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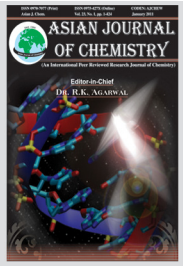

Search of Half Metallicity in VX (X = As, Sb and Bi) Compounds for Spintronic Applications†

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We present electronic and magnetic properties of VX (X = As, Sb and Bi) compounds in zinc blende structure by full potential linear augmented plane wave method using generalized gradient approximation as exchange correlation potential. Our calculations show that these compounds show robust half metallicity with the considerably half metallic gaps in minority spin channel and 100 % spin polarization at Fermi level EF. The total spin magnetic moment for both compounds is found to be 2.0 μB *i.e.* an integer value, which is in accordance with Slater-Pauling rule for governing half metallic compounds.

Key Words: HMF, Density functional theory, Full potential linear augmented plane wave method.

INTRODUCTION

A new spin based electronics or spintronics, which combines magnetic and semiconducting properties within same material has received a considerable attention during the past decades. This new class offers unique opportunities due to spin-dependent effects. Half metallic compound presents metallic behaviour for one spin channel and semiconducting for the second. Therefore, this compound shows 100 % spin polarization at E_F and thus, can be used as spin injectors for magnetic random access memories and other spin-dependent devices.

First of all, Groot *et al.*[1], discovered the half metallicity in NiMnSb, after that many half metallic ferromagnets have been theoretically predicted and some of them have been synthesized in zinc-blende (ZB) phase such as CrAs[2], CrSb[3], MnAs[4] and transition metal doped InAs[5], GaAs[6], BeTe[7], ZnTe[8] and ZnO[9,10] *etc*. The possibility to grow binary CrAs and CrSb compounds in zinc-blende structure epitaxially on GaAs and GaSb substrates[2,3] has motivated us to explore the signature of half matallicty present in similar type of hypothetical compounds such as VX (X = As, Sb and Bi). Here, we are also interested to observe the dependence of half metallic band gap on size of X-atom. Moreover, the simpler structure of these compounds over other spintronic materials, clearly show the importance of this study.

THEORETICAL APPROACH

The space group of the ternary VX in zinc-blende structure is $F\bar{4}3m$. In VX compounds, the V atom is located at (0, 0, 0) whereas X atom is at (½,½, ½). We have employed full potential linear augmented plane wave method based on density functional theory (DFT) for the calculation of electronic and magnetic properties of present compounds. The exchange and correlation (XC) effects were taken in to account within generalized gradient approximation (GGA) formalism in which the parameterization of Perdew-Burke-Ernzerhof (PBE) has been employed to construct the XC potential[11]. The plane wave cut off parameters were decided by $R_{MT}k_{max} = 7$ (where k_{max} is the largest wave vector of the basis set) and $G_{max} = 12$ a.u.$^{-1}$ for fourier expansion of potential in the interstitial region. The **k**-space integration has been carried out using the modified tetrahedron method[12] with 405 **k**-points in the irreducible brillouin zone (IBZ) to obtain self consistency.

RESULTS AND DISCUSSION

In order to have accuracy in results within full potential linear augmented plane wave method, we have optimized the equilibrium lattice parameters of these hypothetical compounds for ferromagnetic configuration in the neighborhood of lattice parameters as calculated by Miao *et al.*[13] and Zhang *et al.*[14]. The optimization curve is presented in Fig. 1 for one of these compounds, VBi. Here, the optimized lattice parameters are defined by the total energy minimum (marked by a vertical arrow) in the optimization plot and the equilibrium values of lattice parameters are listed in Table-1. The calculated total density of states (DOS), shown in Fig. 2, for present compounds are quit similar in nature. The band gap appears in the minority density of states and shows 100 % spin polar-

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ization at E_F for each compound. The density of states for minority spin states shift to higher energies with increase in size of X-atom such that the minority band gap decreases.

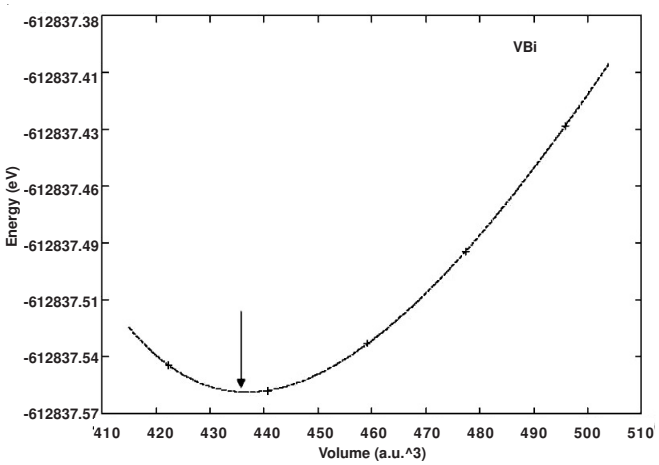

Fig. 1. Optimize lattice parameter for VBi

TABLE-1
OPTIMIZED LATTICE PARAMETERS a(Å), CALCULATED BAND GAP IN MINORITY SPIN E_g (eV), TOTAL AND ATOM RESOLVED SPIN MAGNETIC MOMENTS (μ_B) of VX (X = As, Sb AND Bi) WITHIN GENERALIZED GRADIENT APPROXIMATION

VX	a(Å)	E_g(eV)	M_V (μ_B)	M_X (μ_B)	m_{tot} (μ_B)
VAs	5.70	1.71	1.96	-0.145	2.00
Other (a)	5.60	2.44	-	-	2.00
VSb	6.12	1.47	2.00	-0.156	2.00
Other (a)	6.00	2.19	-	-	2.00
VBi	6.37	1.42	2.10	-0.160	2.00
Other (b)	6.48	1.32	-	-	2.00

(a) Ref. 13, (b) Ref. 14

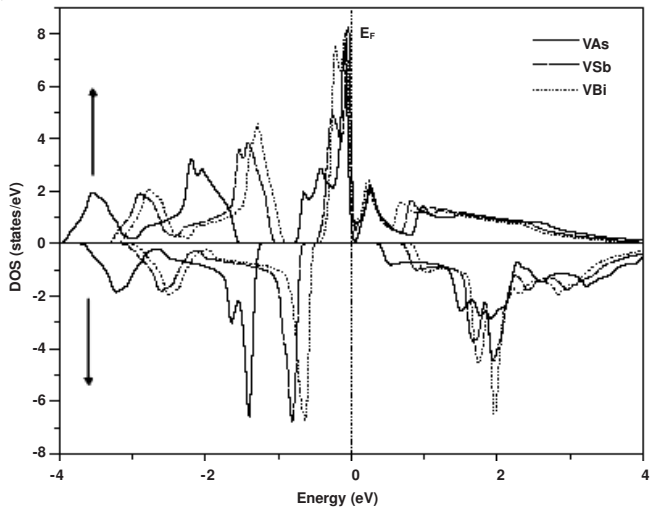

Fig. 2. Calculated total density of states for VX (X = As, Sb and Bi)

The partial density of states analysis for sample compound, VBi depicted in Fig. 3 reveals that the total density of states has main contribution in the vicinity of E_F from V-d states only. These states break in two parts, e_g and t_{2g} states due to crystal field splitting. Bi-*s* and Bi-*p* states are distributed below E_F only. The tetrahedral environment allows V-t_{2g} states to hybridize with Bi-*p* states. This symmetry induces large bonding and antibonding splitting. The position of gap in two split bands is found to be different for both spins such that only for minority spin, E_F falls in the gap. The low lying bonding states have Bi-*p* character where as the antibonding states has V-*d* character mainly. The magnetism comes essentially from V-*d* states, while the half metallic character is due to the Bi-*p* and V-*d* interaction.

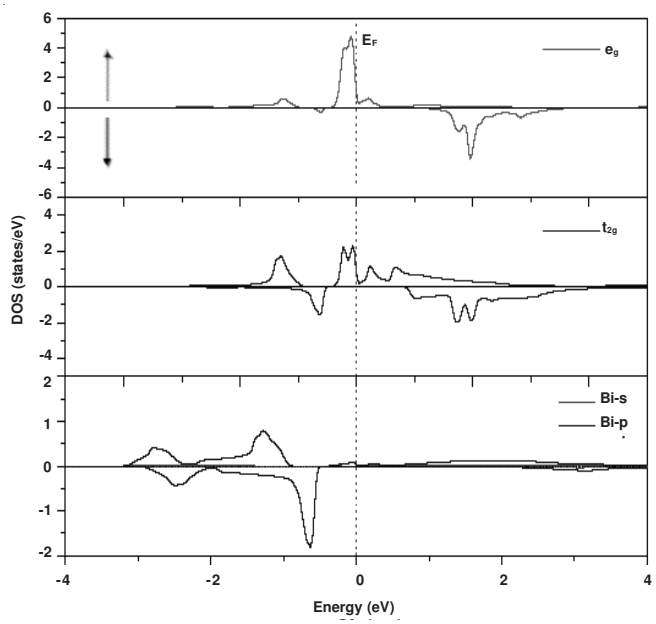

Fig. 3. Spin-polarized density of states for VBi

The total atom resolved spin magnetic moment calculated at optimized lattice parameters for present binary compounds also summarize in Table-1. The corresponding theoretical data from previous calculations[13,14] is also listed for comparison. The large exchange splitting of V atoms leads to the localized spin magnetic moment at V site. The local magnetic moments of VX atoms are (- 2.00 μB), indicating similar electronic environments. The *sp*-atom shows a negligibly small spin moment which is antiparellel to the moment of the transition-metal atoms.

Fig. 4 showed the band structure of VBi, the *s*-states of Bi are located at very low in energy. The full-filled bands in both, majority and minority states at -2.4 eV are due to the bonding V-t_{2g} and Bi-*p* states, which reflects the *p-d* bonding. There is strong dominance of V-t_{2g} states for the majority spin whereas Bi-*p* states participate more actively for the minority spin. The next two bands comprise mainly of V-e_g states at -0.4 eV and 1.0 eV in the majority and minority spin channel, respectively. These bands reflect the nonbonding nature of V-e_g states and are narrow as compared toV-t_{2g} bands. The V-e_g and V-t_{2g} states can be used to measure the strength of important interactions in VX.

Conclusion

It is predicted that the hypothetical zinc-blende-type VX compounds are true half-metallic ferromagnets showing 100 % spin polarization at E_F, with a magnetic moment of 2.0 μ_B. The magnetism comes essentially from the *d* orbitals of V atom in each compound. The minority band gap observed in VX compounds is the fingerprint of the X-*p* and V-*d* interaction. The increase in size of *sp*-element reduces the size of

this gap. It is hoped that the present investigation of half metallic nature in these compounds will stimulate the research in this direction from experiment point of view also.

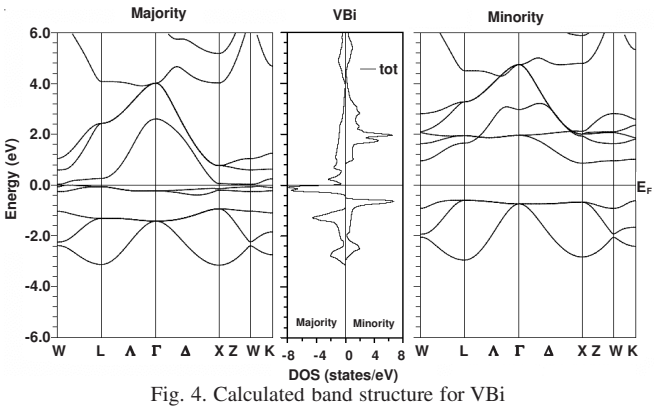

Fig. 4. Calculated band structure for VBi

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