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Effect of Atom Interchange on Half Metallicity of AuMnSn Heusler Compound†

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We have studied the effect of mutual interchange of transition metal atoms on electronic and magnetic properties of AuMnSn Heulser compound using full potential linearized augmented plane wave (FPLAPW) within generalized gradient approximation (GGA). The AuMnSn compound is predicted to be nearly half metallic ferromagnet (HMF) with 72 % spin polarization whereas MnAuSn show the low value of spin polarization (21 %). We have observed lower magnetic moment in MnAuSn (3.48 μ_B) as compared to AuMnSn (4.01 μ_B) which shows the important role of local atomic environment and coordination present in the respective compound.

Key Words: Half metallic ferromagnet, Density functional theory, Full potential linearized augmented plane wave method.

INTRODUCTION

In recent years, spintronics, which uses the spin of electron in addition to its charge, has emerged as rapidly developing field. The prime requirement of spintronics is the presence of high spin polarized charge carriers. In other words, the novel materials with dual properties, conductor for one spin channel and insulator for other, are the need of spintronics. Such materials are known as half metallic ferromagnets. Heusler compounds showing half metallic (HM) ferromagnetism are the ideal candidates for spintronic applications. The ternary XYZ type compounds belong to family of semi Heusler compounds with X and Y as transition metal atoms and Z as a *s* and *p*-element.

The half metallic ferromagnetism found in NiMnSb[1] has boosted the research activities in XYZ compounds from both theoretical and experimental front. In order to find signature of half metallicity, we have carried out band structure calculations of AuMnSn compound. We have also focused our attention to explore the effect of the mutual interchange of transition metal atoms (Au and Mn) on half metallic character.

THEORETICAL APPROACH

Semi Heusler compound AuMnSn crystallizes in $C1_b$ crystal structure with space group $F\bar{4}3m$ such that the Au atom is present at (0 0 0), Mn atom is at (¼ ¼ ¼) whereas Sn atom is located at (¾ ¾ ¾). Moreover, there is a void at (½ ½ ½). Each unit cell consists of three interpenetrating fcc sublattices. The XYZ compound can be viewed as X^{n+} innards a zinc blend YZ^{n-} sublattice. We have employed full potential linearized augmented plane wave method based on density functional theory (DFT) for calculation of present compounds. The exchange and correlation (XC) effects were taken in to account within generalized gradient approximation formalism under the parameterization of Perdew-Burke-Ernzerhof (PBE)[2]. The k-space integration has been carried out using the modified tetrahedron method with 405 k-points in the irreducible brillouin zone (IBZ) to obtain self consistency.

RESULTS AND DISCUSSION

The optimization process shows that ferromagnetic (FM) state is more stable than paramagnetic state for AuMnSn and MnAuSn compounds. The optimized lattice parameters, as listed in Table-1, are in good agreement with available experimental and other theoretical values. The calculated total density of states (DOS) for present compounds is shown in Fig. 1. It is clear from the figure that a band gap appears in the minority density of states just above Fermi level (E_F) for AuMnSn. Fermi level is pinned inside the upper edge of valence band which make this compound a nearly half metallic ferromagnet rather than a complete half metallic ferromagnet. The mutual exchange of transition metal atoms in this compound leads to the abrupt change in electronic and magnetic properties of MnAuSn. The Fermi level crosses the valence band which makes it a poor half metallic ferromagnet. The partial density of states of the both compounds are presented in Fig. 2(a,b).

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TABLE-1
OPTIMIZED LATTICE PARAMETERS A (Å), TOTAL AND ATOM RESOLVED SPIN MAGNETIC MOMENTS (μ_B) OF AuMnSn AND MnAuSn HEUSLER COMPOUNDS WITHIN GENERALIZED GRADIENT APPROXIMATION FORMALISM

XYSn		a	m_X	m_Y	m_{Sn}	m_{tot}
AuMnSn	This work	6.38	0.05	4.01	-0.07	4.01
	Other (a)	6.20	-	4.01	-	4.08
	Exp.(a)	6.32	-	3.80	-	-
MnAuSn	This work	6.29	3.51	0.07	-0.09	3.48
	Other (b)	6.33	4.05	0.02	-0.08	3.80

(a) Ref. 6, (b) Ref. 7

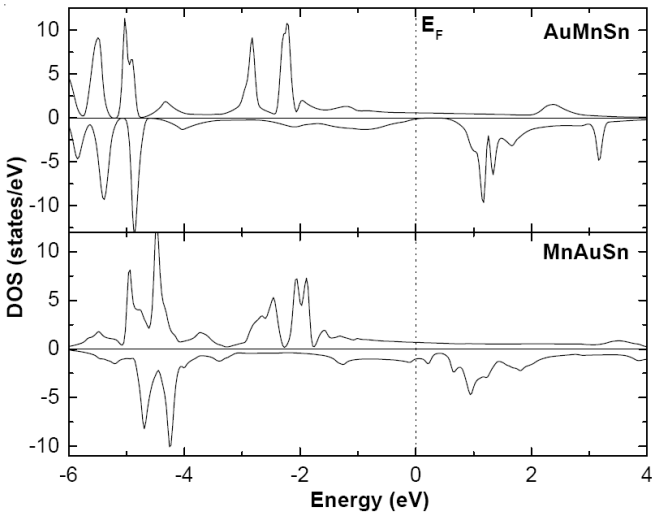

Fig. 1. Calculated total density of states for AuMnSn and MnAuSn at E = 0 eV

The insight study of both compounds reveals that Au dominates mainly in the valence band (VB) below *ca*. -4 eV because of its completely filled 5*d*-orbital. On the other hand, the 3*d*-states of Mn are distributed both in VB and conduction band (CB) due to half filled 3*d*-orbital which makes five unfilled states available for minority electrons. There is very small contribution of the Sn-*s* and Sn-*p* states in the total density of states.

Fig. 3 showed the band structure of AuMnSn compound. There is a clear indirect gap in this compound. The gap is basically due to the covalent hybridization between *d* states of Au and of Mn which leads to the formation of bonding and antibinding states with a gap in between. The spin polarization for AuMnSn compound is found to be 72 % whereas a low value (21 %) of spin polarization is estimated for MnAuSn. The change in electronic structure of MnAuSn is might be due the different local environment for Mn atom in MnAuSn as compared to that in AuMnSn. The spin polarization in AuMnSn can be further enhanced by suitable doping or atomic disorders as it is influenced remarkably by a particular defects/ disorder in Heusler compounds[3,4]. Table-1 lists the calculated total and atom resolved spin magnetic moment of present compounds which is in a fair agreement with corresponding experimental[5] and theoretical value[6,7]. The total spin magnetic moment for AuMnSn is found to be 4.01 μ_B which is in accordance with Slater-Pauling (SP) rule (m_{tot} = Nv-18)) for half metallic compounds. Here NV is accumulated number of valence electrons in the unit cell.

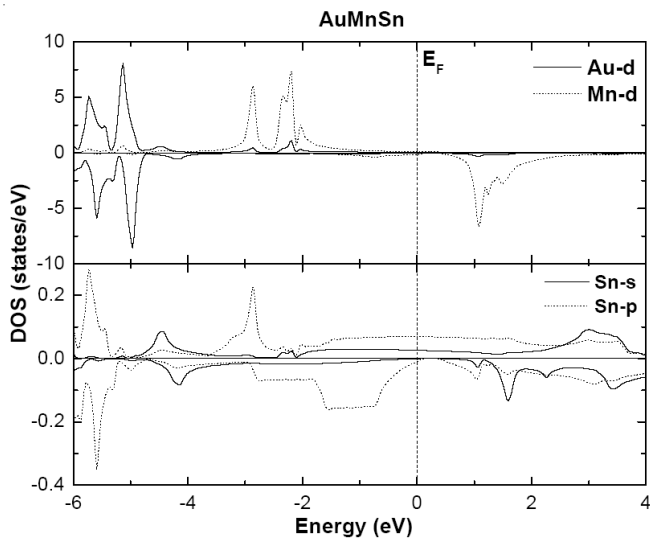

Fig. 2a. Calculated partial density of states for AuMnSn. E = 0 eV represents Fermi level

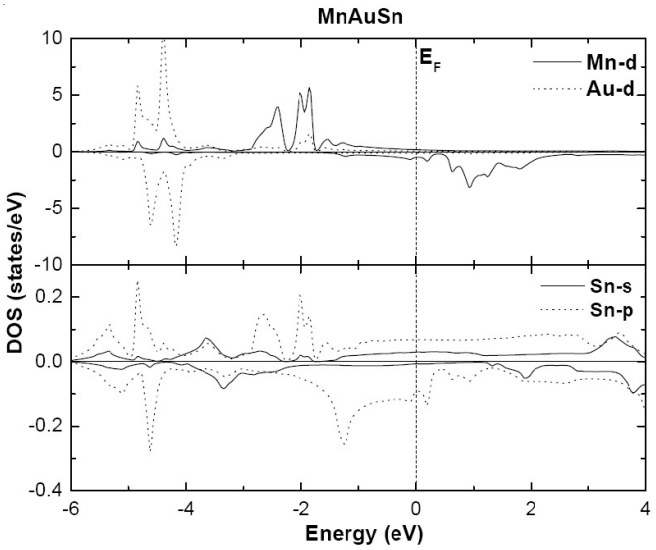

Fig. 2b. Calculated partial density of states of MnAuSn. E = 0 eV represents Fermi level

The total spin magnetic moment for both compounds is mainly carried by Mn atom only due to its large exchange splitting. The small magnetic moment at Au site is attributed to its non-magnetic nature. Tin atom has small magnetic moment which is of induced nature. The negative values of magnetic moment on Sn site clearly indicate that this atom aligned antiparallel to the ferromagnetic Mn atom.

Conclusion

AuMnSn Heusler compound is found to be nearly half metallic ferromagnet with 72 % spin polarization. The mutual interchange of transition metal atoms in AuMnSn results a decrease in spin polarization at Fermi level and hence, there by, reducing the half metallicity which clearly, shows the importance of local site coordination. The magnetic moments of both compounds is mainly carried out by Mn atom which is due to its large exchange splitting. The spin magnetic moment of AuMnSn compound is in accordance with the Slater-Pauling rule. The band structure analysis of AuMnSn compound reveals that there exists covalent hybridization between the

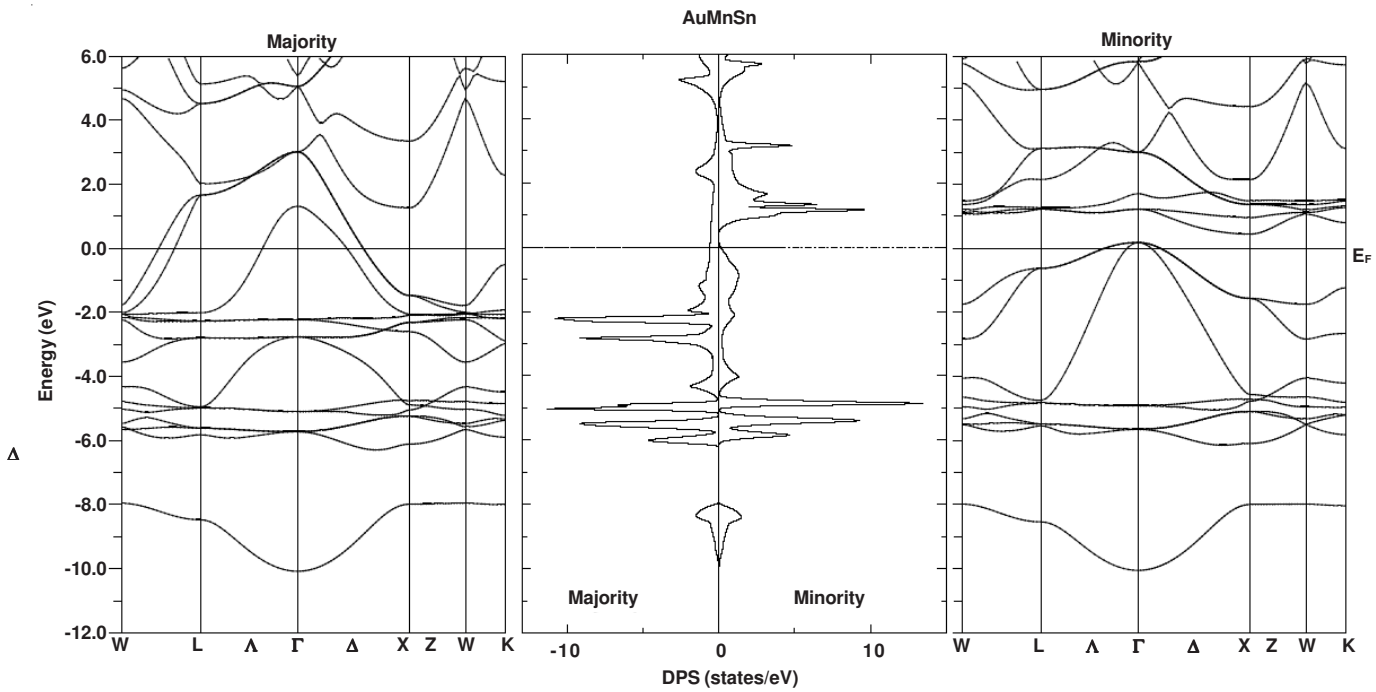

Fig. 3. Band structure of AuMnSn

two transition metals (Au and Mn) atom leads to the indirect band gap at the Fermi level.

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