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Study of electronic and optical properties of vanadium-based double perovskite oxide: Ba_2VNbO_6

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ABSTRACT:
The electronic and optical properties of double perovskite Ba_2VNbTO_6 have been investigated using First-principles density functional theory (DFT). The exchange correlation effects are included through the generalized gradient approximation (GGA) exchange potential. The investigation of electronic properties showed Ba_2VNbO_6 to be semi-metal in spin-up and insulation in spin down. In both spin up and spin down channel, direct band gap along ΓX direction was observed. The real and imaginary parts of dielectric function, refractive index, absorption coefficient and reflectivity are calculated.
KEYWORDS: FP-LAPW, DFT, GGA, DOS, reflectivity, optical, wien2k.

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I. INTRODUCTION

Cation substitutions in simple ABO_3 perovskites lead to a large class of materials including double perovskites, $AA'BB'O_6$. Typically, A-site atoms are alkaline earth metals such as Ba, Sr or a lanthanide and the B atoms are the transition metals. They constitute an important class of materials, characterized by structural distortion from the cubic, space group Fm3m (#225), structure. These distortions are caused by rotations of the BO_6 and $B'O_6$ octahedras to accommodate the A-site cation [1]. Due to their unique properties and potential applications, double perovskite $AA'BB'O_6$ compounds have been investigated massively. Besides perovskites are well known for their applications in different fields of science and technology because of their wide range of electro-optic, mechanical, semiconducting and insulating behavior [2].

Double perovskite oxide Ba_2VNbO_6 was studied early by Musa (2012) and reported as a cubic with (a=7.9559Å) [3]. To our best knowledge, there is no experimental-theoretical combined studies have yet been performed to investigate the crystal structure, electronic, and optical properties of double perovskite oxide Ba_2VNbO_6. Therefore, the current paper describes the detailed study of the electronic and optical properties of Ba_2VNbO_6 by using First-principles density functional theory (DFT).

II. COMPUTATIONAL DETAILS

We have performed the first principle calculations using the WIEN2k code [4] based upon the framework of density functional theory (DFT) [5]. The electronic structure calculation was performed using Tran and Blaha's generalized gradient approximation (GGA) based on the full potential Linearized Augmented Plane Wave (FPLAPW) Method [6]. For a well conversed scf calculation, we used cut off energy= -6.0 Ry, R_{MT} x K_{max} =7 and k-points=1000 to create 10x10x10 k-mesh in the first Brillouin zone. Out of 1000 k-points, 120 irreducible part of k-points were used for first Brillouin zone integration. The charge and energy convergence criteria was set to 0.001 e^- and 0.0001Ry respectively. However the core states are treated relativistically, the semi-core states are treated semi-relativistically by ignoring the spin-orbit (SO) coupling.

The optical properties can be described the dielectric function ε (ω), which is expressed as [7]

$$\varepsilon(\omega) = \varepsilon_1(\omega) + i\varepsilon_2(\omega)$$

The imaginary part $\varepsilon_2(\omega)$ of the dielectric function $\varepsilon(\omega)$ was calculated from the electronic band structure of a solid.

$$\varepsilon_2(\omega)=\left(\frac{\hbar^2e^2}{\pi m^2\omega^2}\right)\sum_{c,v}\int d^3k\langle c_k\mid p^\alpha\mid v_k\rangle\langle v_k\mid p^\beta\mid c_k\rangle x\delta\left(\varepsilon_{c_k}-\varepsilon_{v_k}-\omega\right)$$

Where p is the momentum matrix element between states of band α and β with crystal momentum k. C_k and V_k are the crystal wave functions corresponding to the conduction and valence bands with crystal wave vector k. The real part $\varepsilon_1(\omega)$ of dielectric function can be extracted from the imaginary part using the Kramers- Kroning relation [8]:

$$\varepsilon_1(\omega)=1+\frac{\pi}{2}p\int_0^\infty\frac{\omega'\varepsilon_2(\omega')}{(\omega')^2-\omega^2}d\omega'$$

where p is the principal value of integral. The refractive index $n(\omega)$ and the reflectivity $R(\omega)$ in the crystal are given as [9]

$$n(\omega)=\left[\frac{\sqrt{\varepsilon_1^2(\omega)+\varepsilon_2^2(\omega)+\varepsilon_1(\omega)}}{2}\right]^{\frac{1}{2}}$$

$$R(\omega)=\frac{n+ik-1}{n+ik+1}$$

III. RESULTS AND DISCUSSIONS

Crystal Structure: Ba_2VNbO_6 crystalizes in cubic phase with Fm3m space group. The Ba, V, Nb and O atoms occupy the 8c, 4a, 4b and 24e Wyckoff position in the unit cell with Ba (1/25, 1/25, 1/25), V (0, 0, 0), Nb (1/2, 1/2, 1/2) and O (0.2513, 0, 0), see figure 1(b). The structural optimization based on Murnaghan's equation of state [10] was performed to obtain the relax structure with minimum energy.

The energy versus volume data was fitted to a Murnaghan equation of state to obtain the equilibrium lattice constant (a), the bulk modulus (B) is mentioned in table 1.

Compound	Our Result			Available theor. / expt. Data			References
	a (Å)	B (GPa)	B'	a (Å)	B (GPa)	B'	
Ba_2VNbO_6	8.1168	170.0401	4.7950	7.9559	-	-	[3] theoretical

The output of the volume optimization gives the equilibrium lattice constant, bulk modulus, its pressure derivative etc.

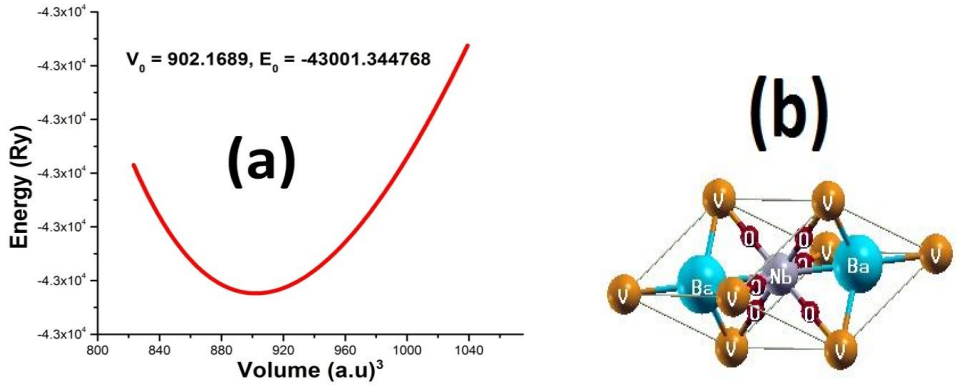

Figure 1: (a) volume optimization plot and (b) crystal structure for Ba_2VNbTO_6

3.1 Electronic properties

The optimal lattice constants obtained were used to study the electronic properties. In order to determine the optical properties, it is necessary to obtain a good description of electronic structure. The contribution of different electronic states in the valance and the conduction band determines the electronic property of the material. This is shown with the help of total and partial density of states in figures 2 to 6 respectively. A closer look on total DOS plot shows that maximum states/eV closest to the Fermi energy is about 9.6 in the spin up channel and in the down channel is about 9.4. Compared to the total states/eV which is about 38 in the spin up channel and 35.05 in the spin down one, the states/eV near Fermi is very low. The system can be interpreted as an insulator in spin down channel and has a mixed conducting state in the spin up channel. The band structure

plot will further reveal this characteristic. From the band structure plot from figure 2 (a) and 2(b), it is seen that in the spin up channel two energy bands appear, one in the conduction band region and another in the valance band region. A direct and an indirect band gap along ΓX direction are observed in the conduction band region with energy gap 1.1 eV and 1.2 eV respectively. Similar band characteristic is observed for valance band region. The direct band gap is along Γ X with energy gap of 1.1 eV while the indirect energy gap is 1.2 eV. In the spin down channel, the Fermi level lies in between the conduction and the valance band. A direct band gap of 1.2 eV is observed. Along ΓX direction an indirect band gap of 1.3 is observed. Unfortunately, there are no experimental nor theoretical results for qualitative comparison. Along the spin up channel, since the Fermi level lies in between the conduction band and the valance band and in addition to DOS results, the system can be interpreted as a semi-metal. In the spin down channel, the band structure shows insulating properties.

From the partial density of states plots figures 3 to 6, it is clear that in the spin up channel, the maximum contribution to the total DOS is due to the f state of Ba (~ 28 eV) and there is an appreciable contribution from d states of Mo and from p state of O. Since Ba has the highest contribution near Fermi energy, therefore the sharp peaks in DOS are mainly due to the f-state electron of Ba. In spin down channel also the maximum contribution to the total DOS is due to the f-state of Ba (~ 24 eV) and there is an appreciable contribution from d states of Mo and from p state of O and d state of V.

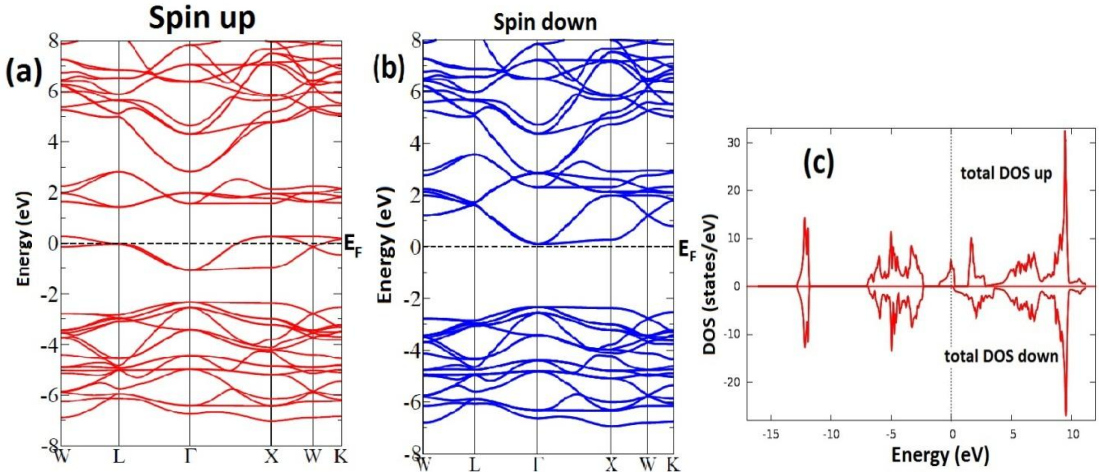

Figure 2: Band structure (a) spin up (b) spin down and total DOS (c) plot for Ba_2VNbO_6

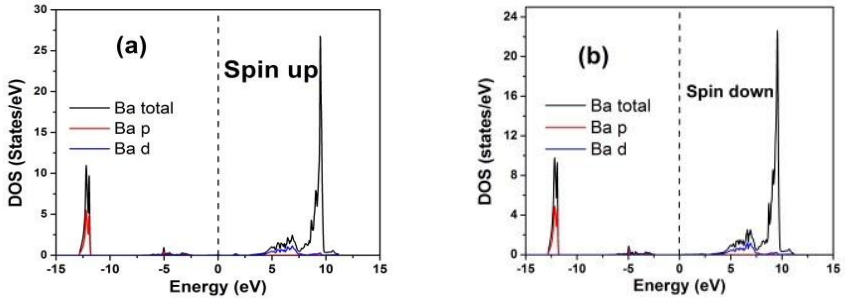

Figure 3: Partial DOS plot of Ba-atom (a) spin up (b) spin down

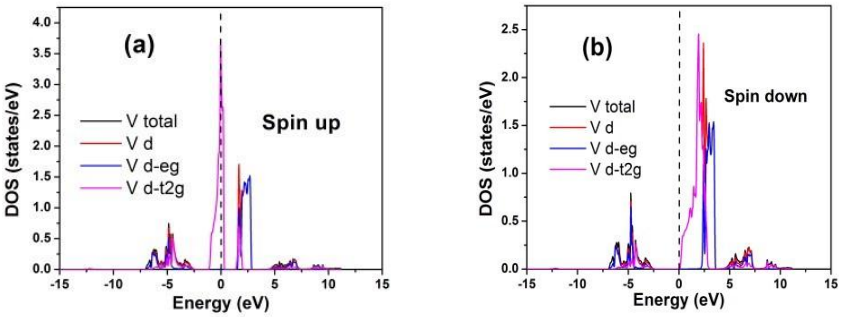

Figure 4: Partial DOS plot of V-atom (a) spin up (b) spin down

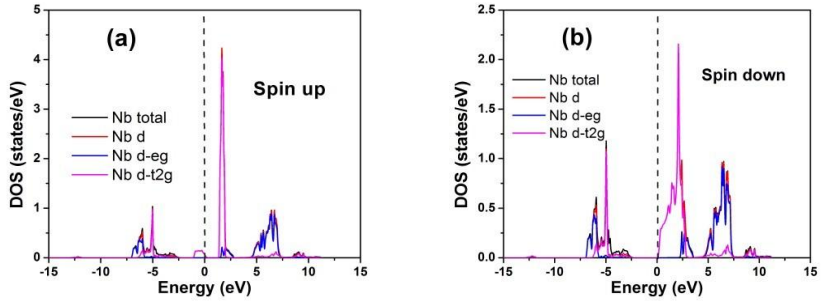

Figure 5: Partial DOS plot of Nb-atom (a) spin up (b) spin down

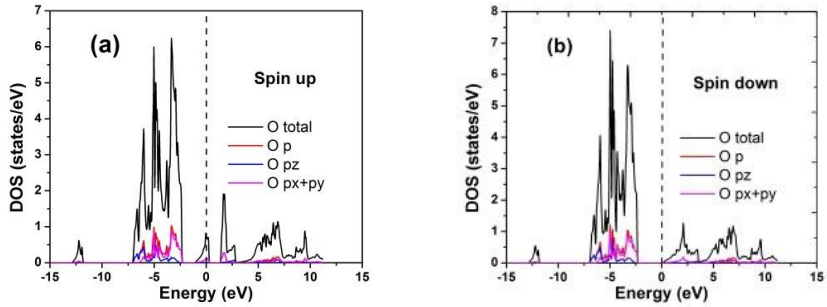

Figure 6: Partial DOS plot of O-atom (a) spin up (b) spin down

3.2 Optical properties

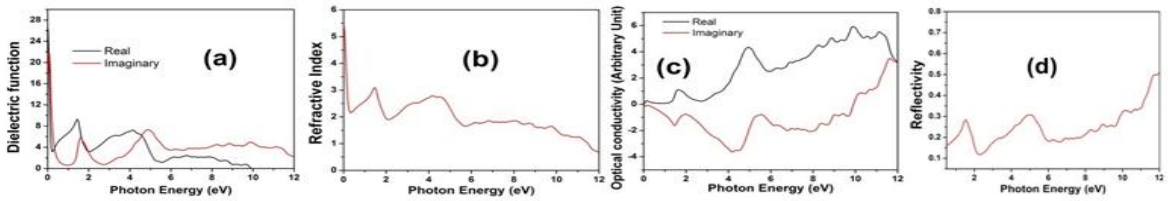

Figure 7: The calculated optical parameters of Ba_2VNbO_6 as a function of the photon energy (eV), (a) dielectric function ε(ω), (b) refractive index n(ω), (c) optical conductivity σ(ω) and (d) reflectivity coefficient R(ω)

The interband transition contribution to the dielectric function represented by ε_2 lies closed to E_F and is flat at approximately 5 eV. The variation of peaks supposed the system possible usage in optoelectronic devices and solar cells. The peak of real part ε_1 which is closed to E_F indicates low contribution from lattice vibration, ε_1 lies at 25. The refractive index reaches a maximum 5.4 at O.2 eV of photon energy. Strong minimum near 3 eV in the reflectivity is observed. A small decrease of the dielectric function with increase in energy is observed. Thus, small absorption and large reflectivity is the characteristics. Real part of optical conductivity increases with photon energy with a maximum near 9.7 eV and imaginary part decreases with increase in photon energy and becomes negative forming a value between 4.2 eV to 8.2 eV and then increases towards zero.

IV. CONCLUSION

First principles calculation have been employed to study the electronic structure and optical properties of double perovskite Ba_2VNbO_6 using full potential linearized augmented plane wave method under generalized gradient approximations within Wien2k. The calculated electronic properties showed Ba_2VNbO_6 to be semi-metal in spin-up and insulation in spin down. In both spin up and spin down channel, direct band gap along with indirect band gap in ΓX direction was observed. The optical properties also indicate a possible application of Ba_2VNbO_6 in optoelectronic devices.

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