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First-Principles Study of the Stabilization and Mechanical Properties of Rare-Earth Ferritic Perovskites (RFeO_3 , $\text{R} = \text{La, Eu, Gd}$)

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Abstract: Current research aims to investigate the mechanical properties of rare earth perovskite ferrites (RFeO_3 , $\text{R} = \text{La, Eu, Gd}$) utilizing density functional theory (DFT) calculations. Using the revised Perdew–Burke–Ernzerhof approximation for solids (PBEsol) approximation, the elastic constants, bulk, Young’s, and shear modulus, Poisson’s ratio, and anisotropic properties are calculated. The quantum theory of atoms in molecules (QTAIM) is employed to analyze the stability of chemical bonds in the structures subjected to an external loading. Based on these calculations, Fe–O and R–O bonds can be considered as nearly ionic, which is due to the large difference in electronegativity of R and Fe with O. Additionally, our results reveal that the charge density values of the Fe–O bonds in both structures remain largely outside of the ionic range. Finally, the mechanical response of LaFeO_3 , EuFeO_3 , and GdFeO_3 compounds to various cubic strains is investigated. The results show that in RFeO_3 by increasing the radius of the lanthanide atom, the mechanical properties of the material including Young’s and bulk modulus increase.

Keywords: density functional theory; quantum theory of atoms in molecules; rare-earth ferritic perovskite; mechanical properties; sound velocity; Debye temperature

1. Introduction

Metal mixed oxides (ABO_3), in particular RFeO_3 ($\text{R} = \text{La, Eu, Gd}$) structures, have been considered as one of the most attractive semiconductors for a wide range of applications such as catalysts, hazardous gases sensors, quantum electromagnets, and microelectronic devices due to their outstanding physical, chemical, mechanical, optical, and magnetic properties [1]. Tang et al. [2] introduced LaFeO_3 perovskite as a potential candidate for using in photocatalytic applications because of its strong absorption in the visible light spectrum. GdFeO_3 possesses ultra-low-temperature thermal conductivity (κ) of 1W/Km at 1 K, which makes it a suitable candidate for the thermoelectric applications [3]. Moreover, it has been known that the EuFeO_3 perovskite has a great performance to use in the microelectronic industry due to its high dielectric constant of 315, and a low dielectric loss of 1.7 [4]. One of the most important applications for these materials is high-temperature electrochemical devices, where the thermal expansion and mechanical properties of the material are crucial [5]. Differences in the thermal and chemical expansion coefficients of the constituent materials introduce compressive or tensile stresses to the compound, which can potentially cause a destruction in the device. Therefore, the effect of such stresses should be investigated on the mechanical properties of the materials. This is

our motivation to study the mechanical properties of RFeO_3 and their response to the external stresses. To predict the mechanical behavior of RFeO_3 , it is important to calculate the parameters such as fracture strength, Young's and shear modulus, and fracture toughness under mechanical loading. In the current study, the mechanical properties of the LaFeO_3 , EuFeO_3 , and GdFeO_3 perovskites in the cubic symmetry are first studied by exerting first-principles calculations based on density functional theory (DFT). In the next step, the topological analysis of electron density is performed utilizing quantum theory of atoms in molecules (QTAIM) to investigate the role of chemical bonds on the mechanical properties of RFeO_3 perovskites.

2. Computational Methods

All calculations in the present study are carried out exploiting the plane-wave pseudopotential procedure within the framework of the density functional theory (DFT) using Quantum ESPRESSO software package [6]. The exchange correlation potential is contemplated by the generalized gradient functional (GGA) with the correction of Perdew–Burke–Ernzerhof approximation for solids (PBEsol) approximation [7]. An optimum cutoff energy of 90 Ry is considered in the all calculations. The integration of the Brillouin zone is carried out with $12 \times 12 \times 12$ k-points using the standard Monkhorst–Pack special grids [8]. The geometry optimizations are done with the Broyden–Fletcher–Goldfarb–Shanno (BFGS) algorithm (for stress minimization). The total energy convergence occurs at the energies less than 1 meV/atom. For geometry relaxation, the force on atom is converged below a threshold of $0.01 \text{ eV } ^\circ\text{A}^{-1}$. Cubic unit cell with the space group $\text{Pm}\bar{3}\text{m}$ containing 5 atoms (Figure 1) is used for the calculations.

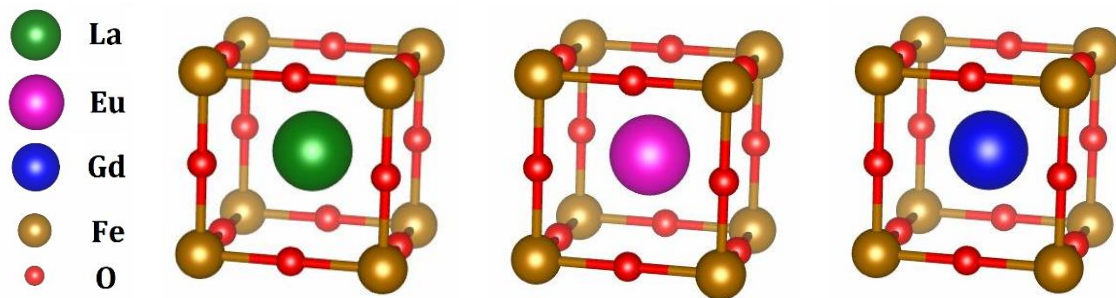


Figure 1. Schematic representation of crystal structures of RFeO_3 ($\text{R} = \text{La}, \text{Eu}, \text{Gd}$).

The elastic constants of cubic RFeO_3 ($\text{R} = \text{La}, \text{Eu}, \text{Gd}$) structures are calculated using continuum mechanics method, which are explained in detail in our previous work [8]. Conforming to this approach, the unit cell is exposed to a series of deformations η based on the crystal structure. The following equation shows how to calculate the elastic energy of a deformed structure:

$$E(\eta_I) = E(0) + V_0 \sum_{I=1}^3 \tau_I^{(0)} \eta_I + \frac{V_0}{2!} \sum_{I,J=1}^3 C_{IJ} \eta_I \eta_J \quad (1)$$

where V_0 , $E(0)$, τ , and C are, respectively, denoting the volume, energy of the equilibrium state, Lagrangian stress tensor, and the elastic stiffness constant. To abbreviation in indexing, we utilize Voigt notation in this equation. Using Equation (1), the elastic constants of the material (C_{ij}) can be calculated as:

$$C_{ij} = \frac{1}{V_0} \frac{\partial^2 E}{\partial \eta_i \partial \eta_j} \quad (2)$$

According to the high-symmetry structure of the cubic phase of RFeO_3 , only three independent elastic constants (C_{11} , C_{12} , and C_{44}) are calculated using Equation (2). The elastic constants for the cubic, orthorhombic, and monoclinic deformations can be obtained using the following deformation

tensors [9]. For each deformation mode, different magnitudes of deformations from −10% to 20% were applied.

$$D_{\text{Cubic}} = \begin{bmatrix} \eta & 0 & 0 \\ 0 & \eta & 0 \\ 0 & 0 & \eta \end{bmatrix}, D_{\text{Ortho}} = \begin{bmatrix} \eta & 0 & 0 \\ 0 & -\eta & 0 \\ 0 & 0 & \frac{\eta^2}{1-\eta^2} \end{bmatrix}, D_{\text{Mono}} = \begin{bmatrix} 0 & \eta & 0 \\ \eta & 0 & 0 \\ 0 & 0 & \frac{\eta^2}{1-\eta^2} \end{bmatrix}$$

3. Results and Discussion

The calculated optimum values for the lattice parameters of the cubic RFeO₃ (R = La, Eu, Gd) structures as well as the previous experimental and theoretical values are given in Table 1. There is befitting compliance between our calculated results with the reported experimental data the literature with a nearly 0.5% underestimation. The weakness of DFT in describing the dispersion forces causes an underestimation in the prediction of the electronic, structural, and physical properties of materials.

Table 1. Comparison between our calculated, and reported the experimental and theoretical results in the literature for the lattice parameters of LaFeO₃, EuFeO₃, and GdFeO₃.

	Experiment Data	Theoretical Data
LaFeO₃	3.89 [10]	3.82
	3.92 [11]	3.92 [5]
	3.93 * [9]	3.95 [12]
EuFeO₃		3.75
	3.68 * [9]	3.83 [5]
GdFeO₃		3.74
	-	3.82 [5]

* Pseudocubic structure.

It can be seen in Table 1, the cell parameter of the unit cells for all three structures decreases by reducing the atomic radius of the central cation. This is in agreement with the other computational studies [5–7,12,13], as listed in Table 1.

In the first step of obtaining the mechanical properties, the elastic constants of RFeO₃ are calculated. These constants are calculated by applying strain in the harmonic region. The relation between the applied strain under three different deformation moods and the total energy changes is presented in Figure 2. The other elastic properties such as bulk modulus, Young’s modulus, shear modulus, and Poisson’s ratio are then identified from the elastic constants [13]. In the Voigt theory, the bulk modulus (B_V), and shear modulus (G_V) can be written as [14]:

$$B_V = \frac{1}{3}[C_{11} + 2C_{12}] \quad (3)$$

$$G_V = \frac{1}{5}[C_{11} - C_{12} + 3C_{44}] \quad (4)$$

While, in Reuss theory, the bulk modulus (B_R), and shear modulus (G_R) are written as [15]:

$$\frac{1}{B_R} = (S_{11} + S_{22} + S_{33}) + 2(S_{12} + S_{13} + S_{23}) \quad (5)$$

$$\frac{15}{G_R} = 4[(S_{11} + S_{22} + S_{33}) - 4(S_{12} + S_{13} + S_{23}) + 3(S_{44} + S_{55} + S_{66})] \quad (6)$$

where S_{ij} , which is entitled the elastic compliance coefficient, is the inverse of C_{ij} . Furthermore, in Hill theory, bulk modulus (B_H), and shear modulus (G_H) are described as follows [16]:

$$B_H = \frac{B_V + B_R}{2} \quad (7)$$

$$G_H = \frac{G_V + G_R}{2} \quad (8)$$

Finally, the Young's modulus (E), and Poisson's ratio (ν) are calculated using Equations (9) and (10), respectively:

$$E = \frac{9BG}{3B + G} \quad (9)$$

$$\nu = \frac{3B - 2G}{2(3B + G)} \quad (10)$$

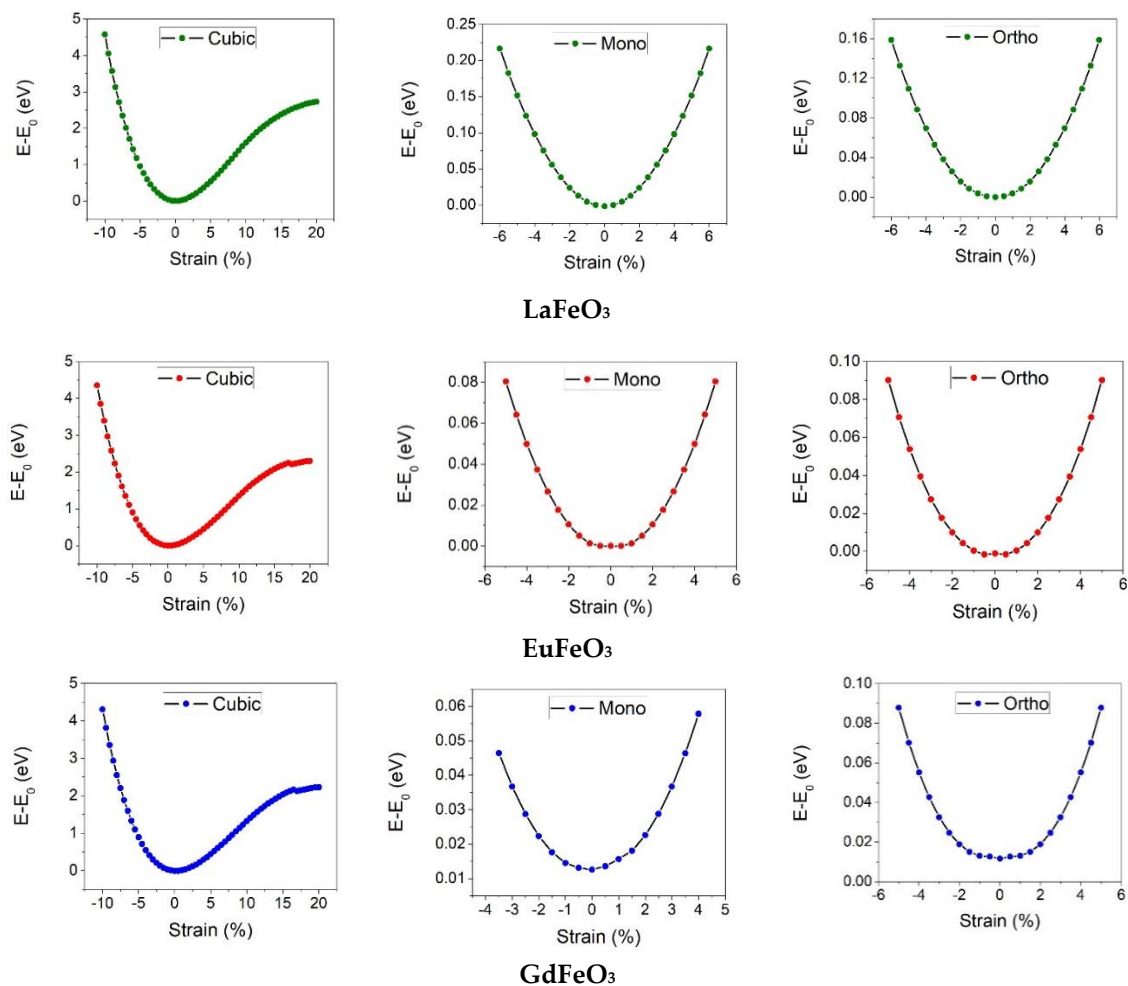


Figure 2. Total energy of LaFeO₃, EuFeO₃, and GdFeO₃ structures as a function of strain under the influence of three types of deformation tensor (E_0 is total energy of equilibrium structure).

The calculated elastic constants of LaFeO₃, EuFeO₃, and GdFeO₃ are reported in Table 2. To the best of our knowledge, there are limited theoretical and experimental efforts on the prediction of the elastic constants of LaFeO₃, EuFeO₃, and GdFeO₃ with the cubic structure. Therefore, to validate our obtained results, we compare the mechanical properties of rare earth Ferritic perovskites with other oxide perovskites. This helps to achieve a better understanding of the mechanical properties of rare earth Ferritic perovskites. Bannikov [17] calculated the elastic constants of C_{11} , C_{12} , and C_{44} , as 286.71,

116.46, and 125.61 for BaVO₃, respectively; all of which are at the same order of the elastic constants of RFeO₃ (R = La, Eu, Gd). In addition, the mechanical properties of SrTiO₃ and SrZrO₃ have been investigated by Shein et al. [18]. They reported the elastic constants $C_{11} = 318.35$, $C_{12} = 100.04$, and $C_{44} = 110.20$ and $C_{11} = 309.71$, $C_{12} = 71.96$, and $C_{44} = 73.78$ for SrTiO₃ and SrZrO₃, respectively [18]. The difference in the results (the values of the elastic constants) can be caused due to the influence of some structural factors in these materials such as structural and relative density, metal-oxygen bond strength and interactions between central cation with the scaffold.

Table 2. Calculated mechanical properties of RFeO₃ (R = La, Eu, Gd).

	C_{11} (GP)	C_{12} (GP)	C_{44} (GP)
LaFeO ₃	278.06	154.63	92.92
EuFeO ₃	242.64	148.81	45.34
GdFeO ₃	215.56	156.80	34.77

Born stability criteria [19] is a valid criterion to investigate mechanical stability of elastic stiffness constants. For cubic structures these criteria are written as:

$$C_{11} > 0, C_{11} - C_{12} > 0, C_{11} + 2C_{12} > 0, C_{44} > 0 \quad (11)$$

According to the Equation (11), all our obtained elastic constants of RFeO₃, as reported in Table 2, are satisfied by Born stability criterion.

Furthermore, the calculated bulk, Young's, and shear modulus and Poisson's ratio for all structures using Equations (3)–(10) are listed in Table 3. As can be seen in Table 3, it is clear that with changing the central cation from the left to the right in the periodic table, the bulk modulus decreases. In each period of the periodic table from left to right, the effective nuclear charge on the outer electrons, and accordingly, the nuclear attraction on the valence band electrons increase. Reducing the atomic radius of the central cation increases the compressibility, which has an inverse relation with the bulk modulus. In Table 4, shear velocity (V_t), compressional velocity (V_l), sound velocity (V_m), and the Debye Temperature (θ_D). The average sound velocity (v_m) is calculated using Equation (12):

$$v_m = \left[\frac{1}{3} \left(\frac{2}{v_l^3} + \frac{1}{v_t^3} \right) \right]^{-\frac{1}{3}} \quad (12)$$

where v_t and v_l are the shear velocity, and compressional velocity, respectively, and are dependent on bulk (B) and shear (G) modulus as follows:

$$v_t = \sqrt{G/\rho} \quad (13)$$

$$v_l = \sqrt{\left(B + \frac{4}{3}G \right) / \rho} \quad (14)$$

The Debye temperature is another physical quantity, which is related to elastic constants, specific heat, and melting point. The relation between Debye temperature and the average sound velocity (v_m) is described in Equation (15):

$$\theta_D = \frac{h}{k} \left[\frac{3n}{4\pi} \left(\frac{N_A \rho}{M} \right) \right]^{\frac{1}{3}} v_m \quad (15)$$

where h , k , N_A , n , M , and ρ represent the Planck's constant, Boltzmann's constant, Avogadro's number, atoms in the cation, molecular mass, and density, respectively. The Debye temperature of RFeO₃ (R = La, Eu, Gd) ranged from 503.1 K for GdFeO₃ to 792 K for LaFeO₃, as can be seen in Table 4. The anisotropy of the Young's and shear modulus of LaFeO₃, EuFeO₃, and GdFeO₃ is illustrated in the form of 3D surface contours in Figure 3 using ELATE code [20]. For an isotropic crystal, one sees a

spherical shape, while a deviation from a spherical shape can directly reflect the degree of the elastic anisotropy in the crystal. It can be seen that the Young's modulus of the LaFeO_3 is strongly anisotropic compared to that of two other structures.

Table 3. Calculated results for bulk, Young, and shear moduli and Poisson ratio of RFeO_3 (R = La, Eu, Gd) structures by Voigt, Reuss, and Hill approaches.

	Averaging Scheme	Bulk Modulus (B) (GPa)	Young's (E) Modulus (GPa)	Shear Modulus (G) (GPa)	Poisson's Ratio (ν)
LaFeO_3	Voigt (V)	195.77	212.24	80.44	0.32
	Reuss (R)	195.77	204.9	77.29	0.32
	Hill (H)	195.77	208.58	78.86	0.32
	Other Work	186.5 [5]			
EuFeO_3	Voigt (V)	180.09	127.1	45.97	0.38
	Reuss (R)	180.09	127.06	45.957	0.38
	Hill (H)	180.09	127.08	45.963	0.38
	Other Work	201.2 [5]			
GdFeO_3	Voigt (V)	176.39	92.17	32.62	0.41
	Reuss (R)	176.39	91.58	32.40	0.41
	Hill (H)	176.39	91.88	32.51	0.41
	Other Work	204.2 [5]			

Table 4. Values of shear velocity (V_t), compressional velocity (V_l), sound velocity (V_m), and the Debye Temperature (θ_D) of RFeO_3 (R = La, Eu, Gd) compounds.

Sample	V_t	V_l	V_m	θ_D
LaFeO_3	3333.8	6470.7	4435.9	792.0
EuFeO_3	2384.1	5463.2	3266.7	594.8
GdFeO_3	1983.0	5148.7	2758.7	503.1

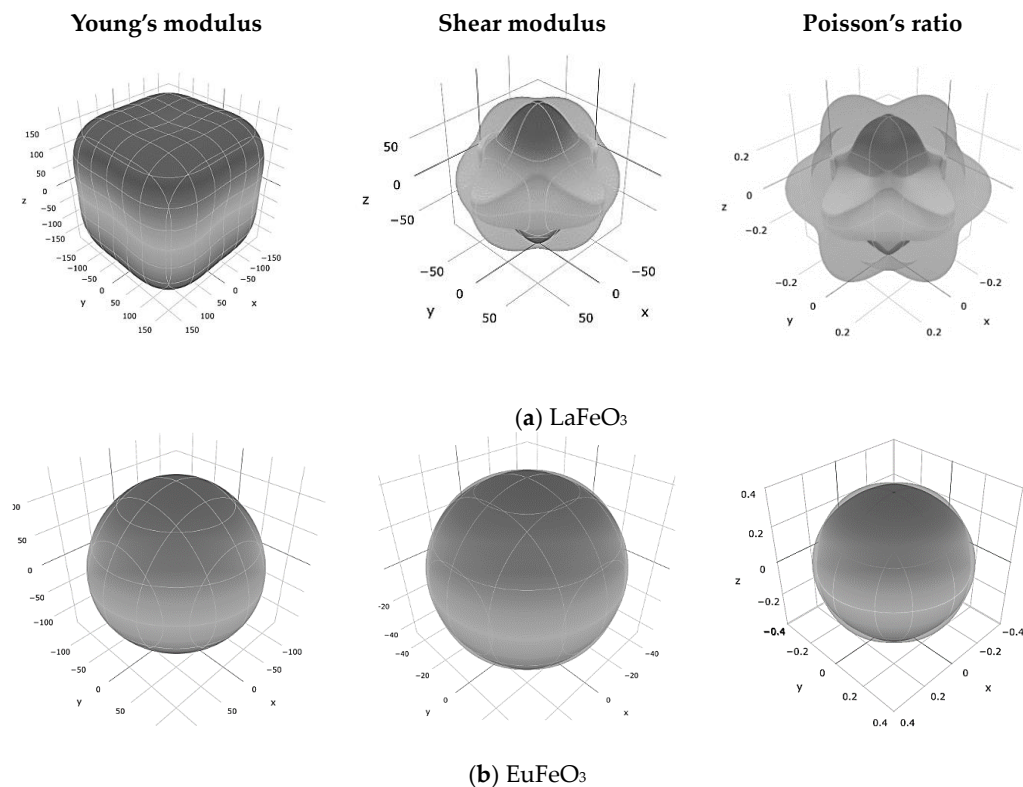


Figure 3. Cont.

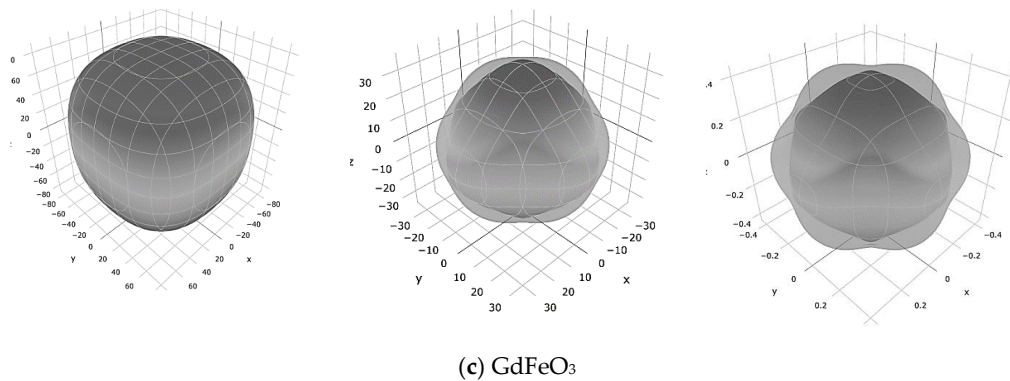


Figure 3. 3D contours of Young's modulus, shear modulus, and Poisson's ratio for (a) LaFeO₃; (b) EuFeO₃, and (c) GdFeO₃.

In this section, the topological analysis of electron density is performed by employing quantum theory of atoms in molecules (QTAIM) to investigate the role of chemical bonds on the mechanical properties of the studied materials [21–23]. A deep understanding between structure (chemical bonds) and mechanical and electronic properties can help to design of low-cost, and scalable materials with enhanced properties. To carry out QTAIM (Bader's analysis), a single-point calculation of the optimized RFeO₃ structure is done to generate the full electron density (Table 5). The simulations are conducted by CRITIC2 code which used the core and valence electron densities as input parameters [24,25]. Firstly, the critical points (CPs) of the electron density are determined by QTAIM analysis. A critical point together with all downward-gradient lines, all of which have their origins in the critical points, constitute an atomic basin, and are the most important of the regions fulfilling the zero-flux condition [26].

Table 5. Properties of electron density critical points of RFeO₃ (R = La, Eu, Gd).

Number and Type of Cps			$\rho(\text{rc})$	$\nabla^2\rho(\text{rc})$	λ_1	λ_2	λ_3
			(e.A−3)	(e.A−5)	(e.A−5)	(e.A−5)	(e.A−5)
LaFeO ₃	Bond	6	0.66	13.33	−2.19	−2.19	17.73
	Bond	12	0.22	2.59	−0.73	−0.68	4.01
	Ring	24	0.12	1.71	−0.20	0.93	0.98
	Cage	8	0.11	1.72	0.29	0.29	1.34
	Cage	3	0.06	0.85	0.24	0.24	0.37
EuFeO ₃	Bond	6	0.73	13.34	−3.07	−3.07	19.49
	Bond	12	0.21	2.75	−0.65	−0.61	4.02
	Ring	24	0.12	1.77	−0.16	0.86	1.08
	Cage	8	0.12	1.82	0.30	0.30	1.22
	Cage	3	0.06	0.80	0.26	0.26	0.26
GdFeO ₃	Bond	6	0.74	13.57	−2.88	−2.88	18.46
	Bond	12	0.2	2.56	−0.69	−0.63	4.02
	Ring	24	0.12	1.75	−0.17	0.85	1.03
	Cage	8	0.12	1.83	0.31	0.31	1.32
	Cage	3	0.06	0.83	0.25	0.25	0.27

There are four types of non-degenerate critical points, which are defined by the number of non-zero eigenvalues of the curvature (Hessian) matrix (λ_i) and the sum of the algebraic signs of λ_i . These four critical points of electron density are: maxima (3, −3), minima (3, +3), and two types of saddle points (3, +1) and (3, −1), which are corresponding to the nuclear positions, cages, rings, and bonds, respectively [26,27]. In solids, atomic basins are equivalent to polyhedral with curved edges and faces. The crystal partitioning can lead to predict the mechanical properties of RFeO₃ on a local scale interdependent with the atoms in the crystal. The analysis is based on variation of hydrostatic pressure

(P) compared to the changes in partition of basin volumes (V_Ω). To calculate the bulk modulus B and its derivative with respect to pressure $B'_0 = \frac{\partial B_0}{\partial P}$, the third-order Birch–Murnaghan (BM) equations of state as [28,29]:

$$P = \frac{3}{2} B_0 \left(\eta^{-\frac{7}{3}} - \eta^{-\frac{5}{3}} \right) \left[1 + \frac{3}{4} (B'_0 - 4) \left(\eta^{-\frac{2}{3}} - 1 \right) \right] \quad (16)$$

here $\eta = V/V_0$ is the ratio of volume V at pressure P to equilibrium V_0 at zero pressure, and B_0 is bulk modulus and $B'_0 = \frac{\partial B_0}{\partial P}$. The analysis is based on the partition of the cell volume (V) into basin volumes (V_Ω), which compress differently upon the application of hydrostatic pressure (P). The local bulk modulus B_Ω and the bulk modulus (B) of the bulk crystal are defined as:

$$B_\Omega = -V_\Omega \left(\frac{\partial P}{\partial V_\Omega} \right) \quad (17)$$

$$B = \sum_{\Omega} f(\Omega) B_\Omega \quad (18)$$

where $f(\Omega)$ is the ratio of total volume (V) to basin volume (V_Ω).

As shown in Table 6, the local bulk modulus is specified for each basin, which is calculated using Equation (17). The incremental amount of the local bulk modulus is maintained by reducing the atomic radius, which is in agreement with our previous results presented in Table 3. The local bulk modulus of Fe and O in changes from one structure to the other one due to the fact that the atomic environment is not the same in the LaFeO_3 , EuFeO_3 , and GdFeO_3 structures. Using Equation (18), the bulk modulus of RFeO_3 ($R = \text{La, Eu, Gd}$) structures are obtained by averaging the local bulk modulus (see Total row of B column), which confirms our previous results in Table 3.

Table 6. The topological charges (Q), volume of each basin, and C index of RFeO_3 ($R = \text{La, Eu, Gd}$).

		V	f (Ω)	B(Ω)	Q(Ω)	OS(Ω)
LaFeO_3	La	17.18	0.308	268.83	2.071	+3
	Fe	7.16	0.128	221.59	+1.475	+3
	O	10.45×3	0.188×3	176.37	-1.182×3	-2×3
	Total	55.70	1.00	210.66	0	0
EuFeO_3	Eu	15.08	0.287	256.59	+1.896	+3
	Fe	6.83	0.130	191.23	+1.527	+3
	O	10.19×3	0.194×3	169.23	-1.141×3	-2×3
	Total	52.54	1.00	196.99	0	0
GdFeO_3	Gd	14.80	0.283	249.64	+1.882	+3
	Fe	6.78	0.130	185.91	+1.537	+3
	O	10.23×3	0.196×3	167.25	-1.139×3	-2×3
	Total	52.29	1.00	193.04	0	0

In addition, as can be seen in Table 6, Q is topological charges of atoms in the crystal, which are calculated using from the integration of each basin corresponding to each atom using Yu and Trinkle method [30]. Obtained charges for each basin help to specify an important parameter that characterizing the whole charge transfer by averaging the ratios between topological charges $Q(\Omega)$ and nominal oxidation states $OS(\Omega)$:

$$C = \frac{1}{N} \sum_{\Omega} \frac{Q(\Omega)}{OS(\Omega)} \quad (19)$$

where Ω denotes each basin and N is the total number of basins. In this equation $C = 1$ means the total ionicity, while $C = 0$ shows total covalency. Table 6 shows the topological volumes, topological charges, and the C indexes are calculated for LaFeO_3 , EuFeO_3 , and GdFeO_3 . The C index is an

important indicator for measure the degree of ionicity of the crystal, where $1-C$ shows the degree of covalency. The ratio between Q (Ω) and OS (Ω) provides a measurement of the deviation from the ideal ionic model for a given basin Ω . The topological charges (Q) are not close to nominal charges ($R^{(+3)}Fe^{(+3)}O_3^{(-2\times3)}$) due to the existence of different topological charges for the same atoms in different atomic environments. The calculated C index is 0.59, 0.55, and 0.57 for $LaFeO_3$, $EuFeO_3$, and $GdFeO_3$ compounds, respectively. Another important mechanical property, which is of great importance in the materials design category, is the elastic limit. The elastic limit is the maximum stress that can be applied on the solid material before the permanent or plastic deformation starts. Prior to the elastic limit, by unloading, the material returns to its original undeformed shape. Passing this limit reduces the material's stiffness and leads to deflections and buckling. This is very important, particularly in thin film applications, where there is a substrate, which strains the film due to the lattice mismatch between the substrate and the thin film. The change of the second Piola–Kirchhoff (PK2) stress with Lagrangian strain is represented in Figure 4 for all $LaFeO_3$, $EuFeO_3$, and $GdFeO_3$ structures. To obtain the Piola–Kirchhoff (PK2) stress, we applied the cubic deformation tensor on the structures. The PK2 is related to the Cauchy (true) stress (σ), and can be obtained from Equation (20) [31]:

$$\Sigma = JF^{-1}\sigma(F^{-1})^T \quad (20)$$

where J is the determinant of the deformation gradient tensor F . The Cauchy stresses are identified based on DFT calculations in the framework of the PBEsol approximation. The maximum stress in this curve is called the ultimate stress and the corresponding strain at this point is called the ultimate strain. The strain range prior to this ultimate strain point is the uniform elastic region of the material. It should be emphasized that the ultimate stress and strain obtained by this method is under the ideal condition, where there is no crystal defect or thermal effects, which are usually present in the real conditions and lower the strength of the material. The ultimate stress and strain values obtained from the PK2 stress curve are given in Table 7. From the PK2 stress, it can be seen that both materials behave in a symmetric manner, which is due to the cubic crystal lattice. In addition, from the steep slope in the compression region, it can be concluded that the structures possess higher resistance in compression compared to tension.

Table 7. Ultimate stresses and ultimate strain of $RFeO_3$ ($R = La, Eu, Gd$) in a, b, and c directions under cubic deformation.

Σ^u (eV/Å).	$LaFeO_3$	$EuFeO_3$	$GdFeO_3$
Σ_a^u	0.126	0.115	0.111
η_a^u	8.5%	8.5%	8.5%
Σ_b^u	0.126	0.115	0.111
η_b^u	8.5%	8.5%	8.5%
Σ_c^u	0.126	0.115	0.111
η_c^u	8.5%	8.5%	8.5%

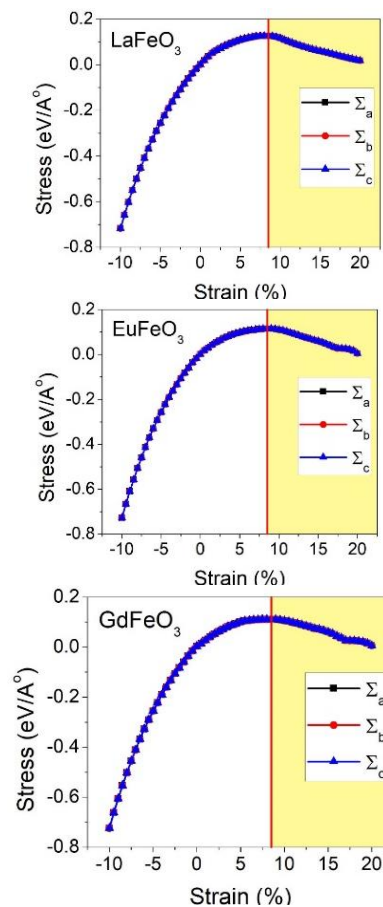


Figure 4. Stress–strain responses of LaFeO₃, EuFeO₃, and GdFeO₃ under cubic deformation.

4. Conclusions

The cubic phase synthesis of the RFeO₃ (R = La, Eu, Gd) structures is very challenging. Recently, some successful methods have been developed to synthesize these materials with cubic structures [6,7]. Therefore, due to the lack of information on the properties of the cubic structures of these materials, theoretical and computational studying of the cubic phases of these materials, and predicting their properties is crucial. In the current study, the mechanical properties of the cubic phase of the RFeO₃ (R = La, Eu, Gd) structures are first investigated using the continuum mechanics approach and density functional theory (DFT). The results of the current research reveal that by increasing the radius of the lanthanide atom in RFeO₃ perovskites, elastic constants increase, and accordingly, the mechanical properties are improved. Then, the quantum theory of atoms in molecules (QTAIM) is utilized to understand the role of chemical bonds on the mechanical properties of RFeO₃ compounds. The QTAIM (Bader's analysis) confirms the DFT results and show when the lanthanide atomic radius increases, the local bulk modulus in the lanthanide basin is enhanced. Moreover, the QTAIM results depict that the EuFeO₃ possesses the highest mechanical isotropy; while LaFeO₃ has the lowest mechanical isotropy. The stress–strain curves of all RFeO₃ (R = La, Eu, Gd) structures show that all these three compounds are deformable up to 8.5% strain, which makes them suitable candidates for flexible electronic and optoelectronic applications.

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