Journal of the Nigerian Society of Physical Sciences

Half-metallic Characteristics of the Novel Half Heusler Alloys XCrSb($X = Ti$, Zr, Hf)

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Abstract

Ab-initio calculations are performed to examine the structural, mechanical, electronic, magnetic and thermodynamic properties of the half-Heusler ternary alloys XCrSb ($X = Hf$, Ti, Zr). In this study, the spin-polarized density functional theory (DFT) method that is spin-polarized with generalised gradient approximation (GGA) are used to perform *ab-initio* calculations to investigate the physical properties of a novel half-Heusler ternary alloys XCrSb ($X = Hf$, Ti, Zr). It was confirmed that the alloys are stable mechanically and exhibit ferromagnetic states (FM). The study reveals that the alloys portray half-metallic character with narrow energy gaps. And it also shows that they have a total magnetic moment of approximately $3\mu_\beta$. From the formation energy calculation, it shows that the alloys can be synthesized experimentally. Also, it was observed that they are mechanically stable. The heat capacities and Debye temperatures were also computed and they show high thermodynamic stability.

Communicated by: E. A. Emile

1. Introduction

The Heusler alloys have been studied extensively in the recent past, and one of the major results is that they are among the best half-metallic ferromagnets (HMF) to achieve 100% spin polarization at room temperature. Density Functional Theory (DFT) has proven to be a reliable tool for calculating electronic structures for many decades, this is due to its simple and usefull approach in approximating the ground state functionals of real many-body electrons. The theory is built on the fact that the properties of many-body interacting system can be seen as a functional of the ground state electron density [1]. From the works of Mehmood et al [2-3], it was gathered that the half-Heusler alloys YZSb ($Z = Cr$, Mn) and RhCrZ ($Z = Si$, Ge) exhibit half-metallic properties within the framework (DFT) among others. Also, the electronic, magnetic and optical properties were equally studied. The field of spintronics is quite different from the conventional electronics in which charges are responsible for transfer of information, whereas in spintronics spins are responsible for the transfer of information. Some of these enhancements and advantages are; increasing the speed of the data processors, drop in the consumption of electric power and the increase in integration density [4 − 6]. The study of half Heusler (HH) alloys present interesting and different magnetic occurances, and this have attracted researchers in re-

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cent time [7 − 15]. Ternary half-Heusler compounds are usually denoted by the chemical formula XYZ, where X is rare-earth metal, Y is transition metal and Z is the main group elements in the periodic table. This area has attracted a lot of attention by many researchers for about a decade now. Relatively, the HH compounds form a big family of materials with several physical properties and applications especially in the areas of opto-electric semiconductors and spintronics [16 − 18], thermoelectiric semiconductors [19 − 21], piezoelectric semiconductors [22] and topological insulators [23, 24]. Considering the half metallic materials, the majority and minority spin-bands exhibit different behaviours. The majority spin band portrays metallic behaviour while the minority spin band displays a semiconductor character with a narrow band gap within the Fermi level. And around the Fermi level, the gap results in a 100% spin-polarization [25, 26]. Since the discovery of the half-metallicity in the (HH) compounds, numerous researchers have done vigorous studies determining the stability of the physical/mechanical, electronic/phonon dispersion and as well as thermodynamic properties using First-Principles calculations. Amoung them are: ZrMnAs [27], PtXBi ($X = Fe$, Co, Mn and Ni) [28], ZrNiPb [29], and XVSb ($X = Fe$, Ni, Co) [30]. The works of Rogl and coworkers [31] provides an extensive review on the mechanical properties of many HH systems, like the XNiSn and XCoSb where $X = Ti$, Zr and Hf. They studied the fracture toughness, hardness/elastic moduli and density-porosity of alloys empirically and theoretically. However, nothing has been mentioned about the replacement of Co atom with Cr atom in the XCoSb series. Considering the industrial uses of chromium, ranging from hardening of steel, chromium plating, leather tanning, as well as industrial catalysts to pigmentation. Therefore, it became imperative in this present study, to predict the physical, mechanical, electronic, magnetic and thermodynamic properties of the novel half-Heusler alloys using ab-initio calculations

2. Methodology

The ab-initio total energy calculations were executed employing the QUANTUM ESPRESSO (QE) as applied in the works of Giannozi [32]. The Projected Augumented Wave pseudo potential was used in the computation [33]. The exchange inter-relationship between electrons, bonding and magnetic features were treated with the GGA-PBE approach. The (HH) alloy XYZ, has an fcc structure, in space group $F − 43m$ No. 216 with its Structurbericht designation of C1 b as recorded in the International Table of Crystallography. The crystal structures for the three alloys are presented in Figure 1. We use the spin-polarized density funtional theory (DFT). The energy cut-off value and the k-points are essential flags (in the input-file) in ensuring the accuracy of the calculations [34]. The k-points are used for the structural optimization and static SCF calculations for the alloys XCrSb ($X = Hf$, Ti and Zr). Convergence tests for the energy cut-off and the k-points are carried out before determining their appropriate values for the calculations. The Monkhorst Pack format with 8 x 8 x 8 framework was used, and the kinetic energy cut-off were fixed to 60Ry for HfCrSb
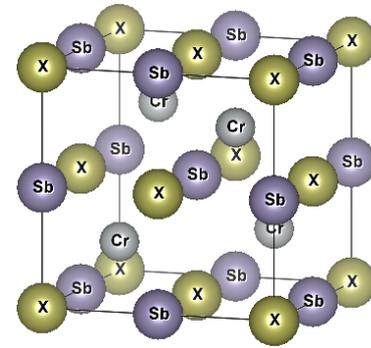

Figure 1. The crystal structure of XCrSb where X=Ti, Zr and Hf.

and ZrCrSb, 65Ry for TiCrSb alloys. The Pseudo-atomic configurations used as valence electrons, in this study, are Hf $5d^2 6s^2$, Ti $3d^2 4s^2$, Zr$4d^2 5s^2$, Cr $3d^5 4s^1$, and Sb $4d^{10} 5s^2 5p^3$ respectively. The ($X = Hf$, Ti and Zr), Sb and Cr occupy the atomic positions 4a(0, 0, 0), 4b($\frac{1}{2}$, $\frac{1}{2}$, $\frac{1}{2}$) and 4c($\frac{1}{4}$, $\frac{1}{4}$, $\frac{1}{4}$) respectively.

3. Results and Discussions

3.1. Structural and Mechanical Properties

Investigating the structural properties of the ground state configuration of the XCrSb compounds (where $X = Ti$, Zr and Hf), firstly, the structural/geometry optimisation was carried out by minimizing the total energy of the alloys with respect to the variation of the lattice parameters. The lattice constant a, the bulk modulus B and its pressure derivative B′ were obtained when the energy-lattice parameter was fitted to the Birch Murnaghan equations of state. These results are presented in Table 1 and the obtained energy-lattice curves for the various alloys are shown in Figure 2. The three HH alloys in different magnetic states were studied in order to ascertain the true nature of the alloys. The results for the ferromagnetic (FM) states, non-magnetic (NM) states as well as for the anti-ferromagnetic (AFM) states were presented in Fig. 3. It is observed that the (FM) states posses the lowest ground state energy for the three HH alloys, hence they are all ferromagnets. It is the ferromagnetic states of these alloys that have been used to compute the other properties in this work. In solids, the elastic constants and some structural features play vital roles in determining the mechanical stability of the material [35]. For cubic phases, the stability is measured by the following criteria $C_{11} + 2C_{12} > 0$, $C_{11} − C_{12} > 0$, , and $C_{11} > 0$ [36]. The alloys are mechanically stable since all the necessary conditions were satisfied, see Table 2. The bulk modulus B, Young Modulus E and shear modulus G are parameters used to quantify the mechanical properties of solids. From Table 1, the results of the B and E show that the deformation resistance decreases in trend from HfCrSb to ZrCrSb to TiCrSb alloys, except for the shear modulus that has a contrary behaviour. An expression to establish the plasticity of a material is given by the $\frac{B}{G}$ ratio. The threshold value for distinguishing between ductility and brittleness of materials is about 1.75 [37]
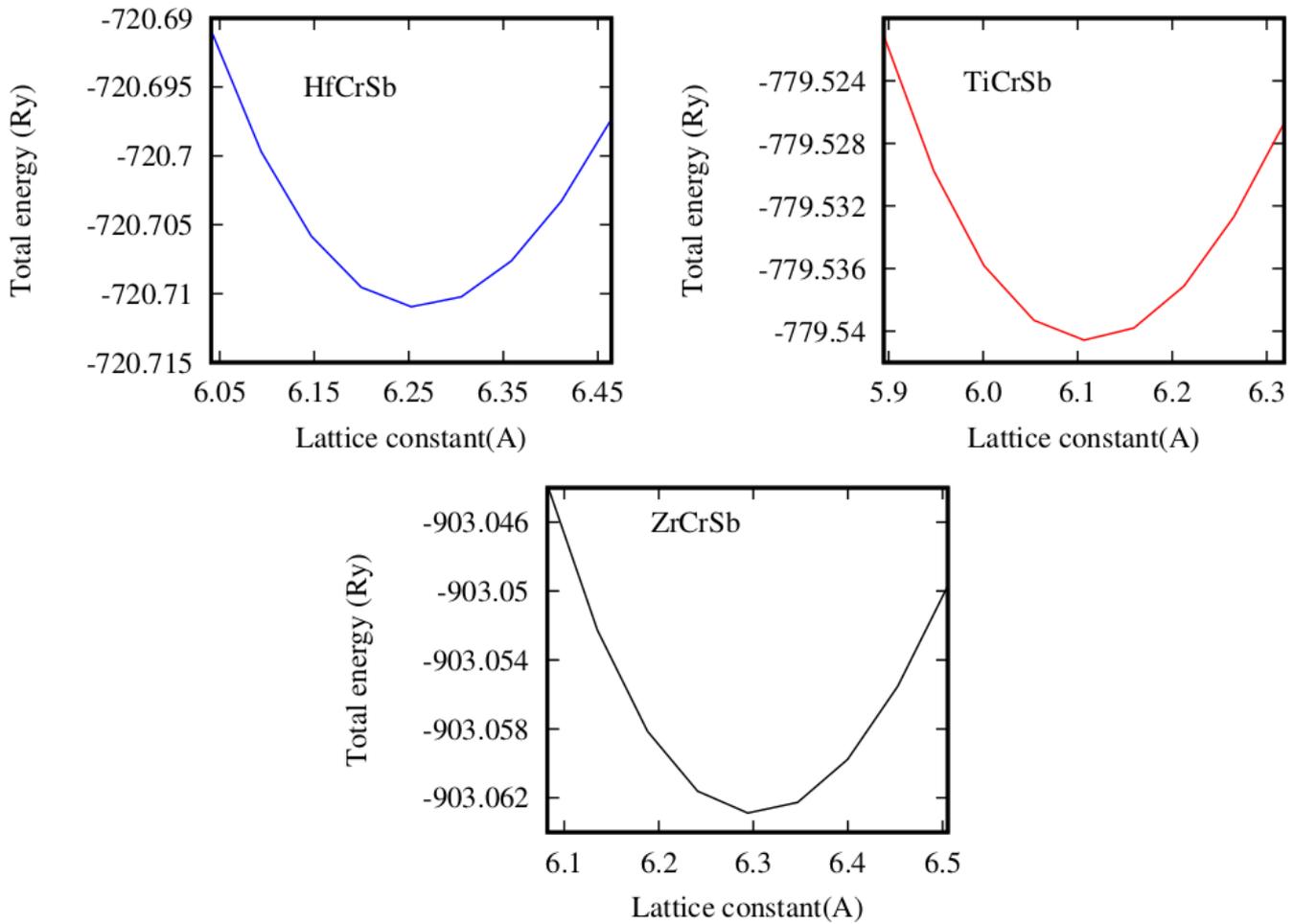
Figure 2. Relationship between total energies per unit cell and lattice parameters for HfCrSb, TiCrSb and ZrCrSb

From our results presented in Table 2, it is obvious that the alloys are ductile in nature since the values of the B/G ratio are more than 1.75. Although, there was no available experimental or theoretical reports on the XCrSb series for comparison, but our results for B, E, and the elastic properties are still within appreciable range when compared with the XCoSb series in literatures [31, 38]. It is observed that the values of the mechanical properties obtained for XCoSb HH alloys are higher than that of XCrSb obtained in this work. This is due to the fact that the bonding during the hybridization of the d-orbital of Cr atom and the d-orbital of X(Ti, Zr and Hf) atom is weak as shown in Figures 7 − 9. The present calculated results of Zener anisotropy A, shows that the three alloys are anisotropic, since the values are approaching 1, which is an indication of high elastic anisotropy. These results were obtained using the relation, from equation (1), as recorded in [39].

$$A = \frac{2C_{44}}{C_{11} - C_{12}} \qquad (1)$$

Another factor that can affect the stability of a material against shear stress is the Poisson′s ratio μ. It reveals the nature of the bonding forces in materials. The value range is of the order 0 ¡ v ¡0.5 [39]. From the results of v in Table 2, it shows that the three alloys are of good plasticity. The Cauchy relation is another parameter which expresses the ductility and brittleness of materials. When the value is positive, the material is considered ductile, otherwise it is brittle. The alloys under consideration are ductile as reported in Table 2. The formation energy Δ H of the alloys were investigated to verify whether they can be synthesized experimentally. The calculation was done using Equation 2:

$$\Delta H = E_t^c - \left(\frac{E_b^{e_1}}{N_a} + \frac{E_b^{e_2}}{N_b} + ... \right) \qquad (2)$$

where E_t^c is the total energy of the alloy, $E_b^{e_1}$ and $E_b^{e_2}$ are the total energies of the constituent elements respectively, and N_a represents the number of atom per cell. From the calcultions, the formation energies of XCrSb ($X = Hf$, Ti, and Zr) are −1.49eV, −1.10eV and −1.0eV respectively. These results confirm that the alloys can be synthesized easily because the enthalpies have negative values.
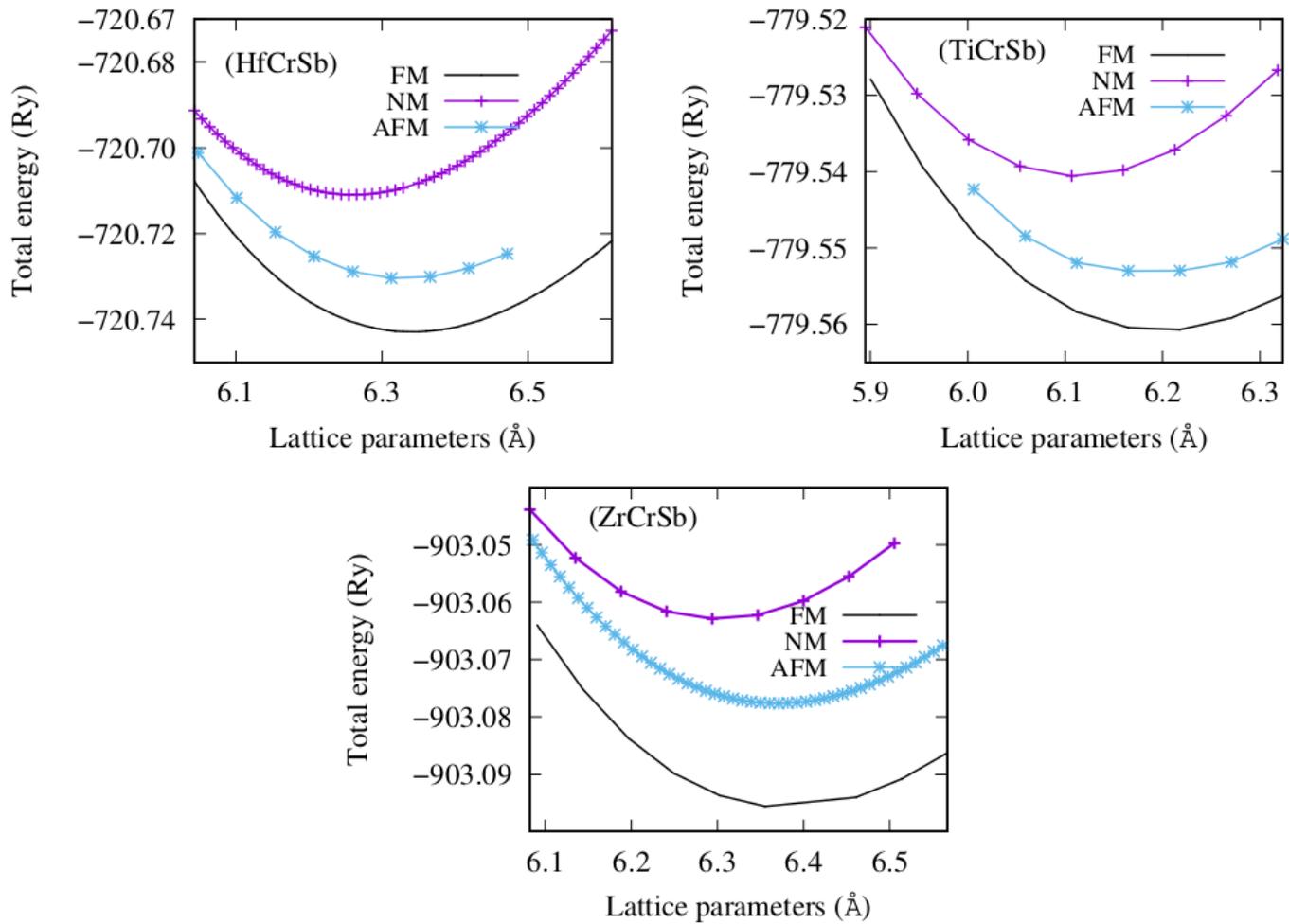
Figure 3. The total energies per unit cell as a function of lattice constants for the Ferromagnetic (FM), Antiferromagnetic (AFM) and Non-magnetic (NM) states of the alloys.

3.2. Electronic and Magnetic Properties

From the crystal structure of the (HH) compounds in Figure 1, the $X(X = Ti$, Zr and Hf) atom forms a tetrahedral position with the Cr atom as the cation at the center. The zincblende sublattice $[CrX]^{3+}$ formed hybridizes with the $[Sb]^{-3}$ ion. With this configuration the Cr atom gains one extra electron added to its initially six valence electrons thereby resulting to seven electrons that occupy the d-orbital. During the filling of the d-orbital, three electrons are left unpaired which constitue the magnetic moment of the alloys. The spin magnetic moment for each of the alloys is approximately 3μ as shown in Table 3. This satisfies the spin magnetic moment predicted by the Slater-Pauling rule [40]. The rule asserts that the total spin magnetic moment per formula unit M_{tot} is given by $M_{tot} = |N_v − 18|$ for (HH) compounds, where N_v is the sum of electrons at the valence. The sum of electrons at the valence for Ti, Zr and Hf are 4 each while that of Cr and Sb are 6 and 5 respectively. Hence the total number of electrons at the valence for each compounds is 15. The total and partial magnetic moments are presented in Table 3.

In order to obtain quantitative results to reveal the half metallic character from the electronic band structure calculations, the spin polarization P was computed for the minority and majority bands. From the three alloys, we have 0ev, 0.25ev for the up and down DOS at the Fermi level respectively. Using Equation (3) for spin polarization [41], we obtained 100% spin polarization in the alloys.

$$P = \frac{Dos\left(E_f\left(up\right)\right) - Dos\left(E_f\left(down\right)\right)}{Dos\left(E_f\left(up\right)\right) + Dos\left(E_f\left(down\right)\right)} \times 100\% \qquad (3)$$

The electronic properties of the three (HH) alloys have been computed in the form of band structures and are presented in Figures $4 − 6$. The (HH) alloys XCrSb ($X = Ti$, Zr and Hf) are found to posses the half-metallic properties since their band structures with the majority spin channels have indirect band gaps while their band structures for the minority spin channels show metallic behaviour. The measured band gaps for TiCrSb, ZrCrSb and HfCrSb are 0.31eV, 0.49eV and 0.42eV respectively. The PDOS for the three compounds have also been computed and are presented in Figures $7 − 9$. The purpose of the PDOS plot is to give insight into the nature of bonding between the orbitals of the individual atoms. The PDOS of the three half

Table 1. The Structural properties: the a (Å), B (GPa), and $B\prime$, energy of formation ΔH(eV), band gap near Fermi energy E_g(eV) and magnetic ground state M_g.

Alloy	a	B	$B\hat{A}\acute{}$	ΔH	E_g	M_g
TiCrSb	6.197	84.96	4.43	-1.10	0.31	FM
ZrCrSb	6.383	95.80	4.65	-1.00	0.49	FM
HfCrSb	6.341	99.66	4.75	-1.49	0.42	FM

Table 2. The mechanical/elastic properties: the C_{11}, C_{12} and C_{44} (GPa), B / G ratio, E (Gpa), Poisson's ratio υ, Zener anisotropy A, and the Cauchy relation.

Alloy	TiCrSb	ZrCrSb	HfCrSb
C_{11}	108.80	112.76	128.29
C_{12}	73.02	69.87	85.33
C_{44}	33.70	30.98	32.33
G	27.38	27.17	27.99
B/G	3.10	3.53	3.56
E	74.17	73.58	76.76
ν	0.35	0.35	0.37
A	1.88	1.44	1.51
$C_{12} - C_{44}$	39.32	38.89	53.00

Table 3. The total and partial magnetic moments of the half-Heusler alloy XCrSb (X=Hf, Ti, Zr).

Alloy	$M_x(\mu_\beta)$	$M_{Cr}(\mu_\beta)$	$M_{Sb}(\mu_\beta)$	$M_{tot}(\mu_\beta)$
TiCrSb	0.2899	2.7133	-0.0025	3.0007
ZrCrSb	0.1835	2.8653	-0.0386	3.0102
HfCrSb	0.1900	2.7696	0.0001	2.9597

Table 4. The specific heat capacity C_v, Debye temperature Θ_D, Zero Point energy E_o, and Debye sound velocity V_s.

Alloy	$C_v(J/Nmol.)$	$\Theta_D(K)$	$E_0(kJ/Nmol.)$	$V_s(m/s)$
TiCrSb	72.33	253	7.11	2302
ZrCrSb	72.63	238	6.69	2232
HfCrSb	73.16	209	5.87	1946

Heusler alloys are some how similar this is due to the fact that they have similar atoms inhabiting the Y and Z atomic sites and the three different atoms inhabiting the X atomic site are in the same group. From the minority-spin channels of the three HH alloys, the t_2g states of Cr atom dominate the region below the Fermi energy while the e_g states dominate in the region above the Fermi energy. Since both states are occupied around the Fermi energy, hence they show metallic character. The gaps seen around the Fermi energy in the majority spin straits for the three half-Heusler compounds are due to the crystal field splitting of the d-orbital of Cr atom into t_2g and e_g. Due to the exchange interactions between the Cr d-orbital and the X(Ti, Zr and Hf) d-orbital, there is depletion of electrons in the majority spin states leading to unoccupied states. This results to the development of half-metallic gap around the Fermi energy. We also observed the bonding states between the Cr d-orbital and the X(Ti, Zr and Hf) d-orbital just below the Fermi energy and the anti-bonding states between the Cr d-orbital and the X(Ti, Zr and Hf) d-orbital just above the Fermi energy. This observation is in line with observations by other researchers who worked on half Heusler alloys. It is also important to investigate the relationship between the magnetic moment and the lattice constant in order to determine the range of lattice constants at which the magnetic moment is preserved. From Figure 10, it is observed that the magnetic moment of $3\mu_\beta$ is preserved within the range of 11.2a.u to 14a.u for three HH alloys

3.3. Thermodynamic Properties

In Solid State Physics, the Debye temperature Θ_D is one basic factor in describing phenomena associated with many physical properties, like melting points, lattice vibration, specific heat, thermal expansion etc. The Θ_D is used for delineating high temperature regions from low temperature regions in solids. Basically, the Θ_D depends on the elastic constants. The Θ_D can be calculated from the average sound velocity, V_m by the expression [42, 43]

$$\Theta_D = \frac{h}{k_B} \left(\frac{3n}{4\pi V_a} \right)^{1/2}_{V_m} \tag{4}$$

$$V_m = \left[\frac{1}{3} \left(\frac{1}{V_t^3} + \frac{2}{V_t^3} \right) \right]^{-\frac{1}{3}} \tag{5}$$

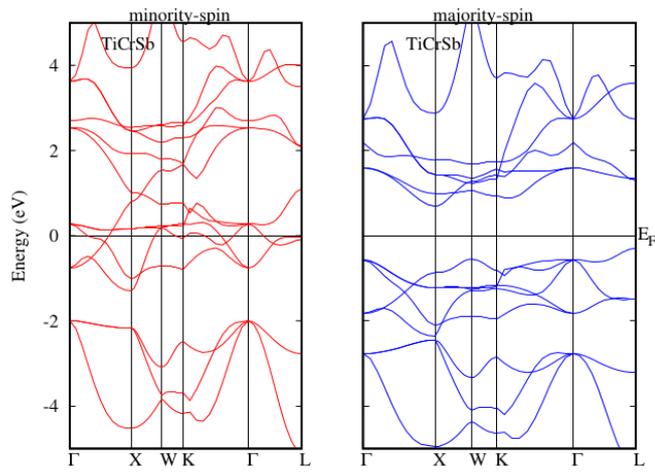$$V_t = \left(\frac{3B + 4G}{3\rho} \right)^{\frac{1}{2}} \tag{6}$$

Figure 4. Band structure of TiCrSb alloy
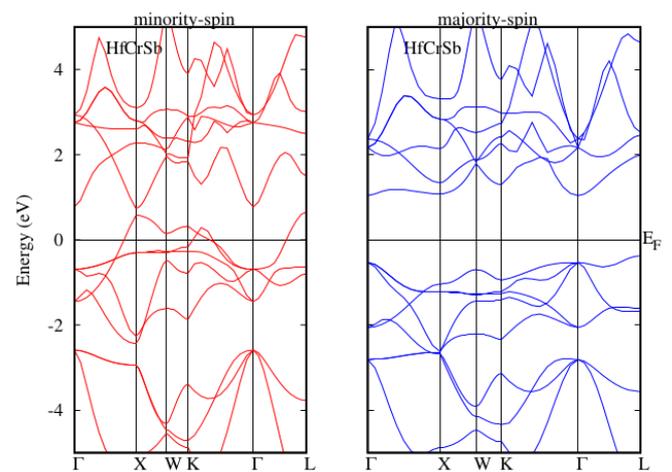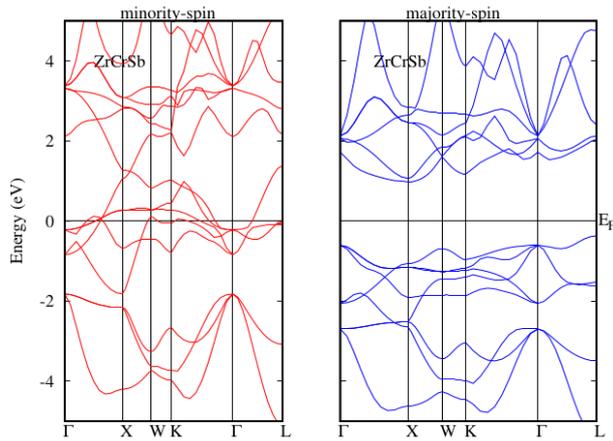

Figure 6. Band structure of HfCrSb alloy

Figure 5. Band structure of ZrCrSb alloy
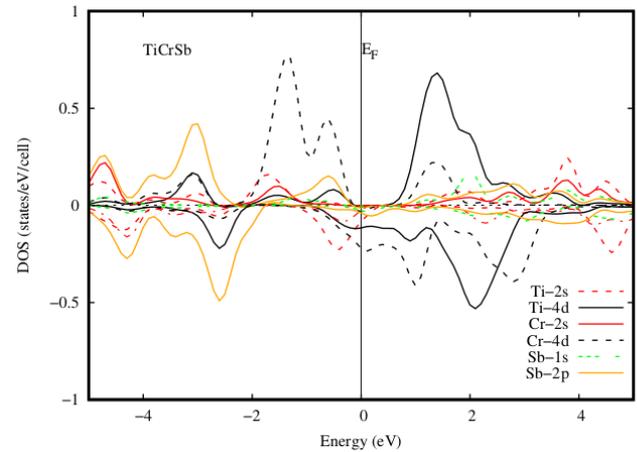

Figure 7. PDOS for TiCrSb alloy

$$A = \frac{2C_{44}}{C_11 - C_12} \tag{7}$$

where B, G and ρ are the bulk modulus, shear modulus and densities of the various alloys respectively. The calculated specific heat capacity, Debye temperatures, Zero Point energy and the Debye sound velocity for the various alloys are presented in Table 4. The Debye temperatures computed in this work are in reasonable range when compared with other half Heuslers [31, 38].

The Debye temperature is related to the strenght of the covalent bonds in solids, that is, the higher the Δ_D of a compound indicates a stronger covalent bond which leads to high melting point. Also, a strong covalent bond is associated with the hardness of the material 44. The other thermodynamic properties such as the enthalpy H, Free energy F , heat capacity at constant volume C_v and the entropy S of the alloys are evaluated by using the QHA. The results are shown in Figure 8. We can see that the C_v of the alloys increases swiftly as the temperature increases, such that at very high temperature it tends to reach the Dulong-Petit terminal point. It was also observed that at very low temperature, C_v is proportional to T^3. The entropy
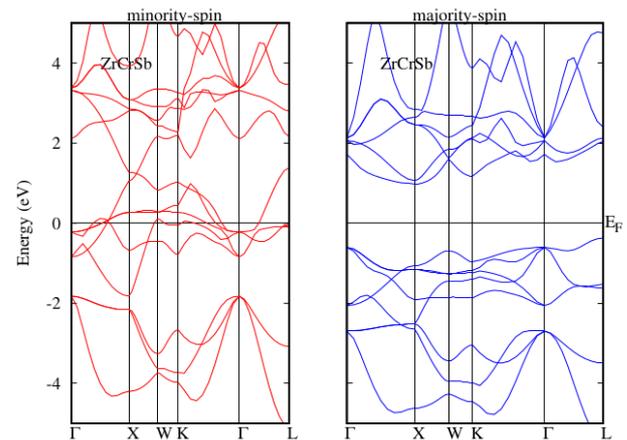

Figure 8. PDOS for ZrCrSb alloy

and enthalpy graphs show that as the temperature increases the values of the properties increased, while the reverse is observed for that of Free energy.
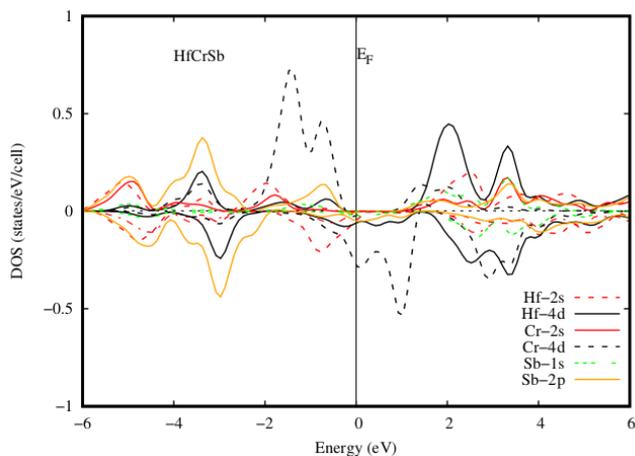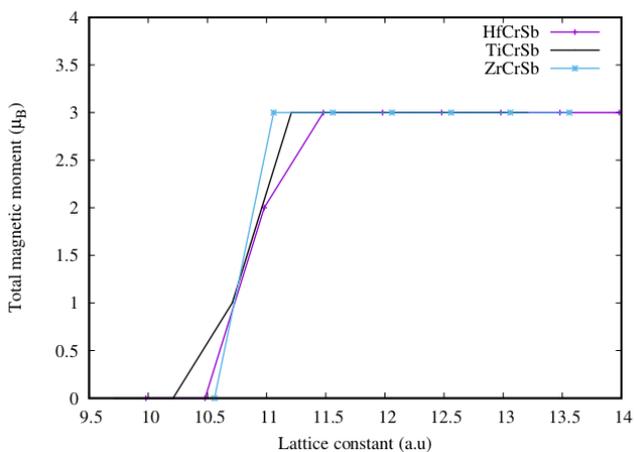
Figure 9. PDOS for HfCrSb alloy

Figure 10. Total magnetic moment per formular unit as a function of lattice constants for the three alloys.

4. Conclusion

The physical properties of a novel (HH) compounds XCrSb (where $X = Hf$, Ti, and Zr) have been investigated using ab-initio calculations. The ferromagnetic state is found to be more stabled and favourable than the antiferromagnetic and non- magnetic states structurally in term of total energy. The alloys are found to be stable from the mechanical stability conditions. Also, the B/G ratio and the Cauchy-relation reveals that the alloys are ductile. The electronic band structure and the DOS calculated reveal that the alloys exhibit half metallic ferromagnetic property and having approximately $3\mu_\beta$ magnetic moment. The total magnetic moment of these alloys is produced through remarkable exchange splitting between the majority-spin states and the minority-spin states of Cr orbital. From Table 3, the Cr atom is found to be the major contributor. Furthermore, the alloys satisfied the Slater-Pauling rule. The alloys are half-metallic in nature with energy-gaps of 0.4196eV, 0.309eV, 0.4946eV for HfCrSb, TiCrSb, and ZrCrSb respectively. Theoretically, it is shown that these new alloys can be synthesized easily experimentally because of their negative formation energies. Finally,

Δ_D and C_v computed for the three HH alloys are within acceptable range when compared with other HH alloys in that series. Finally, the half-metallicity, the stabilty in the ferromagnetic phase and the 100% spin-polarization around the Fermi energy make these alloys promising candidates for future spintronics applications.

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