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Electronic and Magnetic Properties of Insulating Ferromagnetic Semiconductor (Al,Fe) Sb from First-Principles Calculations

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Abstract: *We have investigated the electronic structure and magnetic properties of Fe-doped AlSb using density functional theory within the generalized gradient approximation (GGA)+U schemes. We have shown that the ground state magnetic structure of Fe-doped AlSb is antiferromagnetic. AlSbis the most plausible acceptor among several candidates for p-type conduction and the bound magnetic polarons (BMP) mechanism may be responsible for the origin of the (Al,Fe) Sb ferromagnetism.*

Keywords: *A. Fe doped AlSb; B. GGA+U; C. electronic and magnetic properties; D. first-principles calculation*

PACS Numbers: *71.15.Mb; 75.20.Hr; 71.20.-b; 75.10.-b*

1. Introduction

One of the most central challenges in spintronics is the successful injection of spin-polarized current into a semiconductor [1, 2]. Several approaches have been applied to achieve it and one of the most promising routes is the use of the so-called spin filter materials (SFMs)[3, 4].SFMs are magnetic semiconductors; compounds where there is an energy gap in both spin directions but the band structure is different for the two spin directions leading to magnetic properties. however, most of the potential ferromagnetic materials for spin-filtering are Europium chalcogenides (EuO[5], EuS [6]) or complex oxides (BiMnO3[7]), which are not compatible with mainstream semiconductors. Thus, an insulating ferromagnetic material that is compatible with well-established semiconductors is highly needed. Recently, an insulating ferromagnetic semiconductor (FMS) (Al,Fe) Sb has been reported [8]. By doping Fe in AlSb, they found that a(Al1-x,Fex) Sb sample with an Fe content x of 10% exhibits intrinsic ferromagnetism while being insulating at low temperature, and thus can be used as a spin filter. In this paper, we have performed an ab initio density functional theory study on (Al1-x,Fex)Sb and discussed its ferromagnetic origin.

2. Computational Method

The first-principles calculations were performed by using density functional theory (DFT) method within the Perdew-Burke-Ernzerh of (PBE) generalized gradient approximation (GGA)[9], implemented in the Viennaab initio Simulation Package (VASP)[10]. The strong correlated correction was considered with GGA+U method [11] to deal with the Fe's 3d electrons. The effective onsite Coulomb interaction parameter (U) and exchange interaction parameter (J) are set to be 5.3 eV and1.0 eV for Fe's 3d electrons. These values have been tested and used in the previous experimental and theoretical works [12, 13]. 3s3p for Al, 3d4s for Fe and 5s5p for Sb were treated as valence orbitals in

the calculations. The projector augmented wave (PAW) potential [14] and the plane waves cut-off energy of 300 eV were used. For AlSbunit cell, a Γ-centered Monkhorst-Pack [15] k-point mesh of 5×5×5 was used and the internal atomic coordinates were relaxed until the force was less than 0.01 eV/A. For Fe doped AlSb supercell, a Γ-centered Monkhorst-Packk-point mesh of 3×3×3 was used. The criterion for the total energy was set as 10^{-4}eV.

3. Results and Discussion

AlSb, the host materials of (Al1-x,Fex) Sb, has a cubic crystal structure and space group F-43m, as is shown in figure 1. The experimentally measured lattice constant of AlSb (a=6.136A) was used in our calculations [8] and the internal coordinates were optimized. We first investigate the electronic structure of the pure compound AlSb. In figure 2, the total density of states of the AlSbare depicted. This compound is a non-magnetic semiconductor with a calculated band gap at about 1.1 eV, which is smaller than the experimental data (1.6 eV) [8].The reason is the well-known underestimation band gap of DFT.

We have used two Fe atoms to substitute two Al atoms in a 2×2×2 supercell for constructing

(Al0.9375Fe0.0625) Sb. We have calculated five kinds of Fe-Fe pair configuration of different distances.

(1) The first nearest neighboring two Fe atoms indicating [01],

(2) The second nearest neighboring two Fe atoms indicating [02],

(3) The third nearest neighboring two Fe atoms indicating [03],

(4) The fourth nearest neighboring two Fe atoms indicating [04],

(5) The fifth nearest neighboring two Fe atoms indicating [05], as is shown in figure 3.

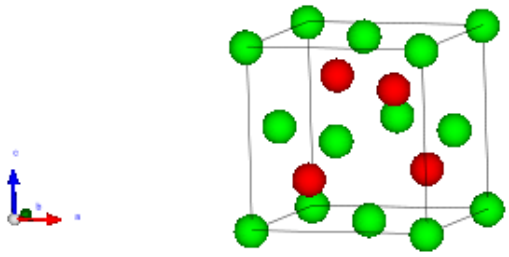

Fig1. *The crystal structure of the AISB unit cell. The green spheres are Al and the red spheres are Sb*

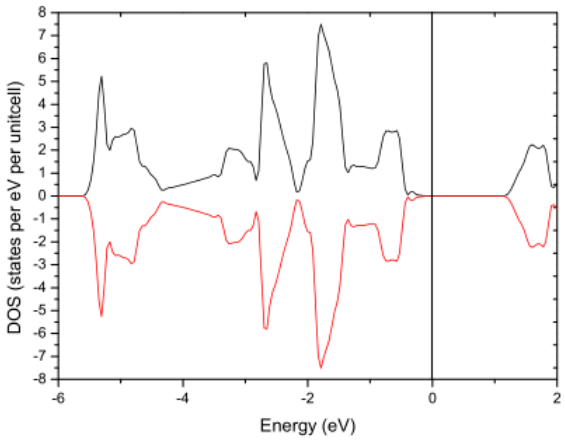

Fig2. *The total density of states of AlSb per unit cell. Black line represent spin up and red line spin down. The energy zero is taken at the Fermi level and indicated by the vertical line.*

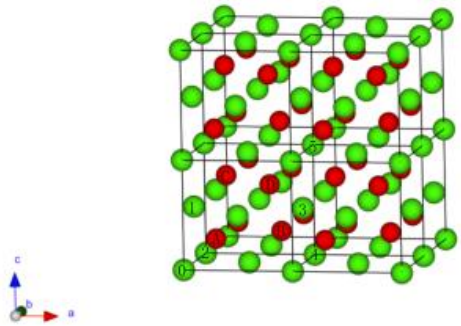

Fig3. *The 2x2x2 supercell of ($Al_{0.9375}Fe_{0.0625}$) Sb. The configurations of Fe-Fe pair indicate [01], [02], [03], [04] and [05]*

TableI. *The total energy (eV) of different configuration of ferromagnetic and antiferromagnetic state of ($Al_{0.9375}Fe_{0.0625}$) Sb*

Configuration	E_{AFM}	E_{FM}	E_{FM}-E_{AFM}
01	-262.1450	-261.6699	0.4751
02	-261.8014	-261.7741	0.0273
03	-261.8208	-261.7529	0.0679
04	-261.9428	-261.7143	0.2285
05	-261.8139	-261.7545	0.0594

Table I lists the total energy of the (Al0.9375Fe0.0625) Sb with ferromagnetic (FM) and anti ferromagnetic (AFM) state for the five configuration. Our calculations show that the total energy of anti ferromagnetic states are always lower than the ferromagnetic states in the considered Fe-Fe pair configuration. This result means that the ground state of stoichiometric (Al0.9375Fe0.0625) Sb is AFM state. However, this result contradicts the experimental report that (Al0.9375Fe0.0625) Sb is a hole-doped ferromagnetic semiconductor. Since Fe atoms are is oelectronic when doped in AlSb, they could not provide the carriers. So we believe that the native point defect maybe one of the origin of the hole carries and may be an important factor for determining the ferromagnetic properties of (Al0.9375Fe0.0625)Sb. Thus we first calculated the defect formation energy of different acceptor defects in the (Al0.9375Fe0.0625)Sb system. There are three kinds of acceptor defects including Al vacancy (VAl), Sb interstitial (Sbint), and Al antisite (AlSb).The defect formation energy Ef is calculated from [16]

$$E_f = E_t - E_b \pm \sum E_a$$

where Et is the total energy of the (Al0.9375Fe0.0625)Sb super cell with an acceptor defect. Eb is the corresponding energy of the (Al0.9375Fe0.0625) Sb super cell with out a defect. Ea is the energy of an isolated atom. Vacancy defect used "+" while interstitial defect "-". Table II lists the formation energy of different defect at different Fe-Fe configurations. The AlSb has the lowest formation energy among these defects for different Fe-Fe configurations and is the most stable defect in (Al0.9375Fe0.0625) Sb.So the source of the hole carriers is most likely Al antisite (AlSb).

TableII. *The calculated formation energy (eV) of different defects at different Fe-Fe configurations*

Configuration	V_{al}	Sb_{int}	Al_{Sb}
01	2.021	1.686	1.014
02	2.041	3.213	1.750
03	2.036	2.959	1.763
04	2.024	3.323	1.443
05	2.342	3.174	1.723

Next, we investigate the influence of hole carriers on the magnetic properties of the (Al0.9375Fe0.0625) Sb. There are many AlSb locations in the (Al0.9375Fe0.0625) Sb super cell. L. D. Anh et al suggest a possible scenario of short-range exchange interactions between Fe-Featoms [8]. Thus, We have calculated FM and AFM energy of four kinds of AlSb locations marked A, B, C and D as is shown in figure 3 for Fe-Fe [01] configuration. As listed in table III, the (Al0.9375Fe0.0625) Sb system prefers FM state only in AlSb @ A congfiguration. The others remain AFM states. We notice that AlSb @A congfiguration is the lowest energy and the most probably stable configuration in the system from our calculation. Considering the local fluctuation of the Fe concentration, we could safely conclude that the nearest neighbor Fe-Fe atoms plus nearest AlSb complex is the one of plausible factor to determine the FM state of (Al0.9375Fe0.0625) Sb system in the experiments.

TableIII. *The calculated energies (eV) of ferro-magnetic (FM) and antiferromagnetic (AFM) state of ($Al_{0.9375}Fe_{0.0625}$) Sb supercell with Alsb at different locations.*

Configuration	FM	A_{FM}	EFM-E_{AFM}
Al_{sb} @A	-260.2963	-260.2923	-0.004
Al_{sb} @B	-259.2759	-259.4206	0.1447
Al_{sb} @C	-259.6920	-259.8853	0.1933
Al_{sb} @D	-259.1451	-259.4172	0.2721

In order to clarify the FM coupling mechanism between the Fe atoms and the nearest AlSb. We investigate the electronic structure of the (Al0.9375Fe0.0625) Sb system with AlSb@A FM state as is shown in figure 4. The Fe3d major orbital is mainly located as deep as 5 eV below the Fermi level and thus cannot accommodate holes. The valence band, which consists mainly of Sb 5p orbital, is located below the Fermi level and have little contribution at the Fermi level. They cannot accept holes either. The impurity bands formed by AlSbis located at the bandgap, revealing that holes are successfully introduced into (Al0.9375Fe0.0625) Sb system. According to the model of bound magnetic polarons (BMP) ferromagnetism [17, 18], a ferromagnetic exchange interaction could be mediated by the impurity band. As is shown in figure 4, the minorun occupied Fe 3d band hybridize with the acceptor states around the Fermi level. In this situation, there is possibility for hole transfer from the acceptor to the magnetic Fe cations. Thus, they form bound magnetic polaron in which Fe-Fe is ferromagnetic coupling. The bound magnetic polaron is localized and extends over only few of magnetic cations. This point can be seen that AlSb impurity band is suffciently narrow in the band gap. We could conclude that the model of bound magnetic polarons (BMP) may be the ferromagnetic exchange mechanism between the Fe atoms in (Al0.9375Fe0.0625) Sb system.

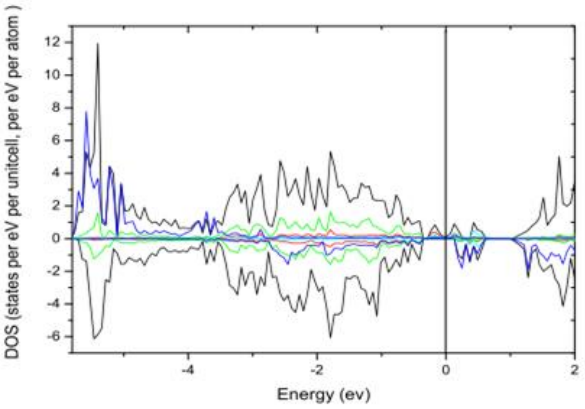

Fig4. *The total averaged (black line) and partial density of states of Sb 5p (green line) and Al 3p (red line) of (Al0.9375Fe0.0625) Sb per unit cell. The partial density of states of Fe 3d (blue line) and Alsb 4p (cyan line) per atorn. The energy zero is taken at the Fermi level and indicated by vertical line.*

4. SUMMARY

In conclusion, we have performed a study of the electronic structure and magnetic properties of Fe-doped AlSb using density functional theory within the GGA+U schemes. We have shown that the ground state magnetic structure of Fe-doped AlSb is antiferromagnetic. AlSbis the most plausible acceptor among several candidates for p-type conduction and the bound magnetic polarons (BMP) mechanism may be responsible for the origin of the (Al,Fe) Sb ferromagnetism.

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