Tuning of Schottky Barriers in Borophene/MoS_2 Van der Waals Heterostructure by External Electric Field

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Abstract. A first principle study of structural properties, band bending and tuning of schottky barrier height (SBH) of borophene/MoS_2 Van der Waals heterostructure has been carried out within the framework of density functional theory (DFT). Studied binding energy shows that the interaction between borophene and MoS_2 is weak. Consequently, both borophene and MoS_2 are preserving their electronic nature in heterostructure. We have calculated the band bending 0.15 eV for borophene and -0.52 eV for MoS_2 in borophene/MoS_2 heterostructure which shows that the metal-semiconductor contact is in between p-type borophene and n-type MoS_2. On the application of external electric field, tuning of schottky barriers has been achieved and metal-semiconductor contact gets transformed into ohmic contact which is important for the fast performance of electronic devices.

INTRODUCTION

The emergence of atomically thin layered materials such as graphene [1] and two-dimensional (2D) semiconductors such as transition metal dichalgogenides (TMDs [2-4] have opened up a window for searching and predicting new members into the families of heterostructures with novel properties to explore the possibility of innovative heterostructure devices. One such material is borophene which is 2D atomic layer of boron atoms. Borophene possess exotic properties including anisotropy and polymorphism [5]. It is the lightest 2D metal [6], which is mechanically strong [7], optically transparent [8], is promising anode material [9] presenting itself to be used in various applications. The borophene (β_{12}) has unique metallic properties which are expected to be useful when integrated into heterostructures with other 2D materials [10]. Vertically stacked heterostructrues incorporating borophene are expected to yield numerous benefits. As an example, 2D metal-semiconductor junctions are likely to enable a range of applications, such as atomically thin Schottky diodes and tunneling transistors [11].

Therefore, in the present work we report first-principles investigation on the structural properties, band bending in pristine borophene/MoS_2 heterostructure and effect of the electric field on the schottky barrier heights (SBH) of borophene contacted MoS_2 Van der Waals heterostructure.

SIMULATION DETAILS

In this study, all calculations which involve geometry optimization and electronic structures etc. are performed within the framework of Density functional theory (DFT) as implemented in the Vienna Ab initio Simulation Package (VASP) [12]. We use the generalized gradient approximation (GGA), in Perdew, Burke, and

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Ernzerhof parametrization [13] to describe the exchange-correlation effects. The electron-ion interactions are taken into account using the Projector Augmented Wave (PAW) method [14]. The cutoff of plane-wave kinetic energy and the convergence of total energy were set to be 700 eV and 10^{-5} eV, respectively, which were tested to achieve sufficiently a high accuracy. To describe the Van der Waals interactions we have made use of the vdW-D2 approach [15]. A 15x9x1 k-point mesh was employed for Brillouin zone integrations. The structural relaxations were performed by computing the Hellmann-Feynman forces using conjugate gradient algorithm within a force convergence of 0. 001 eV/Å. To minimize the lattice mismatch, the supercell contains 1x1borophene and 2x1 MoS_2. A vacuum region of more than 20 Å was taken along the z-axis in order to minimize the interactions of interface with its periodic image.

RESULTS AND DISCUSSIONS

Structural Properties

The top and side views of studied Van der Waals heterostructure of borophene (1x1) and MoS_2 (2x1) are shown in figure 1. Our calculated lattice constants for studied system are a = 3.04 Å and b = 6.09 Å, respectively. Calculated lattice mismatch is 1.1%. In order to check the interlayer interaction of borophene and MoS_2 heterostructure, the binding energy is calculated as E_b:

$$E_b = \left[E_{borophene+MoS_2} - E_{borophene} - E_{MoS_2}\right]/N \tag{1}$$

where, $E_{borophene+MoS_2}$, $E_{borophene}$, E_{MoS_2} and N are the total energy of borophene/MoS_2 composite system, total energy of isolated borophene layer, total energy of isolated MoS_2 layer and total number of atoms in the heterostructure respectively. The calculated binding energy is -0.03eV per atom, which is very weak and is typically representing van der Waals interaction in the considered system for equilibrium interlayer distance 3.23 Å.

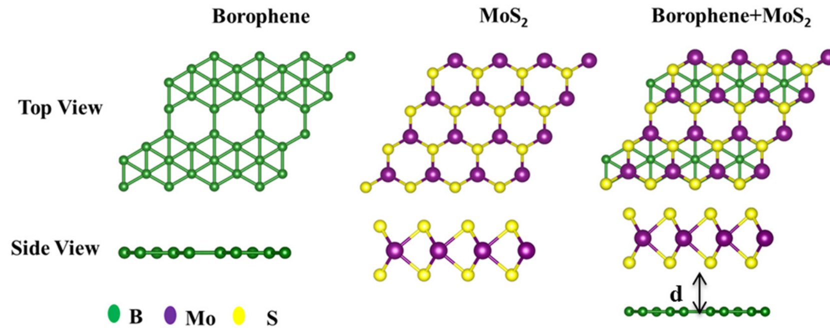

Figure 1. Ball and stick model with respective top and side views of pristine borophene, MoS_2 and their heterostructure (borophene+MoS_2).

ELECTRONIC PROPERTIES

Studied electronic properties for pristine borophene/MoS_2 heterostructure show that borophene interacts with MoS_2 through Van der Waals interactions. Therefore, their intrinsic electronic properties are preserved upon their contact as shown in figure 2 (@E = 0 V/Å). We can observe a small amount of band bending as we move from the region where there are stacked borophene and MoS_2 to the region where only MoS_2 is present [3, 4]. One can obtain the band bending as:

$$\Delta E_F = \Phi_{borophene+MoS_2} - \Phi_P \tag{2}$$

Where, $\Phi_{borophene+MoS_2}$ is the work function of the borophene/MoS_2 and Φ_P is the work function of isolated layers. Band bending in borophene/MoS_2 heterostructure is calculated to be 0.15 eV for borophene and -0.52 eV for

MoS_2. Since $\Delta E_F > 0$ for borophene that means it is p-type contact and $\Delta E_F < 0$ for MoS_2 which shows n-type contact in metal-semiconductor heterostrcuture. From device point of view, it is important to discuss about schottky barrier height (SBH) in metal-semiconductor heterostructure. The vertical schottky barriers for holes or electrons are determined from the energy difference between the Fermi level of borophene and the valence band maximum (VBM) or the conduction band minimum (CBM) of MoS2. We obtained p-type schottky barrier for holes with height of 0.62 eV and n-type schottky barrier for electrons with height of 1.04 eV.

Next we apply external perpendicular electric field, which offers a practical route to tune the schottky barrier heights and can lead to have more efficient carrier injection in electronic devices. On applying perpendicular electric field as high as +1.2 V/Å, VBM of the MoS_2 crosses the Fermi level which shows that SBH for holes has been transformed into p-type ohmic contact. On the other hand, changing the polarity of electric field to -1.2V/Å, CBM of the MoS_2 crosses the Fermi level which shows that the SBH for electrons has been transformed into n-type ohmic contact.

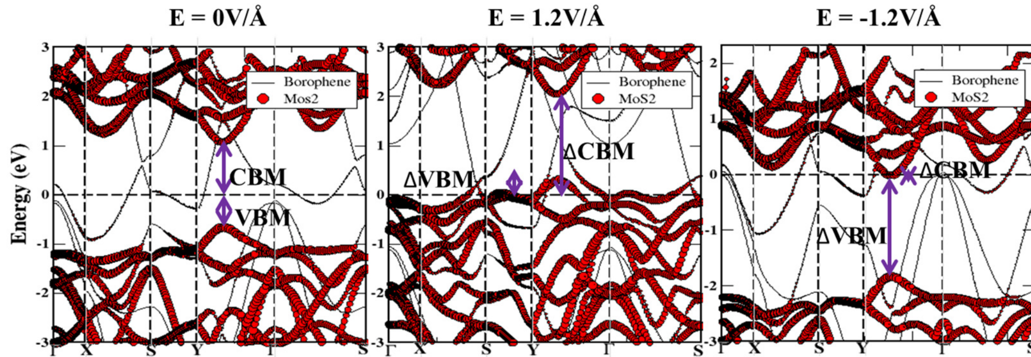

Figure 2. Band structure for pristine borophene/MoS2 and borophene/MoS2 at E = ±1.2V/Å respectively. Width of the bands shows the weight factor. The dashed line at 0 eV represents the Fermi level.

In order to gain further understanding of band structures of borophene/MoS_2 heterostructure, we have analyzed the charge density difference profiles as shown in figure 3.

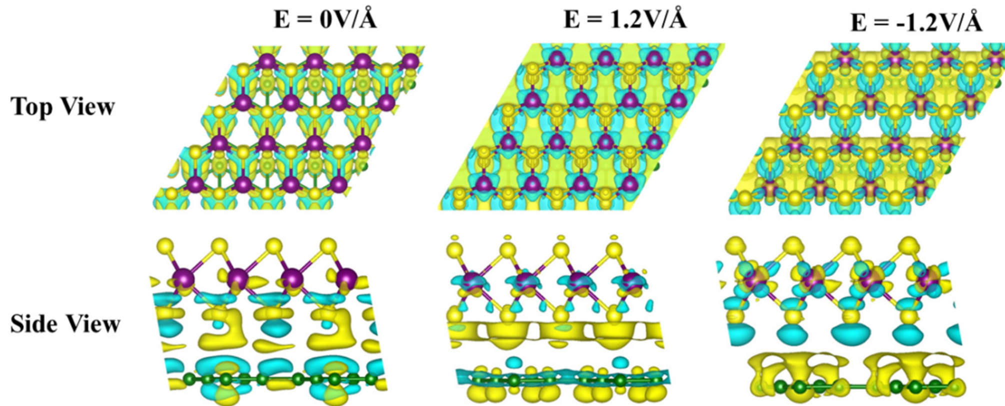

Figure 3. Charge density difference profiles for borophene/MoS_2 heterostructure at different value of external electric field. Isosurface value is set at $1x10^{-3}$ e/Å^{3}. Yellow region shows charge accumulation and blue region shows charge depletion.

The charge density difference can be obtained as:

$$\rho = \rho_{borophene+MoS_2} - \rho_{borophene} - \rho_{MoS_2} \tag{3}$$

Where $\rho_{borophene+MoS_2}$ the total charge density of the heterostructure , $\rho_{borophene}$ is the charge density of borophene and ρ_{MoS_2} is the charge density of MoS_2. We can see in figure 3 that charges get accumulated/depleted on applying positive/negative electric field that results into the change in energy bands on the application of external field.

TABLE 1. Calculated binding energy (**E_b**) per atom, interlayer distance (**d**), SBHs for electrons (**ϕ_e**) and for holes (**ϕ_h**), and band bending ΔE_F for pristine borophene/Mos_2 heterostructure.

System	E_b (eV)	d(Å)	SBH(eV)		Band-Bending ΔE_F (eV)	
			Øe	Øh	Borophene	Mos_2
Borophene/MoS2	-0.03	3.23	1.04	0.62	0.15	-0.52

CONCLUSIONS

In summary, first principles calculations within the framework of density functional theory (DFT) are performed for structural properties, band bending and tuning of schottky barrier height (SBH) of borophene/MoS_2 Van der Waals heterostructure. The interlayer binding energy is weak which is corresponding to the Van der Waals interaction between borophene and MoS_2. Consequently, both borophene and MoS_2 layers preserve their electronic nature upon contact. We have reported the band bending 0.15 eV for borophene and -0.52 eV for MoS_2 in borophene/MoS_2 heterostructure.We have found that on the application of electric field in the range ±1.2V/Å, schottky barrier heights for hole and electron can be tuned to form ohmic contacts which are important for the fast performance of electronic devices.

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