Mechanical Stability, Magnetic and Electronic Properties of Sr$_{1-x}$Ba$_x$FeO$_3$: DFT+U Study

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We provide a thorough study of the structural, elastic, electronic and magnetic properties of the perovskite solid solution Sr$_{1-x}$Ba$_x$FeO$_3$ within the framework of density functional theory (DFT), using the full-potential linearized augmented plane wave plus local orbital FP-(L)APW+lo method. The found results provide predictions for the mixed perovskite solid solution Sr$_{1-x}$Ba$_x$FeO$_3$ ($x = 0.25$, $0.5$, $0.75$) for which no experimental or theoretical data are presently available. These compounds were supposed to have a cubic ferromagnetic structure for all compositions. The GGA-PBE functional was chosen for the prediction of the structural properties, in particular the lattice parameter, the bulk modulus and its pressure derivative as well as the cohesive energy. For testing the mechanical stability of the Sr$_{1-x}$Ba$_x$FeO$_3$ compounds, we have studied their elastic constants and it has been found that these compounds are mechanically stable in their cubic perovskite structure. Several parameters related to the elastic constants have also been predicted, in particular Young’s modulus, the shear modulus, Poisson’s ratio, the anisotropic factor and the Debye temperature ($\theta_D$). For the correct treatment of the high correlation of 3d-iron electrons, the Hubbard correction and TB-mBJ potential were added to the GGA-PBE functional for the analysis of the electronic and magnetic properties of Sr$_{1-x}$Ba$_x$FeO$_3$.

It has been found that they are half-metals with a total magnetic moment of $\sim 4\mu_B$ topics: Sr$_{1-x}$Ba$_x$FeO$_3$, DFT, GGA+U, TB-mBJ potential, elastic constants, half-metallic

1. Introduction

Iron-based perovskites AFeO$_3$ (A = Ca, Sr and Ba) belonging to the ferro-perovskites family represent a small class of compounds that contain an iron atom in a high-valence state of Fe$^{4+}$ [1–8]. These compounds are of great interest in several application fields, particularly in spintronic technology [5, 9], thanks to their high spin-polarization of the conducting charge. Otherwise, compounds whose spin polarization near the Fermi level is 100% are called half-metals [10, 11].

In a ferro-perovskite, the introduction of an “A” element by substitution with a “B” element can improve its electronic and magnetic properties which motivated us to undertake a study with the aim to understand and predict the structural, electronic and magnetic behaviors of Ba$_x$Sr$_{1-x}$FeO$_3$. Matsui et al. have reported that BaFeO$_3$ thin film has a pseudo-cubic perovskite structure with a cell parameter of 0.412 nm [12, 13]. On the other hand, a deposition of BaFeO$_3$ by a pulsed laser on SrTiO$_3$ substrates gave a stoichiometry of cubic BaFeO thin films which are ferromagnetics insulating at room temperature [14, 15]. The magnetocaloric effect (MCE) of BaFeO$_3$ perovskite oxide has been investigated by M. Mizumaki et al. [16] and they found by the application of a small external magnetic field that this compound is a ferromagnetic. Moreover, S. Chakraverty et al. [17] have reported that BaFeO$_3$ has an optical gap of 1.8 eV and a saturation magnetization with a Curie temperature of $3.2\mu_B$/formula unit and 115 K.

SrFeO$_3$ is a metal with a cubic perovskite structure which also characterizes the helical spin order below $T_N = 134$ K [18, 19]. The application of a hydrostatic pressure on this compound promotes its transition between ferromagnetic and antiferromagnetic phases [20, 21]. Furthermore, and according to many theoretical results, SrFeO$_3$ is a ferromagnetic compound [22]. The DFT+U study of the high-pressure ferromagnetic phase transition of BaFeO$_3$ and SrFeO$_3$ under high pressure was the subject of Li et al.’s study [23], in which they found that the cause was the enhanced hybridization.

Cubic iron-based perovskites have a general formula of AFeO$_3$ whose space group is Pm-3m, in which atom positions of different atoms are: A (0.0; 0.0; 0.0), Fe (0.5; 0.5; 0.5) and O (0.0; 0.5; 0.5).

According to our knowledge, there are not only very few experimental but also no theoretical reports on the structural, electronic and magnetic behavior of Ba$_x$Sr$_{1-x}$FeO$_3$. Nevertheless, N. Hayashi et al. [24] have studied the structural and electronic properties of Ba$_x$Sr$_{1-x}$FeO$_3$ cubic
compounds by XRD, ND and magnetization measurements. This study was realized after they have successfully synthesized them.

In their paper, A. Iio et al. [25] have demonstrated that there is a possible application of these perovskites as a sensing electrode material (SE) and as potentiometric yttria-stabilized zirconia (YSZ)-based oxygen sensors for solid-state. Recently, K. Yoshii et al. [26] reported that Sr$_{x}$Ba$_{1-x}$FeO$_{3}$ perovskite is a candidate for magneto-caloric effect (MCE) material.

In the present theoretical work, we focused on the effect of Sr substitution on the structural, mechanical stability, electronic and magnetic behaviors of BaFeO$_{3}$ ferromagnetic cubic perovskite, namely, Sr$_{x}$Ba$_{1-x}$FeO$_{3}$ with $x = 0, 0.25, 0.5, 0.75, 1$.

This paper is organized as follows: in Sect. 2 we give a description of the computational method. In Sect. 3, we show all our results including structural, elastic, electronic and magnetic properties of Sr$_{x}$Ba$_{1-x}$FeO$_{3}$ ($x = 0, 0.25, 0.5, 0.75, 1.0$) with detailed discussion and interpretations. Finally, in Sect. 4, we summarize our conclusions.

2. Computational methods

Structural, elastic, electronic and magnetic properties of Sr$_{x}$Ba$_{1-x}$FeO$_{3}$ (with $x = 0, 0.25, 0.5, 0.75, 1$) were predicted using the first principles full-potential linearized augmented plane wave plus local orbital (FP-$(L)$APW+$lo$) method as implanted in WIEN2K package [27, 28]. The exchange-correlation potentials are treated using the generalized gradient approximation (GGA) of the Perdew, Burke, and Ernzerhof (PBE) functional [29].

The semilocal functionals (LDA or GGA) do not treat electronic and magnetic properties of solid materials with accuracy because they do not consider high correlations between the electrons of the heavy atoms. To resolve this problem, several theoretical models have been proposed. In this work, we have used the Hubbard correction term “$U$” which is added to the GGA-PBE semilocal functional with the already determined value of 3.1 eV [23, 30, 31].

To improve the prediction of the band-gap energies of Sr$_{x}$Ba$_{1-x}$FeO$_{3}$, the modified Becke-Johnson potential by Tran and Blaha (TB-mBJ) [32] has also been used. This choice is motivated by the success of this potential in the prediction of the band-gap energy of solid materials which gives very close values to those of the experimental. The muffin-tin radii for Ba/Sr, Fe and O are taken as 2.20, 1.80 and 1.75 a.u., respectively. The maximum value for partial waves inside the atomic sphere was $l_{max} = 10$. We have used a plane wave cutoff $R_M a K_{max} = 9$ to expand the wave functions in the interstitial region that provides good convergence for the matrix size and 2500 $k$-points in the integration of the Brillouin zone for the convergence of energy eigenvalues. The calculations are obtained with a self-consistent convergence of total energy at $10^{-4}$ Ry.

3. Results and discussion

3.1 Structural properties

To predict the elastic, electronic and magnetic properties of Ba$_{x}$Sr$_{1-x}$FeO$_{3}$ compounds in the cubic structure, it is necessary to determine their structural properties first by determining their cell parameters ($a_0$) as well as the equilibrium volume ($V_0$), the bulk modulus ($B$) and total energy ($E_0$). This property also allows determining the most stable magnetic phase by predicting the total energy of the unit cell (the most stable phase is that of the lowest energy). All this information can be obtained by varying the volume as a function of the unit cell volume by fitting the curve with the Murnaghan equation [33]. We note here that according to our results, SrFeO$_{3}$ and BaFeO$_{3}$ are ferromagnetic compounds because their most stable energies correspond to that of the ferromagnetic phase, which confirms the previous experimental and theoretical results [14, 22, 23].

It is noted that the obtained values of the cell parameters and the bulk modulus for BaFeO$_{3}$ and SrFeO$_{3}$ are very close to those obtained previously. For all compositions ($x = 0, 0.25, 0.5, 0.75$ and 1), it is important to note the absence of any previous results for the heat of formation, as well as the derivative pressure of the bulk modulus. We also note the absence of all comparison results for $x = 0.25, 0.50$ and 0.75.

Figure 1 shows the variation of the lattice constant and the bulk modulus as a function of the Sr composition, where the lattice constant falls with decreasing Sr-composition. This result can be explained by the fact that the atomic radius of Ba is greater than that of Sr-atom and the bonding nature has not changed (no changes in the interatomic distance). Otherwise, bulk modulus increases with concentration ($x$) which proves that the substitution of Sr-atom strengthens the hardness of the crystal system.

![Fig. 1. Comparison between the lattice parameter and bulk modulus for Sr$_{x}$Ba$_{1-x}$FeO$_{3}$ alloys using Vegard’s law as a function of composition $x$.](image-url)
TABLE I

Calculated equilibrium lattice parameter $a$ (Å), bulk modulus $B$ (GPa), pressure derivative of the bulk modulus $B'$ and the cohesive energy (eV/atom) of $\text{Sr}_x\text{Ba}_{1-x}\text{FeO}_3$ for various compositions, compared to some experimental [17, 22] and other theoretical [18, 23, 35, 36] works.

| $x$ | $a$  | $B$   | $B'$  | $E_{\text{coh}}$ |
|-----|------|-------|-------|------------------|
| 0   | 3.96 | 139.01| 4.79  | $-5.57$          |
| 0.25| 3.94 | 141.5 | 4.44  | $-5.63$          |
| 0.5 | 3.91 | 144.32| 5.02  | $-5.61$          |
| 0.75| 3.88 | 147.07| 5.27  | $-5.59$          |
| 1   | 3.85 | 149.2 | 4.83  | $-5.67$          |

*Ref. [17], †Ref. [23], ‡Ref. [36], §Ref. [35], ¶Ref. [22], ⊱Ref. [18]

We also note that the variation of the cell-parameter as a function of $x$ Sr-composition is almost linear and obeys Vegard’s law [34], with marginal upward bowing parameters of $-0.0116$ Å. The variation of bulk modulus as a function of $x$ Sr-composition has also upward bowing which is equal to $-0.9$ GPa. These values were obtained by a second order polynomial fitting of the calculated data. In fact, we find that the bulk modulus of $\text{BaFeO}_3$ is $6.8\%$ higher than that of $\text{SrFeO}_3$. This result suggests the existence of a significant downward bowing of the bulk modulus.

In Table I, we also presented the obtained values of the cohesive energy for all Sr-compositions. This quantity is defined as the difference between the total energy of isolated atoms that form the solid and its unit cell energy:

$$E_{\text{coh}}^{\text{Sr}_x\text{Ba}_{1-x}\text{FeO}_3} = E_{\text{Sr}_x\text{Ba}_{1-x}\text{FeO}_3} - (xE_{\text{Sr}} + (1-x)E_{\text{Ba}} + E_{\text{Fe}} + 3E_{\text{O}}).$$

3.2 Elastic properties

The study of the mechanical stability of a solid material is important and essential to start any other physical study. The elastic model achieves this objective by the prediction of the elastic constants $C_{ij}$. It also makes it possible to predict other related physical quantities for which their knowledge is very valuable, notably the Zener mechanical anisotropy factor $A$, the shear modulus $G$, Young’s modulus $E$, Poisson’s ratio $\nu$ and the Debye temperature. Their relations are given as:

$$A = \frac{2C_{44}}{C_{11} - C_{12}},$$

$$G = \frac{1}{5} (C_{11} - C_{12} + 3C_{44}).$$

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The calculated shear modulus $G$ (GPa), ratio of $B/G$, Young’s modulus $E$ (GPa), Poisson’s ratio $\nu$ and the Zener anisotropy factor $A$ of $\text{Sr}_x\text{Ba}_{1-x}\text{FeO}_3$ for various compositions.

| $x$ | $G$   | $B/G$ | $E$   | $\nu$ | $\varepsilon$ | $A$  |
|-----|-------|-------|-------|-------|---------------|-----|
| 0   | 85.08 | 1.63  | 211.99| 0.25  | 1.59          |     |
| 0.25| 91.17*| 1.74* | 229.65*| 0.26* | 1.55*         |     |
| 0.5 | 90.54 | 1.56  | 223.88| 0.24  | 1.51          |     |
| 0.75| 92.03 | 1.57  | 227.68| 0.24  | 1.43          |     |
| 1   | 93.38 | 1.57  | 231.20| 0.24  | 1.33          |     |
| 102.41* | 1.72* | 257.32*| 0.26* | 1.33* |               |     |

*Ref. [35]

It is important to note that according to Tables II and III, the obtained results of the elastic constants and their related mechanical quantities are in good agreement with the previous works that are available [35].

3.3 Electronic and magnetic properties

The study of the electronic and magnetic properties of $\text{Sr}_{1-x}\text{Ba}_x\text{FeO}_3$ represents the main objective of our work because information about these behaviors is precious to the experimentalists in classifying these materials according to their electronic importance and to propose their possible applications.

The analysis of the band structure and density of states allows to obtain knowledge about any solid material and its classification. The application of the semilocal functional including GGA and LDA makes it possible to precisely identify the nature of the band-gap but the functionals largely underestimate its value as they do not treat with accuracy the systems possessing highly correlated electrons including iron-based materials such as in the case of $\text{Sr}_{1-x}\text{Ba}_x\text{FeO}_3$.

Several theoretical models have been proposed to solve the problem of the large underestimation of the band-gap value by the semilocal functional including the potential of Becke-Johnson modified by Tran and Blaha [32] which is a well-known model. For the treatment of the highly correlated system, the Hubbard correction made to the
The semilocal functional represents a powerful method for this kind of study. In our work, we used the TB-mBJ potential [32] that was brought to GGA+U functional to calculate the band structures of Sr$_{1-x}$Ba$_x$FeO$_3$ which are illustrated in Figs. 3–7, and whose most ideal path (the path which makes it possible to scan the different directions of the first Brillouin zone for a cubic symmetry structure of Pm-3m space group) is given by the following high-symmetry points: \( R - \Gamma - X - M - \Gamma \).

According to the band structures of Sr$_{1-x}$Ba$_x$FeO$_3$, it is noted that the Fermi level passes through the middle of the valence band top for the spin-up states with the presence of a total band-gap (Spin-Up/Dn) which indicates a half-metallic behavior of these compounds. Note also that for BaFeO$_3$, SrFeO$_3$ and Sr$_{0.5}$Ba$_{0.5}$FeO$_3$, the fundamental band-gap is of indirect nature formed by the valence band top located at the \( R \) point of high symmetry and the conduction band...
bottom is located at $\Gamma$ point of high symmetry. However, for the other studied materials in this work (Sr$_{1-x}$Ba$_x$FeO$_3$ with $x = 0.25$ and $0.75$), the fundamental band-gap is of direct nature between the valence band top and the conduction band bottom which are located at the same $\Gamma$ point of high symmetry.

The study of the spin polarization allows the prediction and confirmation of half-metallicity of Sr$_{1-x}$Ba$_x$FeO$_3$ which is identified by the following relation:

$$P = \frac{n(\uparrow) - n(\downarrow)}{n(\uparrow) + n(\downarrow)},$$

where $n(\uparrow)$ and $n(\downarrow)$ are respectively the spin Up and Down densities of states at the Fermi level. The spin polarizations of Sr$_{1-x}$Ba$_x$FeO$_3$ are 100% which confirms the half-metallicity behavior of these compounds. These results confirm previous work for the case of BaFeO$_3$ perovskite [23] and we observe that there is a lack of results for the other studied materials.

Table V summarizes all the obtained results for the band-gap values for different materials studied in this work. Note that for BaFeO$_3$, the band gap value estimated by GGA+U with the TB-mBJ potential is close to that found experimentally, unlike that obtained by GGA+U only. This remark allows us to predict that the obtained values with the TB-mBJ potential added to GGA+U will be close to the experimental values for other compounds once measured. These results make it possible to highlight the importance of these materials and allowed them to be proposed to experimentalists for possible spintronic applications.

| Compound          | Method          | $E_{gHM}$ |
|-------------------|-----------------|-----------|
| BaFeO$_3$         | GGA+U           | 0.68578 (R–$\Gamma$) |
|                  | mBJ             | 2.09064 (R–$\Gamma$) |
|                  | Exp             | 1.8 optical gap |
| Sr$_{0.25}$Ba$_{0.75}$FeO$_3$ | GGA+U           | 0.6525 (R–$\Gamma$) |
|                  | mBJ             | 2.16995 (R–$\Gamma$) |
| Sr$_{0.5}$Ba$_{0.5}$FeO$_3$ | GGA+U           | 0.63486 (R–$\Gamma$) |
|                  | mBJ             | 2.20296 (R–$\Gamma$) |
| Sr$_{0.75}$Ba$_{0.25}$FeO$_3$ | GGA+U           | 0.611191 (R–$\Gamma$) |
|                  | mBJ             | 2.21771 (R–$\Gamma$) |
| SrFeO$_3$         | GGA+U           | 0.54132 (R–$\Gamma$) |
|                  | mBJ             | 2.15921 (R–$\Gamma$) |

Table VI gathers all the obtained results of the partial and total magnetic moments ($\mu_B$) of Sr$_{1-x}$Ba$_x$FeO$_3$ for various compositions.

$$x$$ | $M_{up}$ | $M_{dn}$ | $M_{tot}$ | $M_{int}$ | $M_{nat}$ |
|-------|--------|---------|---------|---------|---------|
| 0     | 0.009  | –       | 3.591   | 0.080   | 0.162   | 4.001   |
| 0.25  | 0.011  | 0.007   | 3.543   | 0.086   | 0.173   | 3.992   |
| 0.5   | 0.010  | 0.006   | 3.539   | 0.092   | 0.174   | 4.005   |
| 0.75  | 0.012  | 0.007   | 3.527   | 0.096   | 0.178   | 4.012   |
| 1     | –      | 0.005   | 3.542   | 0.089   | 0.191   | 4.005   |

The analysis of the density of states makes it possible to understand the formation of the bands and the determination of different states which form these bands. The valence band top and the conduction band bottom are the most important regions for a solid material because they are responsible for most of their physical properties. It can be observed from the Sr$_{1-x}$Ba$_x$FeO$_3$ curves of the density of states (Figs. 8–12) that the valence band top is dominated by a very high contribution of $d$ states of iron in hybridization with $p$ states of oxygen. The conduction band bottom of Sr$_{1-x}$Ba$_x$FeO$_3$ is dominated by $d$ states of iron, strontium and barium.

Table VI gathers all the obtained results of the partial and total magnetic moments which are acquired by GGA+U approximation. We note that the total magnetic moment is calculated according to the number of each atom in the unit-cell [M([x]Ba) + M([1–x]Sr) + M(Fe) + 3M(O) + M(int)]. The values are very close to 4$\mu_B$ due to a strong contribution of the Fe total moment (its value is $\sim$ 3.5$\mu_B$ which is equivalent to 88.5% of the total magnetic moment) whose quantity in the unit cell does not change with the change of the $x$ compositions between Ba and Sr, and for this reason, the magnetic moment changes slightly with the $x$ change. The magnetic moment values of Fe are in agreement with the previously found values [16, 30]. These remarks make it possible to classify these compounds as promising materials for spintronic technology.
4. Conclusion

In this paper, we have studied the structural, elastic, electronic and magnetic properties of Sr$_x$Ba$_{1-x}$FeO$_3$ perovskite (with $x = 0, 0.25, 0.5, 0.75, 1$) using the full-potential linearized augmented plane wave plus local orbital method (FP-(L)APW+lo) in the framework of the density functional theory as implemented in WIEN2K package.

The GGA-PBE exchange-correlations functional was used to study the structural properties such as the lattice constant, bulk modulus, its pressure derivatives and the cohesive energy. We have also predicted the elastic constants $C_{ij}$, the shear modulus and the Debye temperature $\theta_D$. Our results need to be confirmed by future studies due to the lack of any experimental data. These compounds are mechanically stable because their elastic constants satisfy the elastic stability criteria. A linear variation of the lattice constant and the bulk modulus with $x$ Sr-composition has been obtained. GGA+U within TB-mBJ potential were used for the treatment of the electronic and magnetic properties and we found that Sr$_x$Ba$_{1-x}$FeO$_3$ have a half-metallic behavior with a total magnetic moment of $4\mu_B$.

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