Electronic structure calculations of some Cr based spintronic half Heusler alloys

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Abstract. Several XYZ materials with X and Y as 3d and 4d transition metal elements offer half-metallic magnetic properties. In such half-metallic materials there is a band gap at the Fermi energy for the minority spin channel, but not for the majority spin channel. In this work, we present the energy bands and density of states of half-Heusler alloys namely, KCrZ (where Z=S, Se and Te) using first principles full potential linearized augmented plane wave method by applying PBEsol approach of generalised gradient approximation. It is seen that these compounds show half-metallic character with large magnetic moment of about 5.0 μB. Density of states and energy bands are analysed to discuss about the origin of large values of spin moment in such compounds.

1. Introduction
In recent years, half-metallic ferromagnets (HMF) have been studied extensively because of their complete spin-polarized nature and potential applications in spintronics [1-4]. Such materials are best suited as electrode materials for magnetic tunnel junctions, in giant magnetoresistance devices and spin-polarized current injection purposes. Spintronics is very advantageous for high-speed and low energy electronic devices as it uses spin instead of charge for transfer and processing of information. A half-metal exhibits metallic behaviour in one of its spin channels while insulating properties in the opposite spin channel is witnessed. The metallic states are intercepted by Fermi level which lies in the gap of the spin down channel. Hence, half-metals are proved to be ideal materials for fabricating spintronic devices as they show 100% spin-polarized current (according to the Jullière formula [5]). Half-Heusler half-metallic alloys XYZ (where X and Y=transition metals, Z=p-block elements) with 1:1:1 composition show spintronic properties because they contain fully spin-polarized charge carriers at Fermi energy levels and have high spin magnetic moments.

Recently, Barman and Alam [6] have performed first-principles calculations within the density functional theory (DFT) to find the possibility of realizing a topological insulating phase in ZrIrBi. Structural stability and spin–orbit effect on β-LiCrAs and β-LiMnSi have been investigated for spintronic applications by Zhang et al. [7]. Damewood et al. [8] have computed band-gaps and magnetic moments of LiMnZ (Z = N, P, Si) alloys at their strained lattice constants and found HM
behaviours with large semiconducting-type band gaps. In the present study, we have applied the electronic structure calculations to identify new HM compounds suitable for spintronic applications. We have investigated the spin-projected band structures, density of states (DOS) and magnetic moments of KCrZ (Z=S, Se and Te) by first principles density functional calculations.

2. Computational Details
We have employed WIEN2k code [9], based on full potential linearized augmented plane-wave (FP-LAPW) method, to calculate the electronic structure and magnetism in half-Heusler alloys namely KCrS, KCrSe and KCrTe. The exchange and correlation potentials of PBEsol scheme [10] within the generalized gradient approximation (GGA) have been applied for the present investigations. Half-Heusler alloys with formula XYZ crystallize in F-43m symmetry (space group No. 216) with Wyckoff positions 4a (0,0,0), 4d (0.75,0.75,0.75) and 4c (0.25, 0.25, 0.25). Crystal structures of KCrS, KCrSe and KCrTe are shown in Figures 1 (a-c). The values of RMT for K, Cr, S, Se and Te were taken as 2.5Å, where RMT is smallest value of Muffintin (MT) spheres. In present computations, we have selected a grid of 1000 \( k \)-points in the irreducible Brillouin zone (BZ).

3. Results and Discussion

3.1 Electronic Properties
We have derived the electronic properties of KCrZ (Z = S, Se and Te) by applying PBEsol approach within the FP-LAPW theory. The band structures of these alloys in spin-up (left panel) and spin-down (right panel) channels along with total and partial spin-projected DOS curves are shown in Figures 2 (a-c) for KCrZ (Z = S, Se and Te), respectively. KCrZ (Z = S, Se and Te) behave like conductors in up-spin state and semiconductor in spin-down channel, tending to half-metallicity.

The formation of energy bands can be explained by the help of DOS curves. In spin-up state, DOS curves cross the Fermi energy (\( E_F \)) level, while their amplitude vanish around \( E_F \) in spin-down state. The DOS for all the three compounds depict almost similar nature of bonding and antibonding states which result into semiconducting-type band gap in spin down conditions. From DOS curves it can be observed that the d states of Cr atoms contribute majorly in both the spin channels. The lowest valence band (VB) around -14.0 to -13.0 eV is mainly formed due to K-p states and energy bands near -11.0 eV are mainly by chalcogen-s states with small participation of K-p states in both the spin channels. The VB in the vicinity of \( E_F \) is dominated by Cr-d states whereas K-p states are responsible around -4.0 eV to \( E_F \) in spin up channel. The chalcogen-p states are quite dominating around -4.0 to -2.0 eV in spin-up and-down channels with small contribution due to K-p states. The Cr-d electronic states are observed in the CB with peak around 3.0 eV in spin down case.
Figure 2. The spin-up (↑) and spin-down (↓) band structures along with total and partial DOS for half-metallic Heusler alloys (a) KCrS (b) KCrSe and (c) KCrTe using PBEsol scheme of FP-LAPW theory. The $E_F$ level is set to 0 eV.
We found an indirect spin-down gap of 1.40, 1.37 and 1.77 eV for KCrS, KCrSe and KCrTe, respectively. Overlapping of conduction and valence bands in spin-up and band gap in spin-down channels proves half-metallic character.

3.2 Magnetic Properties

In Table 1, we have listed the lattice constants, total and atom specific magnetic moments in a unit cell, energy band-gaps (in spin-down channel) and status of half metallic character for KCrZ with Z=S, Se and Te. Total magnetic moment for all the three alloys is found to be 5.0/μB per formula unit and band-gap in spin-down channel is in the range of visible spectrum indicating the potential application in solar cells within spin-down channel. The computed values of magnetic moments are in reasonable agreement with those reported by Wang et al. [11].

| Alloys       | Present Study | Wang et al. [11] |
|--------------|---------------|------------------|
|              | a (Å)         | M_T (μ_B) | M_K (μ_B) | M_Cr (μ_B) | M_Z (μ_B) | M_int (μ_B) | Band Gap (eV) | HM     | M_T (μ_B) | Band Gap (eV) | HM     |
| KCrS         | 6.90          | 4.999     | 0.06       | 4.39       | -0.13     | 0.67       | 1.40         | Yes    | 5.00      | 2.14         | Yes    |
| KCrSe        | 6.98          | 5.000     | 0.06       | 4.37       | -0.12     | 0.70       | 1.37         | Yes    | 5.00      | 2.09         | Yes    |
| KCrTe        | 7.41          | 5.005     | 0.06       | 4.31       | -0.10     | 0.75       | 1.77         | Yes    | 5.00      | 1.87         | Yes    |

The calculated total magnetic moment is in accordance with the modified Slater-Pauling rule, M_T=(Z_T-8)/μ_B in consonance to Damewood et al. [8], where Z_T is the number of valence electrons in KCrZ (Z=S, Se, Te). In these alloys the K, Cr and X atoms carry one, six and six electrons, respectively, within the covalent electron configuration of K(4s^1), Cr(3d^54s^1), S(3s^23p^4), Se(4s^24p^4) and Te(5s^25p^4) thereby leading to total magnetic moment around 5.0 μ_B in agreement with the previously reported results [11].

4. Conclusions

Density functional theory using PBEsol approach of FP-LAPW method has been used to explore the half metallic character of KCrZ (Z=S, Se and Te). We found a large value of magnetic moment 5.0 μ_B/f.u. and semiconducting type band-gap in spin-down states of KCrS, KCrSe and KCrTe as 1.40, 1.37 and 1.77 eV, respectively. The half-metallic nature provides stabilised spin polarization properties of these compounds.

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