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A First-principles Study on the Surface Half-metallicity and Magnetism of Half-Heusler YCrSb and YMnSb Compounds

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The half-metallicity and magnetism at the (001) surface of half-Heusler-structured YCrSb and YMnSb were investigated using the all-electron full-potential linearized augmented plane wave method within the generalized gradient approximation. Both YSb-terminated surfaces and Cr- or Mn-terminated surfaces were considered for YCrSb and YMnSb. From the calculated local density of states and the total magnetic moments of the systems, the half-metallicity of the YSb-terminated (001) surface for YCrSb was preserved, whereas the surface for YMnSb was almost half-metallic. In contrast, the half-metallicity was destroyed at the Cr- or Mn-terminated surface of YCrSb or YMnSb. The magnetic moments of the Cr and Mn atom at the (001) surface were increased by 28 % and 15 %, respectively, compared to the bulk values due to band narrowing and increased exchange splitting at the surface.

Keywords : half-metal, surface magnetism, first-principles method

1. Introduction

In half metals, a one spin channel is metallic while the other spin channel exhibits semiconducting or insulating properties due to the energy gap at the Fermi energy. By this property, a half-metal has 100 % spin polarization at the Fermi energy and considerable applicability to spintronic devices [1, 2]. A half metal has been used as the spin injection source or ideal electrode for giant magnetoresistance devices (GMRs) [3] as well as for magnetic tunnel junctions (MTJs) [4], spin field effect transistors (FET) [5], etc.

In 1983, de Groot *et al.* [6] predicted half metallicity in a half-Heusler-structured NiMnSb from electronic structure calculations. Since then, half-metallicity has been studied for several materials, including half-Heusler or full-Heusler ternary compounds. Full-Heusler X_2YZ compounds have the $L2_1$ structure, in which four face-centered cubic (fcc) sublattices are interpenetrating. The X atoms are located at 4a (0,0,0) and 4b (1/2,1/2,1/2); the Y atom is located at 4c (1/4,1/4,1/4); and the Z atom can be found at 4d (3/4,3/4,3/4) in Wyckoff coordinates [7]. When the 4b (1/2, 1/2, 1/2) position is vacant, the $L2_1$ structure becomes the $C1_b$-type structure of half-Heusler compounds XYZ [8, 9].

The half-metals of these Heusler structures are structurally compatible with diamond or zinc-blende-structured semiconductors used in conventional electronics; hence, they have attracted considerable attention for practical applications. The Heusler-structured half-metals based on magnetic transition metals, such as Fe, Mn, Co, and Ni have been studied extensively. Among these, Co_2- and Mn_2-based Heusler compounds have attracted considerable attention because of their high Curie temperature and strong magnetism [10-12].

Many studies have been performed on half-Heusler compounds. Recently, Ma *et al.* [13] examined the electronic structures of half-Heusler compounds with X = Cr, Mn, Fe, Co, Ni, Ru, and Rh; Y = Ti, V, Cr, Mn, Fe, and Ni; and Z = Al, Ga, In, Si, Ge, Sn, P, As, and Sb combinations. Among a total of 378 combinations, they reported 45 half-metals and 34 near half-metals with a negative formation energy. If the half-metallic gaps of these materials are small and they have large magnetic moments, it may be difficult to actually synthesize them at room temperature.

Half-metals with large magnetic moments are unsuitable for practical applications in spintronics because they produce large stray fields, which induces large energy loss [14]. Recently, Sattar *et al.* [15] suggested new half-Heusler-structured half-metals, YCrSb and YMnSb, in an

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attempt to find a half-metal with a large half-metallic energy gap and a modest magnetic moment.

Preservation of the half-metallicity at the surface or interface of a half-metal is important for practical applications in spintronics [16-18]. This study examined whether the half-metallicity is maintained at the (001) surface of YCrSb and YMnSb by calculating the electronic structure.

2. Computational Details

The half-Heusler ternary compound consisting of X, Y, and Z can have three different combinations depending on the location of the X, Y, and Z elements. Recently, Sattar *et al.* [15], by the electronic structure calculations, found that among three structural phases of YCrSb and YMnSb, the X_I phase, in which the X, Y, and Z atoms each have a Wyckoff position of 4b (1/2, 1/2, 1/2), 4c (1/4, 1/4, 1/4), and 4a (0, 0, 0), are not only the most stable in energy, but also half-metallic [15] compared to the X_{II} (X at 4a(0, 0, 0), Y at 4b (1/2, 1/2, 1/2), Z at 4c (1/4, 1/4, 1/4)) and X_{III} (X at 4c (1/4, 1/4, 1/4), Y at 4a (0, 0, 0), Z at 4b (1/2, 1/2, 1/2)) phases. The X_{II} and X_{III} phases have 0.018 Ry and 0.084 Ry, and 0.0215Ry and 0.095 Ry higher energy for YCrSb and YMnSb, respectively, than that of the X_I phase.

Therefore, the (001) surface of YCrSb and YMnSb with the X_1 phase in bulk was considered. The lattice constants were chosen to be 6.673 A and 6.565 A for the bulk YCrSb and YMnSb, respectively, according to the calculations by Sattare *et al.* [15]. Two kinds of (001) planes can be found: those terminated with YSb atoms or terminated with Cr or Mn atoms. The electronic structure was calculated for both surfaces. The repeated slabs consisting of 11 layers were adopted to simulate the surfaces. The separation of the slabs was 1.5 times that of the slab thickness. Therefore, the interactions between slabs was negligible. No relaxation or reconstruction on the surface was considered.

To obtain the electronic structure of the surfaces, the Kohn-Sham equation [19] was solved self-consistently in terms of the full-potential linearized augmented plane wave (FLAPW) method [20, 21], as embodied in the Quantum Material Design (QMD)-FLAPW code. The generalized gradient approximation (GGA) of the Perdew-Burke-Ernzerhof type [22] to the exchange-correlation potential was employed. The muffin-tin radii of 2.50 a.u. for the Sb atom, and 2.3 a.u. for the other Cr, Mn, and Y atoms were chosen. The maximal value of the angular momentum, $l_{max} = 8$, was employed to expand the charge density, potential, and wave functions inside the muffin-tin sphere. The number of basis functions was approximately 200 per atom. All core electrons were treated fully relativistically, whereas the valence states were treated scalar relativistically without considering spin-orbit coupling. The self-consistency criterion for the charge- and spin-density convergence was that the difference between the input and output be less than 1×10^{-4} electrons/(a.u.)^3.

3. Results and Discussion

Figure 1 shows the calculated density of states (DOS) projected on atoms in the (001) YSb-terminated surface of the half-Heusler-structured YCrSb compound. The features of the atoms from the center, next to the center, subsurface, and surface layers are shown; the layers are denoted as C, S-5, S-1, and S, respectively. In each panel, the Fermi level was set to zero. The minority electron states are plotted on a negative scale. The (001) YSb-terminated surface of the half-Heusler-structured YCrSb retains the half-metallic properties of the bulk. This was also confirmed by the calculated total magnetic moment of the system being the integer Bohr magneton, 24 μ_B. From the DOS of the center layer Y and Sb atom, an energy band gap of 0.64 eV was estimated for the majority (spin-up) electrons, which is comparable to the value of bulk YCrSb, 0.78 eV calculated by Sattar *et al.* [15]. A comparison of the features of the DOSs of the surface and center-layered Y and Sb atoms showed that they were similar. The energy gap for the surface Y and Sb atoms

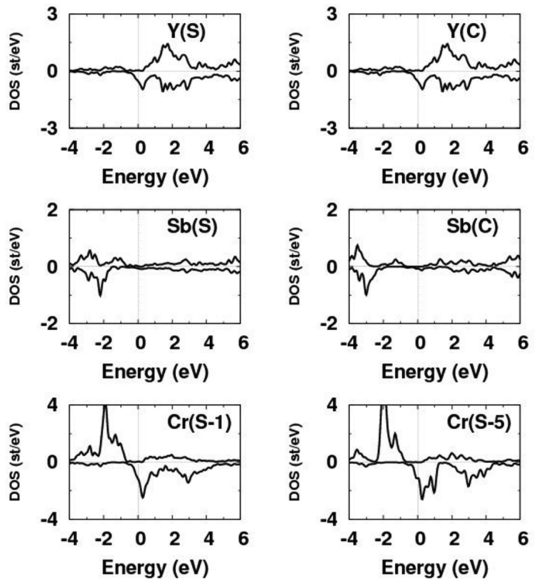

Fig. 1. Atom-projected spin-polarized density of states (DOS) for the chosen atoms of the YSb-terminated YCrSb(001) surface. The spin-down DOS values are multiplied by a negative number, and the Fermi levels were set to zero.

Table 1. *l*–decomposed electrons within muffin-tin spheres on the atoms in each layer of the half-Heusler YSb-terminated YCrSb(001) surface. The magnetic moments (MMs) calculated for the atoms are also given.

	Atom	s (↑/↓)	p (↑/↓)	d (↑/↓)	Total (↑/↓)	MM [μ_B]
YSb-term	Y(S)	0.08 (0.04/0.04)	0.07 (0.04/0.03)	0.60 (0.32/0.28)	0.76 (0.41/0.35)	0.06
	Y(C)	0.09 (0.05/0.04)	0.11 (0.07/0.04)	0.66 (0.38/0.28)	0.87 (0.50/0.37)	0.13
	Sb(S)	1.24 (0.62/0.62)	1.57 (0.78/0.79)	9.94 (4.97/4.97)	12.75 (6.37/6.38)	–0.01
	Sb(C)	1.22 (0.61/0.61)	1.59 (0.76/0.83)	9.95 (4.98/4.97)	13.09 (6.36/6.42)	–0.06
	Cr(S-1)	0.27 (0.15/0.12)	0.23 (0.15/0.08)	4.04 (3.59/0.45)	4.52 (3.88/0.64)	3.24
	Cr(S-5)	0.27 (0.15/0.12)	0.23 (0.15/0.08)	4.06 (3.61/0.45)	4.56 (3.91/0.65)	3.26

was estimated to be 0.60 eV, which is similar to the value of the center layered atoms.

Table 1 lists the calculated partial magnetic moments of each atom type. The values for the bulk-like center layered atoms were 0.13 μ_B for Y(C) and –0.06 μ_B for Sb(C), which are in agreement with those reported for bulks by Sattar *et al.* [15]. Those of the surface Y(S) and Sb(S) atoms were 0.06 μ_B and –0.01 μ_B, respectively. The calculated magnetic moment of Cr(S-5) and Cr(S-1) were the same.

The DOS of the center-layer Cr atom of the Cr-terminated YCrSb (001) system given in Fig. 2 revealed an

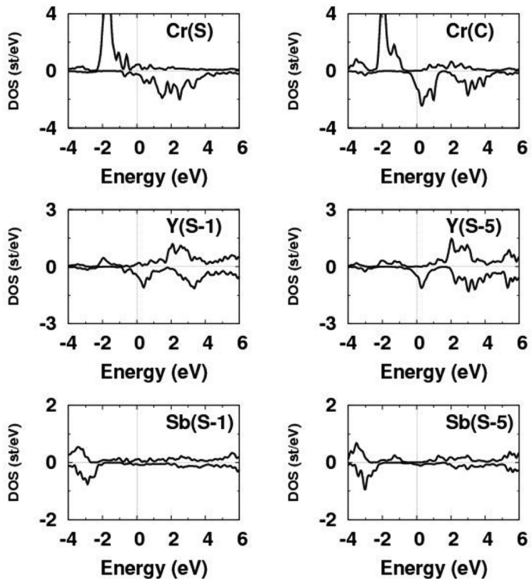

Fig. 2. Atom-projected spin-polarized density of states (DOS) for the chosen atoms of the Cr-terminated YCrSb(001) surface. The spin-down DOS values were multiplied by a negative number, and the Fermi levels were set to zero.

energy gap of approximately 0.60 eV, which is consistent with the calculations by Sattar *et al.* [15]. On the other hand, in the DOS of Cr(S), both the majority and minority spin have a certain DOS value at the Fermi energy, showing that the Cr-terminated YCrSb(001) surface system is not a half-metal. The non-integer value of the total magnetic moment of the system, 24.42 μ_B, confirms that the system is not half-metallic. A comparison of the DOS of the center layer Cr(C) and the surface layer Cr(S) revealed two peaks at 1.0 eV and 3.0 eV in the center layer minority spin electron DOS, whereas a single peak with a peak value at approximately 2.0 eV in the surface layer exists. The peaks with peak values of –2 eV become sharper at the surface layer. This is the effect of typical band-narrowing in the surface layer, resulting in an increase in the average exchange-splitting at the surface; the magnetic moment of the surface Cr atoms is expected to be higher than that of the center Cr atom. In fact, the magnetic moments of atomic Cr atoms in the Cr-terminated YCrSb (001) surface system listed in Table 2 were 3.78 μ_B, which is approximately 15 % larger than the center layer magnetic moment value, 3.28 μ_B.

The atomic DOS of the YSb-terminated YMnSb(001) surface system in Fig. 3 shows that the DOS of the surface layers Y(S) and Sb(S) are similar to those of the center layered Y(C) and Sb(C). On the other hand, the total magnetic moment of this system, 17.99 μ_B, which is almost an integer, shows that the surface layer of this system is virtually half-metallic. Table 3 lists the magnetic moment of each atom for the YSb-terminated YMnSb(001) surface system. The magnetic moment of the Mn(S-5) atom that contributes to the main magnetic moment of the system was 2.93 μ_B, which is comparable to that reported by Sattar *et al.* [15]. The magnetic moment of the sub-

Table 2. *l*–decomposed electrons within muffin-tin spheres on the atoms in each layer of the half-Heusler Cr-terminated YCrSb (001) surface. The magnetic moments (MMs) calculated for the atoms are also given.

	Atom	s (↑/↓)	p (↑/↓)	d (↑/↓)	Total (↑/↓)	MM [μ_B]
Cr-term	Cr(S)	0.26 (0.15/0.11)	0.10 (0.06/0.04)	4.10 (3.91/0.19)	4.45 (4.11/034)	3.78
	Cr(C)	0.27 (0.15/0.12)	0.22 (0.15/0.07)	4.04 (3.61/0.43)	4.54 (3.91/0.63)	3.28
	Y(S-1)	0.10 (0.05/0.05)	0.10 (0.06/0.04)	0.65 (0.35/0.30)	0.85 (0.46/0.39)	0.07
	Y(S-5)	0.10 (0.05/0.05)	0.10 (0.06/0.04)	0.65 (0.38/0.27)	0.86 (0.50/0.36)	0.14
	Sb(S-1)	1.24 (0.62/0..62)	1.59 (0.75/0.84)	9.95 (4.98/4.97)	12.77 (6.34/6.43)	–0.07
	Sb(S-5)	1.22 (0.61/0..61)	1.61 (0.77/0.84)	9.95 (4.98/4.97)	12.79 (6.36/6.43)	–0.06

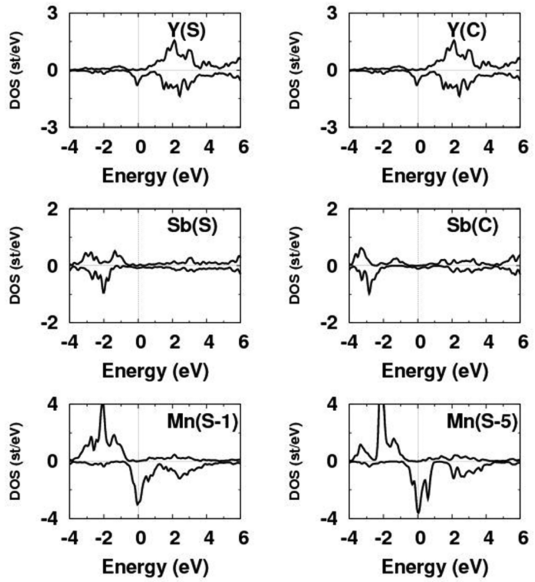

Fig. 3. Atom-projected spin-polarized density of states (DOS) for the chosen atoms of the YSb-terminated YMnSb(001) surface. The spin-down DOS values were multiplied by a negative number, and the Fermi levels were set to zero.

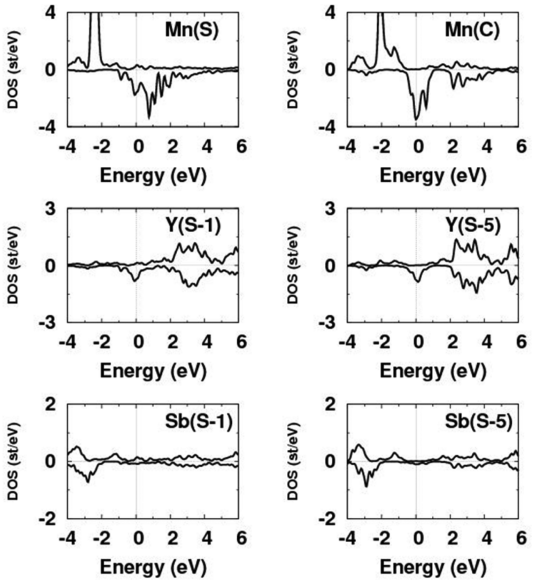

Fig. 4. Atom-projected spin-polarized density of states (DOS) for the chosen atoms of the Mn-terminated YMnSb(001) surface. The spin-down DOS values were multiplied by a negative number, and the Fermi levels were set to zero.

surface layer Mn(S-1) was increased slightly to 2.95 μ_B.

Figure 4 presents the atomic DOS of the Mn-terminated YMnSb (001) surface system. Here, a comparison of the DOS of Mn(C) and Mn(S) showed that the minor peaks due to the surface state are present at the Fermi energy. In addition, the DOS of the surface Mn atom has a typical surface effect due to band narrowing. As a result, the magnetic moment of the surface Mn is 3.61 μ_B, which is significantly higher than that of the center layer Mn atom, 2.83 μ_B, as listed in Table 4. In the case of the Y(S-1) or Sb(S-1) atoms of the remaining surface layer, there was no large difference in the magnetic moment compared to the inner Y(S-5) or Sb(S-5) atoms.

4. Conclusion

Sattar *et al.* [15] identified the half-Heusler-structured ternary compounds, YCrSb and YMnSb, as half-metals in the bulk state by first-principles calculations. In this study, the magnetic and electronic structures of the (001) surfaces of the YCrSb and YMnSb compounds were investigated using the FLAPW band calculation method. For this

Table 3. *l*–decomposed electrons within muffin-tin spheres on the atoms in each layer of the half-Heusler YSb-terminated YMnSb (001) surface. The magnetic moments (MMs) calculated for the atoms are also given.

	Atom	s (↑/↓)	p (↑/↓)	d (↑/↓)	Total (↑/↓)	MM [μ_B]
YSb-term	Y(S)	0.07 (0.03/0.04)	0.08 (0.04/0.04)	0.70 (0.35/0.35)	0.77 (0.33/0.44)	–0.11
	Y(C)	0.09 (0.04/0.05)	0.10 (0.06/0.04)	0.64 (0.30/0.34)	0.83 (0.40/0.43)	–0.03
	Sb(S)	1.24 (0.62/0.62)	1.56 (0.79/0.77)	9.94 (4.97/4.97)	12.74 (6.38/6.36)	0.02
	Sb(C)	1.22 (0.61/0.61)	1.57 (0.77/0.80)	9.96 (4.98/4.98)	13.07 (6.37/6.40)	–0.03
	Mn(S-1)	0.30 (0.16/0.14)	0.24 (0.14/0.10)	5.09 (3.99/1.10)	5.63 (4.29/1.34)	2.95
	Mn(S-5)	0.30 (0.16/0.14)	0.23 (0.14/0.09)	5.10 (3.98/1.12)	5.65 (4.29/1.36)	2.93

Table 4. *l*–decomposed electrons within muffin-tin spheres on the atoms in each layer of the half-Heusler Mn-terminated YMnSb (001) surface. The magnetic moments (MMs) calculated for the atoms are also given.

	Atom	s (↑/↓)	p (↑/↓)	d (↑/↓)	Total (↑/↓)	MM [μ_B]
Mn-term	Mn(S)	0.32 (0.17/0.15)	0.11 (0.06/0.05)	5.07 (4.32/0.75)	5.52 (4.56/0.96)	3.61
	Mn(C)	0.32 (0.17/0.15)	0.25 (0.15/0.10)	5.12 (3.94/1.18)	5.69 (4.26/1.43)	2.83
	Y(S-1)	0.10 (0.04/0.06)	0.11 (0.06/0.05)	0.69 (0.25/0.44)	0.90 (0.35/0.55)	–0.20
	Y(S-5)	0.09 (0.04/0.05)	0.12 (0.07/0.05)	0.65 (0.31/0.34)	0.88 (0.43/0.45)	–0.02
	Sb(S-1)	1.24 (0.62/0.62)	1.60 (0.78/0.82)	9.96 (4.98/4.98)	12.80 (6.38/6.42)	–0.04
	Sb(S-5)	1.22 (0.61/0.61)	1.61 (0.79/0.82)	9.96 (4.98/4.98)	12.81 (6.39/6.42)	–0.03

purpose, a repeated slab model was adopted. Both (001) surfaces terminating with YSb atoms or with Cr atoms or Mn atoms were considered.

Calculations of the atomic density and total magnetic moment of the system showed that the YSb-terminated YCrSb(001) surface system retained the half-metallicity with an integer of the total magnetic moment, 24 μ_B. The half-metallicity was broken for the other systems. On the other hand, the YSb-terminated YMnSb(001) was almost half-metallic with a magnetic moment close to the integer value of 17.99 μ_B. This was attributed to the sufficiently small energy gap of YMnSb in the bulk state, 0.40 eV, which is easily disturbed by surface formation.

The half-metallicity was destroyed in both the Cr-terminated YCrSb(001) and Mn-terminated YMnSb(001) surface systems. This is because of the typical band-narrowing effect that occurs at the surface of the magnetic transition metal. As a result, the exchange-splitting on the surface was increased, and the magnetic moments of the Cr(S) atom and Mn(S) atom on the surface were increased by 15 % and 25 %, respectively, compared to the bulk values.

Acknowledgments

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