Electronic structure of 2D InSe

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1. Introduction

We shows that monolayer InSe combines the best aspects of 3D semiconductors such as higher mobility, shallow dopants and low effective masses into a 2D semiconductor system.

There is presently considerable interest in the layered materials such as the transition metal dichalcogenides (TMDs) and graphene [1,2]. However graphene does not have a band gap. On the other hand, the carrier mobility of TMDs is limited to of order 100 cm2/V.s. Black phosphorus (b-P) is interesting, it has a carrier mobility of order 1000 cm2/V.s [3], but it reacts with water and is an unsuitable semiconductors. Also, substitutional dopant sites in black phosphorus reconstruct and do not dope [4].

There is third class of 2D semiconductors the III-VI materials like GaSe. These have Ga-Ga bonds inside the layer and Se sites on the outside of the layer, and van der Waals bonds between layers [5]. We consider InSe which has an environmental stability better than GaSe. Its carrier mobilities are higher, of order 1000 cm2/V.s, like b-P. This high mobility allows the quantum Hall effect to be observed recently [6]. Here we calculate the band structure of 2D InSe, its band offsets and dopant properties.

2. Method

The calculations are carried out using the plane-wave, density-functional code CASTEP [7]. Norm-conserving pseudopotentials are used with a cut-off energy of 500 eV. The In pseudopotential includes the shallow In 4d core levels in the valence shell. Grimme's method is used to correct the density functional theory (DFT) treatment of the van der Waals interactions. The standard DFT method under-estimates the band gap of semiconductors and insulators. Thus, we use the screened exchange (sX) hybrid density functional [8] to correct these band gap errors. The quasi-particle band gaps are found using the GW method.

3. Results.

Fig. 1(a,b) shows the band structure of an InSe monolayer and bulk using the sX functional. The band gap changes from a direct gap to an indirect gap at the monolayer. The basic ordering of bands is similar to that found by others. We notice that the calculated sX band gap is close to the experimental optical/excitonic band gap value, The difference between the quasi-particle gap and the optical gap is the exciton binding energy, which increases rapidly for small layer numbers due to the reduced screening³⁰.

The band edge states are bonding and anti-bonding along the In-In bond. This means that the band gap does not change much in passing from GaSe to InSe. On the other hand, the band gap of InAs is across the polar In-As bond, and this band gap changes hugely due to the lower In s state than the Ga s state.

The band offsets of InSe with other 2D semiconductors, and with oxides that might be used FETs and its native oxide are parameters of interest. The band offsets calculated within sX are shown in fig 2. The band offset combination of InSe and WSe2 is suitable for use in the tunnel FET.

Fig 2 also shows that HfO2 has a big enough band offset to be used as a gate oxide with InSe.

The dopant energy levels in InSe are summarized in Fig. 3. Fig 4 and 5 shows the atomic configuration of the Zn acceptor and the Cl donor in InSe. Both retain a substitutional character consistent with being shallow.

References

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Fig. 1. Band structure of monolayer InSe



Fig. 2. (Bsand line-ups of InSe and various TMDs and oxides



Fig. 3. Summary of the energy level of substitutional dopants in InSe



Fig. 4. Geometry of the Cl donor in InSe



Fig. 5. Geometry of the Zn acceptor in InSe