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Electronic structure and magnetic properties of the perovskite cerium manganese oxide from ab initio calculations

Saadi Berri [a,b,*], Djamel Maouche [a], Miloud Ibrir [b], Badis Bakri [b]

[a] Laboratory for Developing New Materials and their Characterizations, University of Setif, Algeria
[b] Department of Physics, Faculty of sciences, University of M'sila, Algeria

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ABSTRACT

We have performed first-principle calculations of the structural, electronic and magnetic properties of cerium manganese oxide $(CeMnO)_3$, using full-potential linearized augmented plane-wave (FP-LAPW) scheme within GGA and GGA+*U* approaches. Features such as the lattice constant, bulk modulus and its pressure derivative are reported. Also, we have presented our results of the band structure and the density of states. The results show a half-metallic ferromagnetic ground state for $CeMnO_3$ in GGA+U treatment, whereas semi-metallic ferromagnetic character is observed in GGA. The results obtained, make the cubic $CeMnO_3$ a candidate material for future spintronic application.

1. Introduction

The cubic perovskites with varied compositions and structures have been extensively studied, motivated by their possible applications in numerous industrial and engineering domains [1–5]. They have showed a wide range of attractive properties ferroelectricity [6–8], piezoelectricity [9,10], semiconductivity [11], catalytic activity [12], thermoelectricity [13], superconductivity and metal-insulator transition [14]. As an example ternary oxides of rare earth (Eu, Gd, Tb)CoO_3 type oxides, this series reveal extensive applications in materials science and technology, some of the perovskites (Eu, Gd, Tb)CoO_3 compounds are used as electrode materials for magnetohydrodynamic (MHD) generators [15], for fuel cells [16]. On the other hand, perovskites like $BaMnO_3$ and $SrMnO_3$ have attracted interest in NO removal process as catalysts [17–19].

Lanthanoid-based peroviskite type oxides, such as $LaTMO_3$ (La: Lanthanoid, TM: transition metals), have been well-known as functional inorganic materials having a wide range of application for electrode materials of the alkaline fuel cell [20], ion sensor [21] and gas sensor[22–23]. The structural and electronic transport properties have been predicted for $La_{1-x}Ce_xMnO_3$ [24,25]. Generally, perovskites crystallize in orthorhombic structure, but many studies have depicted the cubic one [26–31].

Recently, half-metallic ferromagnetism has been found in CrO_2 [30], NiMnSb [31], Fe_3O_4 [32], $La_{0.67}Sr_{0.33}MnO_3$ [33], Co_2MnSi [34], Ti_2FeSi [35], Ti_2CoAl [36], NiCr(P, Se, Te, As) [37], Pb_2FeMoO_6[38], and CoFeMnZ (*Z*=Al, Ga, Si, Ge) [39], and nearly 100% high spin-polarization has been observed experimentally in the cases of CrO_2 and $La_{0.67}Sr_{0.33}MnO_3$ materials [40]. Half-metallic ferromagnets (HMF) meet all requirements of spintronics, as a result of their exceptional electronic structure. These materials behave like metals with respect to the electrons of one spin direction and like semiconductors with respect to the electrons of the other spin direction.

The considered $CeMnO_3$ is assumed to have ideal cubic perovskite structure (#221).

* Corresponding author at: Laboratory for Developing New Materials and their Characterizations, University of Setif, Algeria.
Tel.: +21395115576; fax: +213 36 92 72 10.
E-mail address: berrisaadi12@yahoo.fr (S. Berri).

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The cubic unit cell contains one molecule with the Wychoff positions of the atoms that are Ce 1a (0, 0, 0), Mn 1b (0.5, 0.5, 0.5) and O 3c (0.5, 0.5, 0). In the present paper, the structural, electronic and magnetic properties of $CeMnO_3$ compound are reported.

Our main goal in this work is to evaluate and examine the validity of the predictions of half metallicity for $CeMnO_3$ compound. The calculations are performed using ab initio full-potential linearized augmented plane wave (FP-LAPW) scheme within GGA and GGA+U approaches. Our paper is organized as follows. The theoretical background is presented in Section 2. Results and discussion are presented in Section 3. A summary of the results is shown in Section 4.

2. Method of calculations

We have carried out first-principle calculations [41,42] with both the full potential and linear augmented plane wave (FP-LAPW) method [43] as implemented in the WIEN2k code [44] within the density functional theory (DFT). The Perdew–Burke–Ernzerhof generalized gradient approximation GGA [45,46] and GGA+U [47]. In the calculations reported here, we use a parameter $R_{MT}K_{max}=9$, which determines matrix size (convergence), where K_{max} is the plane wave cut-off and R_{mt} is the smallest of all atomic sphere radii. We have chosen the muffin-tin radii (MT) for Ce, Mn and O to be 2.5, 1.8 and 1.6 a.u., respectively. Within the sespheres, the charge density and potential are expanded in terms of crystal harmonics up to angular momenta $L=10$, and a plane wave expansion has been used in the interstitial region. The value of $G_{max}=14$, where G_{max} is defined as the magnitude of largest vector in charge density fourier expansion. The Monkorst-Pack special k-points were performed using 3000 special k-points in the Brillouin zone. The cut off energy, which defines the separation of valence and core states, was chosen as -6 Ry. We select the charge convergence as 0.0001e during self-consistency cycles. The 4f orbital for the Ce atom was treated using the GGA+U approach with the values of $U=$ 7.07 eV, and $J=0.95$ eV(for Ce), and $U=4$ eV, $J=0.87$ eV for the 3d of the Mn [48].

3. Results and discussion

We have calculated the total energy as a function of lattice constant of $CeMnO_3$ compound for the ferromagnetic (FM) state. The plots of calculated total energies versus reduced volume of $CeMnO_3$ compound are shown in Fig. 1. The total energies versus changed volumes are fitted to the Murnaghan's equation of state [49] in order to determine the ground state properties, such as equilibrium lattice constant a, bulk modulus B and its pressure derivative B'. The calculated structural parameters of $CeMnO_3$ compound are reported in Table 1. Until now, an experimental or theoretical lattice constant, the bulk modulus and its pressure derivative value have not been reported. To the best of our knowledge, there are no experimental or theoretical data reported for the bulk modulus and its pressure derivative for the material of interest, and hence our results are predictions. We have also included in Table 1 the bulk modulus and its pressure derivative B' values for $PrMnO_3$ [50], $LaAlO_3$ [51], and $BaTiO_3$ [52] for comparison purpose. Note that the bulk modulus of $LaAlO_3$ and $BaTiO_3$ materials seems to be much larger than that of $CeMnO_3$ in both methods being considered here. This suggests that $CeMnO_3$ compound is less compressible than those materials.

The calculated spin-polarized band structures of $CeMnO_3$ compound at the theoretical equilibrium lattice

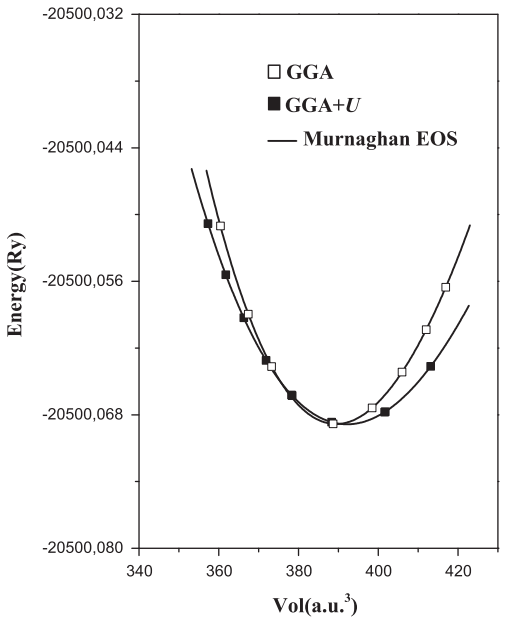

Fig. 1. Volume optimization for the $CeMnO_3$ compound.

Table 1
Lattice constant a(Å), bulk modulus B (in GPa), pressure derivative of bulk modulus B', total and partial magnetic moment (in μ_B) for $CeMnO_3$ compound.

Compound	a	B	B'	$m_{Ce,Pr}$	m_{Mn}	m_O	$m_{interstitial}$	m_{Total}
$CeMnO_3$								
GGA	3.87	141.95	3.83	0.898	3.054	0.053	0.898	4.353
GGA+U	3.91	147.88	3.62	0.988	3.818	−0.046	0.316	4.983
$PrMnO_3$ [50]								
GGA	3.88	–	3.5	2.18	3.23	0.04	0.41	5.94
GGA+U	3.85	–	4.23	2.29	3.35	−0.006	0.37	6
$LaAlO_3$ [51]								
GGA	3.81	193.17	4.29	–	–	–	–	–
$BaTiO_3$ [52]								
EXP	4	162	–	–	–	–	–	–