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An ab initio study of the ferroelectric In₂Se₃/graphene heterostructure.

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Abstract

Using ab initio calculations, we have investigated the electronic structure properties of the ferroelectric α -In₂Se₃/graphene heterostructure. The presence of an intrinsic polarization in In₂Se₃ shifts the Dirac point of graphene above the Fermi level, resulting in a p-type doping, the degree of doping being dependent on the direction of the dipole with respect to the graphene layer. Also, we found that an external electric field can be used to control not only the degree of doping but also the type of Schottky contact, as n-type, p-type or Ohmic.

Keywords: ab initio calculations, ferroelectric, heterostructure

1. Introduction

The isolation of graphene has made possible to highlight a great variety of new physical properties [1, 2] of interest both for fundamental research and for the development of new applications. This discovery opened the way for studying a wide variety of materials with a two dimensional form, such as hexagonal boron nitride [3, 4], silicene [5], germanane [6], transition metal dichalcogenides [7, 8, 9] and certain III-VI compounds [10, 11, 12, 13]. In parallel, materials characterized by ferroelectric and piezoelectric properties are exploited for applications as memories[14], capacitors[15], actuators[16], and sensors[17]. However among

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two dimensional materials these properties are relatively scarce: for instance some theoretical

and experimental studies[18, 19] on transition metal dichalcogenides such as 2H-MoS₂, showed that in-plane piezoelectricity appears for an odd number of few layers. The features of two dimensional materials with piezoelectric and ferroelectric properties have been reviewed recently [20, 21] and for instance it was shown in a recent publication[22] that SnSe can be used as a two-dimensional ferroelectric tunnel junction.

In₂Se₃ compounds are known to be of use in phase change memory, thermoelectric, and photoelectric applications[23, 24]. Also, single and few-layer In₂Se₃ flakes have been obtained on different substrates, such as graphene and mica by van der Waals epitaxy[25]. Recently the 2D semiconductor α -In₂Se₃ has been theoretically[26] predicted and experimentally[27, 28] demonstrated to have both in-plane and out-of plane ferroelectric polarizations. These findings opened a new field concerning the exploration of the properties of 2D ferroelectrics materials, specially when combined with an other bidimensional material to form a van der Waals heterostructure. For instance, Wan et al[29] have recently designed a ferroelectric diode fabricated from graphene and α -In₂Se₃ layers, with an on/off ratio of $\sim 10^5$. Moreover, a non-volatile memory in a hybrid 2D ferroelectric field effect transistor (FeFET) made of ultrathin α -In₂Se₃ and graphene has been realized[30].

Herein, and due to the lack of information about the effect of In₂Se₃ on the properties of graphene, we have conducted DFT calculations to investigate the possibility of an electrostatic doping of graphene by the intrinsic dipole moment of the ferroelectric α -In₂Se₃ layer.

2. Computational details

Our calculations were performed using the Vienna Ab initio Simulation Package (VASP)[31] and the projector-augmented wave method[32]. For the exchange and correlation potential, the generalized gradient approximation of Perdew-Burke-Ernzerhof (GGA-PBE)[33] was used. The cutoff energy for the plane-wave basis set was set to 500 eV. The dispersion correction of Tkatchenko and Scheffler[34] with iterative Hirshfeld partitioning[35] (TS/HI) as implemented recently[36, 37] in VASP was used to describe van der Waals interactions. A 12x12x1 k-mesh was used for the Brillouin zone sampling and a vacuum of 17 Å along the direction perpendicular to the layers was adopted to ensure decoupling between periodically repeated systems. The convergence parameters were set to 0.01 eV/Å for the residual forces on ions and to 10⁻⁶ eV for the total energy.

3. Results and discussion

Due to the inequivalent sides of the ferroelectric layer α -In₂Se₃, two different configurations (noted hereafter C₁ and C₂) can be obtained for the α -In₂Se₃/graphene heterostructure, as shown in figure 1. In the C₁ configuration, the spontaneous out-of-plane electric polarization (P) is pointing towards graphene, while in the C₂ configuration P is pointing away from In₂Se₃. To limit the lattice mismatch between α -In₂Se₃ ($a = 4.06 \text{ \AA}$) and graphene ($a = 2.46 \text{ \AA}$) in our calculations, our simulation cell was built from a 5 x 5 graphene supercell and a 3 x 3 α -In₂Se₃ supercell. After performing a geometry relaxation of the heterostructure, we obtained a lattice parameter of 12.29 \AA , where the α -In₂Se₃ layer is under a biaxial tensile strain of 0.92%, while graphene is under a biaxial compressive strain of -0.08%.

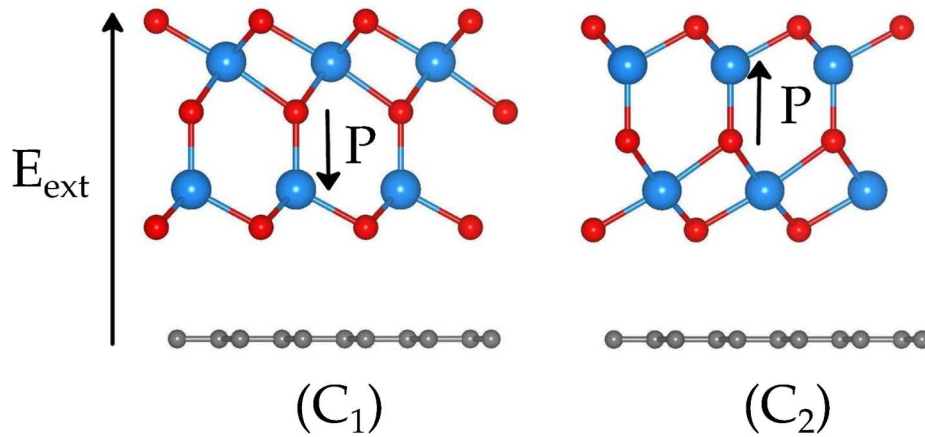


Figure 1: (color online) Side view of the two possible α -In₂Se₃/graphene heterostructure geometries. The red spheres represent the selenium atoms, the blue spheres correspond to indium atoms, and the gray spheres represent the carbon atoms. The black arrow indicate the direction of the out-of-plane ferroelectric polarization (P) of In₂Se₃. A vertical external electric field (E_{ext}) is applied perpendicular to the layers.

Our calculated interlayer distance and binding energy are presented in table 1. The interlayer distance is determined as the selenium-carbon distance along the stacking direction and the binding energy E_b per atom is calculated as $E_b = (E_0 - E_+)/N$, where E_0 is the total energy at equilibrium, E_+ is the total energy when the layers are put at a sufficient distance to avoid interlayer interactions, and N is the number of atoms in the cell. For both configurations, we found a binding energy and an interlayer distance which are typical of van der Waals interactions, similarly to other 2D based heterostructures[38, 39]. Also according to

our calculations, the C_2 heterostructure is slightly more stable than the C_1 heterostructure, by about 1.80 meV/atom (1.14 meV/Å²).

Table 1: Calculated interlayer distance d (in Å) and binding energy E_b (in meV/atom and in meV/Å²) of the α -In₂Se₃/graphene heterostructure .

Geometry	d (Å)	E_b (meV/atom)	E_b (meV/Å ²)
C_1	3.68	20.6	6.19
C_2	3.67	22.4	7.33

Due to the effect of spin-orbit coupling (SOC) on the bandstructure of α -In₂Se₃[11], one may anticipate that the SOC may also affect the electronic structure of the In₂Se₃/graphene bilayer, and more specifically the band alignment. When taking into account the SOC, we found that for both C_1 and C_2 only the VBM (valence band maximum) of In₂Se₃ is affected, with a shift in energy of about 0.02 ~ 0.03 eV. Since the effect of SOC is obviously weak, it will be ignored in the rest of our calculations.

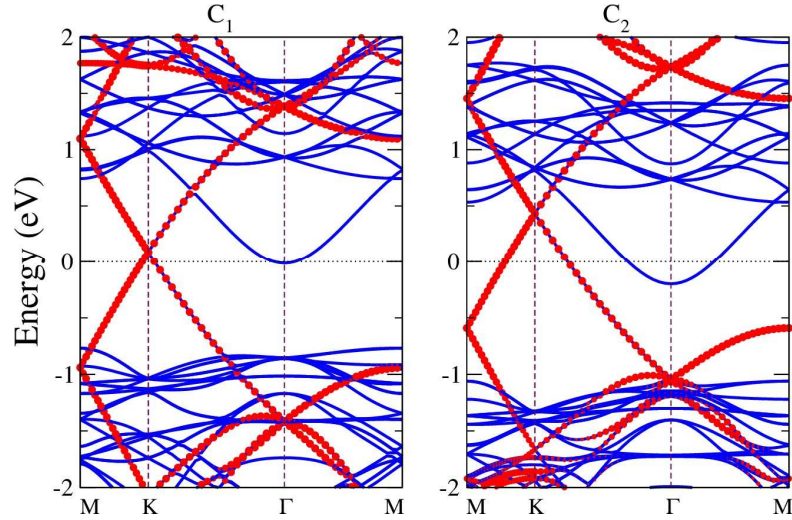


Figure 2: Bandstructure of the C_1 and C_2 configurations of the graphene/ α -In₂Se₃ heterostructure: the projection on the graphene atoms is pictured by red circles, while the projection on the In₂Se₃ layer is denoted by blue lines. The Fermi level is set to 0 eV.

The PBE bandstructure of the two configurations is shown in figure 2. We observe that the Dirac cone of graphene is preserved in the heterostructure, although the graphene layer is p-doped due to the presence of the In₂Se₃ layer. Obviously, the doping level is

dependent on the direction of the polarization of In_2Se_3 : for the C_1 configuration where the intrinsic dipole is directed towards graphene, the Dirac point of graphene and the CBM (conduction band minimum) of In_2Se_3 are shifted relatively to the Fermi energy by ~ 0.09 and -0.013 eV. However, when the intrinsic dipole of In_2Se_3 is in the opposite direction, the shift of the Dirac point of graphene and the CBM of In_2Se_3 relatively to the Fermi energy is much larger, by about 0.43 and -0.21 eV.

In Fig 3, we present our computed electron density difference between the graphene/ α - In_2Se_3 heterostructure and the isolated layers. As expected, the charge redistribution mainly occurs at the interface between the layers, with an accumulation of electrons on the In_2Se_3 layer and a depletion of charges on the graphene layer, which corresponds to the p-doping of the graphene layer observed in Fig. 2. Also, we observe that the charge redistribution is more intense for the C_2 configuration, which pictures a larger charge transfer between the layers than in the C_1 configuration, and confirms the fact that the shift of the Dirac point of graphene is larger for the C_2 arrangement.

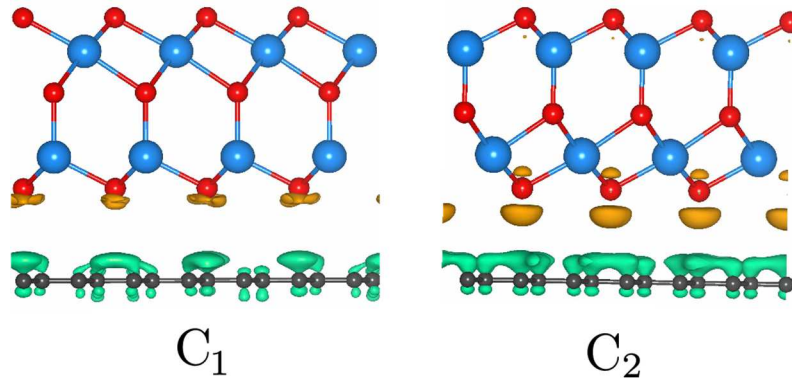


Figure 3: Electron density difference for the configurations C_1 and C_2 of the graphene/ In_2Se_3 heterostructure. The isosurface value for the two configurations is $0.0003 \text{ e}/\text{\AA}^3$, where the accumulation and depletion of electrons are represented in orange and green, respectively.

For the performance of graphene/ In_2Se_3 heterostructures based FET, the investigation of their band offset under the effect of an external electric field is a key point. The evolution of the Dirac point, VBM, and CBM, of graphene and In_2Se_3 , respectively, under the application of an electric field, are shown in figures 4a and 4b. The positive sign of the electric field is defined as shown in figure 1. For the C_1 configuration we found that the p-doping of graphene is increased upon the application of a positive electric field and reduced with the application of a negative electric field to reach neutrality with an applied electric field of less than ~ -0.1

$\text{V}/\text{\AA}$. Concerning the C_2 configuration, the increase and the reduction of the p-doping of graphene under an applied positive and negative electric field is also observed. However, the neutrality between the two materials is not reached even with an applied electric field of $-0.4 \text{ V}/\text{\AA}$ due to the larger p-doping of graphene. In addition to the control of the graphene doping, we found that the application of an electric field modifies the energy gap of In_2Se_3 : when the intrinsic polarization of In_2Se_3 is directed towards graphene, the band gap increases with a positive electric field and is reduced with a negative electric field. When the direction of the intrinsic dipole is switched in the opposite direction of graphene, an inverse behavior is found.

To deepen our analysis, we present in figures 4c and 4d, the evolution of the n- and p-type Schottky contact under the application of the electric field. The Schottky contacts are calculated as the variation of the conduction bands edge (valence bands edge) of In_2Se_3 with respect to the Fermi level of the complex, as $\Phi_{Bn} = E_c - E_F$ and $\Phi_{Bp} = E_F - E_v$. It can be seen from figure 4c (corresponding to the C_1 configuration) that the lines corresponding to Φ_{Bn} and Φ_{Bp} intersect for a value of the electric field of $\sim -0.2 \text{ V}/\text{\AA}$ indicating the presence of the Fermi level in the middle of the band gap, which corresponds to a transition from a n- to a p-type Schottky contact. When the electric field is between $-0.4 \text{ V}/\text{\AA}$ and $-0.2 \text{ V}/\text{\AA}$, the Fermi level has a tendency to move towards the valence bands, indicating the presence of p-type Schottky contact. When the electric field is between -0.2 to $-0.04 \text{ V}/\text{\AA}$, a n-type Schottky contact takes place. For an electric field larger than $-0.041 \text{ V}/\text{\AA}$, the n-type Schottky contact decreases, indicating the transition from a n-type Schottky contact to a Ohmic contact. In the case of the C_2 configuration, an Ohmic contact is found with $\Phi_{Bn} < 0$ even under the application of an electric field. Notice that PBE functional can still reliably predict the trends of the Schottky barrier change[40], despite of its widely known intrinsic bandgap underestimation problem.

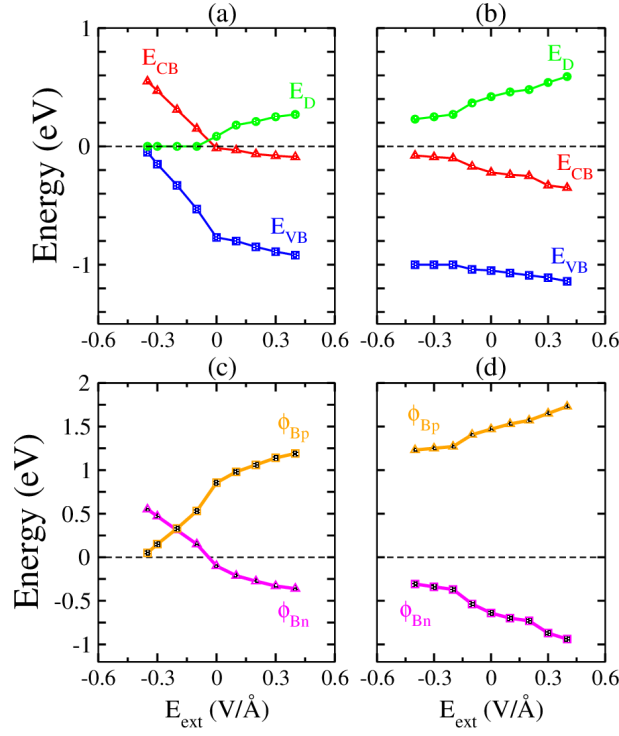


Figure 4: Top panel: evolution the graphene Dirac point (E_D) and the In_2Se_3 VBM (E_{VB}) and CBM (E_{CB}) for the C_1 (a) and C_2 (b) heterostructures under the application of an external electric field. The Fermi level is set to zero. Bottom panel: the evolution of the n- and p-type Schottky barrier height under an applied external electric field for the C_1 (c) and C_2 (d) heterostructures.

4. Conclusion

Using first principle calculations, we have investigated the electronic properties of the ferroelectric $\alpha\text{-In}_2\text{Se}_3$ /graphene heterostructure and demonstrated a different behavior for the two possible configurations. We found that an external electric field can be used as a tool to control the graphene and In_2Se_3 band alignment, and that the Schottky barrier at the interface can be modulated by the direction of the intrinsic polarization of In_2Se_3 with respect to graphene. More generally, the possibility of having of n- and p-doping in the same structure creates the possibility to built a ferroelectric rectifying diode by a graphene/ In_2Se_3 /graphene, which will be the topic of a future investigation.

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