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New Half Metal Perovskite $NbScO_3$ for Spintronic Sensing Applications

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Abstract: Half-metallic ferromagnetic (HMF) materials demonstrate 100% spin polarization at the Fermi level making them promising candidates for spintronic sensing applications. In this work, the full potential linearized augmented plane wave (FP-LAPW) density Functional Theory (DFT) method is used to calculate the electro-magnetic properties of the transition metal perovskite NbScO3 using the generalized gradient approximation (GGA) and the modified Becke-Johnson (mBJ) approximation for the exchange correlations. The electronic band structures for the two spin orientations using GGA, predicts NbScO3 to be a HMF with an integer magnetic moment of 2.0μB and thus a promising candidate for spintronics. The new half metal perovskite shows metallic behaviour in the majority spin and semiconducting in the minority spin channel with a direct Γ− Γ band gap of 1.870 eV. The integer magnetic moment of 2.0μB is also preserved with mBJ exchange potential. The band structure however shows indirect gaps R− Γ and X− Γ of 2.023 eV and 0.780 eV in the minority and majority channels respectively indicating NbScO3 to be a magnetic semiconductor. The results indicate the suitability of NbScO3 for spintronics as the necessary conditions are satisfied. .

Keywords: half metal; band structure; spintronics; sensors; information technology; perovskite

1. Introduction

The rapid technological advancements in the last decade call for a smart and sustainable lifestyle management with sensors playing a vital role [1-3]. Electron spin is fast becoming a very useful tool in sensing devices based on spintronics. Spintronics is the science where the electron spin instead of the charge is used as the information carrier giving us the advantages of low energy consumption, high speed data processing and circuit integration density [4, 5]. Among today's various proposed information transfer methodologies like molecular/nano electronics and quantum technologies, spintronics stands out due to the fact that it is compatible with conventional electronics making it easy to extend the existing well known electronic techniques to spintronic circuits. HMFs due to their exceptional electronic structure satisfy the needs for spintronic applications. The electrons of one spin direction behave like metals and those of the other spin direction act as semiconductors. Recently, quite a few new perovskites have been predicted to be half-metals [6-8].

Transition metals (TM) are especially interesting and a variety of intriguing magnetic properties have been obtained as seen from recent research results. Depending upon the local environment non-magnetic materials have become magnetic due to their presence [9-11]. TM perovskites have piqued the interest of the scientific community due the intriguing nature of the TM ion interplay with the oxide or halide ion [12, 13] with the great possibilities of different electronic and magnetic properties.

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Unlike the majority of pervious research where the TM occupies the B site, in this work we have switched the sites and TM Niobium occupies the A site with some very interesting magneto-electronic results. The aim of the paper is to present comprehensive and precise first principles characterization using DFT_FP-LAPW of the perovskite NbScO3. This has been done for the first time and the results show great potential for use in spintronics and sensing.

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becoming a very useful tool in sensing devices based on spintronics. Spintronics is the science where the electron spin instead of the charge is used as the information carrier giving us the advantages of low energy consumption, high speed data processing and circuit integration density [4, 5]. Among today's various proposed information transfer methodologies like molecular/nano electronics and quantum technologies, spintronics stands out due to the fact that it is compatible with conventional electronics making it easy to extend the existing well known electronic techniques to spintronic circuits.

HMF materials meet all the requirements of spintronics, as a result of their exceptional electronic structure. They behave like metals with respect to the electrons of one spin direction and like semiconductors/insulators with respect to the electrons of the other spin direction. Recently, quite a few new perovskites have been predicted to be half-metals [6-8].

Transition metals (TM) are of special interest and past research results show them to have a range of intriguing magnetic properties and they can even induce non-magnetic materials to become magnetic depending upon the local environment [9-11]. TM perovskites have piqued the interest of the scientific community due the complex nature of TM ion interactions with oxygen or halides [12, 13] and the wide range of possible electronic and magnetic properties.

Unlike the majority of pervious research on TM perovskites, where the TM occupies the B site, in this work we have switched the sites and TM Niobium occupies the A site with some very interesting magneto-electronic results. The purpose of the paper is to give the essential and accurate theoretical characterization using DFT_FP-LAPW of the perovskite $NbScO_3$ which is being investigated for the first time for possible spintronics and sensing applications.

2. Method and materials

The full-potential linearized-augmented plane wave (FP-LAPW) method as implemented in the WIEN2k [14] package is used to calculate the spin polarized ground states of the perovskite $NbScO_3$ within DFT [15]. The Perdew, Burke and Ernzerhof (PBE) [16] generalized gradient approximation (GGA) is used to calculate the optimized structures for a 10×10×10 grid. The optimized lattice constant value is used to evaluate the electronic and magnetic properties with the more accurate mBJ exchange correlation of Trans Blaha [17] at a denser grid of 15×15×15. K_{max} which gives the magnitude of the largest K vector in the plane-wave expansion is set to 8. The muffin-tin radii have been set to 1.60a.u for Sc and O atoms and 2.7a.u for Nb. The tetrahedron method [18] with 120 k points in the IBZ is employed for integrations within the self-consistency cycle (SCF). The convergence tolerance thresholds for SCF is less than 10^{-4} Ry for energy and 10^{-4} for electron charges.

3. Results and discussion

3.1. Structural and electronic

The cubic $NbScO_3$ perovskite has the space group Pm-3m (#221) symmetry and the atoms occupy the positions 1a (0, 0,0), 1b (½, ½,½) and 3c (0,½, ½) sites of Wyckoff coordinates for Nb, Sc and O atoms respectively, as depicted in Figure1 as an inset image.

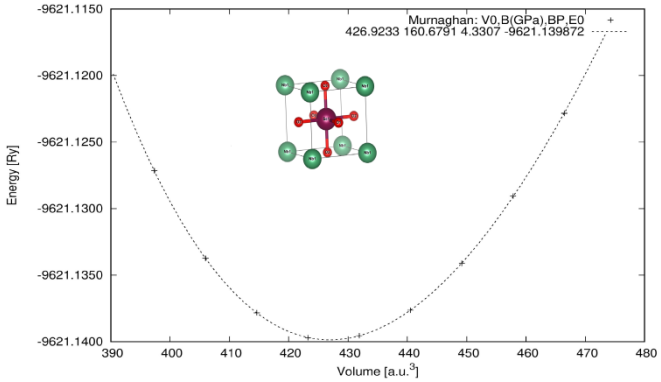
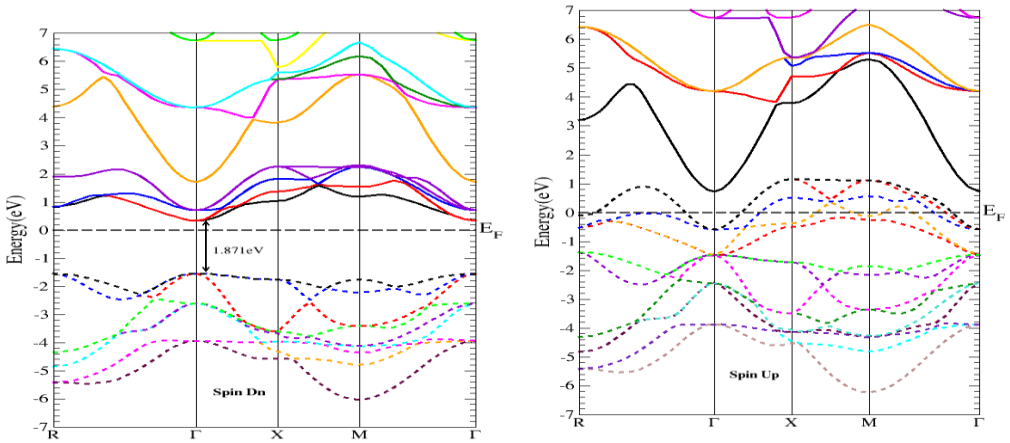


Figure 1. The energy-volume optimization and Murnaghan fit for the perovskite $NbScO_3$.

The lattice constants are optimized using Murnaghan equation of state [19] with only volume optimization as the structure is cubic is required. The energy vs. volume optimization gives the minimum equilibrium energy state lattice parameter and is presented in Figure1. The optimized values of the lattice constant and bulk modulus obtained are 3.985**Å** and 160.679GPa respectively. This lattice constant value of $NbScO_3$ is used with the GGA-PBE and mBJ exchange correlations at denser grids to calculate the electronic band structures along the high symmetry points. The GGA band structure is shown in Figure 2 for both the spin Dn (minority) and spin Up (majority) orientations.

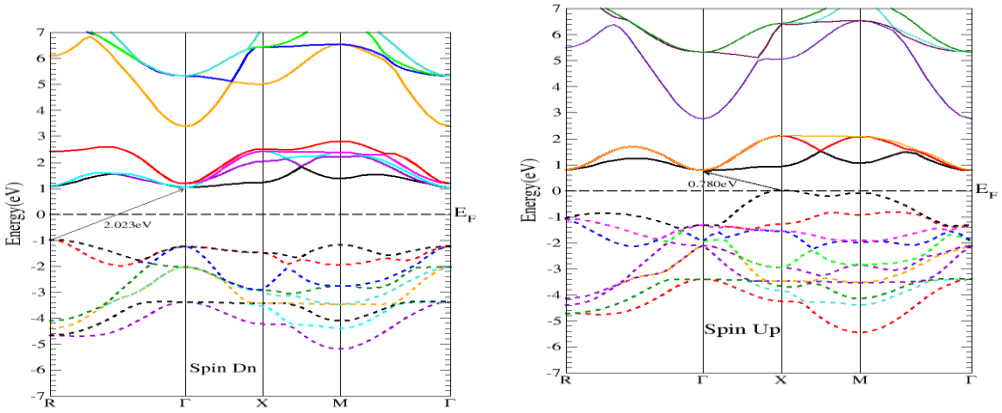


(**a**) (**b**)

Figure 2. The $NbScO_3$ electronic band structures for (a) the minority (Spin Dn) and (b) the majority (Spin Up) channels with PBE-GGA.

We see from the figure that $NbScO_3$ shows typical semi-conducting behavior in the minority spin with a direct Γ−Γ gap of 1.87eV and it is metallic in the majority spin resulting in a half metal ferromagnetic behavior (HMF). HMFs have 100% spin polarization and can intrinsically provide single spin channel electrons, which are very useful in spintronics.

The band structure of $NbScO_3$ with the mBJ exchange potential on the other hand shows it to be a magnetic semiconductor as seen from Figure 3 plots for the spin Dn and spin Up states.



(**a**) (**b**)

Figure 3. The $NbScO_3$ electronic band structures for (a) the minority (Spin Dn) and (b) the majority (Spin Up) channels with mBJ.

The minority spin and majority spin have indirect R–Γ and X–Γ gaps of 2.02 and 0.78eV respectively. Magnetic semiconductors, combine the advantages of both magnets and semiconductors, and form the basis for spintronics. Magnetic semiconductors can be applied for spin generation, injection, and spin manipulation and detection. Since, the mBJ exchange potential gives very reliable and accurate band structures in comparison to that of GGA or hybrid functionals, the correct behavior of $NbScO_3$ would be a magnetic semiconductor.

The half metal gap or spin flip energy E_{HM} is defined here as the minimum energy required to flip a minority-spin electron from the valance band maximum to the majority spin Fermi level. The predicted band gaps and E_{HM} for the GGA and mBJ exchange potential are listed in Table1.

Table 1. The electronic band gaps in the minority and majority spin channels for the $NbScO_3$ perovskite.

$NbScO_3$ Perovskite	**Band Gap (eV)**				E_{HM} (eV)
	Minority (spin Dn)		Majority (spin Up)		
GGA-PBE	**Γ− Γ**	1.871	metallic	No gap	1.547
mBJ	R−Γ	2.023	X−Γ	0.780	0.979

3.2. Magnetic

The band structures plots in the previous section have clearly shown the magnetic nature of NbScO3, and to fully understand the origin and hybridization of the atomic orbitals the total and partial density of states (TDOS/PDOS) are calculated using the mBJ exchange potential and depicted in Figure 4.

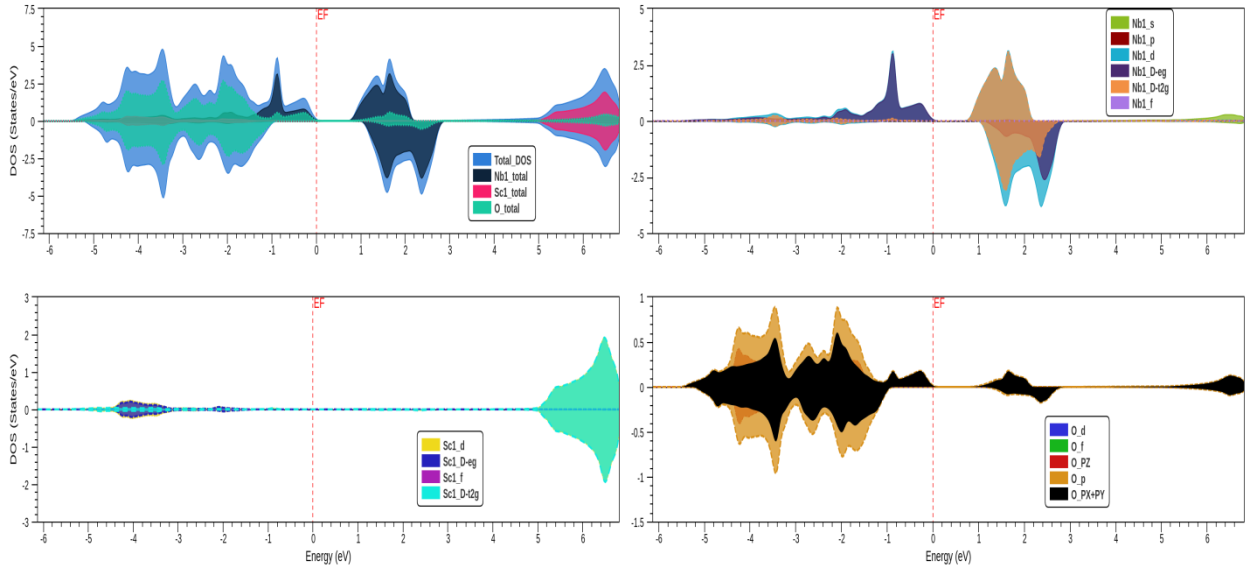


Figure 4. The $NbScO_3$ electronic DOS in both minority (bottom part) and majority (top part) spin channels (a) the TDOS for the compound and the atom constituents (b), (c) and (d) show the PDOS in the different orbitals for the Nb atom, the Sc atom and the oxygen atom respectively.

We clearly see from the plots the semiconducting and magnetic nature of NbScO3. The minority channel shows the wide band gap, with no states at EF (Fermi-energy). Whereas the majority channel has the valence band edge at the Fermi energy and one can say that NbScO3 is an instrinsic magnetic semiconductor. The role of Sc in the magnetism is negligible as indicated by the spin polarized PDOS plot for Sc. The main contribution to the magnetism comes from the 'd' orbital of Nb and the 'Px' and 'Py' orbitals of O2. Also, the significant difference in the majority and minority TDOS can be clearly seen; resulting in the total integer magnetic moment of 2μB typical of HMF as given in Table 2. The Table also lists the atom-wise and interstitial magnetic moments of NbScO3 with the GGA and mBJ exchange correlations..

Table 2. The total and atom projected magnetic moments of the $NbScO_3$ perovskite in units of μ_B.

Exchange	Nb	Sc	O	Intertitial	Total Moment
GGA_PBE	1.8484	0.0126	-0.0761	0.3673	2.0000
mBJ	1.7095	-0.0007	0.0460	0.1533	2.0000

4. Conclusions

In conclusion the FP-LAWP investigation of the perovskite $NbScO_3$ has predicted the system to be a HMF and an intrinsic magnetic semiconductor using the GGA and mBJ exchange potentials respectively. Moreover, the considerable size of the bandgap and magnetic moment obtained confirms the feasibility of $NbScO_3$ for spintronic applications. In addition, the large value of E_{HM} supports the robustness of this system for spintronics and sensing applications, where a significant role is played by the spin of the electrons in the sensor design.

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