

Electronic Structure and Magnetism of CrP/SrBi Interface: A First Principles Study

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(Received 8 June 2007)

We investigated the electronic structure and magnetic properties of zinc-blende CrP/SrBi interface by using the all-electron full-potential linearized augmented plane wave method within the generalized gradient approximation. It is found that the half-metallicity is destroyed when the two half-metals are in contact. Magnetic moments of the atoms forming the supercell differ considerably from the respective values obtained for the bulk structures of the two materials. Cr atoms being and not being in contact with Bi atoms have magnetic moment 3.43 and 2.69 μ_B , respectively. Bi atoms lose their majority electrons which results in their negative polarization. Alkaline Sr atoms are very weakly negatively polarized. The spin distribution within the supercell is such that well separated regions of positive and negative polarization are seen, especially around the layer of P atoms being in contact with the layer of Sr atoms.

Keywords : zinc-blende structured half-metal, interface, electronic structure and magnetism

1. Introduction

Since the first discovery of half-metallicity of Mn-based Heusler alloys in 1983 [1] many half-metallic materials have been proposed, such as half-Heusler alloys, ferromagnetic metallic oxides, dilute semiconductors and transition metal chalcogenides and pnictides with zinc-blende (ZB) structure. The properties of those half-metallic systems were resolved in both experimental and theoretical studies. As far as Cr compounds are concerned, the half-metallicity was found in ZB CrAs [2], CrSb [3] and CrP [4]. According to the recent calculations with the use of all-electron and pseudopotential methods, ZB CrP is half metallic when its lattice constant is exceeded by $\sim 1\text{-}2\%$ (depending on the method of calculations) comparing with its equilibrium value [4]. Therefore, AlP with the lattice constant of 5.53 Å was suggested as a good substrate for growing ZB half-metallic CrP. Recently, it has been predicted that half-metallicity can also be observed in the ZB-structured compounds of alkaline materials with the Bi atom [5]. In the first-principles study of the half-metallic properties of MBi (M=Ca, Sr, Ba) it was found that the equilibrium lattice constant of half-metallic ZB SrBi is 7.76 Å, and the half-metallicity of the compound is sustained until the lattice constant is

compressed to the critical value of 6.67 Å, at which the magnetic moment (MM) of the system is no longer an integer number [5]. Taking into account the above information, namely that the half-metallic lattice constants of ZB-CrP and ZB-SrBi are 5.48 and 7.76 Å, respectively, we can see that the diagonal length of (001) face of CrP unit cell (7.75 Å) is very close to the SrBi unit cell lattice constant. Using 5.49 Å, we obtain a perfect match between CrP and SrBi if we assume that SrBi grows on CrP in [001] direction in such a way that the SrBi unit cell is rotated by 45° with respect to the (001) face of CrP unit cell. Such an approach would make possible to create an interface between two compounds of which both are half metals, but having the insulating energy gap in different spin channels: in SrBi this is majority electron channel [5], and in CrP-minority electrons channel [6]. Considering these half-metallic alloys can be applied to spintronics, it is interesting and desirable to know whether the half-metallic properties are sustained when the two compounds form an interface.

In this paper we present the results of ab initio calculations of the electronic properties of CrP/SrBi system with a special emphasis on the properties of the interface layer, and compare the results with the properties of the two materials not affected by a contact.

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2. Computational Method

The interface was modeled by a supercell consisted of 4 layers of CrP(001) and 4 layers of SrBi(001) as it is shown in Fig. 1. There were 10 atom types in the supercell to which we shall refer hereafter accordingly to the notation indicated in Fig. 1. The layers representing CrP were separated from each other by 1/4 of its lattice constant (2.59 a.u.), and the distances between the other layers were $\sqrt{2}$ times larger (3.66 a.u.). The contacts were created between P(6) and Sr(7) as well as between Cr(1,2) and Bi(10) atoms. The distances between these layers were taken as the average of the two distances mentioned earlier.

The band structure calculations were performed by full-potential linearized augmented plane wave method (FLAPW) [7, 8] as embodied in the QMD-FLAPW code, within generalized-gradient-approximation [9]. This approach allows solving the Kohn-Sham equation [10] for the investigated system. Lattice harmonics with $l \leq 8$ were considered to describe the charge density, potential and wavefunctions inside each muffin-tin sphere within the radii of 1.7 a.u. for P, 2.3 a.u. for Cr, 2.5 a.u. for Sr, and 2.6 a.u. for Bi. More than 1200 LAPW basis functions per each k-point, which corresponds to an energy cut-off of 10 Ry, were used as a variational set. Integration inside Brillouin zone was replaced by summation over 180 k-points inside the wedge of the irreducible Brillouin zone. All core electrons were treated fully relativistically, while valence states were treated scalar relativistically, without spin-orbit coupling [11]. Self-consistency was assumed when the difference between input and output charge densities was less than 1×10^{-4} electrons/(a.u.)³.

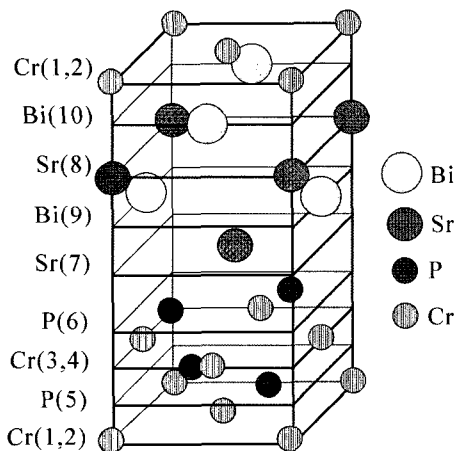


Fig. 1. Schematic view of the ZB-CrP/SrBi supercell together with the notation corresponding to atoms in different layers, as it appears in the text.

3. Results and Discussion

Although both CrP and SrBi are half-metals in their bulk states, they lose the property when an interface is created, which is clearly seen from the local density of states pictures shown in Fig. 2. Only Cr(1,2) layer still exhibits half-metallic properties, and P(5) is nearly half-metallic. A hybridization between Cr(1,2) t_2 and P(5) p orbitals is seen in the LDOS structure at ~ -4.0 and ~ -2.5 eV. There are more localized states around ~ -1.3 eV of e character. This is very similar to what was observed by Pask *et al.* in several ZB Cr pnictides [5]. That means that even though Cr(1,2) atoms are those in direct contact with the Bi(10) atoms of the other material, the nature of interaction between them and P atoms is not much affected. However, the contact between Cr layer of CrP and Bi layer of SrBi affects considerably the electronic properties of Bi atoms. The atom-resolved density of states of Bi(9) and Bi(10) differ considerably one from another. The LDOS of Bi(9), which is not in contact with Cr layer, is characterized by rather narrow bands close to E_F for the both spin channels, and except for the majority spin states at E_F the picture resembles that of ZB-SrBi

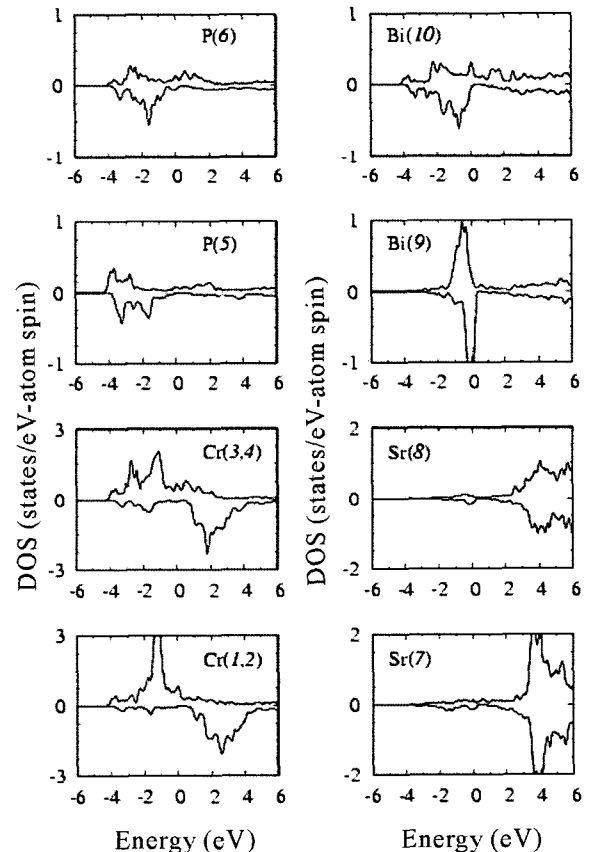


Fig. 2. Atom-resolved local density of states of ZB CrP/SrBi supercell.

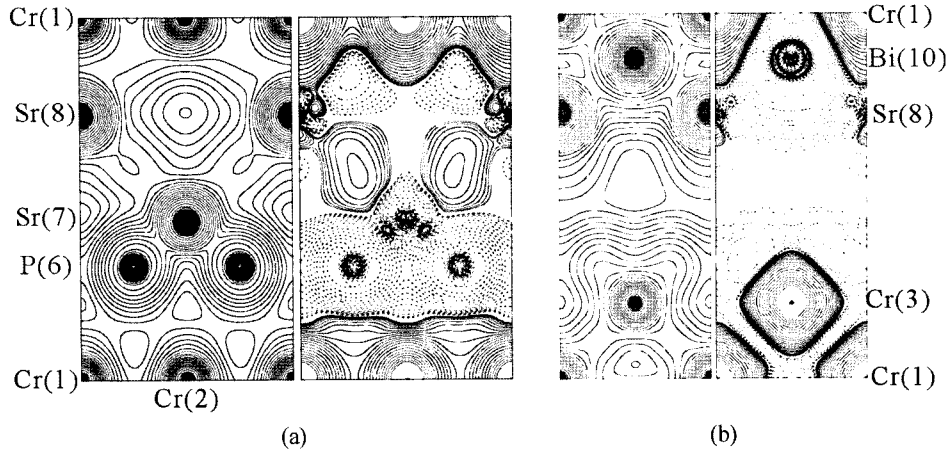


Fig. 3. Charge and spin density distribution within ZB-CrP/SrBi supercell in (a) [110] and (b) [001] direction. Only those atoms which are in the (110) (a) and (001) (b) planes are denoted. The left panels show charge density while the right ones, spin density contour plots. In the spin density contour plots the solid and broken lines represent positively and negatively polarized spin densities, respectively. The lowest contour starts from 1×10^{-3} electrons/a.u.³ and the subsequent lines differ by a factor of $\sqrt{2}$.

bulk [5]. The calculated LDOS for Bi(10) is affected by the contact with Cr(1,2) atoms in a large degree. There are more occupied electronic states, which are additionally much more delocalized in the energy range from -4.0 eV to E_F , which corresponds to the occupied electronic states calculated for Cr(1,2) atoms. In each of the remaining layers of the supercell electronic states at E_F are seen for both spin channels.

In Fig. 3 charge and spin density distribution within the CrP/SrBi unit cell in [110] and [001] directions are shown. From the figure one can see changes are introduced to the electronic properties of CrP and SrBi through creating a contact between them. The interface contact between Cr and Bi layers is a source of a charge transfer from Cr to Bi atom, which is seen in charge density map drawn in [001] direction (Fig. 3(b) left panel). Charges are more localized around Sr atoms in the SrBi layers being farther from the interface than they are in the case of Sr(7) layer facing the layer of P(6) atoms.

Although the studied interface is not half-metallic, its magnetic properties are still interesting. In the spin density contours presented in the right panels of Fig. 3(a) and (b), a long-range magnetic order is seen within the layers of Cr(1,2) and P(5), P(6), as well as in Bi(10). In Cr(1,2) and P(5) and P(6) layers the regions of positive and negative polarization form a flat structures in [110] direction, while in [001] direction the minority electrons channel is surrounded by the negative polarization region coming from the negatively polarized P(5), P(6) and Bi(10) atoms. This kind of polarization structure is not seen within Sr(8) and Bi(9) layers.

Magnetic moments (MMs) of the atoms of the investi-

Table 1. Local magnetic moments (MM) of ZB-CrP/SrBi structure given in units of μ_B .

atom	Cr(1,2)	Cr(3,4)	P(5)	P(6)	Sr(7)	Sr(8)	Bi(9)	Bi(10)
MM	3.43	2.65	-0.18	-0.21	-0.03	-0.01	0.18	-0.28

gated CrP/SrBi supercell are shown in Table 1.

The largest polarizations were found in Cr(1,2) and Cr(3,4) atoms. The atoms have MM equal to 3.43 and 2.65 μ_B , respectively. All other atoms but Bi(9) are negatively polarized. Sr(7) and Sr(8) atoms have very small MM (-0.03 and -0.01 μ_B , respectively). The largest negative polarization is found in Bi(10) atom. In ZB-SrBi the value of MM of Bi atom was found to be equal to 0.61 μ_B [5]. This indicates that the contact with CrP influences the magnetic properties of Bi atom very much. The Bi(9) atom has MM of 0.18 μ_B , that is much smaller than those of the Bi atoms in ZB-SrBi bulk structure. The Bi(10) atom that is in the layer being in direct contact with ZB-CrP loses its charge because a covalent bond with Cr atoms of the adjacent layer is formed, and becomes negatively polarized with MM equal to -0.28 μ_B . This is also confirmed by the LDOS calculated for the Cr(1,2), Bi(9), and especially Bi(10), which due to the hybridization with Cr(1,2) atoms has more occupied minority spin states. This causes that the MM of Bi(10) becomes negative. The MMs of Sr(7) and Sr(8) change much in comparison with ZB-SrBi bulk, in which it was 0.09 μ_B [5]. At the interface the atoms are weakly negatively polarized. The result of these changes is that a sandwich structure of the regions of positive and negative polarization separated by a region of a very weak

polarization appears in ZB CrP/SrBi interface. This structure of spin distribution within this system may quite likely be modified through the change of lattice constant. As it was mentioned earlier, both CrP and SrBi exhibit half-metallic properties only if their lattice constant exceeds a certain minimum (critical) value. Therefore, it is likely that a reduction of the lattice constant will cause a change in the observed localization of majority and minority electrons in certain regions, because of the possibility of stronger interaction between the atoms of the interface. On the other hand, if the lattice constant was larger, half-metallic properties could appear in CrP layers.

4. Conclusions

We calculated the electronic structure and discussed the magnetic properties of ZB-CrP/SrBi interface with the use of FLAPW method within the GGA. From the calculated atom-projected density of states we found that the system created of two half-metals, each of them having the insulating gap in another spin channel, is no longer half-metallic. Only one layer of Cr atoms exhibits half-metallic properties, and its neighbor layer of P atoms is nearly half-metallic with a number of states at the Fermi energy being close to zero for minority electrons. Interaction of Cr atoms of CrP with Bi atoms of the SrBi causes a charge transfer between them. As a result, MM of Cr being in contact with Bi becomes larger than that of Cr atom lying in a deeper layer. Bi atom of the layer in contact with CrP compound is negatively polarized, while

that between Sr layers has positive MM. The alkaline Sr atoms are very weakly negatively polarized. The spin distribution within the supercell is such that well separated regions of positive and negative polarization are seen, especially around the layer of P atoms being in contact with Sr layer. Although the magnetic properties of the investigated interface are interesting, it must be noticed that such an interface would not be good in spintronic applications.

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