physics mechanism in the graphene-based two-dimensional van der Waals heterostructures like as G/MoS_2 heterostructure.

1. Introduction

Graphene [1–4] and other two−dimensional materials such as hexagonal boron nitride (*h*-BN) [5,6], transition metal dichalcogenides (TMDs) [7–9] have attracted considerable interest owing to their extraordinary electronic, optical, transport properties and wide potential applications. Graphene is well-known as a promising material for future applications in the field of nanoelectronics and optoelectronics, such as field effect transistors (FETs), light-emitting diode (LED). However, the absence of an electronic band gap, which is necessary for many application fields, has limited its applications in the electronic devices. Unlike graphene, MoS_2 monolayer, one of the most typical TMDs materials, has a direct band gap semiconductor of 1.8 eV [10], a high on/off current ratio of 10^8, and a high carrier mobility of 200 cm^2/Vs at room temperature, making it a great potential applications in FETs [11] and photodetectors [12]. Recently, the MoS_2 single-layer sheet with honeycomb structure has been successfully synthesized on the Au(111) surface [10,13]. To date, the structural, electronic, mechanical and transport properties of MoS_2 monolayer have been widely studied experimentally and theoretically [9,14–19]. These results showed that the physical properties of MoS_2 monolayer are very sensitive to external conditions like as strain, electric field, and

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pressure. In addition, the indirect-to-direct and semiconductor-to-metal transitions were observed in MoS_2 monolayer under strain and electric field, which opens up its potential applications in the field of nanoelectronics and optoelectronics.

Recently, vertical heterostructure based on graphene and other 2D materials is one of the novel ways to design electronic and optoelectronic devices. Up to date, numerical experimental and theoretical efforts have been made to synthesize and explore new graphene-based heterostructures, such as graphene/phosphorene [20–22],graphene/GaN [23–25], graphene/*h*-BN [26–28]. One can be observed that in these heterostructures, graphene bonds to other 2D materials by the weak van der Walls (vdW) interactions. Thus, the intrinsic electronic properties of both graphene and 2D materials are well preserved upon contacting. Moreover, these graphene-based heterostructures provide more new properties beyond their single components. Currently, the possibility of making vdW G/MoS_2 heterostructure has been synthesized experimentally for memory devices [29], photodetectors [30] and electronic devices [31]. In order to further understand the potential applications of graphene-based heterostructures, we previously studied the electronic properties and Schottky contacts in G/MoS_2 heterostructure in its different stacking configurations [32] and under interlayer coupling [33]. The results showed that the electronic properties and Schottky barrier height in G/MoS_2 heterostructure can be controlled by changing the interlayer distances. Furthermore, the external electric field can also be used to modulate the electronic properties of the graphene-based heterostructures [34–37]. Thus, it is necessary to know more about the possible electronic properties of the G/MoS_2 heterostructure under the electric field.

In this work, we focus on the electronic properties and Schottky barrier height modulation in the G/MoS_2 heterostructure by applying an electric field using the density functional theory. The novel properties of the G/MoS_2 heterostructure can be used to fabricate potential applications in the field of graphene-based electronic and nanoelectronic devices.

2. Computational method details

In this work, all the calculations were performed by using density functional theory (DFT), which is implemented in the Quantum Espresso simulation package [38]. We use the generalized gradient approximation of Predew, Burke, and Ernzerhof (PBE) for the exchange correlation energy. It should be noted that the traditional DFT method overestimates the binding in weakly bonded systems where interactions are mainly of van der Waals type [39,40]. On the other hand, many research effort has been devoted to include vdW forces in the studies of graphene/semiconductors heterostructures, such as graphene/ZnO [41], graphene/phosphorene [37], graphene/SnS [34], graphene/GaN [23]. Therefore, in order to describe a weak vdW interaction, we use the semi–empirical vdW corrected DFT (DFT-D2), which was proposed by Grimme [39]. In DFT-D2 method the vdW interaction was described by adding a semi–empirical dispersion potentials to the conventional DFT energy. In order to describe the electron–ion potential, we use the projected augmented wave (PAW). The kinetic cut–off energy is set to 500 eV for the plane wave expansion. The first Brillouin zone (BZ) sampling of $6 \times 6 \times 1$ MonkhorstPack *k*–point grid is used to perform geometric optimization, whereas the BZ sampling of $9 \times 9 \times 1$ k-point grid is used to perform all the electronic properties calculations. In addition, a large vacuum region of 20 Å is used to avoid artificial interactions between the periodic slabs. All geometric structures are fully relaxed until energy and forces are converging to 10^6 eV and 0.001 eV/Å, respectively.

3. Results and discussion

To study the electronic properties of G/MoS_2 heterostructure, we first studied the electronic properties of freestanding graphene and an isolated MoS_2 monolayer using density functional theory with dispersion-corrected approximation, which was proposed by Grimme [42]. Our calculated lattice parameters of freestanding graphene and isolated monolayer MoS_2 are 2.461 Å, and 3.18 Å, respectively. These results are in good agreement with previous theoretical results [14–16,43] and experimental measurements [2,44]. It can be seen that the lattice mismatch between graphene and MoS_2 monolayer is about 22%. Thus, in order to construct the G/MoS_2 heterostructure, we used a (5×5) supercell of graphene and a (4×4) supercell of MoS_2 monolayer. The lattice mismatch between graphene and MoS_2 monolayer is about 1.8 Å, which has little effects on the electronic properties of graphene and thus do not affect the main electronic properties of the heterostructure. It was confirmed in our previous results [32,33]. Atomic structure of G/MoS_2 heterostructure after relaxation is illustrated in Fig. 1. In this work, we consider only one representative arrangement of G/MoS_2 heterostructure owing to its stable [32]. In this stacking configuration, one C atom of graphene layer located directly on the top of an S atom and one of the graphene hexagonal ring centered above Mo–S hexagonal ring. After relaxation, one can be observed that the graphene layer keeps its planar form. The obtained interlayer distance between graphene and topmost layer of MoS_2 monolayer is 3.34 Å at the equilibrium state. This interlayer distance is very close to other the previous theoretical results in graphene-based van der Waals heterostructures, such as graphene/*h*-BN [45,46], G/MoS_2 [47,48], graphene/ZnO [41,49], graphene/phosphorene [20,37], graphene/arsenene [36], which indicate that graphene layer is bound to the MoS_2 monolayer by a weak vdW interaction. Moreover, in order to evaluate the stability of the G/MoS_2 heterostructure, we next calculate the binding energy per carbon atom in the G/MoS_2 heterostructure. The binding energy can be calculated as follows: $E_b = [E_{G/MoS_2} - (E_G + E_{MoS_2})]/N$, where E_{G/MoS_2}, E_G and E_{MoS_2} are total energy of G/MoS_2 heterostructure, the freestanding graphene, and the isolated MoS_2 monolayer, respectively. N is the number of carbon atoms in calculated supercell ($N = 50$). The obtained binding energy per carbon atom in the G/MoS_2 heterostructure is only -25.1 meV, one also indicates that the graphene is found to interact very weakly with MoS_2 monolayer.