Characterization of Electronic Properties, Exchange Splitting and Ferromagnetic Arrangement in New Ti-Doped BaO

Malika Hachemaoui

Faculty of Sciences, Department of Physics, University of Saida Dr. Moulay Tahar, 20000, Saida, Algeria

Mohamed Meskine

Faculty of Sciences, Department of Physics, University of Saida Dr. Moulay Tahar, 20000, Saida, Algeria

Allel Mokaddem

University Center of Nour Bachir El-Bayadh, 32000, El-Bayadh, Algeria

Bendouma Doumi (✉ bdoummi@yahoo.fr)

Faculty of Sciences, Department of Physics, Dr. Tahar Moulay University of Saida

<https://orcid.org/0000-0003-1563-8587>

Yesim Mogulkoc

Department of Engineering Physics, Ankara University, 06100, Tandogan, Ankara, Turkey

Abdelkader Tadjer

Modelling and Simulation in Materials Science Laboratory, Physics Department, Djillali Liabes University of Sidi Bel-Abbes, 22000, Sidi Bel-Abbes, Algeria

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Characterization of electronic properties, exchange splitting and ferromagnetic arrangement in new Ti-doped BaO

Malika Hachemaoui ^a, Mohamed Meskine ^a, Allel Mokaddem ^{b, c, *}, Bendouma Doumi ^{a, b, **,}, Yesim Mogulkoc ^d, Abdelkader Tadjer ^e

^a Faculty of Sciences, Department of Physics, University of Saida Dr. Moulay Tahar, 20000, Saida, Algeria

^b Instrumentation and Advanced Materials Laboratory, University Center of Nour Bachir El-Bayadh, 32000, El-Bayadh, Algeria

^c University Center of Nour Bachir El-Bayadh, 32000, El-Bayadh, Algeria

^d Department of Engineering Physics, Ankara University, 06100, Tandogan, Ankara, Turkey

^e Modelling and Simulation in Materials Science Laboratory, Physics Department, Djillali Liabes University of Sidi Bel-Abbes, 22000, Sidi Bel-Abbes, Algeria

Corresponding authors

E-mail address:

* mokaddem.allel@gmail.com (Mokaddem Allel)

** bendouma.doumi@univ-saida.dz (Bendouma Doumi)

ORCID : <http://orcid.org/0000-0003-1563-8587> (Bendouma Doumi)

Abstract

We have studied the electronic structures, ferromagnetic properties, half-metallicity and exchange splitting in BaO doped with titanium such as $\text{Ba}_{1-x}\text{Ti}_x\text{O}$ at concentration $x = 0.125$. The structural parameters of BaO and $\text{Ba}_{0.875}\text{Ti}_{0.125}\text{O}$ compounds are calculated with generalised gradient approximation of Wu and Cohen, while their electronic structures, accurate band gaps and magnetic properties are evaluated by the use of the Tran-Blaha-modified Becke-Johnson potential. The changes of lattice parameter and bulk modulus of $\text{Ba}_{0.875}\text{Ti}_{0.125}\text{O}$ are discussed with respect to the BaO. We have found that the $\text{Ba}_{0.875}\text{Ti}_{0.125}\text{O}$ has a wide half-metallic ferromagnetic gap of 2.701 eV and a half-metallic gap of 0.803 eV with integral Bohr magneton of $2 \mu_B$, where its ferromagnetic state is characterised by the main contribution of the direct exchange splitting. Therefore, the $\text{Ba}_{0.875}\text{Ti}_{0.125}\text{O}$ is true half-metallic ferromagnet with spin polarisation of 100 % and appears to be promising material for spintronics applications.

Keywords Electronic structures, Exchange splitting, Ferromagnetic behavior

1 Introduction

Spintronics known as spin electronics is based on the use of the spin of electron plus its charge; it is an attractive field of research into spin-based physical phenomena and electronics [1, 2]. In recent years, the diluted magnetic semiconductors (DMS) have been widely investigated as promising candidates for several spintronics applications. These compounds are characterised by intermediate properties that combine non-magnetic semiconductor and magnetic behaviours, which are obtained by doping non-magnetic semiconductors with magnetic elements for example transition metals and rare-earth [3-5]. The half-metallic ferromagnets DMS with spin polarisation of 100 % have been considered an important class of materials for spintronics because their electronic structures show a semiconductor feature in one direction of spins and a metallic character in the other spin channel [6, 7]. However, spintronics processes the spin of the electron as well as its charge to obtain new functionalities in spin-based devices. The advantages of spintronics devices with respect to the conventional electronics are the non-volatility, high data processing speed, decreased electrical power consumption and high transistor density [8-10].

The barium oxide (BaO) is one of the alkaline-earth-metal binary oxides; it has wide band gap owing to its high ionicity [11]. This compound has several technological applications for example it is used as a buffer layer in the epitaxial growth of multifunctional perovskite oxides directly on silicon [11, 12]. The alkaline-earth-metal binary oxides have been considered as potential materials for spintronics and optoelectronics applications [13-15]. The half-Metallic ferromagnetic property was predicted in the new class of DMS based on C-doped MgO, SrO and BaO [13] and CaO doped with C and N atoms [14]. E. Albanese et al., [15] have investigated magnetic interaction and nature of isolated Nitrogen-dopants in bulk BaO (N-BaO) by the use of first-principles calculations of functional density theory. The BaO is a potential candidate for spintronics according to first-principle study carried out on its half-metallic ferromagnetic behavior under the doping effect of magnetic chromium (Cr) impurities [16].

In this study, we investigated the structural properties, electronic structures, half-metallic ferromagnetic behaviour, exchange splitting and crystal field energy in titanium (Ti)-doped BaO such as $\text{Ba}_{1-x}\text{Ti}_x\text{O}$ compound at concentration $x = 0.125$. The calculations were carried out by the first-principle approaches of full-potential linearised augmented plane-wave (FP-LAPW) method [17] within density functional theory (DFT) [18, 19].

2 Method of calculations

The properties of the BaO and Ba_{1-x}Ti_xO compound at concentration $x = 0.125$ were investigated using the first-principle concepts of the FP-LAPW method and the DFT implemented in WIEN2k code [20]. The structural parameters of BaO and Ba_{0.875}Ti_{0.125}O are determined by the use of the generalised gradient functional of Wu and Cohen (GGA-WC) [21], while the Tran–Blaha-modified Becke–Johnson exchange potential (TB-mBJ) combined with the local density approximation [22, 23] is employed to determine the magnetic moments, exchange constants, exchange splitting, crystal field energy and perfect electronic structures with accurate bands gaps of compounds under study.

The wave functions were extended in the interstitial region to plane waves with a cut-off of $k_{\max} = 8.0/R_{\text{MT}}$, where the $k_{\max}$ is the magnitude of the largest k vector in the plane wave and the R_{MT} is the average radius of the muffin-tin sphere. The charge density is Fourier extended up to $G_{\max} = 14 \text{ (a.u.)}^{-1}$, where $G_{\max}$ corresponds to the largest vector in the Fourier expansion, while the maximum value of the partial waves inside the atomic sphere is $l_{\max}$ equal to 10. The separation of valence and core states is determined by the energy cut-off of -6 Ry. The integration of the Brillouin zone is achieved by employing the Monkhorst-Pack mesh [24], where the $(4 \times 4 \times 4)$ and $(4 \times 4 \times 2)$ k -points are used for BaO and Ba_{0.75}Ti_{0.25}O, respectively. The total energy convergence was set at 0.1 mRy to reach the self-consistent.

Our calculations are based on the conventional BaO lattice in the rock-salt NaCl (B1) structure with space group ($Fm\bar{3}m$) No. 225, where the atoms of barium (Ba) and oxygen (O) are located at the (0, 0, 0) and (0.5, 0.5, 0.5) positions, respectively. We have used the Ba₈O₈ supercell of 16 atoms to create the Ba₇TiO₈ supercell by the substitution of the Ba cationic site at the (0, 0, 0) position with the titanium (Ti) magnetic atom. Therefore, we get the Ba_{0.875}Ti_{0.125}O supercell with concentration $x = 0.125$, which has tetragonal structure with space group of $P4/mmm$ No. 123.

3 Results and discussions

3.1 Structural properties

The structural properties such as the lattice constants (a), bulk modules (B) and their pressure derivatives (B') of BaO and Ba_{0.785}Ti_{0.125}O compounds have calculated by fitting the empirical Murnaghan's equation of state [25]. The obtained results are given in Table 1 with other experimental data [26-29] and theoretical values [11, 16, 30-32]. We have noticed that there are changes in the structural parameters (a) and (B) of Ba_{0.875}Ti_{0.125}O doping material compared to the BaO. This is due to the difference between the ionic radii of the Ba and O atoms. However, the lattice constant of Ba_{0.785}Ti_{0.125}O decreases with respect to the BaO,

leading to the increase of its bulk modulus. Therefore, the $\text{Ba}_{0.785}\text{Ti}_{0.125}\text{O}$ becomes harder than BaO. The behaviours of these two parameters of $\text{Ba}_{0.785}\text{Ti}_{0.125}\text{O}$ compound were observed for BaO doped with Cr [7] and CaO doped with Ti [16]. It should be noted that there are no experimental and theoretical studies on $\text{Ba}_{0.785}\text{Ti}_{0.125}\text{O}$ material in order to compare them with our results of structural parameters.

Moreover, the results of the lattice constant and bulk modulus of BaO are in good concordance with the experimental values [26-28] and theoretical calculations [16] found by GGA-WC [21]. Also, these parameters are better than the theoretical values [11, 16, 30-32] calculated with generalised gradient approximation of Perdew-Burke-Ernzerhof (GGA-PBE) [33] and the local density approximation (LDA) [34] with respect to the experimental values, meaning that the GGA-WC [21] provides good results for the structural parameters. The performance of GGA-WC potential compared to other approximations for determining structural properties results from the fourth order of expansion of its gradient of exchange and correlation functional [21, 35-37].

3.2 Electronic structures and Half-metallic characteristic

Firstly, we have determined the electronic properties of the two BaO and $\text{Ba}_{0.875}\text{Ti}_{0.125}\text{O}$ compounds, and then we have investigated the doping effect of the magnetic Ti impurity on the half-metallic character as well as the origin of ferromagnetic arrangement in $\text{Ba}_{0.875}\text{Ti}_{0.125}\text{O}$. Figs. 1 and 2 show the band structures of BaO and $\text{Ba}_{0.875}\text{Ti}_{0.125}\text{O}$, respectively. The BaO bulk has semiconductor nature as shown in Fig. 1 and there are no electron states at Fermi level because all electrons are linked to the valance band. The valence band maximum and the conduction band minimum occur at the same X high symmetry point, which reveals that BaO has direct gap (E^{XX}). On the other hand, the spin-polarised band structures of $\text{Ba}_{0.875}\text{Ti}_{0.125}\text{O}$ doping system show different behavior of majority-spins bands compared to the BaO bulk due to the injection of the Ti atom of magnetic character. From Fig. 2.b, we see that the minority-spin bands keep the semiconductor feature, but the majority spins become metallic as shown in Fig. 2.a. For majority spins, the metallic character results from the localised magnetic spins of 3d states of Ti around E_F , while the 3d-Ti unoccupied states of minority spins are located at the bottom of the conduction band. Consequently, the $\text{Ba}_{0.875}\text{Ti}_{0.125}\text{O}$ is half-metallic ferromagnetic material. The direct band gap of minority-spin bands located at the X high symmetry point is called the half-metallic ferromagnetic (HMF) gap (G_{HMF}), while the minimum energy located between the valence band maximum and the Fermi level (0 eV) describes the half-metallic (HM) gap (G_{HM}). In the case of the $\text{Ba}_{0.875}\text{Ti}_{0.125}\text{O}$ material, the HM gap corresponds to the absolute value of the maximum

energy of valence bands of minority spins with respect to the Fermi level. The Table 2 summarise the values of direct band gap E^{xx} of BaO, HMF gap G_{HMF} and HM gap G_{HM} of minority-spin bands of $Ba_{0.875}Ti_{0.125}O$ with other theoretical [11, 16, 30, 38, 39] and experimental [40-42] values. The $Ba_{0.875}Ti_{0.125}O$ has direct HMF gap of 2.701 eV situated at the Γ high symmetry point and its HM gap is 0.803 eV located between the valence band maximum and Fermi level. The wide gap of BaO of 3.5 calculated with the TB-mBJ is more improved with respect to the theoretical values [11, 16, 30, 38, 39] found by the GGA-WC [21], GGA-PBE [33] and LDA [34] approximations. The better gap of BaO is due to the performance of TB-mBJ semi-local exchange correlation potential for predicting band gaps of semiconductors and insulators [23, 43, 44].

The projected total and partial densities of states (DOS) of $Ba_{0.875}Ti_{0.125}O$ are given by the Fig. 3 and 4. The $Ba_{0.875}Ti_{0.125}O$ material is doped by the titanium (Ti) transition atom characterised by the 3d electronic levels, which are localised in the gap around E_F as seen in Fig. 4 for majority-spin states. The major contribution of the total-DOS of majority spins at E_F is originated from the contributions of the Ba and Ti atoms. However, the metallic nature of majority-spin states results from the large p-d hybridisation between the p (O) and 3d (Ti) states as shown in Fig. 4. In addition, the 3d states of titanium (Ti) ion are splitted into t_{2g} partially occupied states and e_g empty states due to the octahedral crystal field environment produced by neighbouring oxygen (O) ions. From Fig. 3, we can see clearly that the total-DOS is metallic for the majority spins but a band gap occurs around Fermi level (E_F) for the minority spins. Therefore, the $Ba_{0.875}Ti_{0.125}O$ is half-metallic ferromagnetic with 100 % spin polarisation and it can be considered as a potential compound for spintronics applications.

3.3 Magnetic properties

3.3.1 Magnetic Moments

The origin of magnetism in the compound $Ba_{0.875}Ti_{0.125}O$ is due to the localisation of the partially occupied 3d states of Ti of the majority spins around E_F . The Fig. 4 of partial DOS of majority spins shows that the e_g states are unoccupied, while the t_{2g} states are two-thirds filled which means that they are partially occupied by two electrons. Therefore, the two unpaired electrons created a total magnetic moment of $2 \mu_B$, where the μ_B is the Bohr magneton. The computed total and partial magnetic moments of Ba, Ti and O atoms and in the interstitial sites of $Ba_{0.875}Ti_{0.125}O$ compound are given in Table 3. We have found that the magnetic moment of Ti of $1.778 \mu_B$ is reduced less than $2 \mu_B$ and small magnetic moments are induced at the Ba, O and interstitial sites owing to the p-d interaction. The negative magnetic moment of oxygen (O) means that the interaction is anti-ferromagnetic between the (Ba, Ti) and O

magnetic spins. The ferromagnetic interaction is generated between Ba and Ti owing to their positive magnetic moments.

3.3.2 Exchange couplings

The exchange couplings between the conduction and valence bands and 3d (Ti) states are explained by the $N_0\alpha$ and $N_0\beta$ exchange parameters. The $N_0\alpha$ determines the s-d exchange coupling between the s-type conduction and 3d (Ti) states, whereas the p-d exchange coupling between the p-type valence and 3d (Ti) states is described by the $N_0\beta$. These two important parameters are calculated by using the mean-field theory, given by the following expressions [45, 46] :

$$N_0\alpha = \frac{\Delta E_c}{x \langle s \rangle} \quad (1)$$

$$N_0\beta = \frac{\Delta E_v}{x \langle s \rangle} \quad (2)$$

where the $\Delta E_c = E_c^\downarrow - E_c^\uparrow$ and $\Delta E_v = E_v^\downarrow - E_v^\uparrow$ correspond respectively to the conduction and valence band-edge spin-splittings at Γ high symmetry point of spin-polarised band structures of $\text{Ba}_{0.875}\text{Ti}_{0.125}\text{O}$. The $\langle s \rangle$ is the half computed total magnetic moment per Ti and $x = 0.125$ is the concentration of Ti atom [45]. Table 4 gives the calculated $N_0\alpha$ and $N_0\beta$ exchange parameters of $\text{Ba}_{0.875}\text{Ti}_{0.125}\text{O}$ compound. It shows that the $N_0\alpha$ is positive and $N_0\beta$ is negative, which suggest that the exchange couplings between 3d (Ti) and conduction and valence bands are respectively ferromagnetic and anti-ferromagnetic.

3.3.3 Crystal field energy and exchange splitting

The magnitude of ferromagnetism is measured by the use of other factors such as crystal field energy and direct exchange splitting. The crystal field energy ($\Delta E_{CF} = E_{e_g} - E_{t_{2g}}$) is defined as the difference energies between E_{e_g} and $E_{t_{2g}}$ of e_g and t_{2g} states, respectively. The direct exchange splitting ($\Delta_x(d) = d\downarrow - d\uparrow$) determines the energy separation between the unoccupied ($d\downarrow$) and occupied ($d\uparrow$) peaks of 3d (Ti) states respectively for minority and majority spins. It has been reported that the ferromagnetic state in $\text{Ca}_{0.875}\text{Ti}_{0.125}\text{O}$ compound is mainly contributed by the crystal field energy than that of the exchange splitting [7]. For our $\text{Ba}_{0.875}\text{Ti}_{0.125}\text{O}$ material, the Fig. 4 depicted that the e_g states are located at a high energy compared to the unoccupied ($d\downarrow$) minority-spin states, but the peaks of ($d\uparrow$) and t_{2g} partially occupied states of majority spins occur at the same level with respect to E_F , and

hence, the crystal field energy (ΔE_{CF}) is more dominated than that of the direct exchange splitting $\Delta_x(d)$. This result is revealed by the smaller value of 3.755 eV of the direct exchange splitting compared to the crystal field energy of 4.136 eV as seen in Table 4. This kind of process means that the ferromagnetism state is more favourable by the contribution of the crystal field energy compared to the indirect exchange.

4 Conclusion

We have used the GGA-WC approximation and the TB-mBJ semi-local exchange correlation potential to characterise the structural properties, electronic structures, half-metallic ferromagnetism, exchange constants, crystal field energy and exchange splitting in $\text{Ba}_{1-x}\text{Ti}_x\text{O}$ doped with titanium (Ti) impurity at the concentration $x = 0.125$ such as $\text{Ba}_{0.875}\text{Ti}_{0.125}\text{O}$ compound. The calculated structural parameters of BaO bulk agree with theoretical and experimental results due to the performance of GGA-WC for predicting structural properties. For $\text{Ba}_{0.875}\text{Ti}_{0.125}\text{O}$ compound, the decrease in the lattice parameter leads to the increase in bulk modulus compared to the BaO, these changes result from the size difference between the ionic radii of the Ba atom and the substituted Ti impurity. The calculations of TB-mBJ potential reveal that the BaO has a semiconductor character with wide direct band gap, whereas the $\text{Ba}_{0.875}\text{Ti}_{0.125}\text{O}$ doping compound has a half-metallic ferromagnetic behavior with integral total magnetic moment and spin polarisation of 100 %. The ferromagnetic state in $\text{Ba}_{0.875}\text{Ti}_{0.125}\text{O}$ is more favourable by the crystal field contribution than that of the direct exchange splitting. Therefore, the $\text{Ba}_{0.875}\text{Ti}_{0.125}\text{O}$ doping material is an accurate half-metallic ferromagnet and it can be predicted as a potential candidate for possible applications in semiconductors spintronics.

Disclosure statement

No potential conflict of interest was reported by the author(s).

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Table 1 Calculated lattice constants (a), bulk modules (B) and their pressure derivatives (B') of BaO and Ba_{0.875}Ti_{0.125}O with other theoretical and experimental data.

Compound	a (Å)	B (GPa)	B'	Method
This work				GGA-WC
BaO	5.506	78.60	5.03	
Ba _{0.875} Ti _{0.125} O	5.393	83.35	4.86	
Other calculations				
BaO	5.539 [26] 5.525 [27]	75.6 [28]	5.67 [29]	Experimental
	5.507 [16]	78.59 [16]	4.91 [16]	GGA-WC
	5.594 [11]			GGA-PBE
	5.58 [30]			GGA-PBE
	5.604 [31]	75 [31]	4.1 [31]	GGA-PBE
	5.478 [32]	82.36 [32]	4.21 [32]	LDA

Table 2 Computed direct gap E^{xx} of BaO, half-metallic ferromagnetic gap (G_{HMF}) and half-metallic gap (G_{HM}) of minority-spin bands of Ba_{0.875}Ti_{0.125}O with other theoretical and experimental data.

Compound	G_{HMF} (eV)	G_{HM} (eV)	E^{xx} (eV)	Method	Behavior
This work				TB-mBJ	
BaO			3.476		
Ba _{0.75} Ti _{0.25} O	2.701	0.803			HMF
Other calculations					
BaO			1.884 [16]	GGA-WC	
			2.08 [11]	GGA-PBE	
			2.32 [30]	GGA-PBE	
			2.0 [38]	GGA-PBE	
			2.14 [39]	GGA-PBE	
			3.88 [40] 4.1 [41] 3.985 [42]	Experimental	

Table 3 Calculated total and partial magnetic moments and in the interstitial sites of $\text{Ba}_{0.875}\text{Ti}_{0.125}\text{O}$.

Compound	Total (μ_B)	Ti (μ_B)	Ba (μ_B)	O (μ_B)	Interstitial (μ_B)
$\text{Ba}_{0.75}\text{Ti}_{0.25}\text{O}$	2	1.778	0.002	-0.012	0.234

Table 4 Computed sp-d exchange constants $N_0\alpha$ and $N_0\beta$, crystal field energy ΔE_{CF} and direct exchange splitting $\Delta_x(d)$ of $\text{Ba}_{0.875}\text{Ti}_{0.125}\text{O}$.

Compound	$N_0\alpha$	$N_0\beta$	$\Delta_x(d)$ (eV)	ΔE_{CF} (eV)
$\text{Ba}_{0.875}\text{Ti}_{0.125}\text{O}$	1.344	-2.273	3.755	4.136

Fig. 1 Band structures of BaO.

Fig. 2 Spin-polarized band structures of $\text{Ba}_{0.875}\text{Ti}_{0.125}\text{S}$, (a) Majority spins (*up*) and (b) Minority spins (*dn*)

Fig. 3 Spin-polarized total densities of states (DOS) of Ba, O and Ti atoms and total-DOS in $\text{Ba}_{0.875}\text{Ti}_{0.125}\text{O}$ supercell.

Fig. 4 Spin-polarized partial densities of states of d (Ti), t_{2g} -d (Ti), e_g -d (Ti), p (Ba) and p (O) in $\text{Ba}_{0.875}\text{Ti}_{0.125}\text{O}$ supercell.

Figures

Figure 1

Band structures of BaO.

Figure 2

Spin-polarized band structures of $\text{Ba}_{0.875}\text{Ti}_{0.125}\text{S}$, (a) Majority spins (up) and (b) Minority spins (dn)

Figure 3

Spin-polarized total densities of states (DOS) of Ba, O and Ti atoms and total-DOS in Ba0.875Ti0.125O supercell.

Figure 4

Spin-polarized partial densities of states of d (Ti), t2g-d (Ti), eg-d (Ti), p (Ba) and p (O) in Ba0.875Ti0.125O supercell.