CHAPTER- 4

ELECTRONIC AND MAGNETIC PROPERTIES OF RARE EARTH ANTIMONIDES, NITRIDES AND SEMI-HEUSLER ALLOY

Chapter - 4

Electronic and magnetic properties of rare earth antimonides, nitrides and semi-Heusler's alloy

In this chapter, we present the DOS, energy band structures and magnetic moments for Rare earth antimonides ($LaCrSb_3$, $CeCrSb_3$ and $NdCrSb_3$), Rare earth nitrides (SmN and EuN) and semi-Heusler's alloy NiTbSb. The calculated results will be compared with the experimental results available and also with previously calculated data.

4.1 Rare earth antimonides :

The density of states (DOS) and magnetic moments of the compounds were studied (Sandeep *et al.,* 2010c, 2011a) by using the FP-LAPW method, in the framework of DFT (Kohn and Sham, 1965). We have performed our calculations using the experimentally determined lattice parameters and the atomic positions (Brylak and Jeitschko, 1995) for $RCrSb_3$. Spin polarization has been taken into account. WIEN2k code (Blaha *et al.,* 2001) is used for computations. Since La, Ce and Nd 4*f*-orbitals are rather localized, the 4*f*-electron correlations are expected to be strong. Consequently, the LSDA+U calculations (Anisimov *et al.,* 1997) have been chosen to include the on-site Coulomb interaction. The onsite Coulomb energy (U) and the exchange parameter (J) applied are 0.52 and 0.00 Ry. respectively. We have used 47 *k* points in the irreducible Brillouin zone, and the muffin-tin radii for La, Ce, Nd, Cr, Sb_1, Sb_2, Sb_3 are 2.5, 2.5, 2.5, 2.5 2.35, 2.35 and 2.35 a.u. respectively. The density plane cut-off $R_{MT}*K_{MAX}$ is 7.0, where K_{MAX} is the plane wave cut-off and R_{MT} is the smallest of all atomic sphere radii.

The self-consistency is better than 0.001e/a.u.^{3} for charge and spin density and the stability is better than 0.01 mRy. for total energy per cell.

4.1.1 Results and discussions

The total DOS plots of $LaCrSb_3$ for spin-up and spin-down configurations are shown in Fig. 4.1 (a-d). From the total DOS [Fig 4.1 (a)] of $LaCrSb_3$, peaks are observed at -8.75 eV in the core regions due to Sb- 5*s* states [Fig 4.1 (b)] in both spin up and spin-down configurations. In the semi-core and valence regions (from -5.78 eV upto the Fermi level), peak at -3.2 eV was found due to Cr-3*d* states [Fig 4.1 (c)] in spin-up, while in spin down, peaks were observed at -1.2 eV due to Sb-5*p* states [Fig. 4.1(b)]. The fact that the Cr-3*d* and Sb-5*p* are strongly hybridized (Choi *et al.,* 2007) was also observed in our calculations for spin-up channel [Fig 4.1 (b-c)]. The DOS at and around Fermi level (E_F) were contributed by Sb-5*s*, Sb-5*p* and Cr-3*d* state electrons in both the spin channels. In the conduction region, sharp peaks were observed at 2.0 eV for both spins which were due to localized La-4*f* state electrons [Fig 4.1 (d)]. The exchange-splitting of the Cr-3*d* states were observed to be of the order of 8.0 eV and was the main contributor towards the magnetic moment of the system (Sandeep *et al.,* 2010a; Ghimire *et al.,* 2010a).

The DOS plots of $CeCrSb_3$ are shown in Fig. 4.2 (a-d). In the core region, sharp peaks were observed at -8.8 eV in both spins which were due to the contributions from Sb-5*s* states [Fig. 4.2 (b)]. In the semi-core and the valence region, sharp peaks were observed at -3.25 eV in spin up and -0.95 eV and -1.2 eV in spin down channel. The

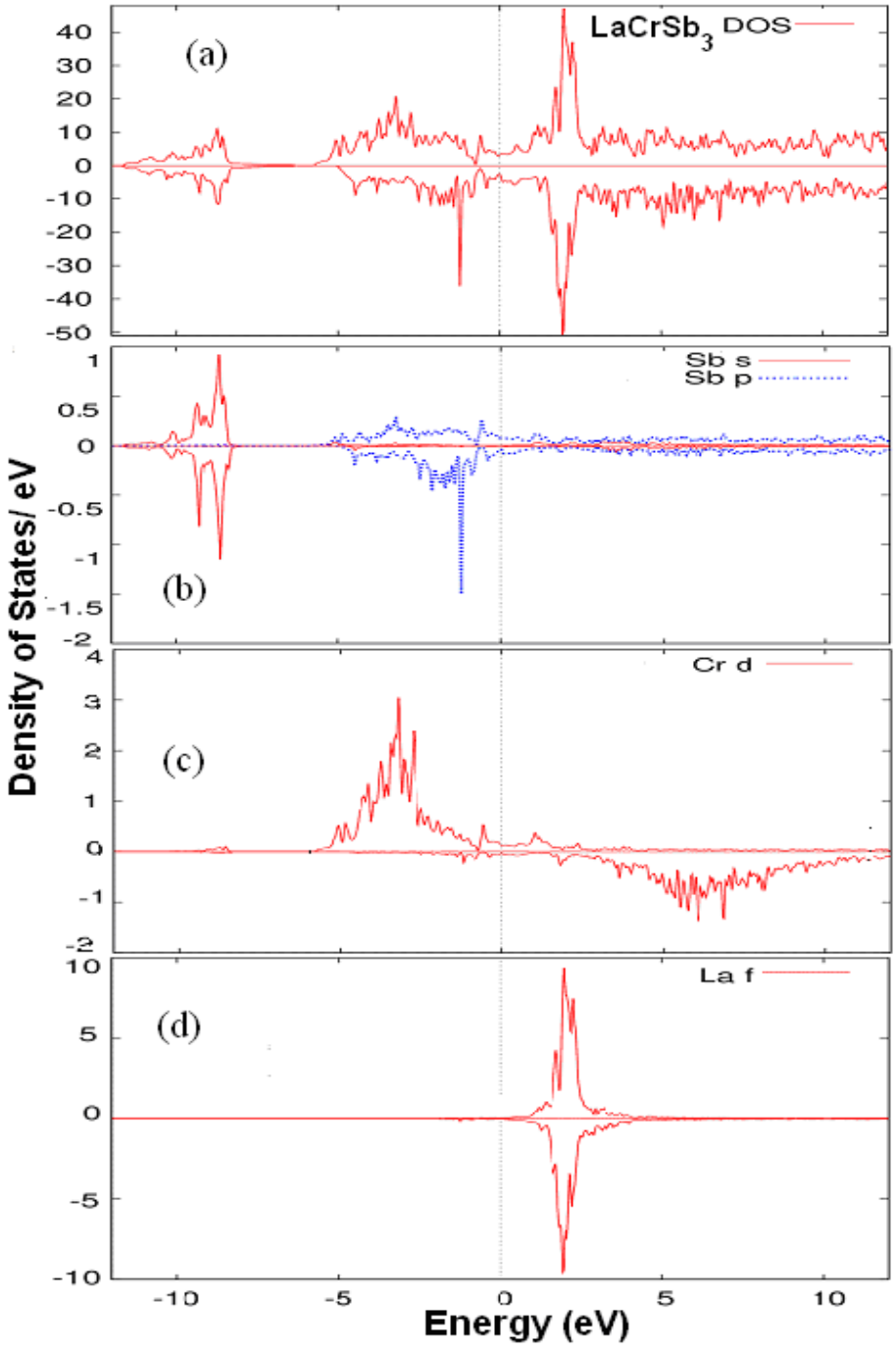

Figure 4.1 (a-d): Total and partial Density of states for $LaCrSb_3$. (E_F=0 eV corresponds to the Fermi level)

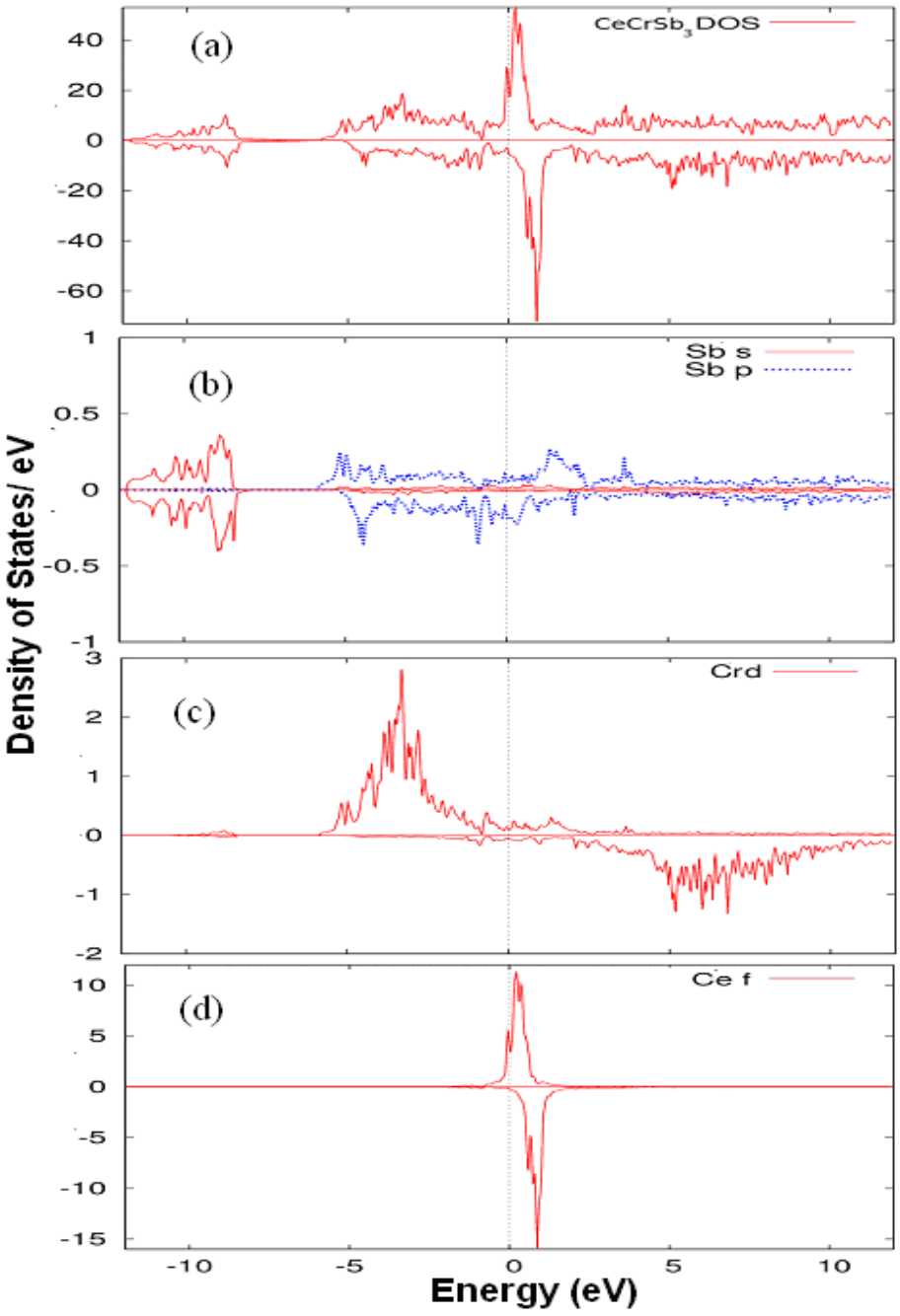

Figure 4.2 (a-d): Total and partial Density of states for $CeCrSb_3$. (E_F=0 eV corresponds to the Fermi level)

major contributor towards the total DOS in this region as shown in Fig. 4.2 (b-c) is Cr-3*d* electrons in spin up while in spin down it is due to Sb-5*p* states. At and above the E_F, Ce-4*f* states were found to contribute in spin up region with a sharp peak at 0.2 eV while in spin down it is observed at 0.9 eV as shown in Fig. 4.2 (d). The Cr-3*d* state electrons as shown in Fig. 4.2 (c) were found to contribute to the total DOS with sharp peaks at -5.1 eV in spin up and 6.9 eV in spin-down. These are responsible for the magnetic ground state of the system. The Sb-5*p* state electrons were observed to be uniformly distributed throughout the valence and the conduction regions. The exchange energy difference between spin up and spin down of Cr-3*d* states is approximately 8.0 eV due to which it gives net magnetic moment in $CeCrSb_3$ (Sandeep *et al.*, 2010d, Wu *et al.*, 2005).

The DOS plots of $NdCrSb_3$ along with the partial DOS of Sb-5*s*, Sb-5*p*, Cr-3*d* and Nd-4*f* are shown in Fig. 4.3 (a-d) respectively. The vertical line at 0.0 eV corresponds to the Fermi level (E_F). From the spin-up configuration peaks were observed below E_F in the valence region at energies of -3.4 eV, -0.5 eV and -0.3 eV. Above E_F in the conduction region, we observe a sharp peak in the spin-up DOS at 0.4 eV as shown in Fig 4.3 (a). The spin down DOS plot has shown the peaks at 1.9 eV and 2.6 eV above E_F and was also observed in the form of thick bands in the spin-down band structures plot (Sandeep *et al.*, 2011a, b). The contributions in the core regions were mainly found to be due to Sb-5s and Sb-5p state electrons as shown in Fig 4.3 (b). The individual DOS contributions by Cr-3*d* atoms of $NdCrSb_3$ are shown in Fig 4.3 (c). It is observed that the total DOS is mainly contributed by the DOS of Nd and Cr atoms. DOS contributions are observed in

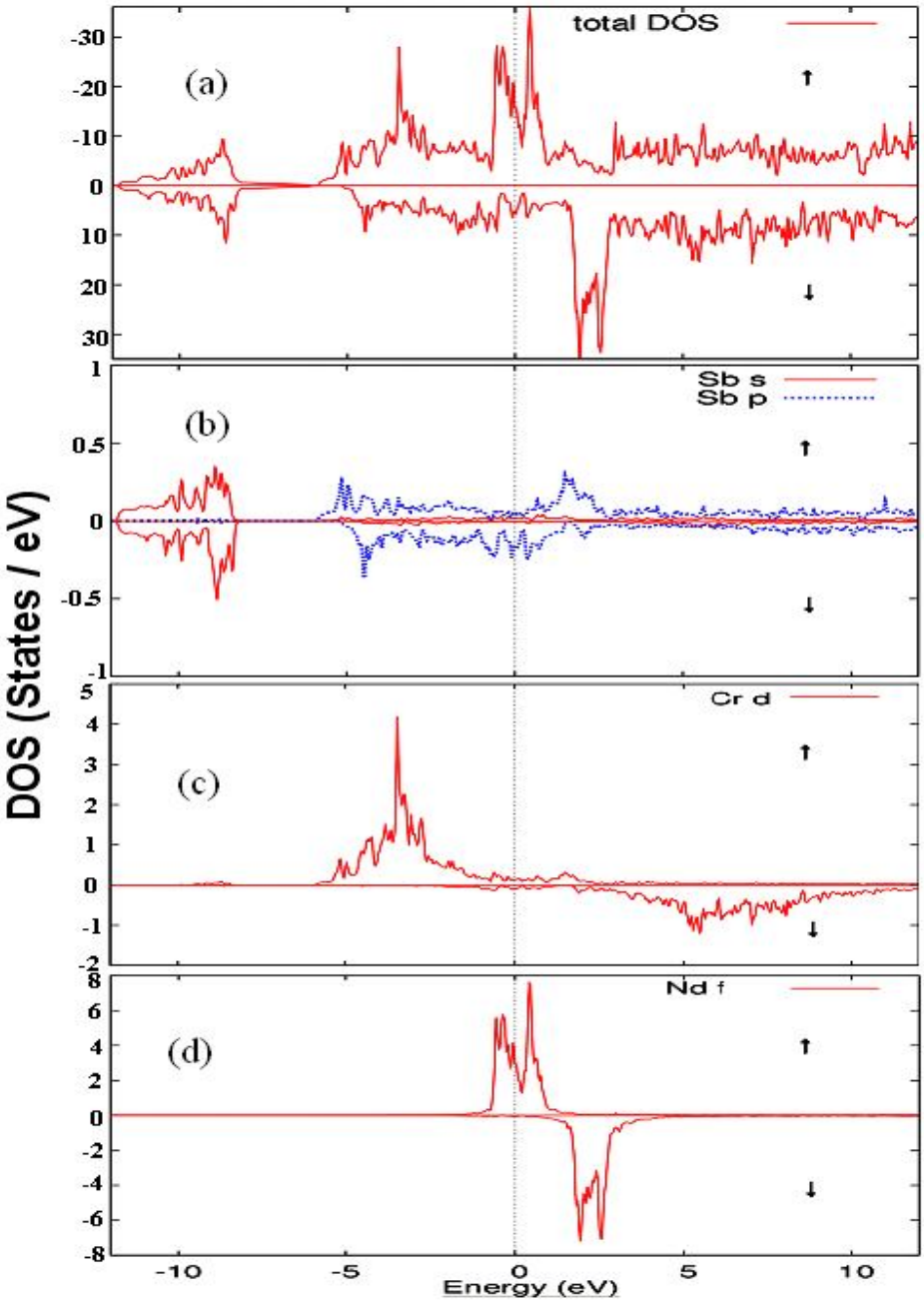

Figure 4.3 (a-d): Total and partial Density of states for $NdCrSb_3$. (E_F=0 eV corresponds to the Fermi level)

Fig 4.3 (c) for Cr-3*d* state electrons in the valence region within -4.4 eV to -2.75 eV with a sharp peak at -3.4 eV below E_F. The highest contribution towards the total DOS of the system is due to the 4*f*-electrons of Nd atom near E_F as shown in Fig 4.3 (d). Towards the total DOS, Sb atoms are found to contribute negligibly as compared to the contributions from electron states of Cr atoms. Exchange splittings of both the Nd-4*f* and Cr-3*d* states were found as shown in Fig. 4.3 (c-d). These splitting were observed to be of the order of 6.0 eV for Cr-3*d* and 2.0 eV for Nd-4*f* respectively.

We have calculated the effective moments of $LaCrSb_3$ and $CeCrSb_3$ to be 3.03 μ_B and 3.73 μ_B respectively. In Table 4.1, we have summarized the total and individual spin moments of $LaCrSb_3$, $CeCrSb_3$ and $NdCrSb_3$. The La individual moment is zero (Hartjes *et al.,* 1997) which is in qualitative agreement with the present calculations. Thus the magnetic behaviour of Cr can be isolated by investigating the properties of $LaCrSb_3$ which does not have 4*f* moments. The moment of Ce atoms is higher than La in $CeCrSb_3$ due to the presence of 4*f* electrons with exchange energy splitting. We observe that, as the rare-earth ion size increases, the moment contributed by the Cr-3*d* decreases. This may be due to the increase in the involvement of the rare-earth 4*f* electrons such that Cr-3*d* bounds to interact only with the Sb-5*p* electrons. We also observe that the magnetic moment increases from $LaCrSb_3$ to $CeCrSb_3$ (Ghimire *et al.*, 2010a; Sandeep *et al.*, 2010 c, d). The results of the individual and effective moments of $LaCrSb_3$ and $CeCrSb_3$ are in qualitative agreement with those of Choi *et al.* (2007), Jackson *et al.* (2001, 2007), Hartjes *et al.* (1997) and Inamdar *et al.* (2008). Hartjes *et al.* (197) have calculated the Ce

Table. 4.1: Total and individual magnetic moments in $LaCrSb_3$, $CeCrSb_3$ and $NdCrSb_3$

Sl. No.	$RCrSB_3$	Magnetic moment of Rare Earth (R)		Magnetic moment of Cr		Total Magnetic moment	
		Present μ_B	Previous μ_B	Present μ_B	Previous μ_B	Present μ_B	Previous μ_B
1.	$LaCrSb_3$	-0.02	0.0 †	4.04	2.81 *	3.03	3.01 ξ 3.68 † † 2.39 *
2.	$CeCrSb_3$	0.78	2.54 †	-	-	3.73	4.06 ξ 3.28 * *
3.	$NdCrSb_3$	3.34	-	3.99	-	5.77	5.2 ξ ξ

† Hartjes *et al.*, (1997); * Choi *et al.*, (2007) ; ξ Inamdar *et al.*, (2008a) ;

† † Jackson *et al.*, (2001); * * Jackson *et al.*, (2007) ; ξ ξ Inamdar *et al.*, (2008b)

moment in $CeCrSb_3$ to be 2.54 μ_B which is contradicting to the present calculation as 0.78 μ_B. This discrepancy may have arise in their calculation due to the localized nature of the 4*f* electrons which has been taken care by using LSDA+U scheme in the present calculations. The magnetic moments observed for $NdCrSb_3$ in our calculations were due to the exchange splitting of Nd-4*f* spin up and spin down channels and Cr-3*d* spin up and spin down channels respectively. The individual magnetic moment of Nd and Cr is 3.34μ_B and 4.0 μ_B respectively. The moment due to Sb atoms is negative. The effective magnetic moment was calculated (Sandeep *et al.,* 2011a, b) out to be 5.77 μ_B for $NdCrSb_3$ which is comparable with the experimental magnetic moment of 5.2 μ_B observed by Inamdar *et al*. (2008).

4.2 Rare Earth Nitrides:

We have performed the spin polarized electronic DOS, band structure and magnetic moment calculations by using first principle FP-LAPW method (Sandeep *et al.*, 2011c; Ghimire *et al.*, 2010b). The lattice parameters were taken to be 5.017 Å for SmN and 5.014 Å for EuN (Aerts *et al.*, 2004). Both the rare earth nitrides SmN and EuN considered in the present work crystallize in the rock-salt structure with space group *Fm3m*. The lattice co-ordinates used for rare earth atom is (0, 0, 0) and nitrogen is (1/2, 1/2, 1/2). There are 2 independent atoms with a total of 2 atoms per unit cell for both SmN and EuN. The radius for the muffin tin sphere was chosen to be 2.5 a.u. for both Sm and Eu and 2.21 a.u. for N respectively. The R_{MT} X K_{MAX} is taken to be 7.00 with G_{min} = 6.34 $a.u.^{-1}$ and G_{max} = 12 $a.u.^{-1}$. A mesh of 1000 *k*-points is chosen which gives 47 *k*-points in the irreducible wedge of the Brillouin zone.

4.2.1 Results and discussions

We are presenting here the results obtained for DOS, band structures and magnetic properties of SmN and EuN in rock-salt phase (Sandeep *et al.*, 2011c). The net magnetic moment is calculated to be 5.0 μ_B/ formula unit and 6.0 μ_B/ formula unit for SmN and EuN respectively. These results agree well with the theoretical results provided by Aerts *et al.*, (2004). It is observed that the total magnetic moments are mainly due to the individual moments of the rare earth atoms (RE = Sm and Eu) along with small positive moments from the interstitials in both SmN and EuN. The N-atom is found with negligible negative moments. The integral values for the magnetic moments also

Table 4.2: Various components of the spin magnetic moments of rare earth nitrides.

Sl. No.	REN	Magnetic moment of Rare Earth (R)		Magnetic moment of N		Total Magnetic moment	
		Present μ_B	Previous μ_B	Present μ_B	Previous μ_B	Present μ_B	Previous μ_B
1.	SmN	5.26	5.22 *	-0.40	-0.24 *	5.00	5.00 *
2.	EuN	6.32	6.30 *	-0.45	-0.30 *	6.00	6.00 *

* Aerts *et al.,* (2004)

confirms the fact these systems are half-metals. The spin magnetic moment is dominated by the 4*f*-state electrons of the rare earth atoms with some hybridisation yielding small contributions from the *s-d* electrons of rare earth atoms and *p*-states of nitrogen atoms (Aerts *et al.,* 2004). This indicates that the *p*-states of nitrogen occurs in the same energy range as the valence rare earth states, allowing hybridization to occur.

Fig. 4.4 (a-c) shows the total and partial DOS plots of SmN (Sandeep *et al.,* 2011c). Two sharp peaks were observed in the majority spin channel below the Fermi level at -0.4 eV and -0.2 eV due to 4*f*- state of Sm [Fig. 4.4 (b)] atoms with a small peak at -1.25 eV due to 2*p* states of N [Fig. 4.4 (c)] atoms. The DOS rises from the valence region cutting the Fermi level E_F to the conduction regions upto 1.1 eV. This behaviour makes the spin-up region metallic. In spin-down configuration, we observe a small peak at -1.0 eV which is only due to 2*p*- state of N [Fig. 4.4 (c)] atoms in the valence region with two sharp peaks in the conduction region at 3.5 eV and 3.9 eV due to 4*f* states of Sm [Fig. 4.4 (b)] atoms. The DOS plot for Sm-4*f* state in Fig. 4.4 (b) shows an exchange splitting of the order of 3.1 eV in spin up and down channel. Fig. 4.4 (d-f) shows the total and partial DOS plots for EuN (Ghimire *et al.,* 2010b). A similar nature of the DOS is seen for Eu-4*f* and N-2*p* in EuN as in the case of SmN. The 4*f* peak of Eu [Fig. 4.4 (e)] atoms was observed at -0.5 eV in the valence region of spin up channel while in the spin down channel, the peak was observed at 4.2 eV of the conduction region. The contribution of N-2*p* states were seen mainly in the valence region for both the spin channels [Fig 4.4 (f)].

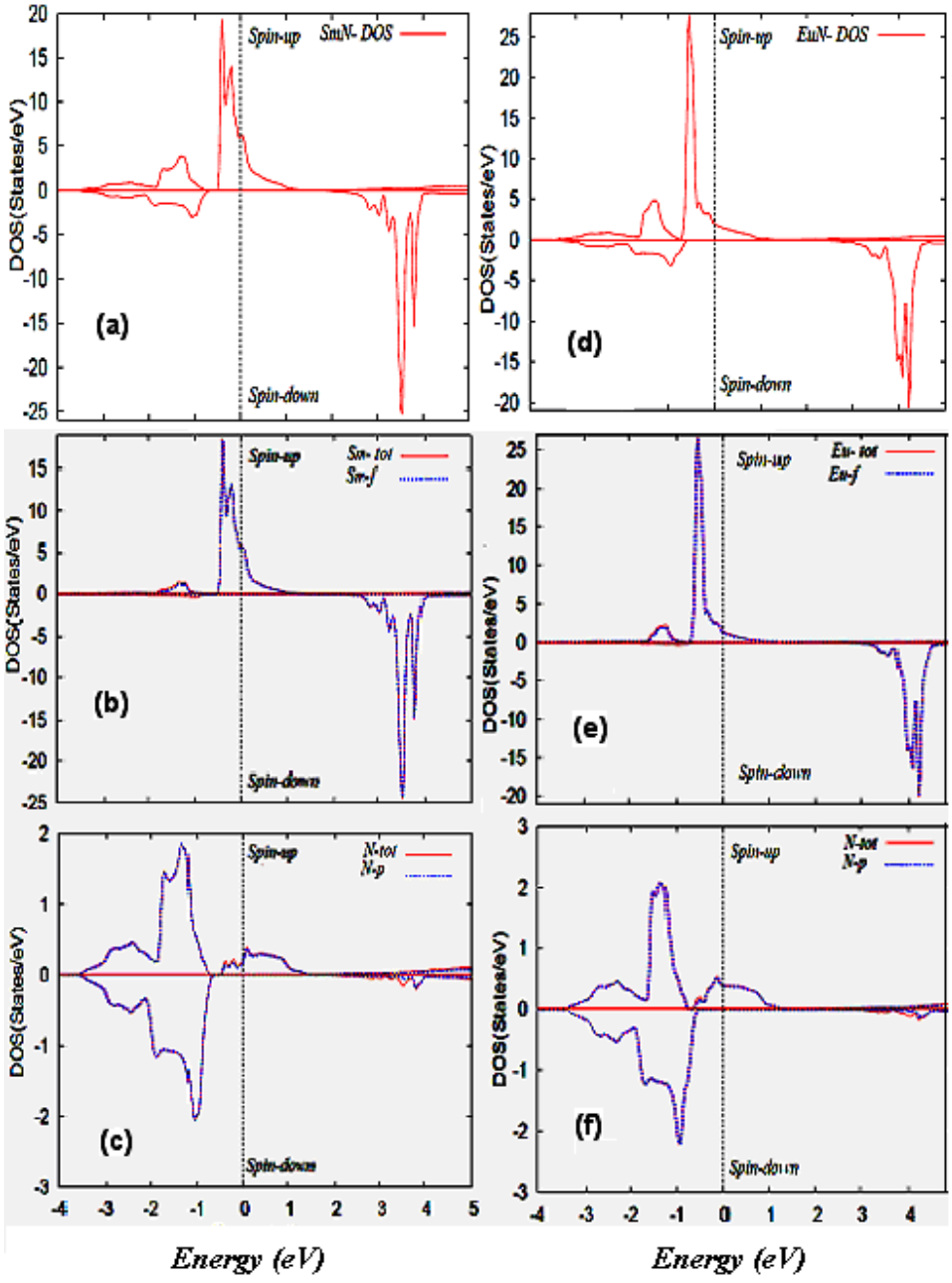

Figure 4.4: Total and partial DOS plots for SmN and EuN. (E_F=0 eV corresponds to the Fermi level)

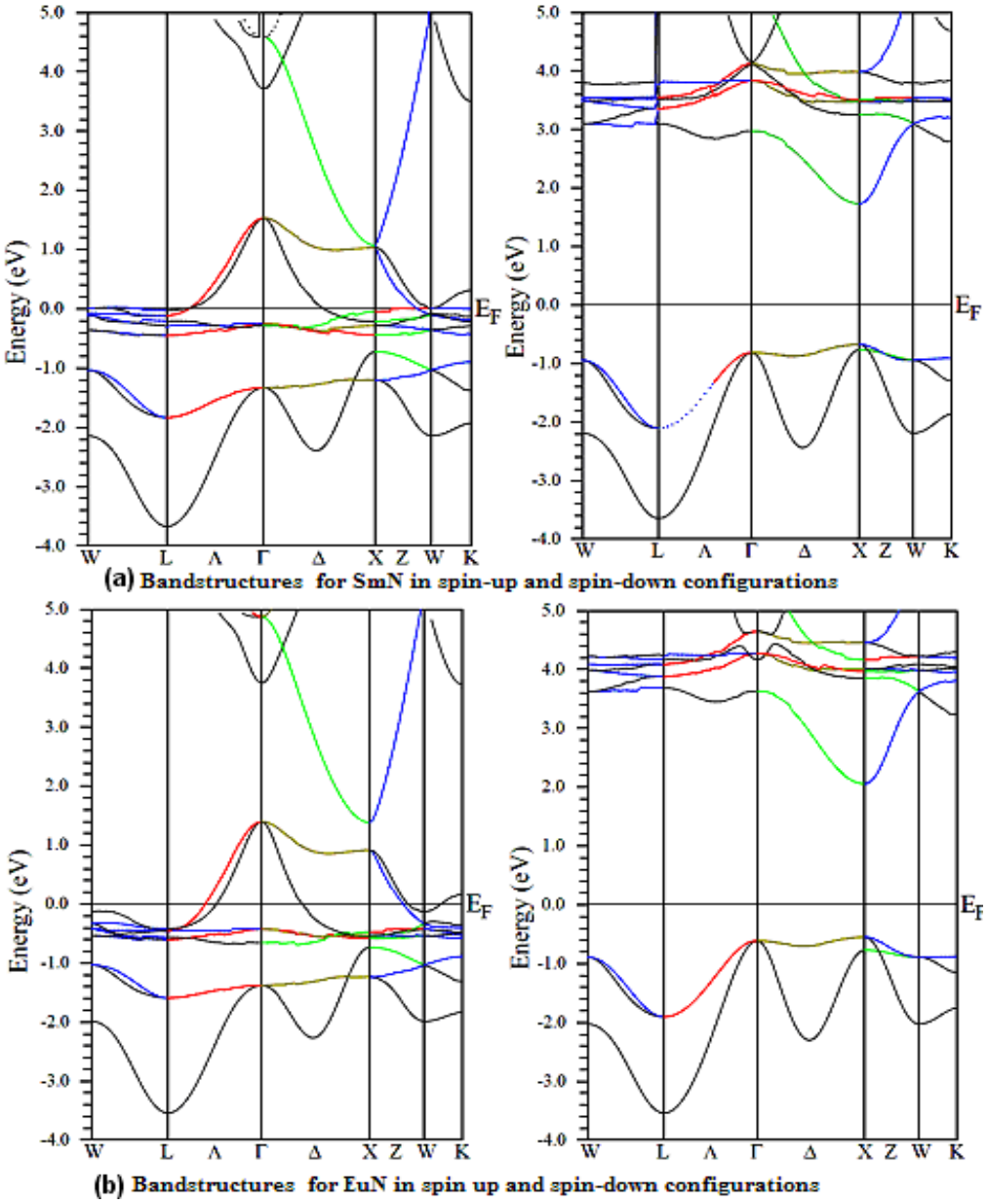

Figure. 4.5: Energy band structures plots of SmN and EuN in spin-up and spin-down configurations. (E_F=0 eV corresponds to the Fermi level)

The peaks due to N-2*p* states at E_F in the spin up channel and around was found to hybridized with 4*f* states of Eu. The DOS plot for Eu-4*f* states in Fig. 4.4 (e) shows an exchange splitting of the order of 4.0 eV in the spin up and down channels. The electronic band structures are shown in Fig. 4.5 for spin-up and spin-down configuration for both SmN and EuN. For SmN, in the spin-up configuration, a typical conducting behaviour is noted where as in the spin-down cofiguration an insulting nature is observed, which clearly suggests the possible half-metallic (HM) nature for SmN (Aerts *et al.*, 2004; Sandeep *et al.*, 2011c; Ghimire *et al.*, 2010b). Further, the DOS informations are also well supplemented by the band structures in both spin-up and spin-down configuration. A band gap of 2.4 eV is observed in the spin down configuration [Fig 4.5 (a-b)]. A weak hybridization between p-states of N with fully occupied *f*-states of Sm is found to occur in the valence region. In the band structure for SmN, it is clear from the figure that the majority spin crosses the Fermi level E_F, whereas the band structures of minority spin have an energy gap of 2.4 eV [Fig 4.5(a)]. As can be seen from the figure, the energy bands near and below E_F up to -4.0 eV are due to the mixing of *d* states of Sm with *p* states of N showing its metallic nature, while the gap between *p* state N and *d* state of Sm like states showing its semi-conducting nature and overall resulting them as half-metallic. Similar analysis is done for EuN where we observe an energy gap of 2.6 eV in the spin down channel and therefore the system is half-metallic [Fig 4.5 b]. Our results on electronic properties of SmN and EuN (Sandeep *et al.*,2011c) are in agreement with the results provided by Aerts *et al.*, (2004).

4.3 Half Metallic semi-Heuslers alloy: NiTbSb

The inter-metallic compound NiTbSb crystallizes in a cubic structure of MgAgAs type with the *f.c.c.* structure. The space group is *F43m*. The Tb and Sb atoms are located at (0,0,0) and (1/2, 1/2, 1/2) forming rock-salt structure arrangement. The Ni atom is located in the octahedral co-ordinated pocket, at one of the cube center positions (1/4, 1/4, 1/4) leaving the other (3/4, 3/4, 3/4) empty Nanda *et al.*, (2003). The optimization of the experimental lattice parameters were performed to determine the optimized lattice parameters which corresponds to the minimum total energy. Integrations in reciprocal space were performed using 10000 *k*-points in the first Brillouin zone (BZ) which corresponds to 504 spatial *k*-points in the irreducible wedge of the BZ. The value for the convergence parameters are taken to be R_{MT} x K_{MAX} = 7, which controls the size of the basis sets consisting of the plane waves. G_{MAX} is chosen to be 12 $(a.u.)^{-1}$ for consistency. Other parameters are chosen as follows: R_{MT} (Ni) = 2.5 a.u, R_{MT} (Tb) = 2.5 a.u, R_{MT} (Sb) = 2.41 a.u. Convergence is achieved with energy tolerance of 10^{-3} Ry.

4.3.1 Results and discussions

For NiTbSb, volume optimization was done (Sandeep *et al.*, 2011d) based on the Murnaghan equation of state (Murnaghan, 1944) using the experimental lattice constants (Kandpal, 2006). The theoretical value of the lattice parameter was calculated using the optimized volume. The optimized value of the lattice constant was used for the DOS, band structures and magnetic moment calculations to predict the electronic and magnetic properties of NiTbSb. The optimized lattice constant of NiTbSb was found 0.8% larger than the experimental lattice parameters (Kandpal, 2006). Fig. 4.6 (a-d) shows the total

and partial DOS plots of NiTbSb in both spin-up and spin-down configurations. Peaks were found below the Fermi level at -9.2 eV, -4.5 eV, -3.2 eV, -1.8 eV and -0.8 eV in spin-up configuration with a negligible DOS in the conduction region [Fig. 4.6 (a)]. The peak at -9.2 eV is found to be due to Sb-5*s* and Ni-3*d* states [Fig. 4.6 (b)] while the peaks at -4.5 eV and -3.2 eV are due mostly to Tb-4*f* [Fig. 4.6 (d)] with few Sb-5*p* and Ni-4*d* (t_{2g}) states [Fig. 4.6 (b-c)]. The peak at -1.8 eV is due to the Tb-5*p* and Tb-6*s* state electrons (not shown). The peaks at -0.8 eV are due to Sb-5*p* and Ni-4*d* state electrons [Fig. 4.6 (b-c)].

In spin-down configuration, sharp peaks are observed at -9.1 eV, -2.9 eV, -1.8 eV, -0.3 eV and 0.0 eV below and at E_F [Fig. 4.6 (a)]. Above E_F, peaks are found at +0.5 eV and +3.4 eV in the conduction region. The peak at -9.1 eV is due to Sb-5*s* states while the peaks at -2.9 eV and -0.3 eV are due to Sb-5*p* and Ni-3*d* electrons. The peaks at -4.5 eV and -3.2 eV in the spin-up case and -0.3 eV, 0.0 eV and 0.8 eV in spin-down case are found to be contributed by the 4*f*-state of Tb atoms. We observe that Ni mainly contributes in the valence band and Tb contributes in the semi-core near and above the Fermi level. The DOS plot of Sb shows that 5*s* states contributes in the core region while 5*p*-states contributes in the semi-core, valence and the conduction region. Hybridization between Ni-3*d*, Tb-4*f* and Sb-5*p* states are found in the semi-core and the valence region below the Fermi level in both spin-up and spin-down configurations. We have observed that in spin-up configurations, there is a band gap of 0.2 eV between the maximum of the valence band and the minimum of the conduction band [Fig. 4.6 (a)]. The minimum of

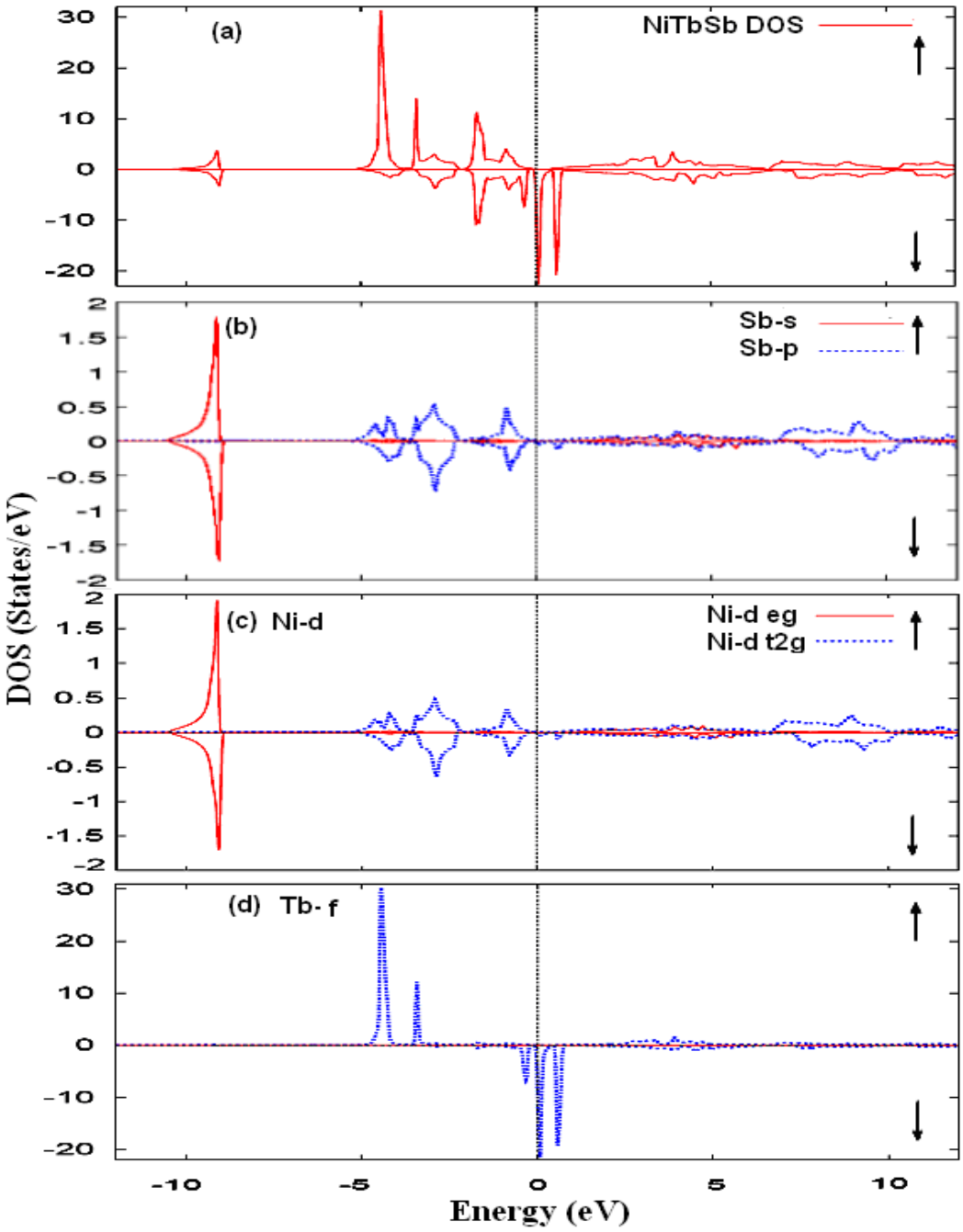

Figure 4.6 (a-d): The spin-dependent total DOS of NiTbSb and partial DOS of Sb-5*s*,5*p* states, Ni-3*d* states and Tb-4*d* states. (E_F=0 eV corresponds to the Fermi level)

the conduction band lies at the Fermi level. In spin-down channel, a sharp peak due to Tb-4*f* state electrons is observed at the Fermi level. The intersection of the total DOS at the Fermi level suggests the metallic nature of NiTbSb in the spin-down channel. Therefore, NiTbSb is predicted to be HMF with a band gap of 0.2 eV in spin-up channel and metallic in spin-down channel. From the partial DOS of Ni, Ni-3*d* states are decomposed into e_g and t_{2g} states [Fig. 4.6 (c)]. It is found that the total *d* contributions in Ni is due to its e_g states in the core regions and due to t_{2g} states in the valence and conduction region. From the band structures plot of NiTbSb with its total DOS shown in Fig. 4.7, the bands are found more concentrated in the valence region when compared to the conduction region, in both the spin-up and spin-down channel. The single band in the core region at -9.2 eV is due to the 5*s* state electrons of Sb atoms in both spin channels. In the valence region, electronic bands are found to occur starting from -5.2 eV upto E_F in the spin-up channel. Bands concentrated at -4.5 eV and -3.2 eV are due to the 4*f* state electrons of Tb and 5*p* state electrons of Sb atom in the spin-up configuration. At -1.8 eV bands are seen to concentrate due to 3*d* state electrons of Ni atoms and 5*p* state electrons of Sb atom. Our observation on the spin up channel shows the energy gap (Γ-X) with a band gap of 0.2 eV (Fig. 4.7). Above and below this gap the 4*f* electrons of Tb atoms were found to contribute in the energy band plot. In the conduction region of the spin-up channel, small contributions were observed from 0.2 eV onwards due to the 5*s* and 5*p* state electrons of Sb along with 3*d*-state electrons of Tb atoms. There is a small shift of energy bands towards the higher energy in the spin-down configuration overlapping the

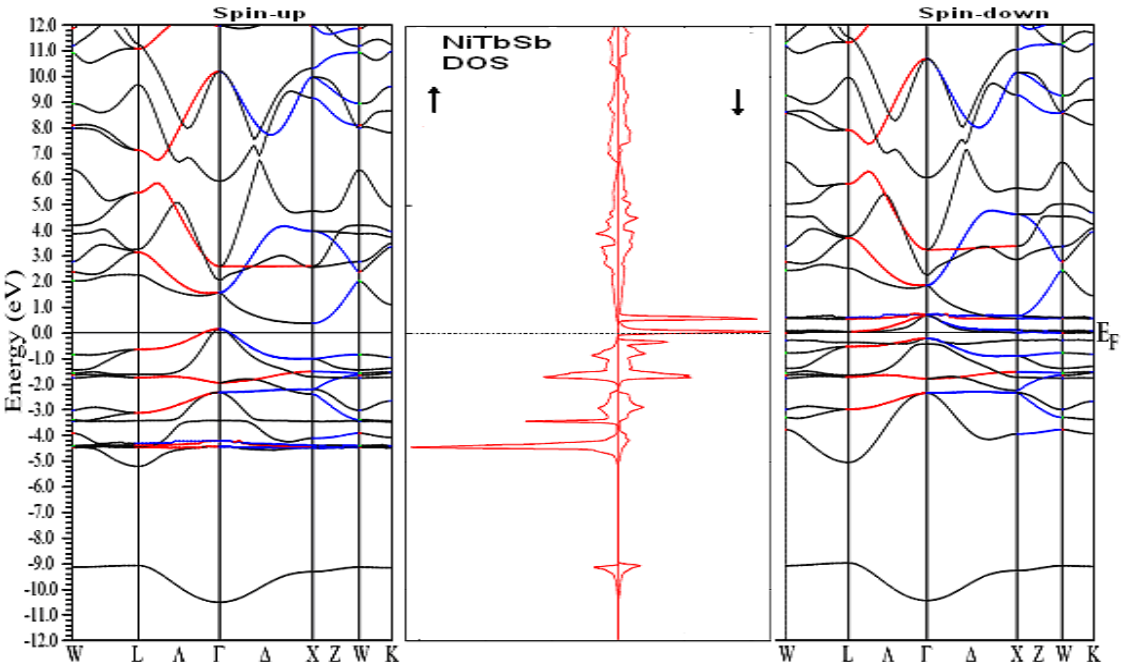

Figure 4.7: Band structures plot of NiTbSb in spin-up (left-panel) and spin-down (right-panel) channel with the total DOS (middle). (E_F=0 eV corresponds to the Fermi level)

Fermi region, when compared to the spin-up configuration. This behaviour of the energy bands makes it metallic in spin-down channel. In the valence region of the spin down channel, bands are less dispersive and concentrations are higher at -2.9 eV (two bands interacting), -1.8 eV and -0.8 eV along different symmetry directions. These are due to the contributions from 3*d*-state electrons of Ni and 5*p* state electrons of Sb. The 4*f* state electrons of Tb were seen to contribute at -0.3 eV in the spin down channel. In the spin down cannel of the conduction region bands are seen mostly just above the Fermi level between 0.1 eV and 1.0 eV due to the 4*f* state electrons of Tb atoms (Kandpal, 2006). The less dispersive bands above the Fermi level in the spin-down regions were due to the contributions from 3*d* state electrons of Tb along with 5*s* and 5*p* state electrons of Sb atoms.

The total magnetic moment is just the difference between the number of spin-up occupied states and the spin-down occupied states. In the HM compounds all states of the spin-down valence band are occupied and thus their total number is an integer and the total magnetic moment is also an integer (Dederichs *et al.*, 2005). The moments of NiTbSb were compared (Table 4.3) with earlier results and were found to support the HMF nature of NiTbSb (Kandpal, 2006). We find that the moments due to individual transition Ni -3*d* and rare-earth (Tb-4*f*) ions are contributing to the total moments of the systems. In Table 4.3, we have summarized the total and species decomposed spin moments of NiTbSb. The magnetic moments of NiTbSb agrees well with the FPLMTO results of Kandpal (2006). From the partial DOS of Ni, Ni-3*d* states are decomposed into

Table 4.3 : Calculated total and individual moments in HMF NiTbSb

Semi Heusler's Alloy	Magnetic moment of Ni		Magnetic moment of Rare Earth (Tb)		Total Magnetic moment	
	Present (μ_B)	Previous (μ_B)	Present (μ_B)	Previous (μ_B)	Present (μ_B)	Previous (μ_B)
NiTbSb	0.063	-	5.813	-	5.983	5.97*

* Kandpal (2006)

e_g and t_{2g} states. It is found that a negligible exchange splitting occurs between e_g up and e_g down states in the core regions and between t_{2g} up and t_{2g} down in the valence and conduction region. Due to this, the resultant moments of Ni are negligible. The moments of NiTbSb is therefore found to be due to the Tb atoms. This is due the exchange splitting between the 4*f* states in both spin-up and spin-down channel which is evident from the DOS of Tb-4*f* states (Fig. 4.6 d). The exchange energy splitting for Tb-4*f* electrons in up and down spin is calculated out to be 5.2 eV. The total magnetic moments of the systems are slightly less than the sum of the moment of individual atoms. It is because, while calculating the electronic and magnetic properties of these compounds, we use the muffin-tin spheres where some of the area is excluded.

CHAPTER- 5

CONCLUSION

Chapter - 5

Conclusions

This thesis is concerned with the study of electronic band structures calculations by using FP-LAPW method. We have calculated the density of states, energy bands and magnetic moments for various systems like Rare earth elements (La, Ce, Pr, Nd, Gd and Lu), Rare earth hexaborides (LaB_6, CeB_6, PrB_6, NdB_6 and SmB_6), Half metallic Rare earth nitrides (SmN and EuN). Rare earth antimonides ($LaCrSb_3$, $CeCrSb_3$, $NdCrSb_3$) and semi Heusler alloy NiTbSb. DOS and band structures result of La and Ce showed metallic behaviour and paramagnetic in nature. In both these elements, the DOS contributions were mainly due to the rare earth-4*f* states in their hexagonal phase. These results were compared with the experimentally obtained XPS and BIS spectra of Lang *et al.* (1981). We have found similar behaviour of DOS and band structures in the case of Pr, Nd and Gd showing that main contributions were from 4*f* state electrons. These results were also in qualitative agreement with the experimentally obtained XPS spectra of Heden *et al.* (1971) and Lang *et al.* (1981) as shown in Fig 3.7. Ferromagnetic ground states for these systems were reported in our results in their hexagonal phase. The magnetic natures of the rare earth elements are due to the 4*f*- unpaired electrons. The atomic picture of 4*f*-electrons which are well localized holds in metals. The fact that some of the bands cross the Fermi level demonstrates that RE= La, Ce, Pr, Nd, Gd and Lu are metals. We have found that LDA+U do not produce significant change in the energy positions of 4*f* states when compared to Shick *et al.* (2000). A ferromagnetic ground states were found for Pr, Nd and Gd through their electronic structure and high magnetic moment value (Kittel, 1996). The La and Lu were found to be

paramagnetic in their ground state. The exchange splittings of spin-up and spin-down and the magnetic moments were found to increase for metals in the series from La to Gd.

The rare earth hexaborides have also been studied with theoretically optimized lattice parameters in which the rare earth 4*f* states were found to be the main contributors in their DOS. Hybridization between the 5*p* states of B atoms with 5*d* states of rare earths were also seen. The present calculations have shown qualitative agreement with the results obtained by Singh *et al.* (2001), Gupta *et al.* (2010), Leger *et al.* (1985) and Bisiani *et al.* (1997). The lattice parameters determined were found with an increment of 0.48%, 0.07%, 0.73%, 0.70% and 0.90% for LaB_6, CeB_6, PrB_6 and NdB_6 and SmB_6 respectively with those of the experimental values. Gupta *et al* (2010) calculated the lattice parameters using GGA as well as LDA approximations. The results obtained in the case of GGA approximation were found closer to the present determination of lattice parameters using LSDA+U approximation. This also points the lack of exchange correlation effect in LDA results.

We have studied the electronic and magnetic properties of $LaCrSb_3$ and $CeCrSb_3$ by using the FP-LAPW method. The ground state of $LaCrSb_3$ and $CeCrSb_3$ shows the ferromagnetic behaviour for the systems due to the exchange splitting between different states of Cr-3*d* and rare-earth 4*f* ions. The exchange splittings of Cr-3*d* state (Raju *et al.*, 1998) in spin up and spin down were explained on the basis of DOS plots. The energy difference between these states showed the variation of magnetic moments in these systems. The Cr moment of these systems were found to be greater than the rare-earth moments. The Cr atom plays a significant role on the magnetic properties of these compounds due to the hybridization between 3*d* states of Cr and 5*p* states of Sb atoms (Choi *et al.*, 2007). The magnetic moments obtained are compared with the experimental results (Hartjes *et al.*,

1997; Choi *et al.,* 2007; Inamdar *et al.,* 2008; Jackson *et al.,* 2001, 2007) and were found to be in qualitative agreement for the total moments of $LaCrSb_3$ and $CeCrSb_3$. The difference on the individual moments for the Ce atoms were observed which can be attributed to the default value of U chosen in our calculation (Wu *et al.,* 2005). The present calculation enables us to conclude that rare earth 4*f* electrons are the major contributor towards the total DOS and the band structures of $NdCrSb_3$ in the spin up configuration at and around E_F. Nd-4*f* states were also found to contribute in the conduction region of the spin down configuration. This supports the bulk ferromagnetic ordering of the spins as suggested experimentally (Inamdar *et al.,* 2008). The 3*d*- state electrons of Cr were also found to contribute significantly in the spin up valence and spin down conduction region to support the ferromagnetic behavior of the system as also confirmed by the magnetic moment (Inamdar *et al.,* 2008). The effective magnetic moment was found to be in qualitative agreement with about 11 % higher than the experimental value. This increase (Wu *et al.,* 2005) in the value of the moment may be due to the default value of U chosen in our calculations.

Rare earth nitrides were studied using theoretically optimized lattice parameters. From the DOS and the band structures plots we observe that there is a small variation of the energy bands and DOS for SmN and EuN. Our observation showed (Sandeep *et al.,* 2011c) that SmN and EuN are showing half metallic behaviours with a minority band gap of 2.4 eV and 2.6 eV respectively. This is consequence of the 2*p* states of nitrogen and 4*f* states of RE occurring in the same energy window, in the vicinity of the Fermi level. This leads to strong hybridization of these states at E_F. With the high magnetic moments and the high DOS in one spin channel these material exhibit, these system finds a continuous range of useful properties particularly with applications in spintronics and spin filtering devices.

Conclusion

We have calculated the optimized value of the lattice constants for HMF NiTbSb using the volume optimization method. The obtained lattice constants were used for the calculations of DOS, band structure and magnetic moments of NiTbSb in zinc-blende structure. From the DOS and band structure results, it is found that NiTbSb has HMF nature which was also reported by Kandpal (2006). The DOS of NiTbSb under study are mainly characterized by the large exchange splitting of the 4*f* states of Tb. This splitting leads to larger localized spin moments at the Tb sites. We also see from the partial DOS [Fig. 4.6 (d)] the exchange splittings of Tb-4*f* states which infact results in the spin-up semiconducting nature of NiTbSb. According to DOS and band-structure calculations, the ferromagnetism is of highly spin-polarized type for NiTbSb [Fig. 4.6]. The value of magnetic moment is 5.983 μ_B and is close to an integral value which is an indication of half-metallicity. The calculated magnitude of the energy gaps in the spin-up configuration for NiTbSb is 0.2 eV along (Γ-X) symmetry directions suggesting the system to be HMF's. Our result when compared with limited earlier results (Kandpal, 2006) is found to be in qualitative agreement for magnetic-moments of NiTbSb. A co-existing semi-metallic state for NiTbSb system was also supported by the results of Ishida *et al.* (1997).

Drawbacks involved in our calculational procedures are like we have used default value of Coulomb potential U in certain cases. It is advised that U be calculated efficienly by the methods given by Madsen and Novak (2007). Volume optimizations were not performed for certain systems which is advisable otherwise.

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RESEARCH PUBLICATIONS

LISTS OF RESEARCH PUBLICATIONS

(I) Journals:

(a) International:

(1) Study of the electronic properties of CrO_2 using density functional theory, M. P. Ghimire, Sandeep and R. K. Thapa, *Mod. Phys. Letts.* **B 24**, 2187-2193 (2010).

(2) Magnetic and Electronic Structure Calculations of Rare-Earth Nitrides, **Sandeep**, M. P. Ghimire and R. K. Thapa, *Jour. Mat. Sci. Engg.* USA. (accepted).

(3) Electronic and magnetic properties of $NdCrSb_3$: A first principles study, **Sandeep**, M. P. Ghimire and R. K. Thapa, *Physica B,* **406**, 1862-1864 (2011).

(b) National:

(1) DOS and Band structures calculations of Transition metals (W and Nb) using FP-LAPW method, R.K.Thapa, M. P. Ghimire, Rosangliana, **Sandeep** and Lalmuanpuia, *Sci. Vis.* **10** 88 (2010).

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(3) Study of Co_2MnAl Heusler alloy as half-metallic ferromagnet, R. K. Thapa, Javad Hashemifar, Morteeza Jamal, D. T. Khathing, P. K. Patra, Indrajit Sharma, Rosangliana, Lalmuanpuia, M. P. Ghimire, **Sandeep** and Dibya Prakash Rai., *Indian Jour. Phys.* **84** (6) 717-721 (2010).

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(6) A study of rare earth elements with emphasis on magnetic and electronic properties, **Sandeep**, M. P. Ghimire and R. K. Thapa, *Int. J. Mat. Phys***. 1, 7**-12 (2010).

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(8) Study of DOS and energy band structures in beryllium chalcogenides, R. K. Thapa, **Sandeep**, M. P. Ghimire and Lalmuanpuia, *Indian Jour. Phys*. **85:** 401-409 (2011).

(9) Study of energy bands and magnetic properties of Co_2CrSi Heusler alloy, Dibya Prakash Rai, M. P. Ghimire, **Sandeep** and R. K. Thapa, *Bull. of Mat. Sc.* India (accepted) 2011.

(10) Magnetic and Electronic properties of Half-metallic NiTbSb: A first principles study, **Sandeep**, M. P. Ghimire, D. P. Rai and R. K. Thapa, *Indian Jour. Phys*. (accepted) 2011.

(II) Conferences:

(a) International:

(1) Magnetic and electronic properties of $CeCrSb_3$, Sandeep, M. P. Ghimire and R. K. Thapa, *International Conference on Physics of Emerging Functional Materials (PEFM-2010)* during September 22-24, 2010, BARC Training School, Mumbai.

(b) National:

(1) Study of Co_2MnAl Heusler alloy as half-metallic ferromagnet, R. K. Thapa, Javad Hashemifar, Morteeza Jamal, D. T. Khathing, P. K. Patra, Indrajit Sharma, Rosangliana, Lalmuanpuia, M. P. Ghimire, Sandeep and Dibya Prakash Rai. *Proceedings of the VI National Conference of PANE*, Tripura University, 2-4 April, 2009.

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(20) Prediction of half-metallic properties in a ferromagnetic Heusler alloy: Co_2CrGa, R. K. Thapa, Dibya Prakash Rai, Amit Shankar, Sandeep and M. P. Ghimire, Conference on theoretical Condensed Matter Physics-2011, Assam University, 3-5th Feb. 2011.

(21) Study of optical properties of beryllium chalcogenides, Lalmuanpuia, Rosangliana Sandeep, M. P. Ghimire and R. K. Thapa, Conference on theoretical Condensed Matter Physics-2011, Assam University, 3-5th Feb. 2011.

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(III) Workshops/ Training Programmes attended:

(1) State Level Workshop on FORTRAN programming, Organized by Department of Physics, Mizoram University, 22^{nd}-24^{th} November 2010.

(2) National workshop on computational physics, Organized by Mizoram University and University of Hyderabad, 14-19^{th} February 2011.

(3) One day State Level Seminar cum Training Programme on Recent Advances in Radiation Physics Department of Physics, Organized by Mizoram University, 15^{th} April 2011.

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- Pre-Ph. D. Course 2010 Grade 'A^+'

Research Experience:

- Completed M. Sc. Project work (on Remote sensing and application) entitled "MODIS products and its study for atmospheric applications" at IIRS, Dehradun, 2005.
- Started research works in Condensed Matter Theory Research group under the guidance of Dr. R. K. Thapa, Department of Physics, Mizoram University, Aizawl, Mizoram since June 2007.
- Calculations of Band structures, magnetic and optical properties.
- Used WIEN-2k code for DOS and band structures calculations.
- Working knowledge of operating systems DOS/WINDOS XP and LINUX: CENTOS 5.0, FORTRAN.

Teaching experience:

- Lecturer in Physics at St. Pauls Higher Secondary School, Aizawl, under the Directorate of School Education, Govt. of Mizoram from 2006 to 2008.
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