Behavior of the cubic double perovskite compound $\text{Pb}_2\text{FeTaO}_6$ through mechanical, electronic and magnetic properties via Ab-initio calculations

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Research Article

Keywords: Perovskite materials, DFT calculations, magnetic properties, TB-mBJ, GGA+U

Posted Date: October 20th, 2020

DOI: <https://doi.org/10.21203/rs.3.rs-87550/v1>

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Abstract

The structural, elastic, electronic and magnetic properties of cubic double perovskite $\text{Pb}_2\text{FeTaO}_6$ have been investigated using self-consistent ab-initio calculation through full-potential linearized augmented plane wave (FP-LAPW) method within the frame work of the spin-polarized density functional theory (DFT), considering generalized gradient approximation (GGA) described by Perdew–Burke–Ernzerhof (PBE), GGA+U and mBJ-GGA. $\text{Pb}_2\text{FeTaO}_6$ is found as ductile material from the elastic calculations. The obtained magnetic results show that $\text{Pb}_2\text{FeTaO}_6$ is stable in the ferromagnetic state; the electronic properties show a half-metallic behavior using GGA and GGA+U and a semiconducting one with TB-mBJ, magnetic moments of each atom are also discussed in this study. These results confirm the use of this compound in spintronic devices.

1. Introduction

Perovskites have the formula ABX_6 , in this type of structure; A represents a large electropositive cation, B is a small transition metal or main group ion, and X is commonly an oxide or halide ion. These materials have received much attention because of their interesting superconductivity, catalytic characteristics, oxygen cathode reduction, and the electro- magnetic properties [1–3]. Double perovskites (DP's) have the general formula $\text{A}_2\text{BB}'\text{O}_6$, proposed by Longo and Ward [4], where A is an alkaline earth, and B and B' are 3d, 4d, and/or 5d transition metals belong to a very broad family of oxide compounds crystallising in the perovskite structure.

Recently, research on this class of materials has increased, since these compounds are used in different range of applications. They have attracted a lot of attention due to their magnetic and electronic properties, including half metallicity, ability to support superconductivity [5], low field magnetoresistance (LFMR) [6–7] and a variety of magnetic structures [8]. All these properties have made this type of materials promising in the technological field such as in hard drives, nonvolatile magnetic random access memory (MRAM) [9] and spintronic devices [10].

The close relation between conduction electrons and magnetic electrons makes an exchange interaction between ions of the same element; this explains the link between the electronic and magnetic properties in double perovskite by scanning the range of different materials with several behaviours from a metallic ferromagnetic or ferrimagnetic to antiferromagnetic or paramagnetic one [11]. There are many studies of half-metallic ferromagnetic compounds due to their potential technological application such as Sr_2CrWO_6 [12], $\text{Sr}_2\text{FeReO}_6$ [13, 14], $\text{Pb}_2\text{FeMoO}_6$ [15], Sr_2FeWO_6 [16], $\text{Sr}_2\text{CoMoO}_6$ [17], $\text{Sr}_2\text{CrMoO}_6$ [18], $\text{Sr}_2\text{FeTiO}_6$ [19] and recently $\text{Sr}_2\text{GdReO}_6$ [20]. $\text{Pb}_2\text{FeTaO}_6$ is among these DP's which has received a lot of interest from the authors Brixel et al [21, 22], they have experimentally worked on the growth of single crystal of this material for studding both of electrical and optical measurements.

Double perovskites (DP's) have different structures, which are mainly related to the difference in charge and the size of cations B_1 and B_2 , if these cations are large enough, they will order three- dimensionally and thus leading to a double unit cell parameter with the space group Fm3m in the ideal cubic case [23]. Through this work, we expect to give details about calculations done by the use of generalized gradient approximations GGA, GGA + U and GGA plus Trans-Blaha-modified Becke– Johnson (TB-mBJ-GGA) exchange correlation method. The structural, electronics and magnetic properties of the cubic (DP) compound $\text{Pb}_2\text{FeTaO}_6$ are calculated with the full-potential linearized augmented plane wave (FP-LAPW) method based on density functional theory (DFT) as implemented in the WIEN2k code.

2. Computational Details

The calculations has been performed by using both full potential and linear augmented plane wave (FP-LAPW) method based on the density-functional theory (DFT) [24, 25] as implemented in the WIEN2K code [26]. For the exchange-correlation contribution, we employ the generalized gradient approximation GGA [24, 25, 27] also the modified Becke– Johnson (TB-mBJ) exchange potential [28, 29] and GGA+U [30], where U is on-site Coulomb interaction correction for treating the exchange-correlation functional in order to generate good magnetic properties. The unit cell for the double perovskite compound $\text{Pb}_2\text{FeTaPO}_6$ is crystallized in the cubic structure space group (225) Fmm, where atomic positions in this unit cell are Pb atoms at (0.25, 0.25, 0.25), Fe at (0, 0, 0.5), Ta at (0, 0, 0) and six O atoms at (0, 0, 0.2531) (Fig. 1).

In this first study which is reported here, we change the first set of guidelines as $R_{\text{mt}}K_{\text{max}}=8.0$ where R_{mt} indicates the smallest atomic sphere radius and K_{max} is the maximum value of the largest K vector in the plane wave expansion and the angular momentum vector

is held at $I_{\text{max}} = 10$. The total Brillouin zone is sampled with 1000 k -points to perform integration over the first Brillouin zone BZ. The self-consistent calculation is considered to have an energy convergence when it reaches 10^{-4} Ry per formula unit. In this calculation, the Fe-3d orbital transition metal is strongly correlated with different U values (where U= 0, 2, 4, 6 and 8 eV).

3. Results And Discussion

3. 1. Structural properties

The present study reports the structural, electronic and magnetic properties of double perovskite $\text{Pb}_2\text{FeTaPO}_6$. We consider the $Fm\bar{3}m$ (no. 225) cubic unit cell containing 40 atomic positions as seen in Fig. 1. The energy of the each unit cell is calculated by the FP-LAPW method within the DFT. To achieve the optimization of structure and geometry of the crystal, Birch Murnaghan's equation of state [31] is used to fit the total energy with the change in the volumes to obtain the equilibrium lattice constant, bulk modulus and its pressure derivative and the stable magnetic structure. The calculated structural parameters of the material are shown in **Table 1**.

Table 1
Calculated values of the total minimum energy, lattice parameter a_0 , bulk modulus B and derivative of bulk modulus B' for nonmagnetic (NM), ferromagnetic (FM) and antiferromagnetic (AFM) state of $\text{Pb}_2\text{FeTaO}_6$.

$\text{Pb}_2\text{FeTaO}_6$	Mag	Energy E_0 (Ry)	a_0 (Å)	B (GPa)	B'
GGA_PBE	NM	-473663.6990	8.16214	187.2281	4.1661
	FM	-473663.7628	8.0338	109.5556	5.6189
	AFM	-473663.7518	7.9737	111.7386	6.7660

Using the GGA-PBE approximation, the calculated total energies as function of unit cell volume were fitted by Birch Murnaghan equation of state [31] as follows:

$$E(V) = E_0 + \frac{B_0}{B'(B'-1)} \left[V \left(\frac{V_0}{V} \right)^{B'} - V_0 \right] + \frac{B_0}{B'} (V - V_0) \tag{1}$$

On **Fig. 2**, the curves of total energy versus volume are shown for GGA approximation. We can see that the curvature of total energy of the ferromagnetic (FM) state is more pronounced than the total energy of antiferromagnetic (AFM) state which gives a positive value of the total energy difference: $\Delta E = E_{\text{AF}} - E_{\text{FM}}$ (see Table 1), so $\text{Pb}_2\text{FeTaPO}_6$ is stable in the FM phase.

The lattice parameters obtained are in good agreement with the experimental results [32]. From the obtained results in **Table 1**, we have found that the total energy of ferromagnetic state is lower than the ones of antiferromagnetic and non-magnetic states for the GGA approximation. It is also important to notice, that there is no experimental reports for the bulk modulus, however there is an experimental one available for $\text{Pb}_2\text{FeTaO}_6$, which is concern the lattice parameter.

3.2. Elastic properties

The study of mechanical properties of materials can play an important role in explicate the structural stability and the binding characteristic [33]. The cubic systems are requisite only three independent elastic constants (C_{11} , C_{12} , and C_{44}) to explain the mechanical stability that is shown in **Table 2**. It is found that all values of elastic constants positive are obey the generalized mechanical Born-Huang mechanical stability conditions $C_{11}-C_{12}>0$, $C_{11}+2C_{12}>0$, $C_{44}>0$ and $C_{12}<B<C_{11}$ [34], which signify the stability of this double perovskite in cubic structure. By Voigt-Reuss-Hill [35-37], we calculated the values of elastic moduli (Bulk modulus (B), Young modulus (Y), as well as the Shear modulus (G)) which have been shown in **Table 2**. The essential mechanical parameter, Young's modulus Y, provides the degree of stiffness of a compound and is clear as the tensile stress to the tensile strain ratio [38]. Higher value of Young's modulus significant that the material as stiffer. It can be calculated by applying the following equation $Y = \frac{E}{1+\nu}$. The calculated value of Y is 254.880 GPa which is very large, for this reason $\text{Pb}_2\text{FeTaO}_6$ will perform as a stiffer material. For the various applications, the performance of the material should be ductile. In order to confirm the brittleness or ductility type of compounds, Poisson's ratio (ν) was calculated whose critical limit is $\nu=0.26$. Upper this critical limit, the material is ductile and under it is brittle. Our result obtained of Poisson's ratio (ν) shows that the double perovskite $\text{Pb}_2\text{FeTaO}_6$ is ductile. Correspondingly, the Pugh

ratio (B/G) also tells us about flexible and fragile behavior of the studied materials whose critical limit is $B/G=1.75$. The values of B/G and ν in the Hill approximation equal 2.496, 0.323 for Pb_2FeTaO_6 respectively, it also confirmed their ductile nature $P=0$ GPa and $T=0$ K. This ductile nature of Pb_2FeTaO_6 is additional verified from Cauchy pressure ($C_p = C_{12} - C_{44}$), its negative value presents fragile nature and positive value as elastic (see Table 2). Moreover, the calculate of elastic anisotropy is given by Zener anisotropy factor,

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

Table 2 The calculated elastic constants (C_{ij}), Cauchy pressure (C_p), Bulk modulus (B), Shear modulus (G), Young's modulus (Y), Pugh's ratio (B/G) all in GPa, Poisson's ratio (ν), anisotropy constant (A) for Pb_2FeTaO_6

Parameters	C_{11}	C_{12}	C_{44}	B_V	B_R	B_H	G_V	G_R	G_H	Y	ν	B/G	A	C_p
Pb_2FeTaO_6	438.41	141.46	71.57	240.44	240.44	240.44	102.33	90.28	96.30	254.88	0.32	2.49	0.48	69.89

For an isotropic material, the value of A is 1, or else, the material is anisotropic. The calculated value of the anisotropy for Pb_2FeTaO_6 is inferior than 1 ($A= 0.482$), therefore, the material will have elastic anisotropic in nature.

3.3. Electronic properties

3.3.1. Band structure energies

In this work, we have done the calculations of both spin-polarized electronic band structure and density of states of the cubic double perovskite Pb_2FeTaO_6 compound at their stability lattice parameters by using the PBE-GGA, TB-mBJ and GGA + U approximation. The band structures of Pb_2FeTaO_6 compound along the high symmetry directions of the first Brillouin zone are illustrated in Fig 3 for GGA approximation, in Figs 4 and 5 for GGA+U and TB-mBJ respectively. Based on both approximations (GGA and GGA + U), It is evident to note that the energy bands in the valence band cut the Fermi level in the minority -spin states (spin-down case), whereas they are located bottom the Fermi level in majority -spin states (spin-up case), confirming the complete half-metallic characteristic of this compound. Even as the band structure in the minority and majority spin, the configurations shows that, our compound has a space of a semiconductor character between the valance and conductor band using TB-mBJ -GGA approximation. The half-metallic gap (E_{HM}) is known as the minimum between the lowest energy of spin-up and spin-down conduction bands with esteem to the Fermi level, and the absolute values of the maximum energy of majority-spin and minority-spin valence bands [39, 40]. The calculated E_{HM} value with the GGA + U approximation is improved with respect to the GGA approximation; consequently, this improvement is due to the complete relating of 'd' orbitals by GGA + U approximation. Unluckily, no experimental information is existing for this compound to compare. We hope that these results will promote further experimental of this material for different chemical and physical applications.

3.3.2. Electronic density of states

The electronic structure of our compound can be describe during its electronic density of states (DOS) in specify. Figs 3, 4 and 5 shows the total density of states (TDOS) of the cubic double perovskite Pb_2FeTaO_6 compound, where the results confirm the half-metallic character that is proved before by the electronic structure investigations. The Partial Density of States (PDOS) is explicating more the bonding nature of our materials. The rustles of partial density of states (PDOS) of the FM double perovskite Pb_2FeTaO_6 calculated by GGA, GGA+U and TB-mBJ have been plotted in Fig. 6, respectively. From these results, we can observe the offered of a great exchange splitting between spin-up and spin-down electrons in the environs of Fermi level (E_F); in detail, the full-filled orbitals are reported in 3d-Fe states for both majority-spin and minority-spin cases, while the partial-filled orbitals are the 2p-O states of both spin-up and spin down. For Pb_2FeTaO_6 compound, when $U = 4, 6$ and 8 eV, GGA + U approximation indicates a semiconductor behavior for both spins directions, and we remark the same observation for TB-mBJ approximation, we also noticed the increased energy gap value when we increased the value of U (see Table 3). But for $U = 2$ eV; this compound change its behavior from semiconductor to half-metallic character, with a semiconductor behavior for the spins-up ones and with a gap value of energy equivalent to 2.98 eV and however possesses a metallic behavior in the spin-down. The figures illustrate the results obtained for our material double perovskite using the GGA, GGA + U, and mBJ-GGA approximations, where the E_F is indicated by a perpendicular dash line as located at 0.0 eV. The energy spectrum from -7.50 to $+0.40$ eV is essentially dominated by 3d-Fe orbitals of spin-up and spin-down directions with a petite

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occupy the spin-up region approximately at the Fermi level, whereas the

matching 3d-Fe states of spin-up states are mostly dotted in the energy range from -1.95 to +0.40 eV, confirming that 3d-Fe electrons are responsible for the creation of the half-metallic ferromagnetism character within the cubic $\text{Pb}_2\text{FeTaO}_6$ compound. In fact, we observe that the conduction band is mainly assembled by the electrons majority-spin and minority-spin 2p-Pb, 3d-Fe and 3d-Ta orbitals.

Table 3 Calculated energy gap in electron volt (eV) for $\text{Pb}_2\text{FeTaO}_6$ using different approximations GGA, GGA + U (U = 2, 4, 6, 8eV) and TB-mBJ.

$\text{Pb}_2\text{FeTaO}_6$	GGA	GGA+U					mBJ
Energy gap E_g (eV)	0 eV	2 eV	4 eV	6 eV	8 eV		
	--	--	0.812	1.645	1.997		

In order to improve the effect of the parameter U on the double perovskite structure; we have plotted the half-metallic energy versus Hubbard parameter on **Fig. 7**. As we see the maximum of E_{HF} is obtained for U = 2 eV which is beneficial for our choice of this parameter and ensures the half-metallic behavior of $\text{Pb}_2\text{FeTaO}_6$.

3.4. Magnetic properties

In this section, we have investigated the magnetic properties for our double perovskite oxide, because the magnetic interaction plays an essential role in the modern study as well as the importance of magnetic materials in our days as person in different application similar to medicine and the home activity [41-46]. The results relating to the total, local and interstitial magnetic moments for $\text{Pb}_2\text{FeTaO}_6$ calculated using GGA, GGA + U and mBJ-GGA is assembled in Table 3. This study shows that the total magnetic moment for the $\text{Pb}_2\text{FeTaO}_6$ compound is 4.00 μ_B , proving the ideal half-metallic property of this compound, where the important contribution of the total magnetic moment is due to iron atom (See **Table 4**). Therefore, these remarks are essentially due to the incompletely filled layer 3d, which confers a magnetic moment to the transition metals ions. With the use of GGA + U approximation, with a change in U_{eff} values from 2 to 8 eV for analysis the transition metals (Fe) 3d orbital partially filled, we clearly observe that the greatest magnetic moment for Fe (3.27 μ_B), is obtained with U = 2. In addition, we can observe from **Table. 4**, that the total magnetic moment is practically the same for $\text{Pb}_2\text{FeTaO}_6$ and we find the maximum values of magnetic moment for iron atom when we use the TB-mBJ potential (3.52 μ_B).

Table 4 Calculated total (μ^{Cell}), local and interstitial (μ^{inter}) magnetic moments in the units of (μ_B) for $\text{Pb}_2\text{FeTaO}_6$ with GGA, GGA+U and TB-mBJ approximations.

$\text{Pb}_2\text{FeTaO}_6$	GGA	GGA+U				mBJ
		2 eV	4 eV	6 eV	8 eV	
	0.04008	0.0474	0.02728	0.01984	0.01808	0.01432
	3.1602	3.2759	3.1140	3.0620	3.0120	3.5205
	-0.08147	-0.09515	0.01329	0.02868	0.03302	0.00006
	0.56002	0.6330	0.43268	0.4497	0.49228	0.24048
	0.33327	0.13599	0.41254	0.43997	0.44481	0.28026
	4.0121	3.9971	4.0001	4.0002	4.0002	4.00015

4. Conclusion

In summary, we have calculated the structural, elastic, electronic, and magnetic properties of the double perovskite $\text{Pb}_2\text{FeTaO}_6$ by using the full-potential linearized augmented plane wave (FPLAPW) in the framework of the density functional theory (DFT) within the generalized gradient approximation (GGA), GGA + U and TB-mBJ. It is found that $\text{Pb}_2\text{FeTaO}_6$ is mechanically stable and performs ductility property from the elastic constants .It is also found that the magnetic phase stability of the cubic double perovskite $\text{Pb}_2\text{FeTaO}_6$ compound is ferromagnetic (FM) arrangement, confirming the most stable ground state of this material. The GGA

approximation allows remarking a half-metallic behavior for $\text{Pb}_2\text{FeTaO}_6$ with metallic character in spin down and direct semiconductor gap energy in spins up equal 2.98 eV and included magnetic moment total to 4.0 μ_B . The majority essential part of $\text{Pb}_2\text{FeTaO}_6$ double perovskite compound magnetic total moments is afford by Fe ion. The electronic properties calculated with GGA + U shows a semiconductor character of $\text{Pb}_2\text{FeTaO}_6$ material for U = 4,6 and 8 eV and also when we using the TB-mBJ with band gap equal 0.812, 1.645, 1.997, 1.811 eV respectively, but half-metallic behavior at U = 2 eV with the use of GGA-PBE. Therefore; as a result, the calculation electronic and magnetic properties shows that this compound has a technological potential for spintronic application in materials sciences.

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Figures

Figure 1

Crystal structure of $\text{Pb}_2\text{FeTaO}_6$.

Figure 2

Calculated total energy (Ry) as a function of volume for Pb₂FeTaO₆ in nonmagnetic (NM), ferromagnetic (FM) and antiferromagnetic (AFM) phase using GGA.

Figure 3

Calculated total density of states and band structure of Pb₂FeTaO₆ using GGA.

Figure 4

Calculated total density of states and band structure of $\text{Pb}_2\text{FeTaO}_6$ using GGA+U.

Figure 5

Calculated total density of states and band structure of $\text{Pb}_2\text{FeTaO}_6$ using TB-mBJ.

Figure 6

Calculated total and partial density of states of Pb₂FeTaO₆ using GGA, GGA + U, and TB-mBJ; the Fermi level is set to zero.

Figure 7

Half-metallic energy (EHF) versus U values of the double perovskite cubic Pb₂FeTaO₆.