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# An ab initio study of the ferroelectric In<sub>2</sub>Se<sub>3</sub>/graphene heterostructure.

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#### Abstract

Using ab initio calculations, we have investigated the electronic structure properties of the ferroelectric  $\alpha$ -In<sub>2</sub>Se<sub>3</sub>/graphene heterostructure. The presence of an intrinsic polarization in In<sub>2</sub>Se<sub>3</sub> 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

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and experimental studies[18, 19] on transition metal dichalcogenides such as  $2H-MoS_2$ , 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.

In<sub>2</sub>Se<sub>3</sub> compounds are known to be of use in phase change memory, thermoelectric, and photoelectric applications[23, 24]. Also, single and few-layer In<sub>2</sub>Se<sub>3</sub> flakes have been obtained on different substrates, such as graphene and mica by van der Waals epitaxy[25]. Recently the 2D semiconductor  $\alpha$ -In<sub>2</sub>Se<sub>3</sub> 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  $\alpha$ -In<sub>2</sub>Se<sub>3</sub> layers, with an on/off ratio of ~10<sup>5</sup>. Moreover, a non-volatile memory in a hybrid 2D ferroelectric field effect transistor (FeFET) made of ultrathin  $\alpha$ -In<sub>2</sub>Se<sub>3</sub> and graphene has been realized[30].

Herein, and due to the lack of information about the effect of  $In_2Se_3$  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  $\alpha$ -In<sub>2</sub>Se<sub>3</sub> 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  $10^{-6} \text{ eV}$  for the total energy.

#### 3. Results and discussion

Due to the inequivalent sides of the ferroelectric layer  $\alpha$ -In<sub>2</sub>Se<sub>3</sub>, two different configurations (noted hereafter C<sub>1</sub> and C<sub>2</sub>) can be obtained for the  $\alpha$ -In<sub>2</sub>Se<sub>3</sub>/graphene heterostructure, as shown in figure 1. In the C<sub>1</sub> configuration, the spontaneous out-of-plane electric polarization (P) is pointing towards graphene, while in the C<sub>2</sub> configuration P is pointing away from In<sub>2</sub>Se<sub>3</sub>. To limit the lattice mismatch between  $\alpha$ -In<sub>2</sub>Se<sub>3</sub> (a = 4.06 Å) and graphene (a= 2.46 Å) in our calculations, our simulation cell was built from a 5 x 5 graphene supercell and a 3 x 3  $\alpha$ -In<sub>2</sub>Se<sub>3</sub> supercell. After performing a geometry relaxation of the heterostructure, we obtained a lattice parameter of 12.29 Å, where the  $\alpha$ -In<sub>2</sub>Se<sub>3</sub> 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  $\alpha$ -In<sub>2</sub>Se<sub>3</sub>/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 In<sub>2</sub>Se<sub>3</sub>. A vertical external electric field (E<sub>ext</sub>) 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<sub>2</sub> heterostructure is slightly more stable than the C<sub>1</sub> heterostructure, by about 1.80 meV/atom (1.14 meV/Å<sup>2</sup>).

Geometry	d(Å)	Eb(meV/atom)	Eb(meV/ Å <sup>2</sup> )
<b>C</b> <sub>1</sub>	3.68	20.6	6.19
C <sub>2</sub>	3.67	22.4	7.33

Table 1: Calculated interlayer distance d (in Å) and binding energy Eb(in meV/atom and in meV/Å<sup>2</sup>) of the  $\alpha$ -In<sub>2</sub>Se<sub>3</sub>/graphene heterostructure .

Due to the effect of spin-orbit coupling (SOC) on the bandstructure of  $\alpha$ -In<sub>2</sub>Se<sub>3</sub>[11], one may anticipate that the SOC may also affect the electronic structure of the In<sub>2</sub>Se<sub>3</sub>/graphene bilayer, and more specifically the band alignment. When taking into account the SOC, we found that for both C<sub>1</sub> and C<sub>2</sub> only the VBM (valence band maximum) of In<sub>2</sub>Se<sub>3</sub> 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/ $\alpha$ -In<sub>2</sub>Se<sub>3</sub> heterostructure: the projection on the graphene atoms is pictured by red circles, while the projection on the In<sub>2</sub>Se<sub>3</sub> 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  $In_2Se_3$  layer. Obviously, the doping level is dependent on the direction of the polarization of  $In_2Se_3$ : for the C<sub>1</sub> 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/ $\alpha$ -In<sub>2</sub>Se<sub>3</sub> 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<sub>2</sub>Se<sub>3</sub> 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 C2 configuration, which pictures a larger charge transfer between the layers than in the C1 configuration, and confirms the fact that the shift of the Dirac point of graphene is larger for the C2 arrangement.



Figure 3: Electron density difference for the configurations  $C_1$  and  $C_2$  of the graphene/In<sub>2</sub>Se<sub>3</sub> heterostructure. The isosurface value for the two configurations is 0.0003 e/Å<sup>3</sup>, where the accumulation and depletion of electrons are represented in orange and green, respectively.

For the performance of graphene/In<sub>2</sub>Se<sub>3</sub> 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<sub>2</sub>Se<sub>3</sub>, 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<sub>1</sub> 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  $\sim -0.1$ 

V/Å. 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 V/Å 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<sub>2</sub>Se<sub>3</sub>: when the intrinsic polarization of In<sub>2</sub>Se<sub>3</sub> 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 ptype 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<sub>2</sub>Se<sub>3</sub> 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<sub>1</sub> configuration) that the lines corresponding to  $\Phi_{Bn}$  and  $\Phi_{Bp}$  intersect for a value of the electric field of ~ -0.2V/Å indicating the presence of the Fermi level in the midle 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 V/Å and -0.2 V/Å, 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 V/Å, a n-type Schottky contact takes place. For an electric field larger than -0.041 V/Å, the n-type Schottky contact decreases, indicating the transition from a n-type Shottky contact to a Ohmic contact. In the case of the C<sub>2</sub> 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<sub>2</sub>Se<sub>3</sub> VBM  $(E_{VB})$  and CBM  $(E_{CB})$  for the C<sub>1</sub> (a) and C<sub>2</sub> (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<sub>1</sub> (c) and C<sub>2</sub> (d) heterostructures.

#### 4. Conclusion

Using first principle calculations, we have investigated the electronic properties of the ferroelectric  $\alpha$ -In<sub>2</sub>Se<sub>3</sub>/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<sub>2</sub>Se<sub>3</sub> band alignment, and that the Schottky barrier at the interface can be modulated by the direction of the intrinsic polarization of In<sub>2</sub>Se<sub>3</sub> 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<sub>2</sub>Se<sub>3</sub>/graphene, which will be the topic of a future investigation.

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