Electronic And Magnetic Properties Of $NdVSb_3$: A First Principles Study

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Abstract. The electronic density of states (DOS) and magnetic moments of rare-earth antimonides ($NdVSb_3$) has been studied by the first principles full-potential linearized augmented plane wave (FP-LAPW) method based on density functional theory (DFT). For the exchange–correlation potential, the GGA+U method is used. The effective moments of $NdVSb_3$ was found to be 4.50 μ_B. The exchange-splittings of V-3*d* state electrons and 4*f*-states of Nd atoms were analyzed to explain the magnetic nature of these systems. The V atom plays a significant role on the magnetic properties due to the hybridization between V-3*d* and Sb-5*p* state orbitals. The results obtained are compared and found to be in qualitative agreement with the available results.

Keywords: Rare-earth antimonides; DFT; DOS; Magnetic moment.
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INTRODUCTION

The magnetic exchange mechanisms and spin-correlations mediated by itinerant electrons have attracted renewed interest in the last few years in the emerging field of spin electronics [1]. Due to the anisotropy in structure, and display of complex magnetic interaction $RVSb_3$ is a material of interest which has major technological applications in spin electronics, Read Head, magnetic RAM, nano-systems etc [2-3]. We calculate the DOS and magnetic moments of $NdVSb_3$ using first principles density functional theory using FP-LAPW method.

COMPUATIONAL DETAIL

We have performed our calculations using the experimentally determined lattice parameters and the atomic positions [4] for $NdVSb_3$. For rare earth elements, the 4*f*-electron correlations are expected to be strong. Consequently, the GGA+U calculations have been chosen to include the on-site Coulomb interaction. The onsite Coulomb energy (U) applied is 0.51 Rydberg (Ry.) for the Nd and 0.15 Rydberg (Ry.) for V respectively [5]. We have used 47 *k* points in the irreducible Brillouin zone, and the muffin-tin radii are 2.5 2.5, 2.27, 2.27 and 2.27 for Nd, V, Sb_1, Sb_2, Sb_3 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 muffin-tin radii. The self-consistency is better than 0.001 e/a.u.^{3} for charge density and spin density and the stability is better than 0.01 mRy. for total energy per cell. For computations of DOS and magnetic moments, WIEN2k code [6] is used.

RESULTS AND DISCUSSIONS

The total DOS for $NdVSb_3$ is shown in Fig. 1 The regions are contributed by the Sb-5*s* and Sb-5*p* state electrons in both spin channels. In the valence regions DOS contributions were observed due to V-3*d* state electrons in spin-up channel. Sharp peak due to V-3*d* state electrons were observed at 1.5 eV in the spin-up channel [Fig 1(c)]. At Fermi level contribution of Nd-4*f* state electrons were highest in the spin-up channel. The splitting of the DOS in the spin-up and spin-down

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channels were found to occur for both V-3*d* and Nd-4*f* states which contribute to the magnetic nature of the compounds and were supported by the individual magnetic moments calculated [Table 1]. The magnetic moment calculated showed that the Nd-4*f* state is the main contributor towards the total magnetic moment of the system with moment equal to 3.37 μ_B which is in qualitative agreement previous calculated moment [7] of Nd in $NdVSb_3$. In addition we have presented the individual contributions of moments from V atom and Sb atoms. We have observed that the individual magnetic moment of V atom in $NdVSb_3$ is higher by 28 % when compared to the experimental moment calculated by Hartjes *et al.* [7]. Thus the total moment of the system was found to be higher by 21% in the present study. The lower magnetic moment could be explained on the basis of hybridization between the states of Sb-5*p* and V-3*d* which leads to a less prominent splitting of the 3*d* states giving rise to lower magnetic moment for V atoms.

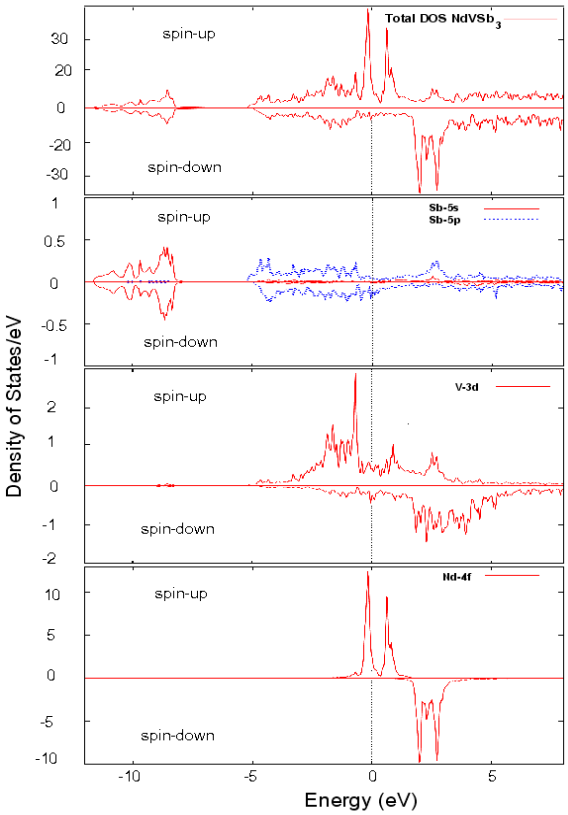

FIGURE 1. Total and partial DOS plots of $NdVSb_3$ in spin-up and spin-down configurations.

TABLE 1. Total and partial magnetic moments of $NdVSb_3$

	Nd	V	Sb1	Sb2	Sb3	Total
Our Results	3.37	2.14	-0.06	-0.10	-0.03	4.50
Previous results	3.27[7] 3.62[7]	1.53[7]				3.54[7]

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