The Theoretical Studies of the structural, electronic and Magnetic Properties of the Co_2CrGe

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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 (GGA) is used for structural study where as Local spin density approximation (LSDA) for electronic calculation. First principles structure optimizations were done through total energy calculations at 0K by the full potential linearized augmented plane wave (FP-LAPW) method as implemented in WIEN2K code.

Keywords-component; GGA, half-metallicity, DOS and band structure

I. INTRODUCTION

Strontium titanate ($SrTiO_3$) is one of the most studied oxides of the ABO_3 perovskite type structures, due to its great technological importance. Many interesting phenomena such as colossal magnetoresistance, high-*Tc* superconductivity, multiferroicity, and ferroelectricity are observed in complex oxides. Since most of the interesting complex oxides have perovskite structure, $SrTiO_3$ is an ideal starting point for their study. It has been widely used for integration with other oxides into heterostructures. The Ferromagnetic materials are of great interest to materials science, because their structure is relatively simple reflects various properties: electronic, and magnetic. The properties of these materials have made possible the development and manufacture of various technological devices. Studies of these new materials are of great importance to obtain information on their physical properties in order to improve their devices for their immediate applications.

Many new concepts of modern condensed matter and the physics of phase transitions have been developed while investigating this unique material.[**1–2]** SrTiO3 has applications in the fields of ferroelectricity, optoelectronics and macroelectronics. It is used as a substrate for the epitaxial growth of high temperature superconductors. SrTiO3 exhibits a very large dielectric constant. In comparison with SiO_2, $SrTiO_3$ has almost two orders of magnitude higher dielectric constant and may as well offer a better replacement for SiO_2 in Si-based nanoelectronic devices. $SrTiO_3$ has found usage in optical switches, grain-boundary barrier layer capacitors, catalytic activators, waveguides, laser frequency doubling, high capacity computer memory cells, oxygen gas sensors, semiconductivity, etc.[**3–4]**

II. COMPUTATIONAL DETAILS AND CRYSTAL STRUCTURE

The density functional calculations presented here were done using two methods. The ambient pressure electronic structure and optical properties were obtained using the linearized augmented plane wave (LAPW) method [5] This is an all electron full potential method. These calculations were performed using the WIEN2k package[6]We usedLAPW sphere radii of 2.65, 2.70, 2.65, 2.55, and 2.30 bohrs, for Ba, I, Br, Cl, and F, respectively. We employed well converged zone samplings and basis sets including local orbitals for the semicore states of Ba and to relax linearization errors[7] Relativity was treated at the scalar relativistic level. We used the experimental lattice parameters[8-10]and relaxed the internal coordinates using the generalized gradient approximation (GGA) . The multipole exapansion of the crystal potential and the electron density within muffin tin (MT) spheres was cut at *l*=10. Nonspherical contributions to the charge density and potential within the MT spheres were considered up yo *lmax*=6. The cut-off parameter was RKmax=7. In the interstitial region the charge density and the potential were expands as a Fourier series with wave vectors

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up to Gmax=12a.u-1. The MT sphere radii(R) used were 2.35a.u. for Co, 2.35a.u. for Cr and 2.21a.u. for Ge. The number of k-points used in the irreducible part of the brillouin zone is 286.

The full Heusler structure consists of four penetrating fcc sublattices with atoms at X1(1/4, 1/4, 1/4), X2(3/4, 3/4, 3/4), Y(1/2,. 1/2, 1/2) and Z(0, 0, 0) positions which results in L21 crystal structure having space group Fm-3-m as shown in Fig. 1.

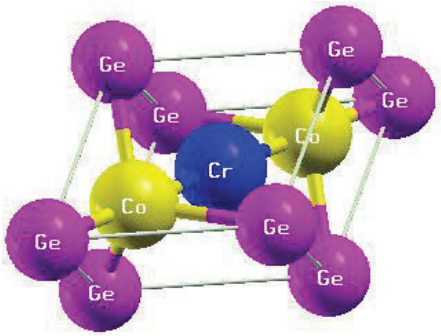

FIGURE 1. Unit Cell Structure of Co2CrGe.

II. RESULTS AND DISCUSSIONS

The volume optimization was performed using the lattice constant by taking the experimental one. The calculated total energies within GGA as function of the volume were used for determination of theoretical lattice constant and bulk modulus. The bulk modulus was calculated using the Murnaghan's equation of state [11]. The calculated values of lattice constant and bulk modulus are presented in Table I. The figure 2 show, the curves of variation of total energy according to the volume of the cell unit for the

We can see that in both cases of calculation, our phase is presented in the form of the most stable phase. Thus, in what follows of our calculations, we choose to treat the properties of the three compounds in this phase

TABLE I. Lattice constant and Bulk modulus.

Lattice Constants a_o (Å)			Bulk Modulus B(GPa)	**Equilibrium Energy (Ry)**
Previous	Calculated	?(a_o)		
5.740[12]	5.77	0.03	250.437	-11873.836

In conclusion, these three materials can present ferromagnetic properties, in spite of the absence of the magnetic elements.

From the figure 3 and 4 we have the projection of the partial densities of state calculated with the LSDA of Co_2CrGe. Generally, one notices according to the two configurations of spin, spin-high and spin-low presented, a remarkable difference between the states. We can note that, there is a shift of the spades in the states of Co between the two directions of spin that indicates that the origin of magnetism in these materials is due to orbital the d of Co in these materials. The Cr-d gives almost an exchange splitting type pattern as shown in Fig. 3(c). The sharp peaks appear at the fermi level in spin up region for Cr-d atoms. The contribution of Co-d atoms are very small at the conduction region. The hybridization between the Co-d and Cr-d atoms are appear between 3.5eV and 5.5eV, which responsible for the creation of magnetic moment. According to Fig. 5 the indirect band gap along the G-X symmetry for Co2CrGe is 0.24eV. For Co2CrGe the Fermi energy (EF) lies in the middle of the gap of the minority-spin states, determining the half-metal character [Fig. 4(a)]. The formation of gap for the half-metal compounds was discussed by Galanakis *et al.* [13] for Co2MnSi, 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.

We calculated the total magnetic moment by using the LSDA approximation .the total magnetic moment of the cell unit is broken up into contribution of the spheres atomic and of the interstitial area, magnetic moments total and partial of our material are represented below in table II One notices that the moment magnetic total of each material considered takes its origin of the magnetic moment of the anion which is the nitrogen with a weak contribution of the magnetic moments of the cations. It is noticed that the value of the total magnetic moment of Co_2CrGe is whole ˜ 4 (μB).

TABLE II. Total and partial magnetic moments.

Magnetic Moment μ_B of Co_2CrGe				
Previous				
	Co	Sr	Ge	total
4.00[14]	0.932	2.122	-0.029	3.999

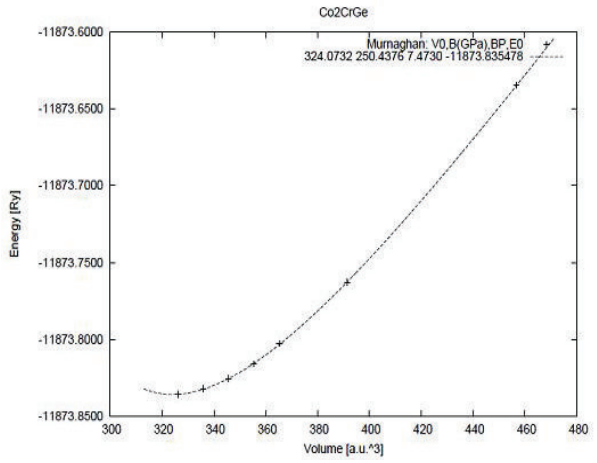

FIGURE 2. Volume optimization of Co2CrGe.

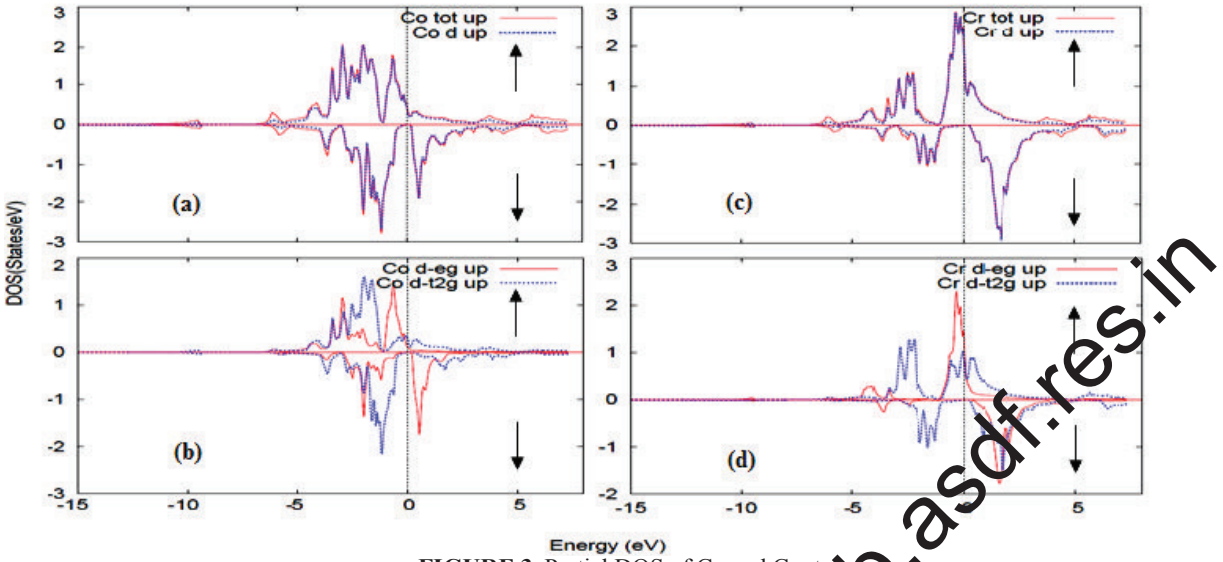

FIGURE 3. Partial DOS of Co and Cr atoms.

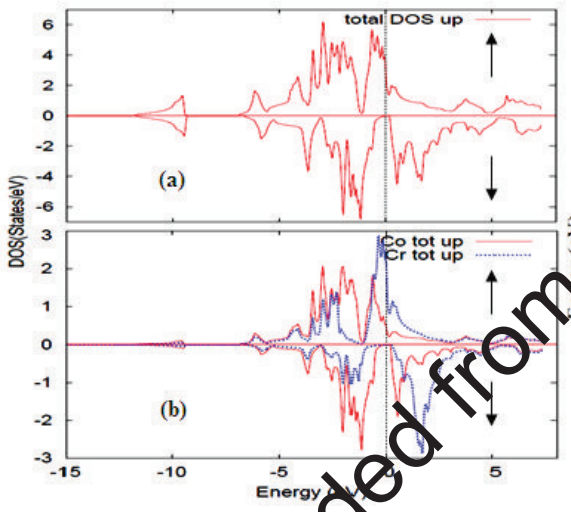

FIGURE 4. Total DOS of Co_2CrGe

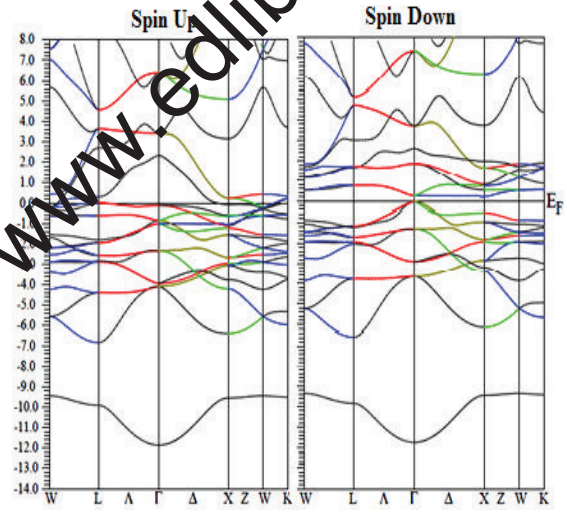

FIGURE 5. Band Structure.

III. 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 Co2CrGe 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 being very small and the contribution is very less in the total magnetic moment. We have investigated the possibility of appearance of half-metallicity in the case of the full Heusler compound Co2CrGe which shows 100% spin polarization at EF. The existence of energy gap in minority spin (DOS and band structure) of Co2CrGe is an indication of being a potential HMF. This is also evident from the calculated magnetic moment for Co2CrGe is 3.9999μB. The calculated result is in qualitative agreement with the integral value, supporting the HMF.

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