Journal of Theoretical and Applied Physics
a SpringerOpen Journal

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Electronic and magnetic properties of a full-Heusler alloy Co_2CrGe: a first-principles study

D P Rai[1*], A Shankar[1], Sandeep[1], M P Ghimire[2] and R K Thapa[1]

Abstract

The structural, electronic, and magnetic properties of Co_2CrGe, 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 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 Co_2MnAl [5] and Co_2CrSi [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 = Co, Y = Mn, Z = Ge, Sn)-type Heusler compounds using a first-principles study and reported HMFs [7]. Rai et al. also studied the electronic and magnetic properties of Co_2CrAl and Co_2CrGa 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 Co_2FeZ (Z = Al, Si, Ga, and Ge) using the X-ray diffraction and extended X-ray absorption fine structure (EXAFS) techniques. Using EXAFS, they found that the compounds Co_2FeGa and Co_2FeGe 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 Co_2CrGe.

Computation detail

The full-potential linearized augmented plane wave (FP-LAPW) method (WIEN2K) [10] was applied to the band structure calculations of Co_2CrGe. 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 $l_{max} = 6$. The cutoff parameter was $RK_{max} = 7$. In the interstitial region, the charge density and the potential were expanded as a Fourier series with wave vectors up to $G_{max} = 12$ 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 = Co, Y = Cr, and Z = Ge) was used. The full-Heusler structure

* Correspondence: dibyaprakashrai@gmail.com
[1]Department of Physics, Mizoram University, Aizal 796004, India
Full list of author information is available at the end of the article

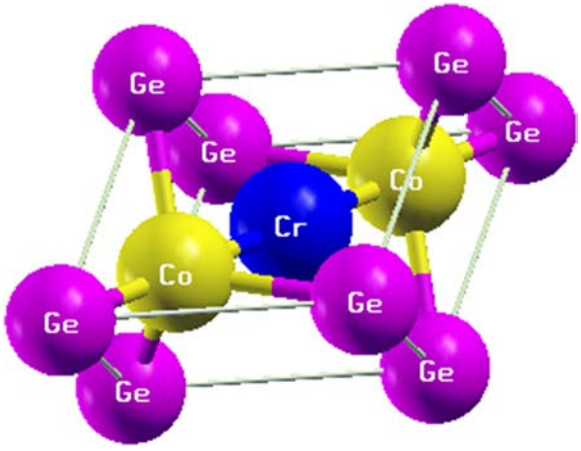

Figure 1 Unit cell structure of Co_2CrGe.

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 Fm-3-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 state [13]. The calculated values of the lattice constant and bulk modulus are presented in Table 1.

Table 1 Lattice constant, bulk modulus, and equilibrium energy

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

The calculated bulk modus is 250.4376 GPa, and its pressure derivative is found to be 7.4730 for Co_2CrGe. The optimized lattice constant for Co_2CrGe is 5.770 Å, and the change in the lattice constant of Co_2CrGe with that of the previous result [14] is 0.030. As the experimental results are not available, we have compared the calculated results of Co_2CrGe with its homologous systems like Co_2MnGe and Co_2CrGa. Rai et al. calculated the lattice constants of Co_2MnGe and Co_2CrGa 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.$^{-3}$ 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.

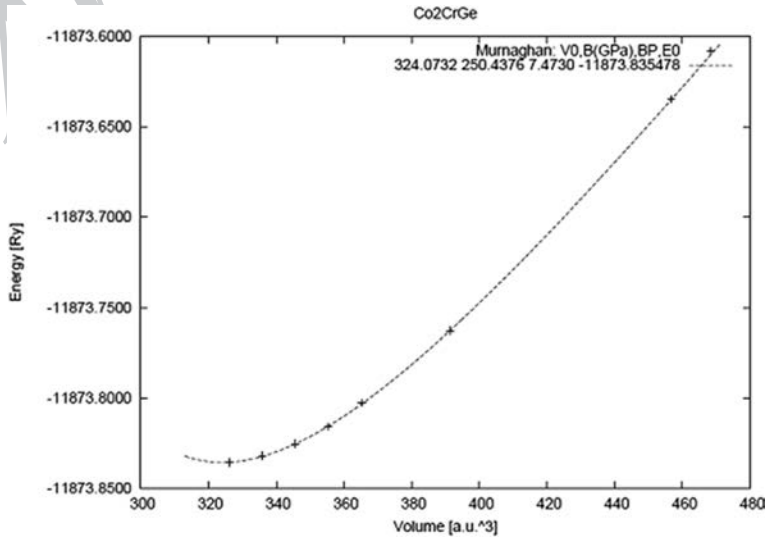

Figure 2 Volume optimization of Co2CrGe.

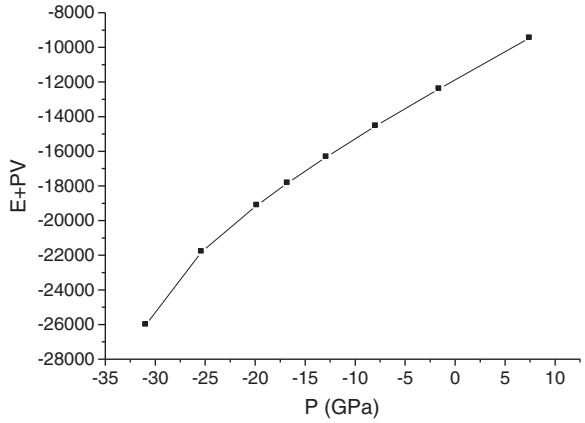

Figure 3 Evaluation of magnetic moment, energy gaps, and lattice constants with the valence electrons.

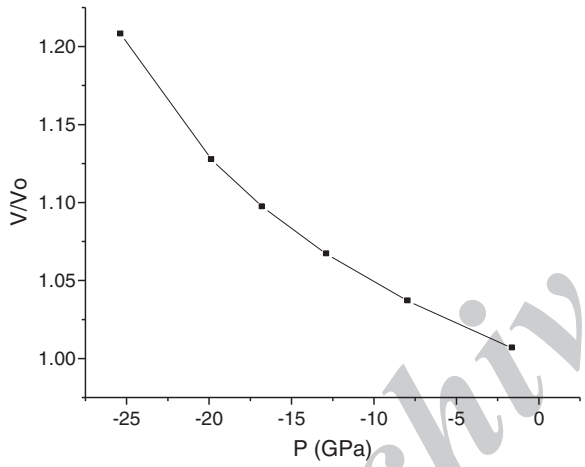

Figure 4 Enthalpy (*H*) versus pressure derivative.

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 ↑ and ↓ 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 Co_2CrGe system which shows 100% spin polarization at E_F (Table 3). According to our result, the compound Co_2CrGe 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, Co_2CrGe 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

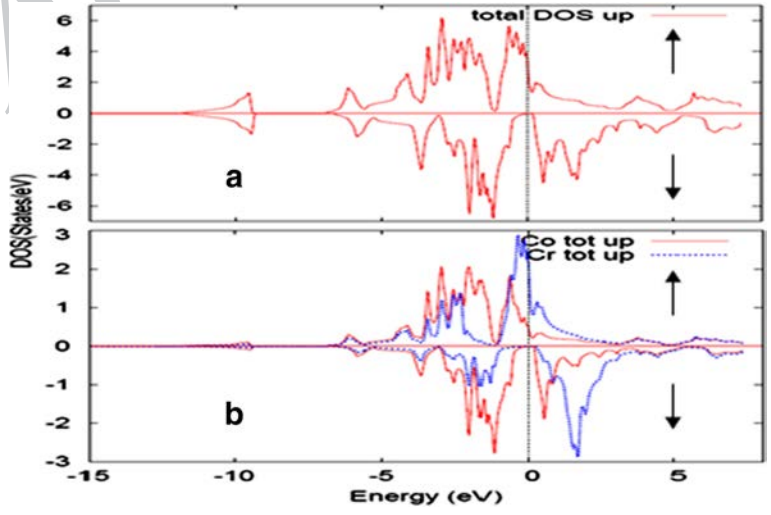

Figure 5 Change in volume versus pressure derivative.

Table 2 Total and partial magnetic moments

Magnetic moment (μ_B) of Co_2CrGe				
Previous	Calculated			
	Co	Cr	Ge	Total
4.00 [14]	0.932	2.122	−0.029	3.999

Table 3 Energy gap and spin polarization of Co_2CrGe

Energy gap E_g (eV)			Spin polarization		
E_{max} (Γ)	E_{min} (X)	ΔE	$\rho\uparrow(E_F)$	$\rho\downarrow(E_F)$	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 Γ-X symmetry for Co_2CrGe is 0.24 eV. For Co_2CrGe, 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 Co_2MnSi, 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 Co_2MnGe and Co_2CrGa are 0.60 [7] and 0.38 eV [8], respectively. It is seen that the energy gap is smaller for Co_2CrGe as compared with those for Co_2MnGe and Co_2CrGa 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 μ_B for Co_2CrGe as expected for the half-metallic systems. The magnetic moments of its homologous systems like Co_2MnGe and Co_2CrGa are 5.004 μ_B [7] and 3.075 μ_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].

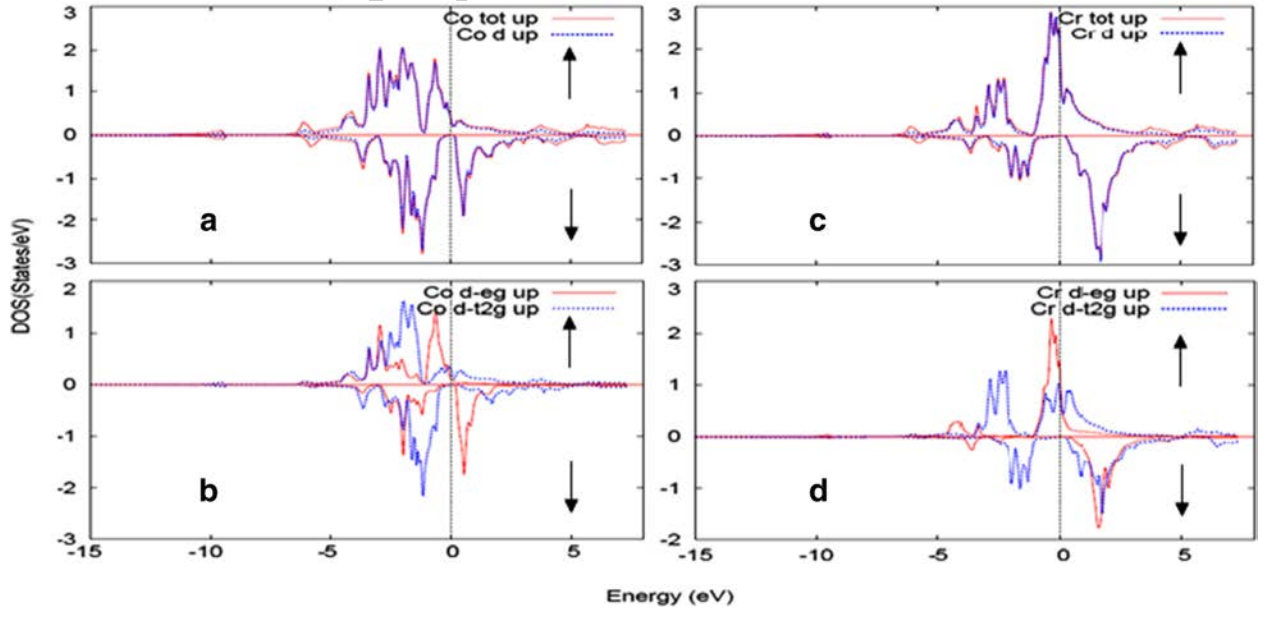

Figure 6 Total DOS.

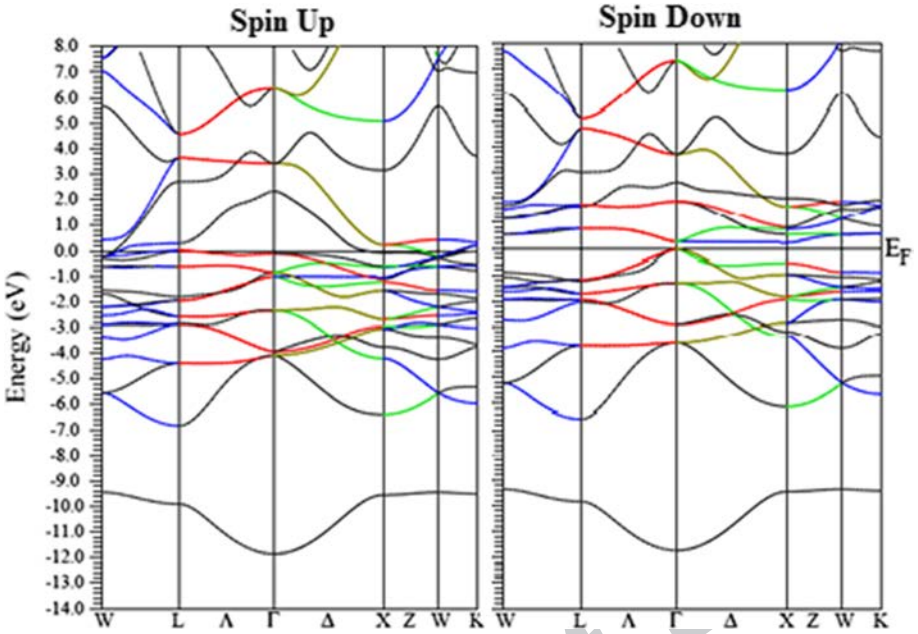

Figure 7 Partial DOS of Co and Cr atoms.

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 Co_2CrGe 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 Co_2CrGe which shows 100% spin polarization at E_F. The existence of the energy gap in the minority spin (DOS and band structure) of Co_2CrGe is an indication of being a potential HMF. This is also evident from the calculated magnetic moment for Co_2CrGe which is 3.9999 μ_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 Co_2CrGa, Co_2CrGe, and Co_2MnGe. The case is just reverse for the lattice constants. The calculated energy gap of Co_2CrGe is small as compared with the energy gaps of Co_2CrGa and Co_2MnGe.

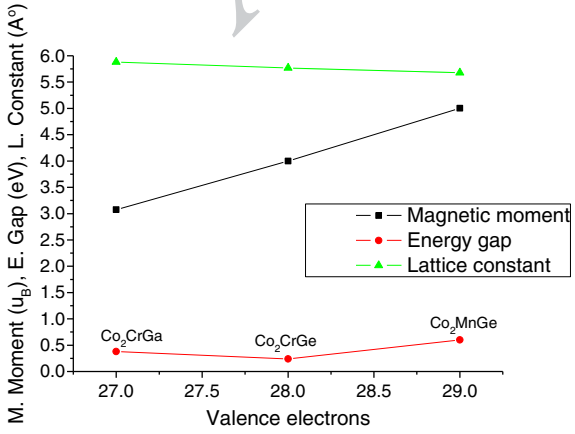

Figure 8 Band structure.

Competing interests
The authors did not provide this information.

Authors' contributions
The authors did not provide this information.

Acknowledgment
DPR acknowledges the DST Inspire Research Fellowship, and RKT acknowledges the research grant from UGC (New Delhi, India).

Author details
[1]Department of Physics, Mizoram University, Aizal 796004, India. [2]National Institute for Materials Sciences, Tsukuba-Shi, Ibaraki 305-0044, Japan.

Received: 30 October 2012 Accepted: 30 October 2012
Published: 11 January 2013

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doi:10.1186/2251-7235-7-3
Cite this article as: Rai *et al.*: **Electronic and magnetic properties of a full-Heusler alloy Co_2CrGe: a first-principles study.** *Journal of Theoretical and Applied Physics* 2013 **7**:3.