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Electrically tunable band gap of the 1T-MoS_2 based heterostructure: A first-principles calculation

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ABSTRACT

First-principles density functional theory (DFT) calculations are performed on the structural and electronic properties of the 1T-MoS_2/BN van der Waals (vdW) heterostructures under an external electric field (E-field). Our results reveal that the 1T-MoS_2/BN vdW heterostructure has a direct band gap of 0.39 eV in the raw. The results also imply that electrons are likely to transfer from MoS_2 to BN monolayer due to the deeper potential of BN monolayer. It is also observed that, by applying an E-field, ranging from 0.0 to +0.50 V/Å, the band gap decreases from 0.39 eV to zero. Through partial density of states (PDOS) plots, it is revealed that, d and p orbitals of Mo, S, B, and N atoms are responsible for the significant variations of band gap. These obtained results predict that, the electric field tunable band gap of the 1T-MoS_2/BN vdW heterostructures carries potential applications for nanoelectronics and spintronic device applications.

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1. Introduction

Graphene, as a typical monolayer honeycomb structure, has got wide interest. A large number of researches have verified its superior properties than conventional materials [1–3]. Two-dimensional (2D) materials will have potential applications for future nanoscale devices [4,5]. However, the 2D materials still face important challenges, such as growth of large areas, the integration in current Si-based nanotechnologies, which seriously restricts its practical application. In this aspect, searching substitutable 2D materials, which have supereminent chemical and physical properties, is under significant research interests [6–9]. Among those 2D materials, 1T-MoS_2 monolayer has attracted much interest and demonstrated to be powerful in future nanoscale devices [10–12]. Quite different from 1T-MoS_2, BN monolayer has a large direct band gap and has been widely studied [13,14]. These studies give useful information to produce potential applications in electronic and optoelectronic devices.

Discovery of new 2D materials, has stimulated the scientific community to study and analyze the van der Waals (vdW) heterostructures, which consisted of different types of different 2D materials. It has been suggested in previous studies that, the vdW heterostructures having unique chemical and electronic properties, such as graphene/BN [15,16], graphene/TMD [17,18], phosphorene/TMD [19], holds wide range of technological applications. In order to facilitate the vdW heterostruc-

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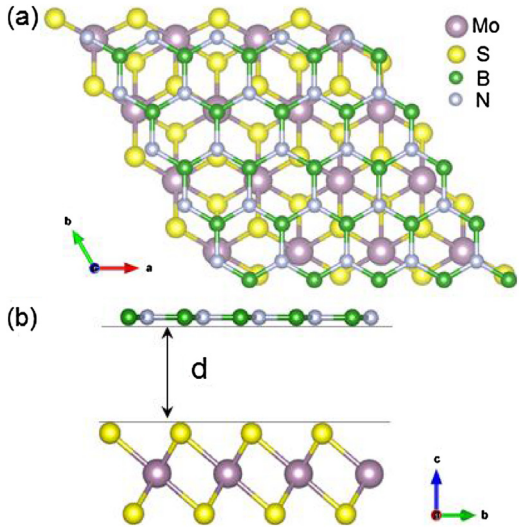

Fig. 1. The 1T-MoS_2/BN vdW heterostructures of (a) top and (b) side views. The interlayer distance (d) changes along the c-axis. (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article).

tures to be utilized for spintronic device applications, it is crucial to modulate the band gap with the help of geometrical strain or an external electric field (E-field) [20–25]. Monolayer 1T-MoS_2 and h-BN contain similar atomic structures but showing different characteristics; it is worthwhile to investigate the 1T-MoS_2/BN vdW heterostructures and unique electronic properties different form pristine 1T-MoS_2 and BN would be expected.

In this study, we try to investigate electronic structures of the 1T-MoS_2/BN vdW heterostructures under the application of an external E-field. First-principles study calculations have been performed on the 1T-MoS_2/BN vdW heterostructures and aforementioned properties have been investigated comprehensively. Without any E-field, an indirect band gap of 0.39 eV is shown. With an external E-field, very interesting phenomena have been observed. A tunable band gap, ranging from 0.39 to 0.0 eV, has been observed and the decreasing tendency presents a parabola-like relationship with the E-field. Our obtained results can enable the electronic properties of the 1T-MoS_2/BN vdW heterostructures to be modified for desired engineering applications, particularly spintronic and nanoelectronics device applications.

2. Method

The electronic and magnetic properties in this paper are performed by the density functional theory (DFT) implemented in the VASP code [26]. The Perdewe-Burkee-Ernzerhof (PBE) of exchange-correlation calculations with the generalized gradient approximation (GGA) are used [27]. The projector-augmented wave (PAW) potentials [28] are used with a 450 eV cut-off energy. The vdW correction (DFT-D2) within the PBE functional proposed by Grimme is applied [29]. A set of $5 \times 5 \times 1$ k-points are used. The lattice constants of 2D-BN and 1T-MoS_2 are 2.503 and 3.160Å. The 1T-MoS_2/BN vdW heterostructure is made up of a $4 \times 4 \times 1$ 1T-MoS_2 monolayer (48) and a $5 \times 5 \times 1$ BN monolayer (50 atoms), as shown in Fig. 1(a) and (b). The 1T-MoS_2/BN vdW heterostructures having only 1.2% lattice disparity, which has little effects on the electronic properties in the vdW heterostructure. To simulate the 1T-MoS_2/BN vdW heterostructure, a vacuum of 20 Å along the z-direction is added. Geometry relaxation was processed until, the given structures were fully optimized, and the Hellmann–Feynman forces less than 0.01 eV/Å and the total change in energy less than 10^{-6} eV was obtained.

3. Results and discussion

Firstly, we explored the electronic structure of pristine BN and 1T-MoS_2 monolayer. The 1T-MoS_2 monolayer shows the metallic characteristic and the BN shows a direct band gap of 4.50 eV, as shown in Fig. 2(a) and (b). These results are consistent with previous reports [11,30]. These results verified the reliability of our methods. We calculated the adsorption energy for the 1T-MoS_2/BN bilayer in order to verify the stability of given systems using following expression;

$$E_b = E_T - (E_{MoS2} + E_{BN})$$

where E_T is the total energy of the 1T-MoS_2/BN vdW heterostructure; E_{MoS2} and E_{BN} are the total energies of pure 1T-MoS_2 and BN monolayers. Based on calculated binding energies, as shown in Fig. 3, the binding energy changes demanding on the distance between 1T-MoS_2 and BN monolayers and gets the lowest value of −0.067 eV at an equilibrium distance of $d_0 = 4.80$ Å. Moreover, we calculate the plane averaged charge density differences and electrostatic potentials of the vdW

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