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Research Article

STUDY OF HALF-METALLIC PROPERTIES IN CO2CrSb USING GGA AND LSDA

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ABSTRACT
Based on the density functional theory (DFT) calculations, the electronic and magnetic properties of Heusler compound Co_2CrSb were investigated. The system Co_2CrSb were treated with generalized gradient approximation (GGA) as well as local spin density approximation (LSDA). Co_2CrSb gives the 100% spin polarization at E_F. Co_2CrSb is the most stable Half-Metallic Ferromagnets (HMF). But the energy gap when treated with GGA is much larger as compared with the system treated with LSDA. We have also found that the increase in the total magnetic moments in GGA. Based on the calculated results we have predicted the half-metal ferromagnetic character for Co_2CrSb.

Key Words: *GGA, LSDA, DOS, band structure, HMF, spin polarization.*
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INTRODUCTION

In 1983, de Groot discovered half-metallic ferromagnetism in semi-Heusler compound NiMnSb [de Groot et al. (1983)] by using first-principle calculation based on density functional theory. After that, half-metallicity attracted much attention [Katsnelson et al. (2008)] because of its prospective applications in spintronics [Zutic et al. (2004)]. Recently rapid development of magneto-electronics intensified the research on ferromagnetic materials that are suitable for spin injection into a semiconductor [Ohno (1998)]. 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 E_F [Zutic et al. (2004), de Boeck et al. (2002)]. Ishida *et al.* [Ishida et al. (1982)] have also proposed that the full-Heusler alloy compounds of the type Co_2MnZ, (Z=Ge, Sn), are half-metals. Heusler alloys have been particularly interesting systems because they exhibit much higher ferromagnetic Curie temperature than other half-metallic materials [Webster et al. (1988)]. Rai *et al.* [Rai et al. (2010), Rai et al. (2011)] investigated the ground state study of Co_2MnAl and Co_2CrSi using LDA+U and LSDA method respectively. The preparation and characterization of bulk Co_2MnZ (Z=Si, Ge, Ga and Sn) to be used as targets for pulsed laser deposition (PLD) of magnetic contacts for spintronic devices [Manea et al. (2005)]. Rai and Thapa investigated the Electronic Structure and Magnetic Properties of X_2YZ (X=Co, Y=Mn, Z=Ge, Sn) type Heusler Compounds by using A first Principle Study and reported HMFs [Rai and Thapa (2012)]. Rai et al. (2012) also studied the electronic and magnetic properties of Co2CrAl and Co2CrGa using both LSDA and LSDA+U and reported the increase in band gap, hybridization of d-d orbitals as well as d-p orbitals when treated with LSDA+U. In our present work, we have studied the structural, electronic and magnetic properties of Co_2CrSb using full potential linearized augmented plane wave (FP-LAPW) method.

COMPUTATION DETAIL

A computational code (WIEN2K) [Blaha et al. (2001)] based on FP-LAPW method was applied for structure calculations of Co_2CrSb. GGA was used for the exchange correlation potential. 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 l_{max}=6 . The cut-off parameter was RK_{max}=7. In the interstitial region the charge density

and the potential were expands as a Fourier series with wave vectors up to G_{max}=12 $a.u^{-1}$. The number of k-points used in the irreducible part of the brillouin zone is 286. The Muffin Tin sphere radii (RMT) for each atom are 2.45 a.u. for Co, 2.45 a.u. for Cr and 2.31 a.u. for Sb.

CRYSTAL STRUCTURE

Heusler alloy [Heusler (1903)] with chemical formula Co_2CrZ (Z = Sb). The full Heusler structure consists of four penetrating fcc sublattices with atoms at Co1(1/4,1/4,1/4), Co2(3/4,3/4,3/4), Cr(1/2,1/2,1/2) and Z(0,0,0) positions which results in L_{21} crystal structure having space group Fm-3-m as shown in Fig. 1.

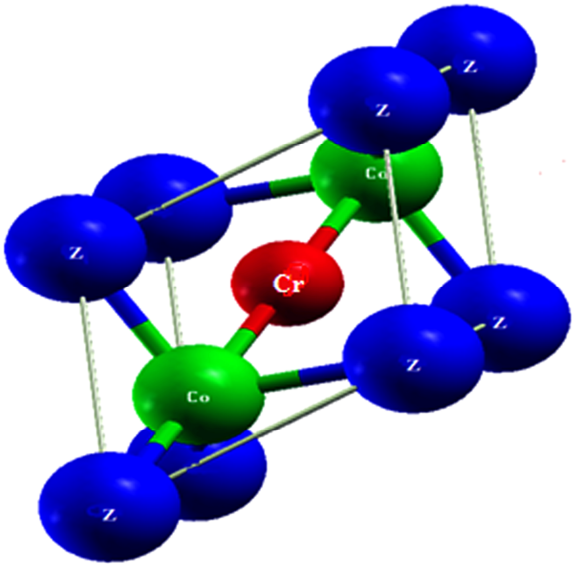

Figure 1: Unit cell Structure of Co_2CrZ: Co(green), Cr(red) and Z(blue) generated by xCrysden package.

RESULTS AND DISCUSSIONS

Structural optimization for Co_2CrSb

Systematic calculations of the electronic and magnetic properties of the Heusler compounds Co_2CrSb were carried out in this work. The results of the electronic properties calculations are compared to study the effect of the different kinds of atoms and valence electron concentration on the magnetic properties and in particular the band gap in the minority states. The electronic properties were calculated using GGA and LSDA respectively. The optimized lattice constant, isothermal bulk moduli, its pressure derivative are calculated by fitting the total energy to the Murnaghan's equation of state [Murnaghan (1944)]. The optimized lattice parameters were slightly higher than the experimental lattice parameters, the change in lattice parameters are given by $\Delta(a_o)$. It is confirmed that the ferromagnetic configuration is lower in energy in case of the systems Co_2CrSb [Table 1]. The results of the structural optimization are shown in Fig. 1. The detail values of the optimized Lattice parameters and bulk moduli are given in Table 1.

Spin Polarization and half-metallic ferromagnets

The electron spin polarization (P) at Fermi energy (E_F) of a material is defined by equation (1) [Soulen et al. (1998)].

$$P = \frac{\rho\uparrow(E_F) - \rho\downarrow(E_F)}{\rho\uparrow(E_F) + \rho\downarrow(E_F)} \qquad (1)$$

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 [**Ozdogan et al. (2006)**]. The electrons at E_F are fully spin polarized (P=100%) when $\rho\uparrow(E_F)$ or $\rho\downarrow(E_F)$ equals to zero. In present work, we have studied the system Co_2CrSb shows 100% spin polarization at E_F [Table 2]. According to our results, the compound Co_2CrSb is interesting as it shows large DOS at the E_F of $\rho\uparrow(E_F)$ =2.5 states/eV within both GGA as well as LSDA.

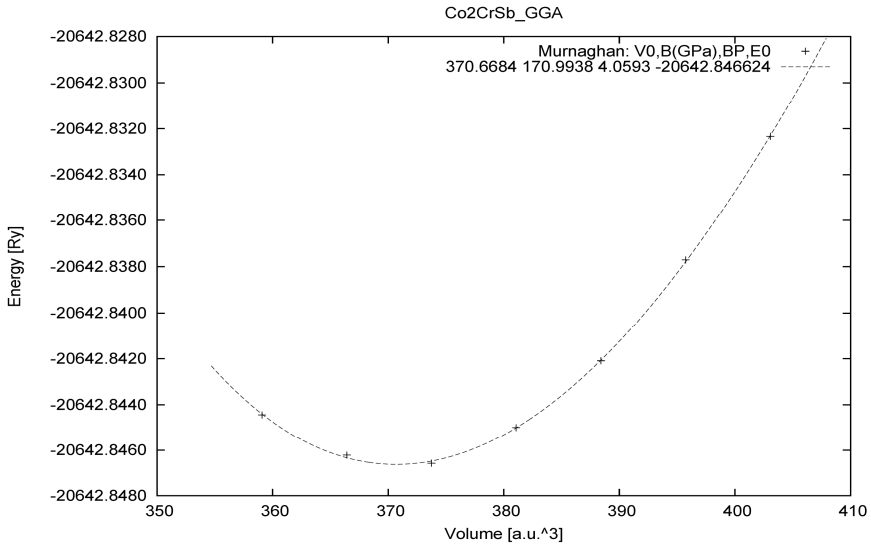

Figure 2: Volume optimization of Co2CrSb

Table 1: Lattice parameters, Bulk modulus and Equilibrium energy.

Compounds	**Lattice Constants a_o (Å)**			**Bulk Modulus**	**Equilibrium**
	Previous	**Calculated**	**$\Delta(a_o)$**	**B(GPa)**	**Energy (Ry)**
Co_2CrSb	6.011[a]	6.034	0.023	170.763	-20642.8466

[a]***Ref :*** **M. Gilleßen (2009)**

Fig.3 summarizes the results of the DOS which were calculated using LSDA. As Compared to LSDA, GGA increases the exchange splitting between the occupied majority and the unoccupied minority states and thus to larger gap for Co_2CrSb [Fig. 5]. According to Figs. (4, 6) the indirect band gap along the Γ-X symmetry for Co_2CrSb are 0.25 eV and 0.45 eV using LSDA and GGA respectively. Incase of both LSDA and GGA the Fermi energy (E_F) lies in the middle of the gap of the minority-spin states, determining the half-metal character [Figs. (5, 6)].

Table 2: Energy gap and Spin polarization

Tools	**Energy gap E_g (eV)**			**Spin Polarization**		
	$E_{max}(\Gamma)$	**$E_{min}(X)$**	**ΔE**	$\rho\uparrow(E_F)$	$\rho\downarrow(E_F)$	P%
LSDA	-0.25	0.00	0.25	2.50	0.00	100
GGA	-0.25	0.20	0.45	2.40	0.00	100

The formation of gap for the half-metal compounds was discussed by **Galanakis *et. al.* (2002)** for Co_2MnSi, 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.

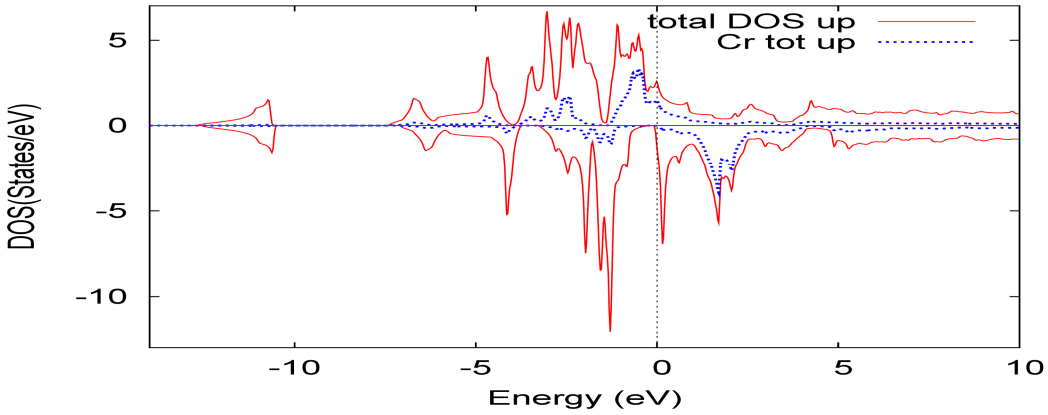

Figure 3: Total DOS of Co2CrSb using LSDA

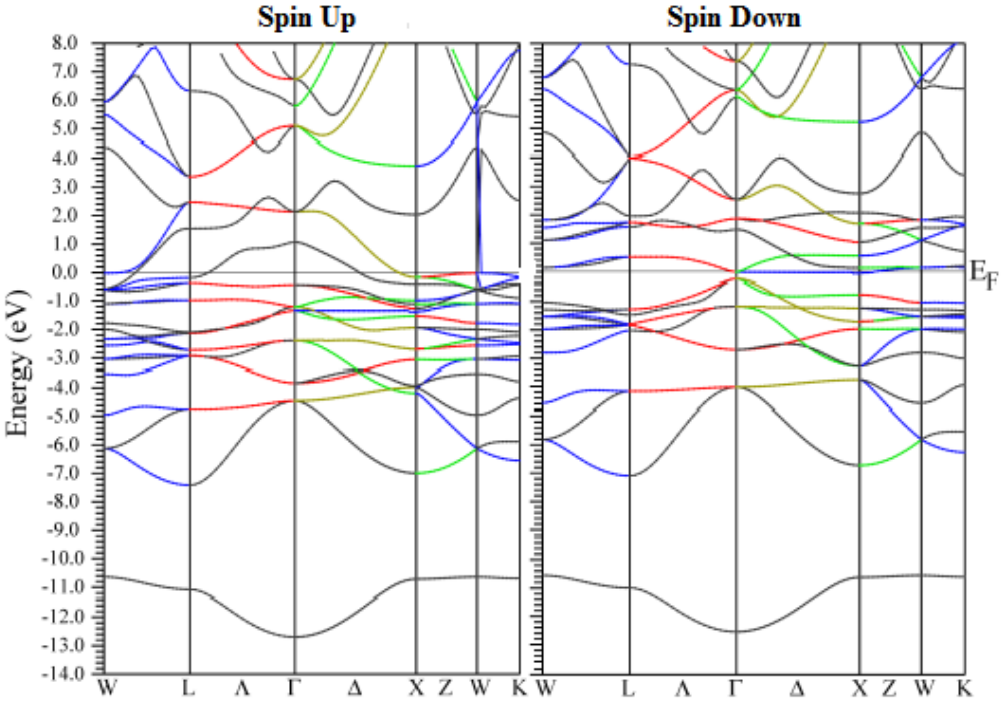

Figure 4: Band structure using LSDA

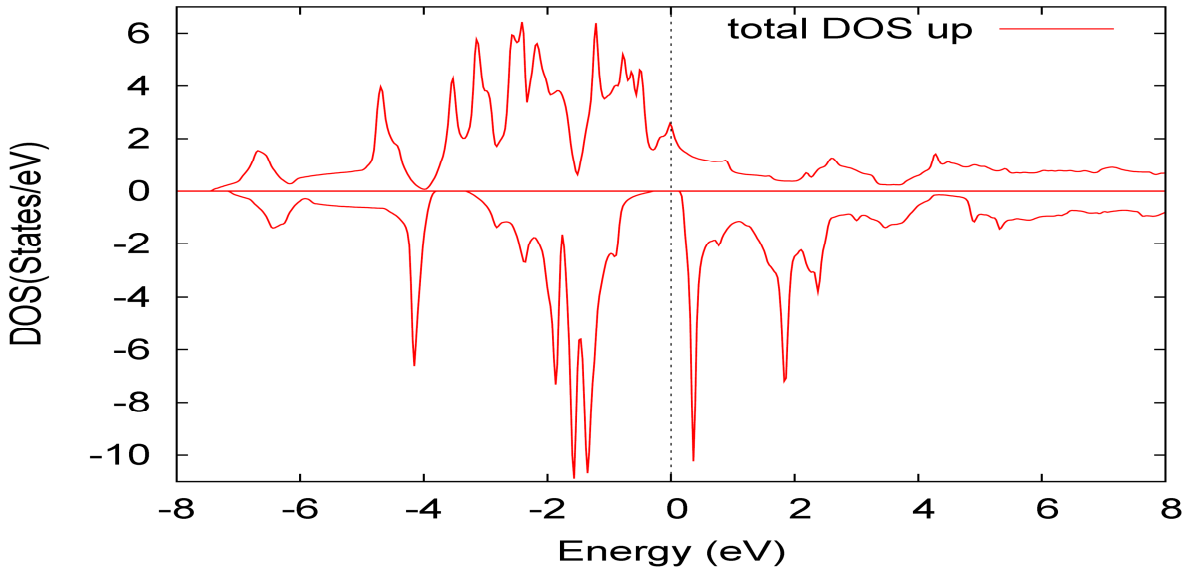

Figure 5: Total DOS using GGA

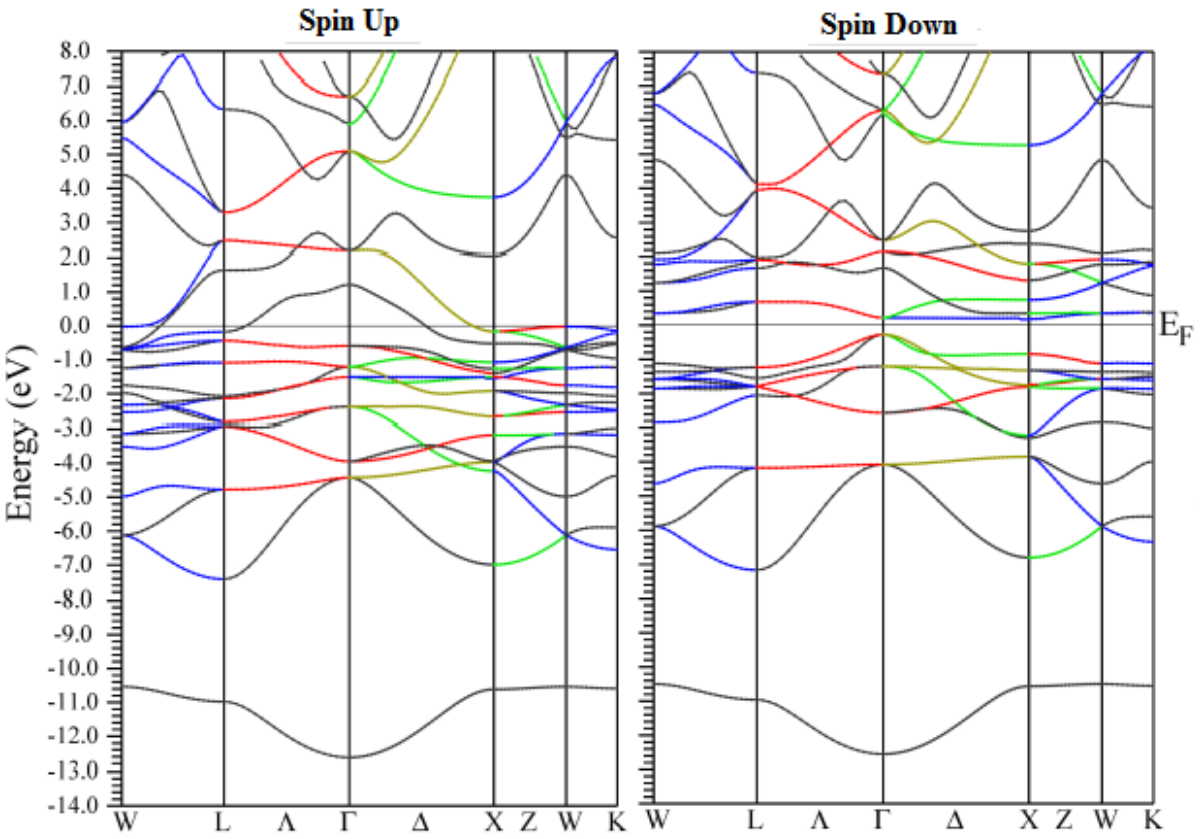

Figure 6: Band structure using GGA

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 3. It is shown in Table 3 the calculated total magnetic moment is almost an integer value in case of Co_2CrSb as expected for the half-metallic systems. It is found that the partial as well as the total magnetic moment increases in GGA as shown in Table 3. We have found that the Co sites contribute much more to the magnetic moment in the Sb compound 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 3 the Sb atoms carry a negligible magnetic moment, which does not contribute much to the overall moment. We have also noticed that the partial moment of Sb atoms aligned anti-parallel to 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 Z sites are mainly due to polarization of these atoms by the surroundings, magnetically active atoms as reported by Kandpal *et al.,* (2006).

Table 3: Total and partial magnetic moments

Tools	**Magnetic Moment μ_B**				
	Previous	**Calculated**			
		Co	**Cr**	**Z**	**Total**
LSDA	5.023[a]	1.039	2.778	-0.010	4.939
GGA		1.058	2.853	-0.014	4.999

[a]***Ref :*** **M. Gilleßen (2009)**

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 structures of Co_2CrSb were calculated using FP-LAPW method. The calculated results were in good agreement with the previously calculated results. The GGA gives wider gaps as well as the higher value of magnetic moment as compared to LSDA and the half-metallicity is more stable in Co_2CrSb is the most stable HMF. For Ferromagnetic compounds the partial moment of Z being antiparallel to the Co and Cr atoms. We have investigated the possibility of appearance of half-metallicity in the case of the full Heusler compound Co_2CrSb which shows 100% spin polarization at E_F. The existence of energy gap in minority spin (DOS and band structure) of Co_2CrSb is an indication of being a potential HMF. As well as the integral value of magnetic moment is also the evident of HMF. The calculated magnetic moment are in qualitative agreement with the integral value, supporting the HMF.

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REFERENCES

de Groot R. A., Mueller F. M., Van Engen P. G., and Buschow K. H. J. (1983) New Class of Materials: Half-Metallic Ferromagnets. *Physical Review Letters*, **50**(25)**,** 2024–2027.

Katsnelson M. I., Irkhin V. Y., Chioncel L., Lichtenstein A. I., and de Groot R. A. (2008) Half-metallic ferromagnets: From band structure to many-body effects. *Review of Modern Physics*, **80**(2), 315–378.

Zutic I., Fabian J. and Das Sarma S. (2004) Spintronics: Fundamentals and applications *Review of Modern Physics*, **76**(2), 323.

Ohno H. (1998) Making Nonmagnetic Semiconductors Ferromagnetic. *Science* **281**(5379), 951.

Van Roy de Boeck W., Das J., Motsnyi V., Liu Z., Lagae L., Boeve H., Dessein K. and Borghs G. (2002) Technology and materials issues in semiconductor-based magnetoelectronics. *Semiconductor Science Technology*, **17**(4), 342.

Ishida S., Akazawa S., Kubo Y. and Ishida J. (1982) Band theory of Co_2MnSn, Co_2TiSn and Co_2TiAl. *Journal of Physics F: Metal Physics*, **12**(6)**,** 1111**.**

Webster P. J. and Ziebeck K. R. A. (1988) *Alloys and Compounds of d-Elements with Main Group Elements. Part 2*(*Landolt B¨ornstein New Series*, Group III, Vol. 19, Pt.c) ed H R J Wijn (Berlin: Springer) 75–184.

Rai D. P., Hashemifar J., Jamal M., Lalmuanpuia, Ghimire M. P., Sandeep, Khathing D. T., Patra P. K., Sharma B. I., Rosangliana and Thapa R. K. (2010) Study of Co2MnAl Heusler alloy as half metallic Ferromagnet *Indian Journal of Physics*, **84**(5), 593-595.

Rai D. P., Sandeep, Ghimire M. P. and Thapa R. K. (2011) Study of energy bands and magnetic properties of Co2CrSi Heusler alloy *Bulletin of Material Sciences*, **34**(6), 1219-1222.

Manea A. S., Monnereau O., Notonier R., Guinneton F., Logofatu C., Tortet L., Garnier A., Mitrea M., Negrila C., Brandford W. and Grigorescu C. E. A. (2005) *Journal of Crystal Growth* **275**(1-2), e1787-e1792.

Rai D. P. and Thapa R. K. (2012) Electronic Structure and Magnetic Properties of X_2YZ (X=Co, Y=Mn, Z=Ge, Sn) type Heusler Compounds by using A first Principle Study, *Phase Transition: A Multinational Journal*, iFirst, 1-11.

Rai D. P., Sandeep, Ghimire M. P. and Thapa R. K. (2012) Electronic tructure and magnetic properties of Co_2YZ (Y=Cr, V=Al, Ga) type Heusler compounds: A first Principle Study,
International Journal of Modern Physics B **28**(8), 1250071

Blaha P., Schwarz K., Madsen G. K. H., Kvasnicka D. and Luitz J. (2001) "WIEN2k, An augmented plane wave + local orbitals program for calculating crystal properties," Karlheinz Schwarz, Techn. Universität, Wien, Austria, 3-9501031-1-2.

Heusler F. **(1903)** Kristallstruktur und Ferromagnetismus der Mangan-Aluminium-Kupferlegierungen. *Verh. Dtsch. Phys. Ges.* **12**, 219.

Murnaghan F. D. **(1944)** The Compressibility of Media under Extreme Pressures. *Proc. Natl. Acad. Sci. USA* **30**(9), 244.

M. Gilleßen (2009) *Von der Fakult¨at f¨ur Mathematik, Informatik und Naturwissenschaften der RWTH Aachen University zur Erlangung des akademischen Grades eines Doktors der Naturwissenschaften genehmigte Dissertation.*

Soulen Jr. R. J., Byers J. M., Osofsky M. S., Nadgorny B., Ambrose T., Cheng S. F., Broussard P. R., Tanaka C. T., Nowak J., Moodera J. S., Barry A. and Coey J. M. D. (1998) Measuring the Spin Polarization of a Metal with a Superconducting Point Contact. *science* **282**(5386), 85.

Ozdogan K., Aktas B., Galanakis I. and Sasioglu E. (2006) Influence of mixing the low-valent transition metal atoms (Y,Y*=Cr,Mn,Fe) on the properties of the quaternary $Co_2[Y_{1-x}Y^*_x]$. *arxiv: cond-mat/0612194v1 [cond-mat.mtrl-sci]*.

Kandpal H. C., Fecher G. H. and Felser C. (2006) Calculated electronic and magnetic properties of the half-metallic, transition metal based Heusler compounds. *Journal of Physics D: Applied Physics*, **40**(6)**,** 1507-1523.

Galanakis I., Dederichs P. H. and Papanikolaou N. (2002) Slater-Pauling behavior and origin of the half-metallicity of the full-Heusler alloys. *Physical Review* B **66**(17), 174429.