

Investigation of half-metallicity of GeKMg and SnKMg by Using mBJ potential method

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Abstract. The electronic structures, magnetic properties and half-metallicity of GeKMg and SnKMg half-Heusler compounds have been investigated by the first-principles calculations based on the density functional theory. The spin-polarized calculations using full-potential linearized augmented plane-wave (FP-LAPW) method was utilized for the study of the compounds. The modified Becke-Johnson (mBJ) exchange potential was employed for a better description of the half-metallic response of the two compounds. We have found that GeKMg and SnKMg alloys are half-metallic ferromagnets with the magnetic moment of $1 \mu_B$ per formula unit at equilibrium lattice constant.

1. Introduction

Half-metallic ferromagnets (HMF) which shows metallic behaviour in one spin channel while the other spin channel shows semiconductor or insulator behaviour at the Fermi level have gained a lot of interest due to their unique properties and potential applications in spintronic devices. Materials like these are important to scientific researchers due to their potential device applications such as non-volatile magnetic random access memories (MRAM), magnetic sensors [4-6] and of spin-injector materials because their electronic structure is metallic in only one of the two spin channels, which results in complete (100%) spin polarization at the Fermi level. The concept of half-metallic ferromagnets was first introduced by de Groot et al. [1, 2], on the basis of band structure calculations in NiMnSb and PtMnSb half-Heusler compound and since then more HM ferromagnets have been predicted theoretically or confirmed experimentally in some classes of compounds such as the half-Heusler alloys, the full-Heusler alloys, the perovskites [9], the magnetite [10-12] and the zinc-blende (ZB) [8] and wurtzite transition-metal pnictides [3] and chalcogenides [8].

Because of their high Curie temperatures and structural similarity to conventional semiconductors with zinc-blende structure HM ferromagnets with half-Heusler and full-Heusler structures have gained research interest e.g., the full-Heusler compounds Co_2MX ($\text{M} = \text{Mn, Fe and Cr; X} = \text{Si, Ge and Sn}$) with $L2_1$ structure have been found to be HM ferromagnets by some theoretical and experimental research groups [35-39]. The half-Heusler compounds, CoMnX ($\text{X} = \text{P, As and Sb}$) [6,42] FeCrSb , FeMnSb [42] and NiCrZ ($\text{Z} = \text{P, Se and Te}$) and NiVAs [43-45] have also been predicted to be HM ferromagnets. Theoretically, the above-room-temperature ferromagnetism in NiCrZ and NiVAs were predicted by Şaşıoğlu et al. [45].

In this paper, we have adopted a method based on density functional theory (DFT) to investigate electronic and magnetic properties of GeKMg and SnKMg half-Heusler alloys with Cl_b -type structure by using Perdew-Burke-Ernzerhof generalized gradient approximation (GGA) [13]. Even though the ground state is well described by GGA, the values of the band gaps are sometimes underestimated. And so electronic properties are analysed further using the modified Becke Johnson potential (mBJ) calculations for improved values of the band gaps [14]. The exchange potential, introduced by Becke and Johnson, [19] was modified by Tran and Blaha. [15] The modified Becke-Johnson (mBJ) potential is given by



$$V_{mBJ}(r) = cV_x^{BR}(r) + (3c - 2) \frac{1}{\pi} \sqrt{\frac{5}{12}} [2t(r) / \rho(r)]^{1/2}$$

where $V_x^{BR}(r)$ is the Becke-Roussel exchange potential, [47] (r) is the electron density and $t(r)$ is the Kohn-Sham kinetic energy density. In the above equation, $c = A + B\sqrt{g}$ where g is the average of $|\nabla\rho / \rho|$ over the volume of the unit cell, and A and B are parameters adjusted to produce the best fit to the experimental values of the semiconductor band gaps. Radi A. Jishi [40] has shown that using the modified Becke-Johnson exchange potential with $A = 0.4$ and $B = 1.0 \text{ bohr}^{1/2}$, the calculated band gaps of MAPbI_3 , MAPbBr_3 , RbPbI_3 , and CsPbX_3 ($X = \text{Cl, Br, I}$) are in excellent agreement with experimental values. [41]

2. Computational method

In this paper, in order to investigate the structural stability and potential half-metallicity of half-Heusler compounds GeKMg and SnKMg we use the first-principles calculations to systematically investigate their electronic, magnetic and structural stability.

The spin-polarized density functional theory (DFT) calculations are performed with WIEN2k code [15-16]. The generalized gradient approximation (GGA) in Perdew Burke-Eenzehof generalized gradient approximation (GGA) [13,17] is used to describe the exchange correlation energy. The mBJ (modified Becke Johnson) potential [19-21] is used to get a more accurate representation of the DOS and band structures and comparisons were made with the results from PBE-GGA and mBJ calculations. A mesh of $12 \times 12 \times 12$, consisting of 286 special k points are set in the Brillouin zone (10000 k points in the full BZ) of irreducible wedge for the integrations within the modified tetrahedron method [23]. The cut off parameter for the plane wave was set to $K_{\text{max}} \times R_{\text{mt}} = 7.0$ where K_{max} is the uttermost value of the reciprocal lattice vector in plane wave function and R_{mt} is the smallest muffin tin sphere radii. The value of G_{max} is 12 where G_{max} is the largest vector value in charge density Fourier expansion. These parameters ensure good convergences for the total energy.

3. Results and discussions

3.1. Crystal Structure.

Half-Heusler compounds, which have the chemical formula XYZ, crystallize in the face-centered cubic C1b structure with the space group F-43m [24]. In this structure, X, Y and Z atoms occupy $(1/4, 1/4, 1/4)$, $(0, 0, 0)$ and $(1/2, 1/2, 1/2)$ sites, respectively, and $(3/4, 3/4, 3/4)$ site is empty. To get the equilibrium lattice constants of the half-Heusler alloys GeKMg and SnKMg , we calculate the total energy as a function of lattice constants for the three possible atomic arrangements as in Table 1. The α -phase is used for calculations of the electronic and magnetic properties as it has the lowest minimized energy. Fig.2 shows optimized volume of GeKMg at equilibrium lattice constant in the α -phase and the lattice parameters at constant equilibrium is 7.26 \AA for GeKMg and 7.61 \AA for SnKMg by using Murnaghan equation [18]. The equilibrium lattice constants, bulk modulus, energy we calculated are displayed in Table 2.

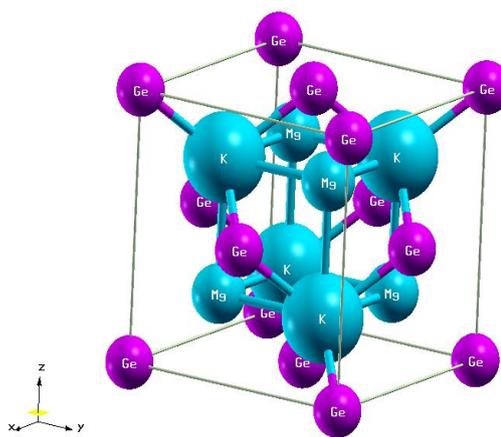


Figure 1. Unit Cell of cubic C1b-type structure for GeKMg in α -phase.

Table 1. Atomic arrangements of X,Y and Z atoms in three phases.

Phase	X	Y	Z
α	$\frac{1}{4}, \frac{1}{4}, \frac{1}{4}$	0,0,0	$\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$
β	0,0,0	$\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$	$\frac{1}{4}, \frac{1}{4}, \frac{1}{4}$
γ	$\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$	$\frac{1}{4}, \frac{1}{4}, \frac{1}{4}$	0,0,0

Table 2. Computed equilibrium lattice constant with bulk modulus and energy with previous calculation*[26].

Compound	GGA (\AA^0)	GGA (\AA^0)*	Bulk Modulus (Gpa)	Energy (Ryd)
GeKMg	7.26	7.22	21.2	-5803.059
SnKMg	7.61	7.57	18.392	-13963.145

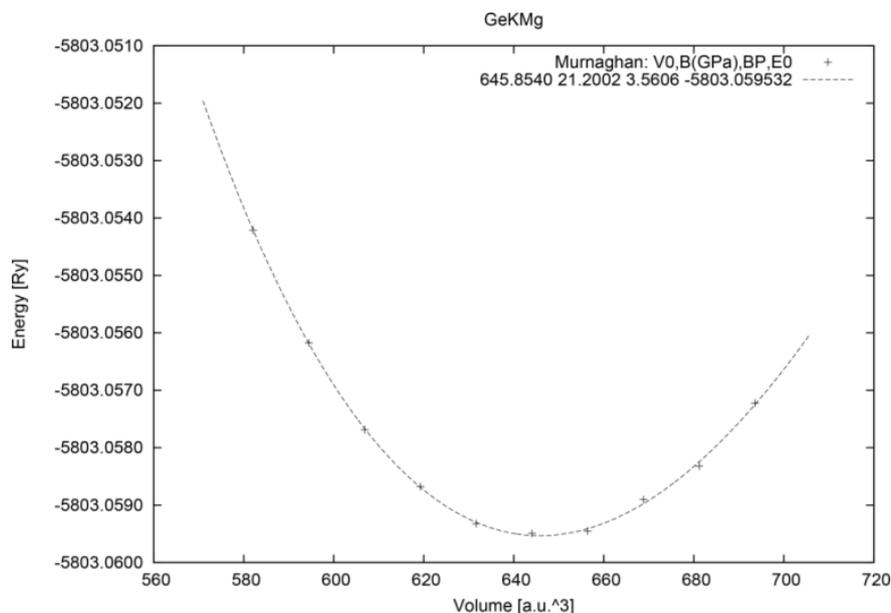


Figure 2. Total energy as a function of volume at equilibrium lattice constant for GeKMg in α -phase.

3.2 Electronic and magnetic properties.

Fig. 3 presents the spin polarized total density of states (DOS) of GeKMg and SnKMg at their respective equilibrium lattice constants in GGA and mBJ configurations. One can see that for GeKMg in both GGA and mBJ there is an energy gap around the Fermi level in the majority-spin (spin-up) channel while the minority-spin (spin-down) channel is strongly metallic, that is to say, it exhibit a true HM characteristic with 100% spin-polarization around the Fermi level. However for SnKMg structure the energy gap around the Fermi level in the majority-spin (spin-up) channel is not exactly around the Fermi level indicating that it is nearly half metallic in GGA. But for mBJ configurations Fermi level lies in between the energy band gap in majority-spin channel thereby showing a half metallic character.

It can easily be observed that the total DOS is mainly contributed by the Ge-p states while the d and p states of K and Mg respectively contributes to the DOS near the Fermi level. Fig. 3 also shows that, for GeKMg the energy gaps around the Fermi level in the majority-spin channel are about

0.32 eV(GGA) and 1.05 eV (mBJ) and for SnKMg 0.49 eV(GGA) and 1.1 eV(mBJ) which are similar to NiMnSb (0.5 eV) and CoMnSb (1 eV) [35]. Meanwhile, the HM gap [31–33], which is the minimum between the bottom energy of majority (minority) spin conduction bands with respect to the Fermi level and the absolute values of the top energy of majority (minority) spin valence bands, is 0.1 eV and 0.39 eV for GeKMg in mBJ and GGA respectively and 0.14 eV for SnKMg in mBJ. The different physical properties of GeKMg and SnKMg are given in Table 3. The calculated spin-projected partial DOS of GeKMg and SnKMg in the ferromagnetic state at the equilibrium lattice constant is shown in Fig. 3. The partial DOS of some states such as s and d states of Ge are omitted as their contribution is very small. Comparing the total and partial DOS with the band structure we can see that, for both majority- and minority-spin channels, the lowest band mainly originates from the Ge-p states and the bands around 6 eV are mainly formed by the K-d state. However, these states are located far from the Fermi level and the spinsplitting is very weak, so that their contribution to the form of half-metallicity in GeKMg and SnKMg is very small. The half-metallicity is mainly from the spin polarization of the Ge-p, K-d and Mg-p.

Fig. 5 shows the respective band structure plots of GeKMg and SnKMg in GGA and mBJ in both spin channels along with total DOS. In the valence region of the spin up and spin down channels, the bands are mostly due to the Ge-p states in both GeKMg and SnKMg. The bands in the conduction regions are mostly due to K-d electrons states in both cases of GeKMg and SnKMg. For GeKMg in GGA and mBJ the width of the energy gap EG is the difference in energies of the maximum occupied band at the symmetry point Γ in the valence band and the minimum unoccupied band in the conduction region at a symmetry point Γ which gives a direct band gap. And in the case of SnKMg in GGA and mBJ the energy gap is also along the symmetry point Γ respectively giving a direct band gap. For GeKMg in GGA and mBJ the direct band gap obtained are 0.32 eV and 1.05 eV respectively. Similarly for SnKMg in GGA and mBJ a direct band gap obtained along the symmetry point Γ are 0.49 eV and 1.1 eV respectively. When mBJ potential calculations are employed it is observed that the valence bands shift downwards while the conduction band shifts upwards resulting in a wider band gap.

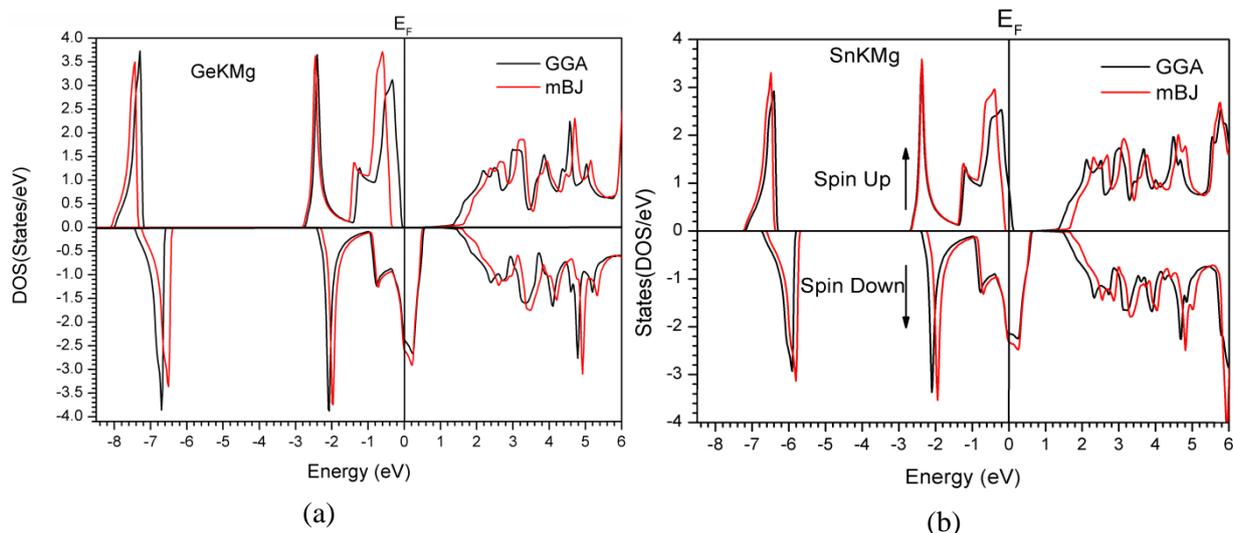


Figure 3. Total DOS of GeKMg (a) and SnKMg (b) in GGA and mBJ at the lattice equilibrium constant.

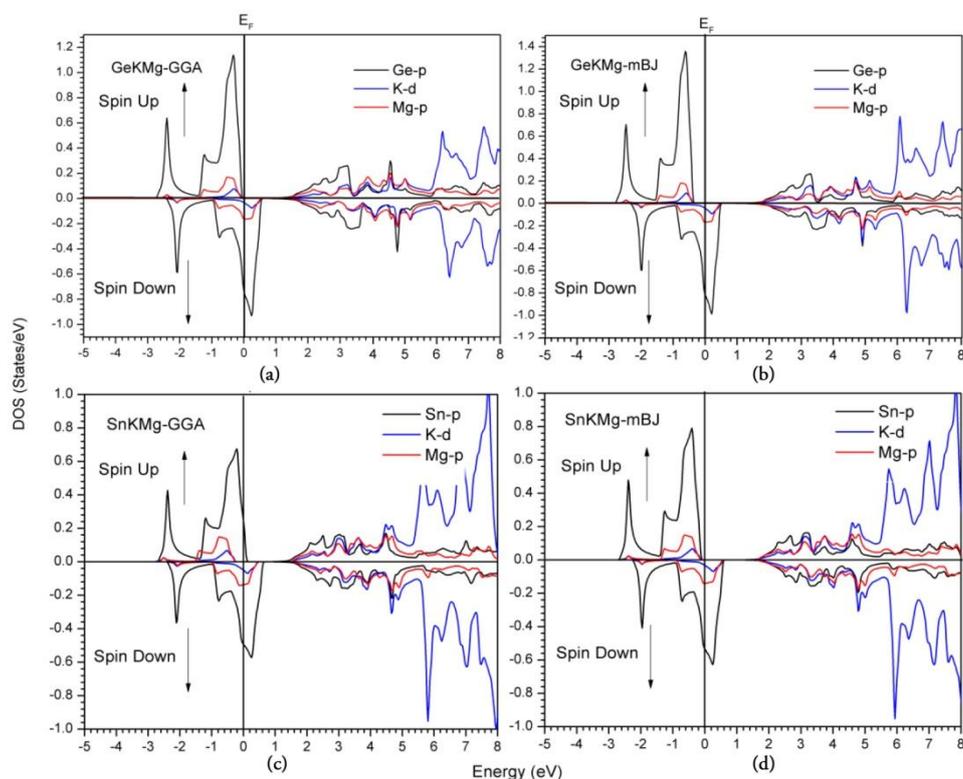


Figure 4. (a) Partial DOS of GeKMg in GGA (b) Partial DOS of GeKMg in mBJ (c) Partial DOS of SnKMg in GGA and Partial DOS of SnKMg in mBJ.

Table 3. Different physical properties of GeKMg and SnKMg at equilibrium lattice constant in the α -phase, V_{XC} is the exchange correlation potential, V_{BM} is the valence band maxima, C_{BM} is the conduction band minima, E_{BG} is the energy band gap, E_{HM} is the half-metallic gap, M is magnetic moment, * gives the value of previous calculation [26].

Material	V_{XC} (eV)	V_{BM} (eV)	C_{BM} (eV)	E_{BG} (eV)	E_{HM} (eV)	M (μ_B)	M^* (μ_B)	Result	Result*
GeKMg	GGA	-0.1	0.22	0.32	0.10	0.99	1.00	HM	HM
	mBJ	-0.39	0.66	1.05	0.39	1.00	-	HM	-
SnKMg	GGA	0.07	0.56	0.49	-	0.90	0.81	Not HM	Not HM
	mBJ	-0.14	0.96	1.1	0.14	1.00	-	HM	-

Table 4. gives the calculated total and partial magnetic moments for GeKMg and SnKMg at the optimized equilibrium lattice constants. The calculated total magnetic moment per formula unit is $0.99 \mu_B$ and $1 \mu_B$ for GeKMg in GGA and mBJ respectively. While The calculated total magnetic moment per formula unit is $0.90 \mu_B$ and $1 \mu_B$ for SnKMg in GGA and mBJ respectively. It can be seen that the atomic spin moment mainly originates from the Ge and Sn atom in GeKMg and SnKMg respectively. Therefore from the observed magnetic moments we can conclude that GeKMg is a half metal in both GGA and mBJ while for SnKMg half metallicity is observed only in mBJ.

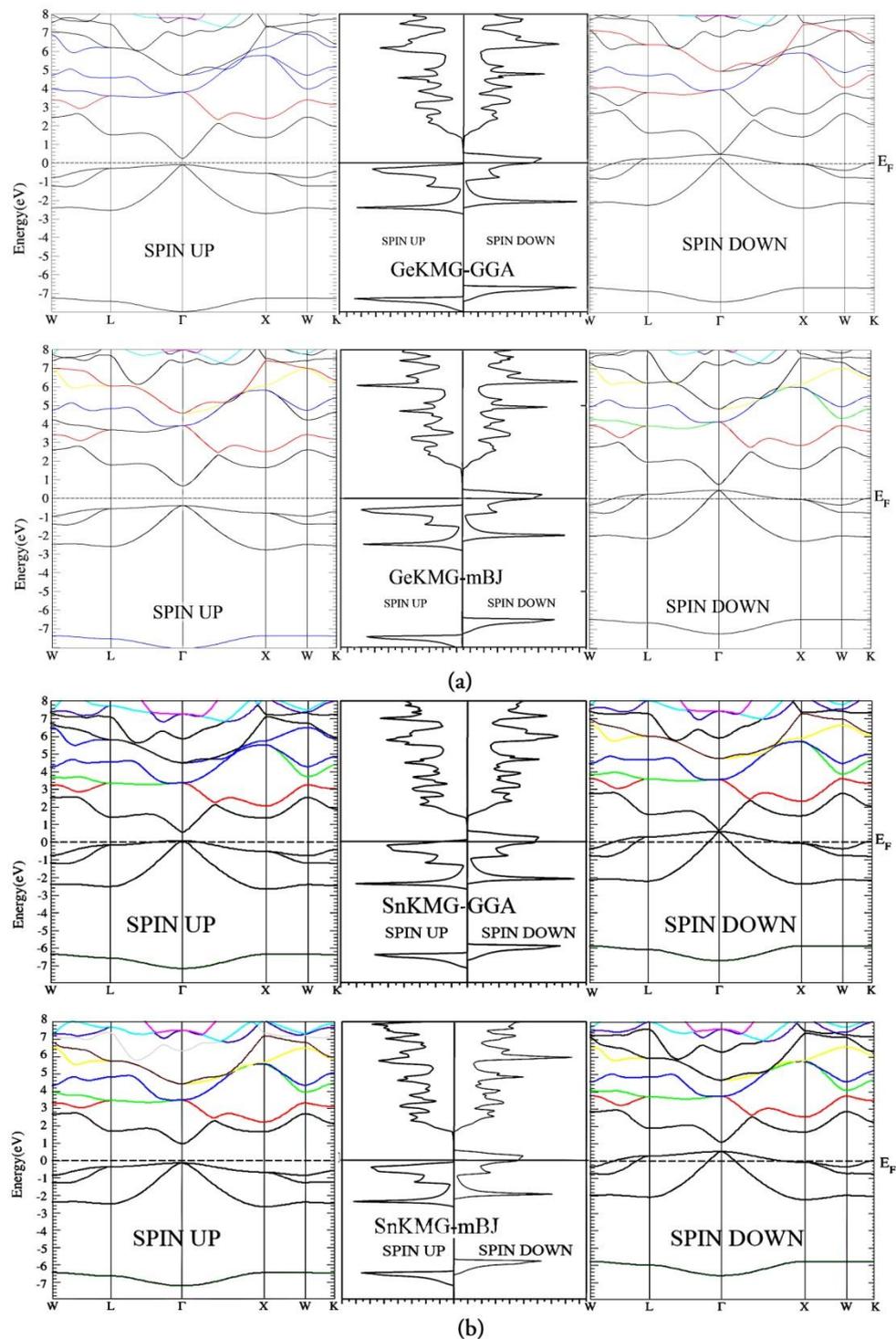


Figure 5. Band Structures of GeKMg (a) and SnKMg (b) in GGA and mBJ with DOS.

Table 4. Total magnetic moment M_{tot} (μB) and local magnetic moments (μB) of GeKMg and SnKMg in GGA and mBJ values. M_{I} (μB) is the magnetic moment of the interstitial region, M_{tot}^* [26] is the previous calculation. V_{XC} is the exchange –correlation potential.

Compounds	V_{XC}	m_{Ge} (μB)	m_{K} (μB)	m_{Mg} (μB)	M_{I} (μB)	M_{tot} (μB)	M_{tot}^* (μB)
GeKMg	GGA	0.41	0.03	0.03	0.51	0.99	1.00
	mBJ	0.45	0.03	0.01	0.45	1.00	-
SnKMg	GGA	0.25	0.03	0.03	0.57	0.90	0.81
	mBJ	0.29	0.02	0.03	0.64	1.00	-

4. Conclusion

To summarize, we have investigated the structural, electronic and magnetic properties GeKMg and SnKMg compounds with half-Heusler structure by using the full potential linearised augmented-plane wave (FP-LAPW) code based on density functional theory implemented with the WIEN2k package. GGA approximation is first used to get a view of the electronic structures and mBJ potential methods are employed to get a better description of the energy band gaps. GeKMg showed half-metallicity with HM gaps of 0.1 eV (GGA) and 0.39 eV (mBJ) while SnKMg showed half-metallicity only in the mBJ configuration with HM gap of 0.14 eV. The calculated magnetic moment, 1 μB per formula unit for both GeKMg and SnKMg, mainly originates from the Ge (Sn) atom.

Acknowledgement

The author (T. Malsawmtluanga) would like to extend his sincere appreciation to Condensed Matter Theory Research Group, Physics Department, Mizoram University and especially to Benjamin Vanlalruata, a brilliant contributor to the group who recently passed away.

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