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# Electronic and magnetic properties of a full-Heusler alloy $\text{Co}_2\text{CrGe}$ : a first-principles study

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## Abstract

The structural, electronic, and magnetic properties of  $\text{Co}_2\text{CrGe}$ , a Heusler alloy, have been evaluated by first-principles density functional theory and compared with the known experimental and theoretical results. Generalized gradient approximation is used for structural study, whereas local spin density approximation is used for electronic calculation. First-principles structure optimizations were done through total energy calculations at 0 K using the full-potential linearized augmented plane wave method as implemented in the WIEN2K code.

**Keywords:** GGA, half metallicity, DOS, band structure

**PACS:** 70, 71.5.-m, 71.15.Mb, 71.20.Be

## Background

In 1983, de Groot discovered half-metallic ferromagnetism in the semi-Heusler compound  $\text{NiMnSb}$  [1] using first-principles calculation based on density functional theory. Heusler alloys are the ternary intermetallic compounds with composition  $X_2YZ$ , where X and Y are transition elements (Ni, Co, Fe, Mn, Cr, Ti, V, etc.) and Z is III, IV, or V group elements (Al, Ga, Ge, As, Sn, In, etc.). One of the promising classes of materials is the half-metallic ferrimagnets (HMF), 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]. After that, half metallicity attracted much attention [3] because of its prospective applications in spintronics [4]. The electronic and magnetic properties of  $\text{Co}_2\text{MnAl}$  [5] and  $\text{Co}_2\text{CrSi}$  [6] using local spin density approximation (LSDA) show the half metallicity at the ground state. Rai and Thapa investigated the electronic structure and magnetic properties of  $X_2YZ$  ( $X = \text{Co}$ ,  $Y = \text{Mn}$ ,  $Z = \text{Ge}$ ,  $\text{Sn}$ )-type Heusler compounds using a first-principles study and reported HMFs [7]. Rai et al. also studied the electronic and magnetic properties of  $\text{Co}_2\text{CrAl}$  and  $\text{Co}_2\text{CrGa}$  using both LSDA and LSDA+U and reported the increase in bandgap and hybridization of  $d$ - $d$  orbitals as well as  $d$ - $p$  orbitals when treated with LSDA+U

[8]. Blake et al. studied the compounds  $\text{Co}_2\text{FeZ}$  ( $Z = \text{Al}$ ,  $\text{Si}$ ,  $\text{Ga}$ , and  $\text{Ge}$ ) using the X-ray diffraction and extended X-ray absorption fine structure (EXAFS) techniques. Using EXAFS, they found that the compounds  $\text{Co}_2\text{FeGa}$  and  $\text{Co}_2\text{FeGe}$  crystallize in the  $L2_1$  structure [9]. In this present work, we report the result of generalized gradient approximation (GGA) and LSDA of the bulk electronic structure and magnetic properties of  $\text{Co}_2\text{CrGe}$ .

## Computation detail

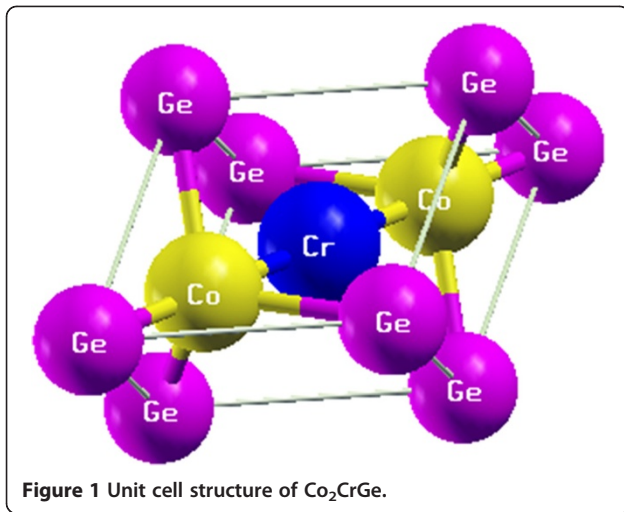
The full-potential linearized augmented plane wave (FP-LAPW) method (WIEN2K) [10] was applied to the band structure calculations of  $\text{Co}_2\text{CrGe}$ . GGA [11] and LSDA were used for the exchange correlation potential. The multipole expansion of the crystal potential and the electron density within muffin tin (MT) spheres were cut at  $l = 10$ . Nonspherical contributions to the charge density and potential within the MT spheres were considered up to  $l_{\text{max}} = 6$ . The cutoff parameter was  $RK_{\text{max}} = 7$ . In the interstitial region, the charge density and the potential were expanded as a Fourier series with wave vectors up to  $G_{\text{max}} = 12 \text{ a.u.}^{-1}$ . The MT sphere radii ( $R$ ) used were 2.35 a. u. for Co, 2.35 a.u. for Cr, and 2.21 a. u. for Ge. The number of  $k$  points used in the irreducible part of the Brillouin zone is 286.

## Crystal structure

Heusler alloy [12] with chemical formula  $X_2YZ$  ( $X = \text{Co}$ ,  $Y = \text{Cr}$ , and  $Z = \text{Ge}$ ) was used. The full-Heusler structure

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consists of four penetrating fcc sublattices with atoms at  $X_1(1/4, 1/4, 1/4)$ ,  $X_2(3/4, 3/4, 3/4)$ ,  $Y(1/2, 1/2, 1/2)$ , and  $Z(0, 0, 0)$  positions which results in a  $L_{21}$  crystal structure having space group  $\text{Fm-}3\text{-m}$  as shown in Figure 1.

## Results and discussions

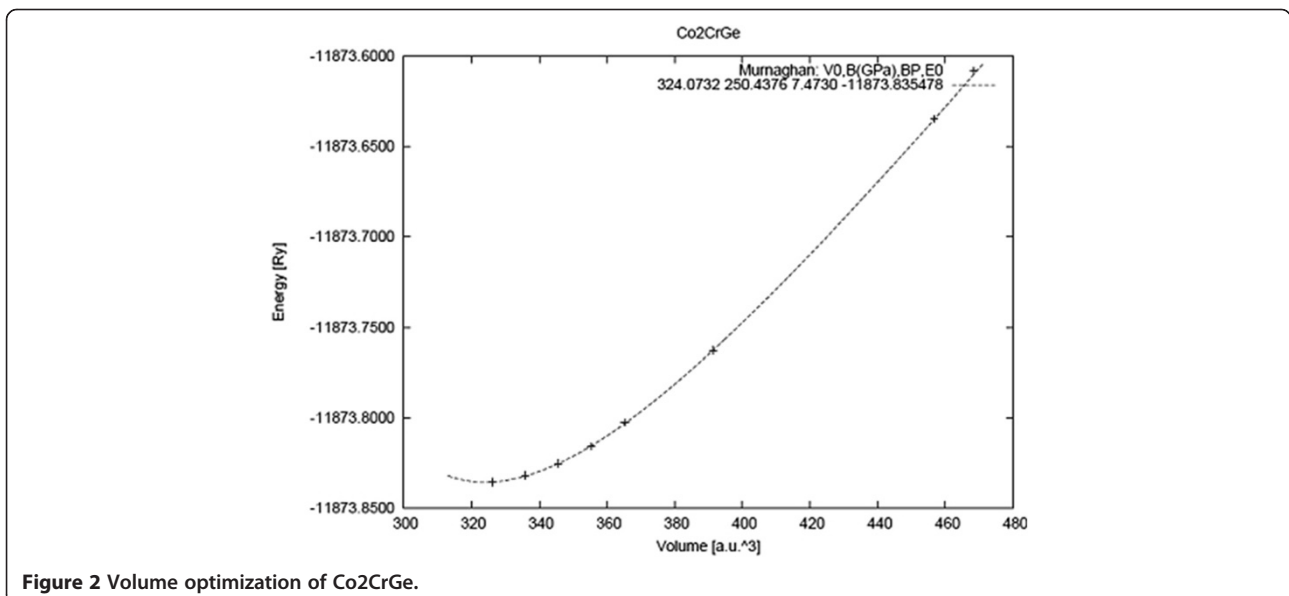
The volume optimization was performed using the lattice constant by taking the experimental one (Figure 2). The calculated total energies within GGA as a function of the volume were used for the determination of the theoretical lattice constant and bulk modulus. The bulk modulus was calculated using Murnaghan's equation of

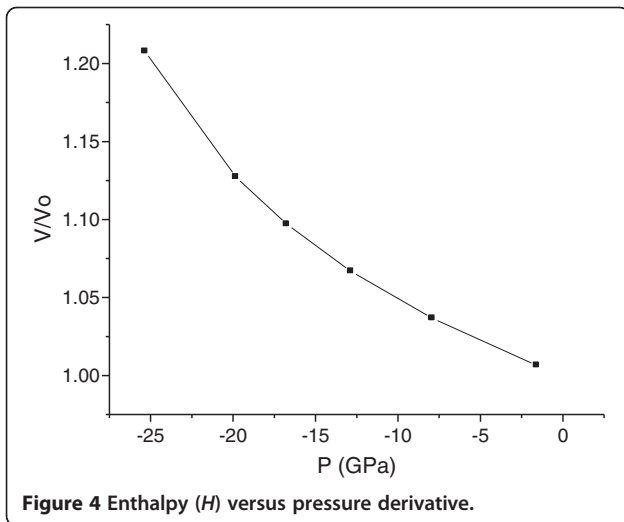
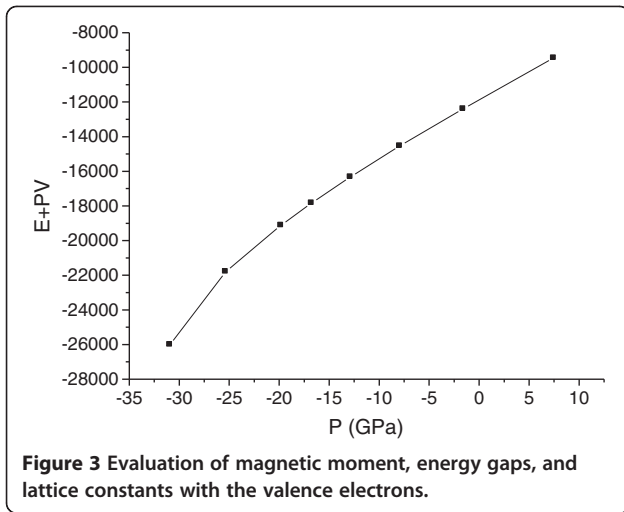
**Table 1** Lattice constant, bulk modulus, and equilibrium energy

Lattice constants $a_o$ (Å)			Bulk modulus $B$ (GPa)	Equilibrium Energy (Ry)
Previous	Calculated	$\Delta(a_o)$		
5.740 [14]	5.770	0.030	250.4376	-11873.8355

state [13]. The calculated values of the lattice constant and bulk modulus are presented in Table 1.

The calculated bulk modulus is 250.4376 GPa, and its pressure derivative is found to be 7.4730 for  $\text{Co}_2\text{CrGe}$ . The optimized lattice constant for  $\text{Co}_2\text{CrGe}$  is 5.770 Å, and the change in the lattice constant of  $\text{Co}_2\text{CrGe}$  with that of the previous result [14] is 0.030. As the experimental results are not available, we have compared the calculated results of  $\text{Co}_2\text{CrGe}$  with its homologous systems like  $\text{Co}_2\text{MnGe}$  and  $\text{Co}_2\text{CrGa}$ . Rai et al. calculated the lattice constants of  $\text{Co}_2\text{MnGe}$  and  $\text{Co}_2\text{CrGa}$  using GGA which are 5.678 Å [7] and 5.8794 Å [8], respectively (Figure 3). The optimized lattice parameter was slightly higher than the experimental lattice parameters; the change in lattice parameters is given by  $\Delta(a_o)$ . As shown in Figures 4 and 5, the volume derivative decreases with the increase in pressure; on the other hand, the enthalpy ( $H$ ) is increasing and finally reaches -9452.0364 Ry at a stable volume of 324.0732 a.u.<sup>-3</sup> and a pressure derivative of 7.4730. The values of total and local moments are given in Table 2 in comparison with the earlier results. In order to understand the formation of magnetic properties, it is necessary to consider their density of states (DOS) and band structure.





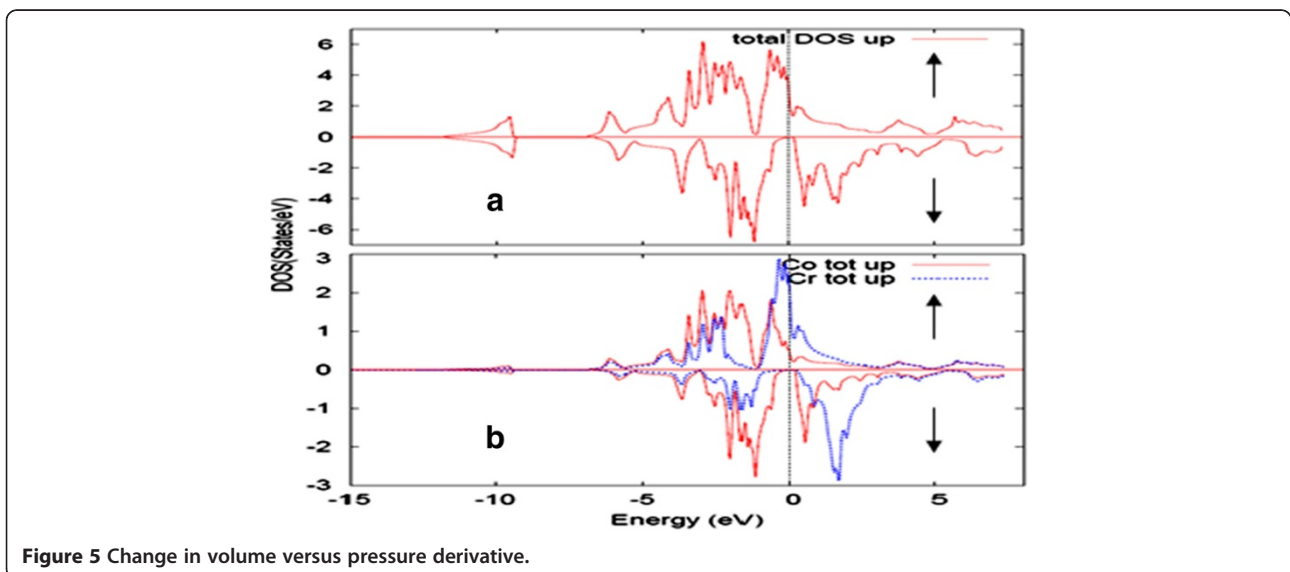
### Spin polarization and half-metallic ferromagnets

The electron spin polarization ( $P$ ) at Fermi energy ( $E_F$ ) of a material is defined by Equation 1 [15].

$$P = \frac{\rho_{\uparrow}(E_F) - \rho_{\downarrow}(E_F)}{\rho_{\uparrow}(E_F) + \rho_{\downarrow}(E_F)}, \quad (1)$$

where  $\rho_{\uparrow}(E_F)$  and  $\rho_{\downarrow}(E_F)$  are the spin-dependent density of states at the  $E_F$ . The  $\uparrow$  and  $\downarrow$  assigns the majority and the minority states, respectively.  $P$  vanishes for paramagnetic or anti-ferromagnetic materials even below the magnetic transition temperature. It has a finite value in ferromagnetic materials below Curie temperature [16]. The electrons at  $E_F$  are fully spin polarized ( $P = 100\%$ ) when  $\rho_{\uparrow}(E_F)$  or  $\rho_{\downarrow}(E_F)$  is equal to zero. In the present work, we have studied the  $\text{Co}_2\text{CrGe}$  system which shows 100% spin polarization at  $E_F$  (Table 3). According to our result, the compound  $\text{Co}_2\text{CrGe}$  is interesting as it shows large DOS at the  $E_F$  of  $\rho_{\uparrow}(E_F) = 3.00$  states/eV (Table 3). The reason for this large value is that  $E_F$  cuts through strongly localized states of Cr- $d$ , whereas the contribution of Co- $d$  states to  $\rho_{\uparrow}(E_F)$  is very small as illustrated in Figure 6b. On the other hand,  $\rho_{\downarrow}(E_F) = 0.00$  states/eV for both Co and Cr atoms; according to this,  $\text{Co}_2\text{CrGe}$  is a half metal which gives 100% spin polarization at  $E_F$ .

Figures 6 and 7 summarize the results of the DOS which were calculated using LSDA. It is shown in Figure 7a,c that the majority contribution of DOS is from the  $d$  states of Co and Cr atoms. The Cr- $d$  gives almost an exchange splitting-type pattern as shown in Figure 7c. The sharp peaks appear at the Fermi level in the spin up region for Cr- $d$  atoms. The contribution of Co- $d$  atoms is very small at the conduction region. The hybridization between the Co- $d$  and Cr- $d$  atoms appears between 3.5 and 5.5 eV, which is



**Table 2 Total and partial magnetic moments**

Previous	Magnetic moment ( $\mu_B$ ) of $\text{Co}_2\text{CrGe}$			
	Calculated			Total
	Co	Cr	Ge	
4.00 [14]	0.932	2.122	-0.029	3.999

**Table 3 Energy gap and spin polarization of  $\text{Co}_2\text{CrGe}$**

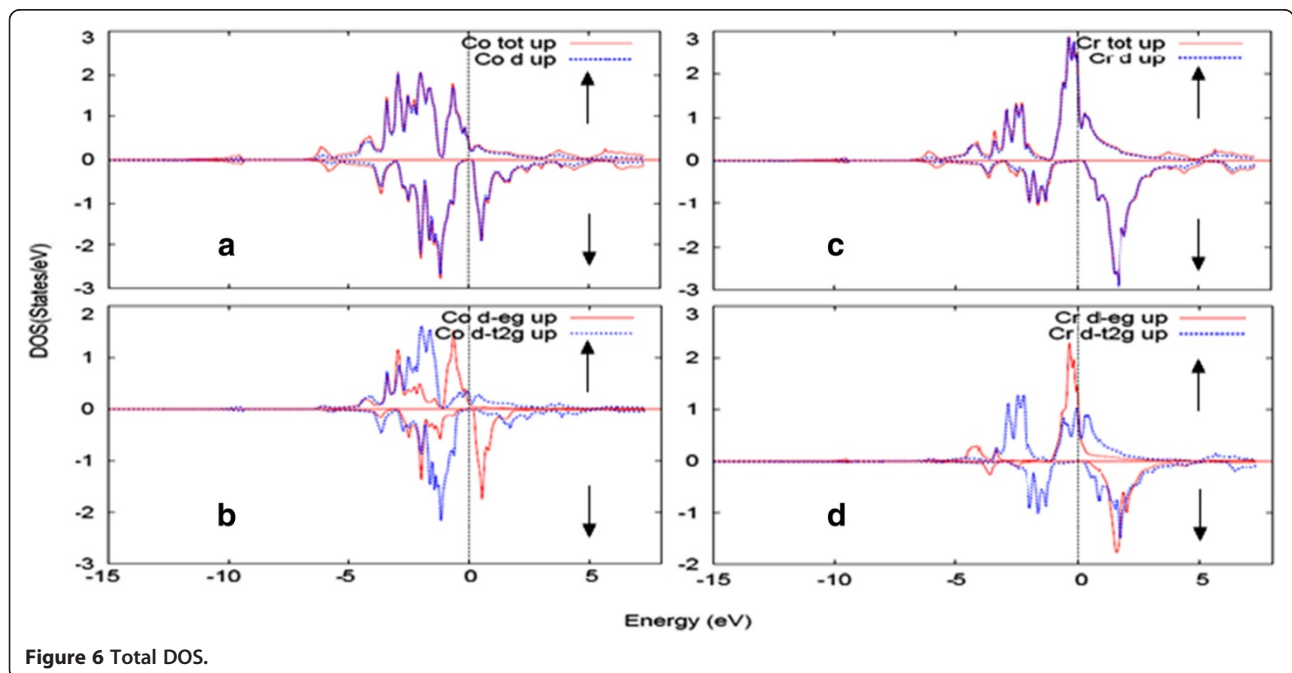
Energy gap $E_g$ (eV)			Spin polarization		
$E_{\text{max}}$ ( $\Gamma$ )	$E_{\text{min}}$ (X)	$\Delta E$	$\rho_{\uparrow}(E_F)$	$\rho_{\downarrow}(E_F)$	P%
0.24	0.00	0.24	3.00	0.00	100

responsible for the creation of magnetic moment. According to Figure 8 the indirect bandgap along the  $\Gamma$ -X symmetry for  $\text{Co}_2\text{CrGe}$  is 0.24 eV. For  $\text{Co}_2\text{CrGe}$ , the ( $E_F$ ) lies in the middle of the gap of the minority spin states, determining the half-metal character (Figure 6a). The formation of gap for the half-metal compounds was discussed by Galanakis et al. [17] for  $\text{Co}_2\text{MnSi}$ , which is due to the strong hybridization between Co- $d$  and Mn- $d$  states, combined with large local magnetic moments and a sizeable separation of the  $d$ -like band centers. The energy gaps of its homologous systems like  $\text{Co}_2\text{MnGe}$  and  $\text{Co}_2\text{CrGa}$  are 0.60 [7] and 0.38 eV [8], respectively. It is seen that the energy gap is smaller for  $\text{Co}_2\text{CrGe}$  as compared with those for  $\text{Co}_2\text{MnGe}$  and  $\text{Co}_2\text{CrGa}$  as shown in Figure 3.

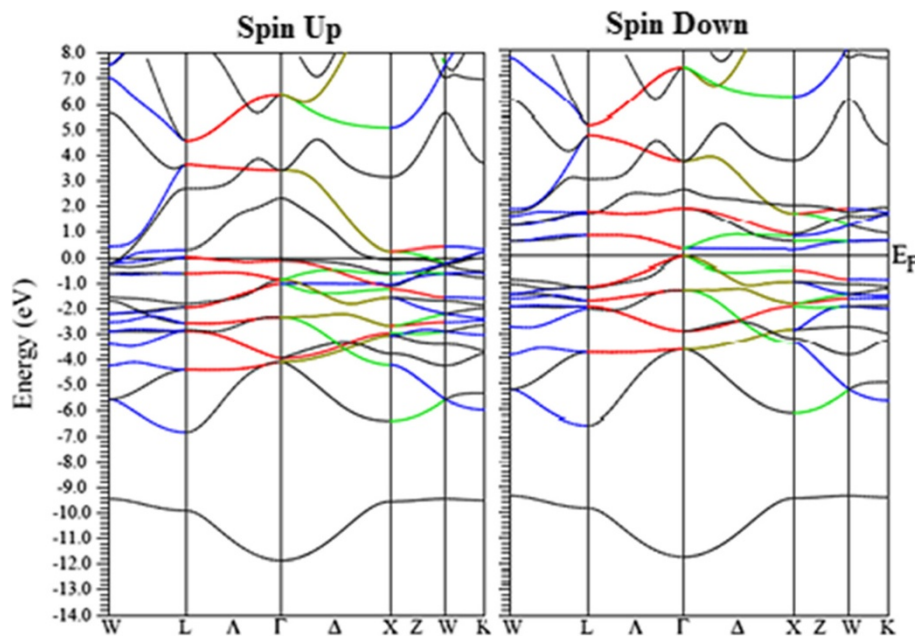
**Magnetic properties calculated in the LSDA**

Starting with the compound under investigation, all the information regarding the partial, total, and the previously calculated magnetic moments are summarized in Table 2. It is shown in Table 2 that the calculated total magnetic moment is almost an integer value 3.999  $\mu_B$  for  $\text{Co}_2\text{CrGe}$  as expected for the half-metallic systems. The magnetic moments of its homologous systems like  $\text{Co}_2\text{MnGe}$  and  $\text{Co}_2\text{CrGa}$  are 5.004  $\mu_B$  [7] and 3.075  $\mu_B$  [8], respectively.

In most cases, the calculated magnetic moments are in good agreement with the previous results. We have found that the Co sites contribute much less compared with the Cr sites; this is because Cr- $d$  states show exchange splitting. The same observation was also reported and explained by Kandpal et al. [18] because of the indirect connection between the specific magnetic moment at Co and the hybridization arising from the interaction between the electrons at the Co sites with the neighboring electrons in the Co  $t_{2g}$  states. As shown in Table 2, the Ge atom carries a negligible magnetic moment, which does not contribute much to the overall moment. We have also noticed that the partial moment of Ge atoms aligned anti-parallel to the Co and Cr moments of the systems. It emerges from the hybridization with the transition metals and is caused by the overlap of the electron wave functions. The small moments found at the Ge sites are mainly due to the polarization of these atoms by the surroundings, magnetically active atoms as reported by Kandpal et al. [18].



**Figure 6 Total DOS.**



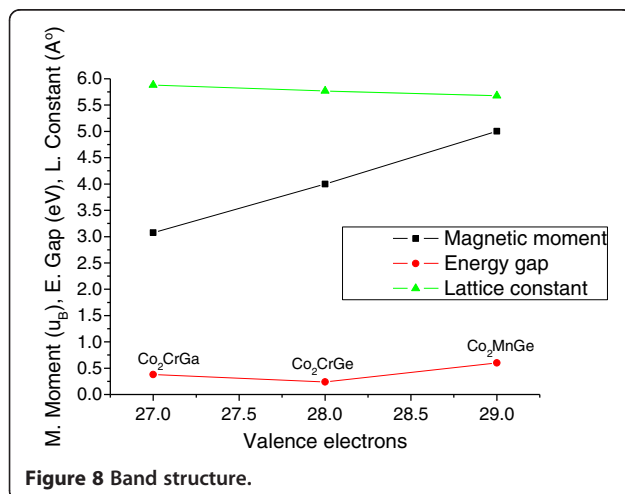
**Figure 7** Partial DOS of Co and Cr atoms.

The change of lattice constants, energy gap, and magnetic moments with respect to valence electrons are given in Figure 3.

### Conclusions

We have performed the total energy calculations to find the stable magnetic configuration and the optimized lattice constant. The DOS, magnetic moments, and band structure of  $\text{Co}_2\text{CrGe}$  were calculated using FP-LAPW method. The calculated results were in good agreement with the previously calculated results. For ferromagnetic compounds, the partial moment of Ge is very small, and the contribution is also very small in the total magnetic

moment. We have investigated the possibility of appearance of half metallicity in the case of the full-Heusler compound  $\text{Co}_2\text{CrGe}$  which shows 100% spin polarization at  $E_F$ . The existence of the energy gap in the minority spin (DOS and band structure) of  $\text{Co}_2\text{CrGe}$  is an indication of being a potential HMF. This is also evident from the calculated magnetic moment for  $\text{Co}_2\text{CrGe}$  which is  $3.9999 \mu_B$ . The calculated result is in qualitative agreement with the integral value, supporting the HMF. It is shown in Figure 3 that the magnetic moment is increasing with the valence electrons for  $\text{Co}_2\text{CrGa}$ ,  $\text{Co}_2\text{CrGe}$ , and  $\text{Co}_2\text{MnGe}$ . The case is just reverse for the lattice constants. The calculated energy gap of  $\text{Co}_2\text{CrGe}$  is small as compared with the energy gaps of  $\text{Co}_2\text{CrGa}$  and  $\text{Co}_2\text{MnGe}$ .



**Figure 8** Band structure.

### Competing interests

The authors did not provide this information.

### Authors' contributions

The authors did not provide this information.

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