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Ab-initio study of optoelectronic and magnetic properties of the orthorhombic $NdMnO_3$ perovskite

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ABSTRACT

Using the full potential linear augmented plane wave (FPLAPW) method based on density functional theory (DFT), we have studied the structural, electronic, optical and magnetic properties of the orthorhombic perovskite oxide $NdMnO_3$, with both generalized gradient approximation (GGA) and GGA+U approaches, where U is on-site Coulomb interaction correction. We have analyzed the structural parameters, total and partial densities of states. The results show a half-metallic ferromagnetic ground state for NdMnO3 in GGA+U due to the strong hybridization effect between Mn 3d and Nd 4 f states The integer value of the total magnetic moment is one of the significance of the half metallic nature of this material. Furthermore, we have computed optical properties of $NdMnO_3$; we found pronounced peaks occurring in different parts of the spectrum. The results obtained, make the orthorhombic $NdMnO_3$ a promising candidate for application in spintronics and opto-electronics.

1. Introduction

Perovskite-type oxides (ABO_3) are very important materials which have attracted considerable attention, because they exhibit exceptional properties such as, ferromagnetism [1–6], ferroelectricity [7–10], piezoelectricity [11–14], and semiconductivity. ABO_3 has been effectively used for a number of applications, including non-volatile memories, micro electro-mechanical systems (MEMS) [15–18], multi-state memory elements [19], heterogeneous catalysts [20–21], magneto-resis-tance colossal [22] and in spintronic domains [23,24]. Generally, ABO_3 materials are half-metallic (HM), which are important in spintronic devices because of their spin-polarized conductivity. So, the energy gap in one spin channels of HM materials is insulated, whereas metallic behavior is observed in the second spin channels. Therefore, determination of HM compounds is important.

Recently, the multiferroic manganites $REMnO_3$ have attracted great scientific attention due to their manifestations of interesting and significant coupling between the magnetic and electric order parameters [24–27]. These new properties have undergone a new start to the perovskite materials, especially the magnetic oxides ($AMnO_3$ or the $AFeO_3$). The magnetic properties are important factors for better understanding of the oxide behavior. The study of perovskite $NdMnO_3$ has been motivated by the reporting that $Nd_{0.7}Sr_{0.3}MnO_3$ has the largest Colossal Magneto Resistance (CMR) effect among the manganites [28,29].

Based on first-principle calculations, in this letter, we investigate electronic structure and optical properties of the orthorhombic perovskite oxide $NdMnO_3$. These properties are evaluated by using GGA and GGA+U approximations, where U is Hubbard parameter for considering the Coulomb repulsion between the highly localized 3d/4f electrons. It is important to notice that there are no theoretical data available for $NdMnO_3$ compound and this is why, we are motivated to study this material theoretically.

2. Calculation

The calculations were performed in the present work using Kohn–Sham equations [30] which are solved to calculate the structural, electronic and magnetic properties of the orthorhombic perovskite $NdMnO_3$, using the WIEN2K code [31,32]. It is based on the full-potential linearized augmented plane wave method [33].

Basis functions were expanded as combinations of spherical harmonic functions inside non-overlapping spheres around the atomic sites (MT spheres) and in Fourier series in the interstitial region. The valence wave functions, inside the spheres are expanded up to $l_{max}=10$. Reciprocal space integration is carried out with a k mesh of $5\times4\times6$, giving rise to 120 K-points in the irreducible Brillouin zone, which is found to be sufficient to achieve convergence.

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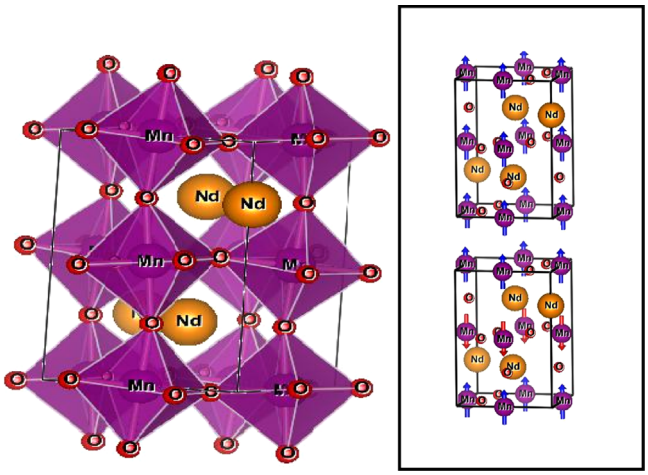

Fig. 1. (Color online) Cristal structure and magnetic configuration with the orthorhombic polyhedron MnO_6 of $NdMnO_3$ compound. The ferromagnetic (FM) phase at the top and the anti-ferromagnetic (AFM) phase at the bottom.

Table 1
Calculated resultants (equilibrium lattice parameters: a(Å), b [Å],c [Å], bulk modulus B (GPa)), its pressure derivative (B') and the Volume of cell [Å^3] of orthorhombic Pnma $NdMnO_3$ obtained with GGA and GGA+U.

Parameters	GGA	GGA+U	Experimental data	
a [Å]	5.794	5.732	5.792 [a]	5.711 [c]
b [Å]	7.927	7.649	7.564 [a]	7.589 [c]
c [Å]	5.068	5.271	5.421 [b]	5.411 [c]
Volume of cell [Å^3]	232.826	235.361	237.521	–
Pressure derrivative (B')	4.261	4.468	–	–
Bulk modulus B(GPa)	173.330	197.242	–	–

[a] Ref.[41].
[b] Ref.[42].
[c] Ref.[43].

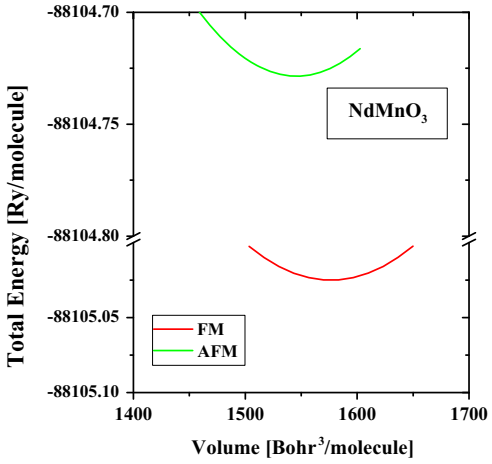

Fig. 2. (Color online) The total energy (Ryd) of the orthorhombic $NdMnO_3$ as a function of the unit cell volume [Å^3] for: both configurations ferromagnetic (FM) and anti-ferromagnetic (AFM) phases using GGA.

The wave functions in the interstitial region were expanded in plane waves with a cutoff of $k_{max}=8/R_{MT}$ (where R_{MT} is the average radius of the MT spheres). The muffin-tin radius R_{MT} is based on two conditions: (i) no core charge leaks out of MT spheres and (ii) no overlapping is permitted between spheres. The muffin-tin (MT) radii of Nd, Mn and O were chosen to be 2.4, 1.80 and 1.6 Bohr, respectively.

The lattice constants and bulk modulus are calculated by fitting the total energy versus volume according to the Murnaghan's equation of state [34]. For the exchange correlation functional, we have used the GGA [35] as well as the GGA+U [36–38]. In this formalism; the 4f orbital (for Nd) was treated using the GGA+U approach with the values of U= 8 eV and U=4 eV for the 3d of Mn [39].

3. Results and discussions

3.1. Structural properties

In order to obtain the equilibrium lattice constant and the bulk modulus for the orthorhombic $NdMnO_3$ in ferromagnetic phase (FM) and antiferromagnetic one (AFM), we performed the structural