Structural, electronic and thermodynamic properties of half-metallic Co$_2$CrZ (Z = Ga, Ge and As) alloys: First-principles calculations

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**Abstract**

Using first principles calculations, the structural, electronic, and magnetic properties of ferromagnetic half-metallic full-Heusler Co$_2$CrZ (Z = Ga, Ge and As) alloy via the FP-LAPW method in the generalized gradient (GGA) and GGA+U approximations are compared with other experimental and theoretical results. The calculated equilibrium lattice constants were in qualitative agreement with the previous results. The existence of the energy gap in the minority spin (DOS and band structure) of Co$_2$CrZ (Z = Ga, Ge and As) are an indication of being a potential half-metallic ferromagnetic HMF. The half-metallicity of the obtained material may prove useful for applications in spin-polarizers and spin-injectors of magnetic nanodevices. The calculated total spin magnetic moments are almost exactly that expected from Slater-Pauling rule. Thermal effects on some macroscopic properties of Co$_2$CrZ (Z = Ga, Ge and As) are predicted using the quasi-harmonic Debye model, in which the lattice vibrations are taken into account. The variations of the primitive cell volume, volume expansion coefficient, bulk modulus, heat capacity and Debye temperature with pressure and temperature in the ranges of 0–20 GPa and 0–3000 K, respectively are obtained successfully.

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1. Introduction

Heusler alloys (HA) have attracted a significant attention due to their interesting physical properties promising various practical applications in the fields of smart materials and magneto-electronics [1]. Indeed, certain Co$_2$Y-where Y is transition elements (Ni, Co, Fe, Mn, Cr, Ti, V, etc.) -based full-Heusler alloys (FHA) is predicted to be ferromagnetic and half-metallic i.e., compounds for which only one spin channel presents a gap at the Fermi level, while the other has a metallic character, leading to 100% carrier spin polarization at the Fermi energy ($E_F$) [2]. Half-metallicity has attracted much attention because of its prospective applications in spintronics [3]. Therefore, fabrication and investigation of the electronic structure and physical properties of Co$_2$Y-based FHA are of fundamental and technological interests.

The important aspect of the half-metallic Heusler alloys is their unique magneto-optical (MO) properties: a discovery of giant Kerr rotation in half-Heusler PtMnSb alloy opens the way for applications in MO reading-recording. [4] Optical
and MO properties of a number of half-metallic FHA’s have been investigated theoretically and experimentally. [5] Rai and Thapa [6] have investigated the electronic structure and magnetic properties of Co2MnZ (Z = Ge, Sn)-type Heusler compounds using first principles calculations [6].

In the present work, we investigate and discuss the bulk electronic structure, magnetic and thermodynamic properties of Co2CrZ (Z = Ga, Ge and As) alloys using the density functional first-principles calculations on the basis of the full-potential linear muffin-tin orbital (FP-LMTO) and the generalized gradient approximation (GGA) for the exchange correlation term.

The manuscript is organized as follows: in Section 2, we give details of the computational methodology and structural models. Section 3 contains the results and discussion and Section 4 summarizes the conclusion.

2. Method of calculations

The calculations reported here were carried out using ab initio full-potential linear muffin-tin orbital (FP-LMTO) method [7–10] as implemented in the Lmtart code [11]. The exchange and correlation potential was calculated using the generalized gradient approximation (GGA) [12] and GGA+U. By means of the option of the effective Coulomb-exchange interaction (\( U_{\text{eff}} = U - J \)) used here for the calculations, the values \( U_{\text{eff}} = 1.59 \) eV and 1.92 eV for Cr(3d) and Co(3d), respectively. The FP-LMTO is an improved method compared to previous LMTO techniques, and treats muffin-tin spheres and interstitial regions on the same footing, leading to improvements in the precision of the eigenvalues. At the same time, the FP-LMTO method, in which the space is divided into an interstitial regions (IR) and non-overlapping muffin-tin spheres (MTS) surrounding the atomic sites, uses a more complete basis than its predecessors. In the IR regions, the basis set consists of plane waves. Inside the MT spheres, the basis sets is described by radial solutions of the one atomic sphere method [13]. The self-consistent calculations are performed up to 35 special irreducible Brillouin zone (IBZ) using Blochl's modified tetrahedron method [13]. The calculated total energies within GGA as a function of the volume were used for determination of theoretical lattice constant and bulk modulus. Equilibrium lattice constant, isothermal bulk modulus, and its pressure derivative are calculated by fitting the calculated total energy to Murnaghan’s equation of state [14].

The plot of energy versus volume is shown in Fig. 1. The volume corresponds to the lowest energy is used to determine equilibrium lattice constant. We summarize the calculated structural parameters and bulk modulus Co2CrZ (Z = Ga, Ge and As) systems in Table 1 using the GGA and GGA+U approaches.

It is clear from the table that our calculated results using GGA+U Co2CrGe(As) alloy are in good agreement with the available calculated data. To the best of our knowledge, there are no comparable studies in literature. We have compared the calculated results of Co2CrGe(As) with its homologous systems like Co2MnGe, Co2CrGa and Co2FeGe. The experimental lattice parameters of Co2MnGe and Co2CrGa are 5.743 Å [21] and 5.805 Å [15], respectively. Uvarov et al. have calculated the lattice constants of Co2FeGe alloy using GGA and GGA+U which are 5.75 Å [22]. The bulk modulus given by GGA+U for Co2CrAs is in reasonable agreement with other theoretical calculations [20]. While, the bulk modulus given by GGA+U is smaller than that corresponding GGA for the three compounds.

3. Results and discussion

3.1. The crystal structure

Experimentally, Heusler alloys crystallizes at ambient conditions in the cubic L21 structure (space group Fm–3m) with chemical formula X2YZ (X = Co, Y = Cr and Z = Ga, Ge and As). The X atoms are placed on 8a X (1/4,1/4,1/4), 4a Y (1/2,1/2,1/2) and 4b Z (0,0,0) positions.

The calculated total energies within GGA as a function of the volume were used for determination of theoretical lattice constant and bulk modulus. Equilibrium lattice constant, isothermal bulk modulus, and its pressure derivative are calculated by fitting the calculated total energy to Murnaghan’s equation of state [14].

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3.2. Magnetic moment and half-metallicity

The calculated total moment of Co2CrZ (Z = Ga, Ge and As) within the muffin-tin spheres of the relevant Co, Cr, and Z(Ga, Ge and As) atoms for the Heusler compounds are shown in Table 2, which agrees with the Slater–Pauling curve quite well. In half-metallic Heusler alloys, the Fermi level locates in the minority energy gap, so their magnetic moments are integral values and can be described by the S–P curve of N = 24, where N is total number of the valence electrons and 24 means that there are 12 occupied spin-down states per unit cell as has already been reported in Ref. [25]. For 3d transition metals and their binary compounds, the total spin magnetic moment \( m^S \) shows the well-known Slater–Pauling behavior [26]. Thus the Co2CrZ(Z = Ga, Ge and As) alloys are with 28, 29 and 30 valence electrons, respectively. For example, the N for Co2CrGa is 28Co(3d44s2) + Cr(3d44s2) + Ga(4s4p3) = 27, it has the total magnetic moment of 3 \( \mu_B \). The replacement of Ga by Ge and As leads to increase the total magnetic moment (Cr magnetic moment down) to 2.993, 3.936 and 4.90 \( \mu_B \) (1.427, 2.002 and 2.578 \( \mu_B \)) using GGA in Co2CrZ(Z = Ga, Ge and As) alloys. The Co magnetic moment increases along Ga–Ge–As series.
due to decreasing of Co–Cr hybridization for minority spin states.

The local spin magnetic moments on the non-transition metal atoms Ga(Ge and As) is small and aligned antiparallel to that of the Co and Cr atoms. The calculated $m_{\text{tot}}^{s}$ for GGA+U approach is almost exactly that expected from Slate Paulin $m_{\text{tot}}^{s}$Co$_2$CrZ ($Z$ = Ga, Ge and As) = 3.156, 4.004 $\mu_B$ and 5.01 $\mu_B$, respectively. While, the calculated $m_{\text{tot}}^{s}$ using GGA approximately is different. Thus, Rai et al. [17] have reported the total magnetic moment of the alloy $m_{\text{tot}}^{s}$Co$_2$CrZ ($Z$ = Ga, Ge and As) = 3.03, 3.999 and 4.891 $\mu_B$, respectively [17]. Tung et al. [24] have calculated for Co$_2$CrGe the total magnetic moment of $m_{\text{tot}}^{s}$(Co$_2$CrGe) = 3.997 $\mu_B$.

These values for the magnetic moments of the Co$_2$CrZ ($Z$ = Ga, Ge and As) have obtained using GGA (GGA + U) are in good agreement with the previous results shown in Table 2.

### 3.3. Spin polarization and half-metallic

The spin polarization of a magnetic material is defined by

$$P_N = \frac{N_\uparrow - N_\downarrow}{N_\uparrow + N_\downarrow}$$

where $N_\uparrow$ and $N_\downarrow$ are the number of $\uparrow$ spin and $\downarrow$ spin states at $E_F$, respectively. Under this definition, $P_N$ measures the spin imbalance of mobile electrons. It has also been defined, alternatively, as the net fractional spin polarization near $E_F$. In this case, we denote it by $P$ to distinguish from $P_N$, with

$$P = \frac{d_\uparrow - d_\downarrow}{d_\uparrow + d_\downarrow}$$

where $d_\uparrow$ and $d_\downarrow$ are the density of states (DOS) of $\uparrow$ spin and $\downarrow$ spin channels at $E_F$, respectively. $P$ can therefore be directly determined from the DOS.

The spin polarization $P$ would then vary from −1.0 to 1.0 only. For the half-metallic materials, $P$ equals to either −1.0 or 1.0. The calculated $\uparrow(E_F)$, $d_\uparrow(E_F)$ and $P$ for the Heusler compounds are shown in Table 3. In the present work, we studied the Co$_2$CrGe alloy which shows 100% spin polarization at $E_F$ (Table 3). According to our result, the compound Co$_2$CrGe is interesting as it shows large DOS at the $E_F$ of $d_\uparrow(E_F) = 1.71$ states/eV (Table 3). The reason for the big value is that $E_F$ cuts through strongly localized states of Cr-d, whereas the contribution of Co-d states to $d_\downarrow(E_F)$ is very small as shown in Fig. 2a. On the other hand, $d_\uparrow(E_F) = 0$ states/eV for both Co and Cr atoms;
Table 1
Lattice constants $a$ and bulk modulus $B$ correspond to experimental results and other theoretical calculations of $\text{Co}_2\text{Cr}_Z(Z = \text{Ga, Ge and As}).$

<table>
<thead>
<tr>
<th>$\text{Co}_2\text{Cr}_Z$</th>
<th>Lattice constant $a$ (Å)</th>
<th>Bulk modulus $B$ (GPa)</th>
<th>Pressure derivative $B'$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\text{Co}_2\text{CrGa}$</td>
<td>GGA 5.735</td>
<td>213.26</td>
<td>4.21</td>
</tr>
<tr>
<td></td>
<td>GGA+U Previous. 5.805</td>
<td>190.40</td>
<td>4.49</td>
</tr>
<tr>
<td></td>
<td>GGA+U Present. 5.879</td>
<td>262.69</td>
<td>7.47</td>
</tr>
<tr>
<td>$\text{Co}_2\text{CrGe}$</td>
<td>LSDA 5.608</td>
<td>250.71</td>
<td>4.63</td>
</tr>
<tr>
<td></td>
<td>GGA 5.742</td>
<td>203.94</td>
<td>4.53</td>
</tr>
<tr>
<td></td>
<td>GGA+U Previous. 5.743</td>
<td>250.43</td>
<td>7.47</td>
</tr>
<tr>
<td>$\text{Co}_2\text{CrAs}$</td>
<td>GGA 5.727</td>
<td>248.78</td>
<td>2.74</td>
</tr>
<tr>
<td></td>
<td>GGA+U Previous. 5.785</td>
<td>179.44</td>
<td>4.79</td>
</tr>
</tbody>
</table>

$\text{Co}_2\text{CrGa}$: Ref [15].
$\text{Co}_2\text{CrGe}$: Ref [16].
$\text{Co}_2\text{CrAs}$: Ref [17].
$\text{Co}_2\text{CrGa}$: Ref [18].
$\text{Co}_2\text{CrGe}$: Ref [19].
$\text{Co}_2\text{CrAs}$: Ref [20].

Table 2
Total and partial magnetic moments of $\text{Co}_2\text{Cr}_Z(Z = \text{Ga, Ge and As}).$

<table>
<thead>
<tr>
<th></th>
<th>Co</th>
<th>Cr</th>
<th>Z</th>
<th>total</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\text{Co}_2\text{CrGa}$</td>
<td>GGA 0.804</td>
<td>1.427</td>
<td>-0.042</td>
<td>2.993</td>
</tr>
<tr>
<td></td>
<td>GGA+U 0.791</td>
<td>1.778</td>
<td>-0.057</td>
<td>3.156</td>
</tr>
<tr>
<td>Other calc [23]</td>
<td>0.758</td>
<td>1.651</td>
<td>-0.053</td>
<td>3.051</td>
</tr>
<tr>
<td></td>
<td>0.737</td>
<td>1.602</td>
<td>-0.064</td>
<td>3.03</td>
</tr>
<tr>
<td>$\text{Co}_2\text{CrGe}$</td>
<td>GGA 0.976</td>
<td>2.002</td>
<td>-0.018</td>
<td>3.936</td>
</tr>
<tr>
<td></td>
<td>GGA+U 0.944</td>
<td>2.213</td>
<td>-0.044</td>
<td>4.004</td>
</tr>
<tr>
<td>Other calc [24]</td>
<td>0.932</td>
<td>2.122</td>
<td>-0.029</td>
<td>3.999</td>
</tr>
<tr>
<td>[23]</td>
<td>0.950</td>
<td>2.129</td>
<td>-0.033</td>
<td>3.997</td>
</tr>
<tr>
<td>$\text{Co}_2\text{CrAs}$</td>
<td>GGA 1.13</td>
<td>2.598</td>
<td>0.048</td>
<td>4.90</td>
</tr>
<tr>
<td></td>
<td>GGA+U 1.099</td>
<td>2.656</td>
<td>0.019</td>
<td>5.01</td>
</tr>
<tr>
<td>Other calc [17]</td>
<td>1.066</td>
<td>2.578</td>
<td>0.044</td>
<td>4.891</td>
</tr>
<tr>
<td>[20]</td>
<td>1.98</td>
<td>2.95</td>
<td>0.07</td>
<td>5.00</td>
</tr>
</tbody>
</table>

Table 3
Energy gap and spin polarization of $\text{Co}_2\text{Cr}_Z(Z = \text{Ga, Ge and As}).$

<table>
<thead>
<tr>
<th>$\text{Co}_2\text{Cr}_Z$</th>
<th>Energy gap band $E_g$ (eV)</th>
<th>Spin polarization</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>$E_{\text{max}}(\uparrow)$</td>
<td>$E_{\text{max}}(\downarrow)$</td>
</tr>
<tr>
<td>$\text{Co}_2\text{CrGa}$</td>
<td>GGA 0.071</td>
<td>0.439</td>
</tr>
<tr>
<td></td>
<td>GGA+U 0.154</td>
<td>0.595</td>
</tr>
<tr>
<td>Other calc [17]</td>
<td>0.0</td>
<td>0.28</td>
</tr>
<tr>
<td></td>
<td>0.0</td>
<td>0.28</td>
</tr>
<tr>
<td>$\text{Co}_2\text{CrGe}$</td>
<td>GGA –0.076</td>
<td>0.208</td>
</tr>
<tr>
<td></td>
<td>GGA+U –0.119</td>
<td>0.493</td>
</tr>
<tr>
<td>Other calc [21]</td>
<td>0.0</td>
<td>0.24</td>
</tr>
<tr>
<td></td>
<td>0.0</td>
<td>0.24</td>
</tr>
<tr>
<td>$\text{Co}_2\text{CrAs}$</td>
<td>GGA –0.633</td>
<td>–0.105</td>
</tr>
<tr>
<td></td>
<td>GGA+U –0.246</td>
<td>0.108</td>
</tr>
<tr>
<td>Other calc [17]</td>
<td>–0.50</td>
<td>–0.10</td>
</tr>
<tr>
<td></td>
<td>–0.50</td>
<td>–0.10</td>
</tr>
</tbody>
</table>
Fig. 2. Spin-projected total and partial DOS for (a) Co$_2$CrGa, (b) Co$_2$CrGe, and (c) Co$_2$CrAs.
Fig. 3. Band structure for (a) Co$_2$CrGa, (b)Co$_2$CrGe and (c)Co$_2$CrAs.
The non-equilibrium Gibbs function $G^\text{n}(V, P, T)$ is expressed as:

$$G^\text{n}(V, P, T) = E(V) + PV + \text{Avib}(\theta(V); T)$$  \hspace{1cm} (4)

where $E(V)$ is the total energy per unit cell for Co$_2$CrGe, $PV$ is the constant hydrostatic pressure condition, $\theta(V)$ is the Debye temperature, and the vibrational Helmholtz free energy $\text{Avib}$ can be written as:

$$\text{Avib}(\Theta; T) = n k T \left[ \frac{9 \Theta}{8 T} + 3 \ln \left(1 - e^{-\Theta/T}\right) - D \left(\Theta/T\right) \right]$$  \hspace{1cm} (5)

where $n$ is the number of atoms per formula unit, $D(\Theta/T)$ is the Debye integral. For an isotropic solid [32]

$$\Theta = \frac{R}{6 \pi^2 V^{1/2} n} f(\sigma) \left(\frac{B_S}{M}\right)$$  \hspace{1cm} (6)

where $M$ is the molecular mass per unit cell and $B_S$ is the adiabatic bulk modulus. The non-equilibrium Gibbs function $G^\text{n}(V, P, T)$ as a function of $(V; P, T)$ can be minimized with respect to volume $V$ as:

$$\left[ \frac{\delta G^\text{n}(V, P, T)}{\delta V} \right]_{P,T} = 0$$  \hspace{1cm} (7)

The thermal properties such as internal energies, entropy, heat capacity at constant volume $C_V$, and thermal expansion $\alpha$ are taken as:

$$U = n k T \left[ \frac{9 \Theta}{8 T} + 3D \left(\Theta/T\right) \right]$$  \hspace{1cm} (8)

$$S = n k \left[ 4D \left(\Theta/T\right) - 3 \ln \left(1 - e^{-\Theta/T}\right) \right]$$  \hspace{1cm} (9)

$$C_V = 3n k \left[ 4D \left(\Theta/T\right) - 3 \Theta/T \right]$$  \hspace{1cm} (10)

$$\alpha = \frac{\gamma c_v}{B_S V}$$  \hspace{1cm} (11)

Here $\gamma$ is the Grüneissen parameters which are given by the following equation [27]:

$$\gamma = - \left( \frac{d \ln \Theta(V)}{d \ln V} \right)$$  \hspace{1cm} (12)

The thermal properties are determined in the temperature range from 0 to 3000 K, where the quasi-harmonic model remains fully valid. The pressure effect is studied in the 0–20 GPa range.

The dependence of the primitive cell volume on the temperature using GGA is shown in Fig. 4. The volume increases almost linearly with increasing temperature. For a given temperature $T = 300$ K and zero pressure,
the primitive cell volume alters with increasing pressure via GGA for Co$_2$CrZ ($Z = \text{Ga}, \text{Ge}$ and As) alloys to be 321.62 $\mu$m$^3$, 323.11 $\mu$m$^3$ and 318.95 $\mu$m$^3$, respectively.

The second-order polynomial fitting of $V$–$P$ data gives the following equations at $T = 300$ K, for three alloys:

$$V(P) = 321.6243 - 1.4801P + 0.0118P^2 \text{(Co}_2\text{CrGa)}$$  \hspace{1cm} (13)

$$V(P) = 323.1179 - 1.5513P + 0.0143P^2 \text{(Co}_2\text{CrGe)}$$  \hspace{1cm} (14)

$$V(P) = 318.952 - 1.2812P + 0.0076P^2 \text{(Co}_2\text{CrAs)}$$  \hspace{1cm} (15)

The variations in thermal expansion coefficient ($\alpha$) with temperature and pressure are shown in Fig. 5. It is shown that, at a given pressure, $\alpha$ increases sharply with increasing of temperature up to 400 K. When $T > 500$ K, $\alpha$ gradually approaches a linear increasing with enhanced temperature and the propensity of increment becomes very moderate, which means that the temperature dependence of $\alpha$ is very small at high temperature. As shown in Fig. 5, for $T > 600$ K and $P = 20$ GPa, Co$_2$CrGe has a fairly constant thermal expansion $\alpha = 2.87 \times 10^5$ K$^{-1}$. For a given temperature, $\alpha$ decreases drastically with increasing of pressure. Using GGA, at 300 K and zero pressure, the $\alpha$ values for Co$_2$CrZ ($Z = \text{Ga}, \text{Ge}$ and As) are $2.4367 \times 10^5$ K$^{-1}$, $3.089 \times 10^5$ K$^{-1}$ and $1.385 \times 10^5$ K$^{-1}$ respectively.

The fit equations to third-order polynomial for $\alpha$–$T$ data at zero pressure and for $\alpha$–$P$ data at $T = 300$ K are given as:

$$\alpha(T) = 9.3927 \times 10^3 + 1.0518 \times 10^3 T - 1.24857^2 + 4.478 \times 10^{-4} T^3 \text{ (} P = 0 \text{ GPa)}$$  \hspace{1cm} (16)

$$\alpha(P) = 2.4367 \times 10^5 + 5.1029 \times 10^2 P - 2.0109 \times 10^4 P^2 + 4.076P^3 \text{ (} T = 300 \text{ K)}$$  \hspace{1cm} (17)

Fig. 5. Variation of the thermal expansion coefficient with temperature at different pressures for (a) Co$_2$CrGa, (b)Co$_2$CrGe and (c)Co$_2$CrAs.

Fig. 6 shows the variation of the bulk modulus versus temperature. The compressibility is practically constant between 0 and 300 K for $T > 600$ K then it decreases linearly with increasing temperature. For a given temperature, the bulk modulus increases with increasing pressure. The effect of increasing pressure and decreasing temperature on the bulk modulus are nearly the same. At zero pressure and $T = 300$ K, the bulk modulus for Co$_2$CrZ ($Z = \text{Ga}, \text{Ge}$ and As) are 214.21 GPa, 201.2 GPa and 246.63 GPa, respectively.
The bulk modulus–pressure relations are obtained by fitting the B–P data at \(T=300\) K to the following third-order polynomials for \(\text{Co}_2\text{CrZ} (Z = \text{Ga, Ge and As})\) alloys:

\[
\text{Co}_2\text{CrGe} \begin{cases} 
\alpha(T) = 7.056 \times 10^4 + 7.412 \times 10^2 T - 0.5047^2 + 1.045 \times 10^{-4} T^3 \quad (P = 0\ \text{GPa}) \\
\alpha(P) = 3.089 \times 10^5 - 6.418 \times 10^3 P + 1.527 \times 10^2 P^2 - 2.455P^3 \quad (T = 300\ \text{K})
\end{cases}
\]

(18, 19)

\[
\text{Co}_2\text{CrAs} \begin{cases} 
\alpha(T) = 4.3724 \times 10^3 + 5.6809 \times 10^2 T - 0.5977T^2 + 1.76 \times 10^{-4} T^3 \quad (P = 0\ \text{GPa}) \\
\alpha(P) = 1.385 \times 10^5 - 5.962 \times 10^2 P - 17.827P^2 + 0.3408P^3 \quad (T = 300\ \text{K})
\end{cases}
\]

(20, 21)

The variation of heat capacity \(C_V\) at constant volume versus temperature at 0, 5, 10, 15 and 20 GPa pressures is shown in Fig. 7. With increasing temperature, \(C_V\) values increase rapidly at a lower temperature, then increase slowly at high temperature [33,34], which is common to all alloys at high temperature. It is found that when \(T < 600\) K, \(C_V\) depends on both temperature and pressure (\(C_V\) is proportional to \(T^3\) [35]). From 0 to about 800 K, \(C_V\) increases exponentially and then at high temperature approaches approximately 99.5 J mol\(^{-1}\) K\(^{-1}\) for the three compounds. Using GGA, at zero pressure and 300 K, \(C_V\) is 48.64 mol\(^{-1}\) K\(^{-1}\), 82.46 mol\(^{-1}\) K\(^{-1}\) and 85.49 J mol\(^{-1}\) K\(^{-1}\) for the \(\text{Co}_2\text{CrZ}(Z = \text{Ga, Ge and As})\) alloys, respectively.
4. Conclusion

In this work, we have investigated the electronic structure and magnetism of three half-metallic full-Heusler compounds, Co$_2$Cr$Z$ ($Z$ = Ga, Ge and As) with a high-ordered structure using full-potential linear muffin-tin orbital (FP-LMTO) method within the generalized gradient GGA and GGA+U approximation, framework based on the density functional theory (DFT). The systems show perfect half-metallic character with semiconducting minority spin band structure, which has zero electronic density of states at Fermi level. The energy gap in minority spin channel is a direct gap at point $\Gamma$. The total magnetic moment of the Co$_2$Cr$Z$ ($Z$ = Ga, Ge and As) are 3.156, 4.004 and 5.01 $\mu_B$, respectively. The results are in good agreement with the Slater–Pauling rule. We have investigated the possibility of appearance of half-metallicity in the case of the Co$_2$CrZ ($Z$ = Ga, Ge and As) system that shows 100% spin polarization at $E_F$. The existence of energy gap in minority spin DOS and band structure) is an indication of being a potential HMF. As well as the integral value of magnetic moment is also the evident of HMF. Through the quasi-harmonic Debye model, the dependences of the lattice constant, bulk modulus, thermal expansion parameter, heat capacity and Debye temperature on temperature and pressure have been obtained successfully. It is hoped that our new results for Co$_2$CrZ ($Z$ = Ga, Ge and As) will be confirmed experimentally and theoretically in future.

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