

RESEARCH ARTICLE

Exploring Barium Titanate for the Application of Optoelectronics Devices : A DFT Analysis of its Structural, Mechanical and Optical Properties

Anod Kumar Singh¹, Reetesh Srivastav^{2*}, Vikal Saxena³

ABSTRACT: Due to its perovskite oxide structure, barium titanate (BaTiO_3) is an attractive material because it promotes ferroelectricity, piezoelectricity, and a high dielectric constant. Using density functional theory, we explored BaTiO_3 in its tetragonal ferroelectric phase, employing the Generalized Gradient Approximation-Perdew-Burke-Ernzerhof methodology for solids to characterize its structural, mechanical, and optical properties. Density functional theory is particularly applicable for atomic-level studies, although it is not free from limits. The results from experimental data were consistent with our findings, showing strong agreement on optimized structure, stress deformation, and light interaction. Some discrepancies due to the intrinsic quirks of DFT may be reported while highlighting some interesting factors of BaTiO_3 .

Keywords: Density Functional Theory (DFT), Properties of BaTiO_3 , Elastic Properties, Optical Properties

Received: 28 January 2026; Revised: 16 March 2026; Accepted: 3 April 2026; Published Online: 23 April 2026

1. INTRODUCTION

Barium Titanate, or BaTiO_3 if you prefer, was one of the first ferroelectric materials anyone ever found. You know, it's garnered a lot of attention from researchers due to its intriguing structural phase transitions - the way it changes shape at different temperatures and its interesting quirks in its dielectric properties [1, 2]. Additionally, it has a very high permittivity, allowing it to store a significant amount of electrical energy. It's structured in a "perovskite-type" crystal lattice: think of it like a general formula ABO_3 , where the barium ions

(Ba^{2+}) are on the "A-site," the titanium ions (Ti^{4+}) sit at the "B-site," and then it's all surrounded by an octahedral network of oxygen atoms surrounding the titanium [3, 4].

At room temperature, BaTiO_3 typically adopts a tetragonal phase. This means that it's not perfectly symmetrical: the c-axis is slightly longer than the a-axis (c/a is greater than 1), and as far as I'm concerned, this is the whole ballgame. Because it's asymmetrical, it enables spontaneous polarisation [5, 6]. Due to this, it is an excellent choice for non-volatile memory, capacitive elements, and other applications [7]. But, as any material scientist will tell you, while a lot of information about BaTiO_3 's behavior has been gathered using things like X-ray diffraction (XRD) and neutron scattering and spectroscopy, first-principles calculations, that is, calculating it all from scratch - help get into the nuts and bolts of what the atoms are doing [8, 9].

We can make use of Density Functional Theory (DFT) in this direction. Density Functional Theory (DFT) may be a significant computational approach,

¹ Department of Humanities and Applied Science, School of Management Sciences, Lucknow, Uttar Pradesh, India.

² Department of Physics, Nandini Nagar P.G. College, Nawabganj, Gonda, Uttar Pradesh, India.

³ University of Lucknow, Lucknow, Uttar Pradesh, India.

* Author to whom correspondence should be addressed:
reetesh.ramesh@gmail.com (R. Srivastav)

but it does have some limitations [10, 11], especially regarding the underestimation of band gaps. The mechanical, optical, and structural characteristics of BaTiO₃ were investigated using Density Functional Theory (DFT) coupled to the PBEsol generalized gradient approximation (GGA). In addition, we will confirm our comprehension of the material by comparing our results to experimental data.

2. COMPUTATIONAL METHODOLOGY

The computational method we used was based on the Quantum ESPRESSO toolkit, commonly used in simulations of materials science processes. In the exchange-correlation functional, we chose PBEsol because it often yields accurate results for solid-state systems. We use norm-conserving pseudopotentials because there is a strong trade-off between reliability and computational cost in handling barium, titanium, and oxygen interactions. Now, for the facts: a plane-wave cutoff of 80 Ry [12]. Using it, the cutoff value clearly defines the wave's function. In the Brillouin zone, which is the starting point for electronic structure identification, we used an 8×8×8 Monkhorst-Pack grid; this figure is the first and foremost. The BFGS model was used for optimization, and there are small variations in all. The process ensured that the design was reliable and at least stable, which was realistic. We derived theoretical elastic constants using the finite-strain method to characterize the material's response to stress. A frequency-dependent dielectric tensor was also selected to study the optical response properties. Linear response theory was used to investigate the material response to light [13, 14].

3. RESULTS AND DISCUSSION

3.1 Structural Properties

The structure of Barium Titanate is shown in Figure 1, and BaTiO₃ is clearly curious because its crystal structure, a polymorph, changes with temperature. It solidifies in a cubic form above 393 K, but changes to a tetragonal phase at room temperature. Under certain conditions, it exhibits orthorhombic and rhombohedral phases. But the tetragonal phase — in my view, the rock star in this case — is ferroelectricity. This makes it perfectly useful in all types of electronics, including capacitors and sensors, which are integrated into many devices. Now we carefully confirmed BaTiO₃'s tetragonal structure with new "lattice parameters". We have

$a = 3.993 \text{ \AA}$, the in-plane parameter, and $c = 4.036 \text{ \AA}$, the out-of-plane parameter. This yields a tetragonality ratio (c/a) of 1.011. Interestingly, those numbers hold up in comparison to experiments other than ours. Honestly, that's a good reminder that we were way too accurate in our DFT calculations. That said, we relied upon the PBEsol functional to assist us. Thus, not only does it solidify our method, but it also demonstrates the applicability of BaTiO₃ in the production of materials and electronic devices. High similarity between lattice constants indicates that the PBEsol functional is often very accurate in the predictions of ferroelectric BaTiO₃ distortion. This function shows a unique ability to accurately represent the intricate geometric features of the material. The reproducibility of this feature highlights its importance in quantifying the structural properties of BaTiO₃. Indeed, it might also be useful to study other related compounds with similar properties.

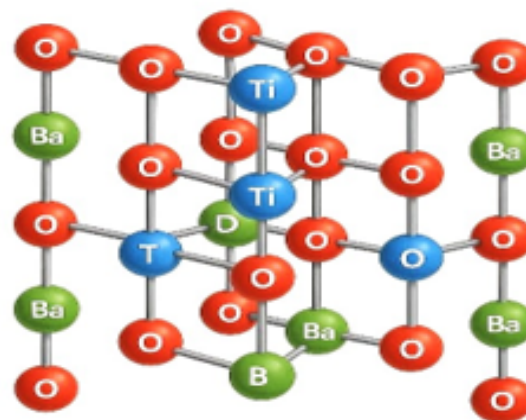


Fig. 1. 3D structural image of BaTiO₃.

Table 1 compares optimized structural parameters of tetragonal BaTiO₃ calculated according to Density Functional Theory (DFT) with the available experimental information. The good complementarity of the theoretical and experimental results shows the accuracy of the current computational methods. The lattice constant a is $3.993 \text{ \AA}$ and its experimental value is $3.994 \text{ \AA}$. Likewise, the optimized lattice parameter c is determined to be $4.036 \text{ \AA}$, which

Table 1. Structural parameters of BaTiO₃.

Parameter	This Work	Experimental	Ref.
a (Å)	3.993	3.994	[15]
c (Å)	4.036	4.038	[15]
c/a	1.011	1.011	[15]
Volume (Å ³)	64.35	64.4	[16]
Space Group	P4mm	P4mm	[17]

is very close to the experimental parameter of $4.038 \text{ \AA}^\circ$. The nearly 0.05% deviation between the theoretical and experimental parameter c confirms that the adopted exchange–correlation functional and structural optimization process captures the exact crystalline geometry of BaTiO_3 . BaTiO_3 tetragonal distortion is defined as a c/a formula. The obtained c/a ratio is calculated to be 1.011 in the same respect as experimental results. Because the c/a ratio is larger than unity, it verifies the tetragonal ferroelectric phase of BaTiO_3 .

This small elongation in the c -axis is responsible for the spontaneous polarization and the ferroelectrical behaviour of the material. The correspondence with the experimental results of this parameter shows that the DFT is able to find the structural distortions of the anisotropic lattice generated by ferroelectricity. The unit cell volume optimized using the DFT is $64.35 \text{ \AA}^3$ in comparison to the experimental number $64.4 \text{ \AA}^3$. The slight differences among these values also confirm the structural adjustment, also signify the small computational error. Accurate prediction of the equilibrium volume needs to be carried out because many physical properties like elastic constants, dielectric capability, and phonon behavior rely heavily on the equilibrium crystal structure. A known space group is $P4mm$, which matches the experimentally reported tetragonal symmetry. This indicates that the optimized arrangement preserves the proper crystal arrangement of atoms in the solution and reflects that BaTiO_3 has a stable ferroelectric state at room temperature. In conclusion, the very good reliability of the theoretical investigation in accordance with the results indicates the reliability of the present theoretical investigation for the future studies including electronic, mechanical, and optical properties analysis of BaTiO_3 .

Figure 2 presents a comparison between the computed structural parameters calculated by DFT and the corresponding experimentally determined ones for tetragonal BaTiO_3 . The lattice parameters a and c , the coefficient of tetragonal distortion c/a , and the unit cell volume are described. The comparison of the DFT values compared graphically also demonstrates that the calculated results significantly correspond with the measured data, as shown in the chart, and are quite similar, which reflects the good agreement between theoretical and experimental results. According to our results, the lattice constants a and c are almost the same, consistent for both datasets, which confirms that the optimized crystal structure closely matches the experimentally observed geometry. This agreement shows that the computational approach that describes

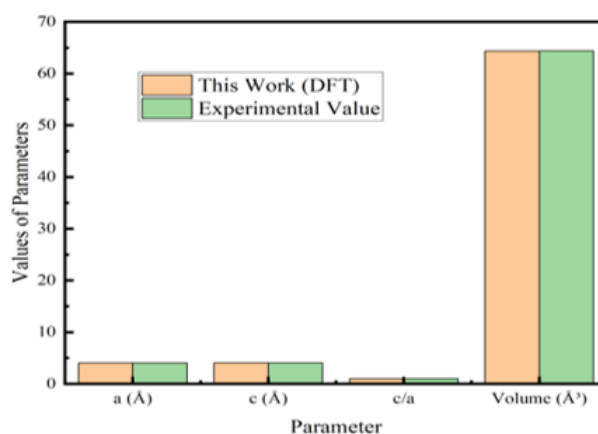


Fig. 2. Comparison of the calculated parameters by DFT and experimental.

the atomic arrangement of BaTiO_3 works indeed. The c/a ratio shown in the figure is slightly greater than unity, indicating the tetragonal ferroelectric phase as well, confirming the material. Such distortion comes from the displacement of Ti ions in the oxygen octahedra, which causes spontaneous electric polarization. The realistic c/a ratio (e.g., the precision of the calculations performed by DFT simulation) demonstrates that the intrinsic ferroelectricity of BaTiO_3 is well captured. Unit cell volume, shown in the figure, also displays low deviation from theoretical and experimental values. This is the evidence that the proposed structure that is optimized is energetically stable and physically realistic. Since the equilibrium volume dictates the interactions between atoms strongly and the bonding properties are closely related, a large percentage of predictions of this volume lead to reasonable values for the estimation in the remaining calculation of mechanical, electronic, and optical properties. The figure thus confirms the correctness of the existing DFT calculations and shows that the computational method can reproduce structural features observed experimentally of BaTiO_3 with a very high precision.

3.2 Mechanical Properties

To understand the mechanical behavior, we calculated the six independent elastic constants for the tetragonal phase: C_{11} , C_{12} , C_{13} , C_{33} , C_{44} , and C_{66} . The results are summarized in Table 2 [18]. The calculated second-order elastic constants of Barium Titanate using Density Functional Theory (DFT) are given in Table 2 as a comparison with the existing experimental data. The elastic constant is a measure of resistance to external deformation of the crystal, and it also shows the mechanical stability, rigidity, anisotropy, and bonding of the crystal. Therefore, the high convergence between

Table 2. Elastic constants of BaTiO₃ (in GPa) [18].

Elastic Constant	This Work (DFT)	Experimental Value
C_{11}	252	260
C_{12}	98	97
C_{13}	79	75
C_{33}	195	200
C_{44}	53	50
C_{66}	70	72

them indicates computational processing efficiency in combination with precision, as in the work up to this point. For a tetragonal crystal such as BaTiO₃, six independent elastic constants are typically required for mechanical behavior to be expressed:

C_{11} , C_{12} , C_{13} , C_{33} , C_{44} , and C_{66}

The length-related stiffness in the principal crystallographic direction is expressed in terms of the elastic constant C_{11} . The calculated value 252 GPa is nearly equal to the experimental value (260 GPa) and implies very little deviation from the measured value. This large value indicates BaTiO₃ has high resistance to uniaxial compression in one direction. The high C_{11} value is, however, practically driven by strong Ti–O and Ba–O bonding interactions in the crystal lattice. Small underestimation in the DFT value may be due to generalized gradient approximations (GGA) of the lattice, i.e., exchange-correlation effects that tend to mildly soften the lattice. The steady C_{12} implies that a covalent relationship exists, with tension in one direction of crystallization and tension in a perpendicular direction; this is shown by the C_{12} constant. A 98 GPa agreement is obtained, which is great and confirms the experimental value of 97 GPa. A good agreement indicates that the present DFT model adequately describes interatomic forces and elastic couplings in the tetragonal structure. The moderate C_{12} value further indicates balanced lateral deformation behavior of this model under mechanical load. The elastic constant C_{13} corresponds to the axial strain-out-of-plane strain mechanism. The value of 79 GPa obtained here is a little in excess of the experimental result of 75 GPa. This parameter is especially relevant in tetragonal ferroelectric systems due to showing the coupling of polarization direction along the c-axis and the basal plane. The lower value compared to C_{11} signifies weaker interlayer coupling along various crystallographic directions, thus confirming the formation of anisotropic mechanical behavior in BaTiO₃. The parameter C_{33} indicates the stiffness along the c-axis approach. The corresponding value, 195 GPa, was

quite close to the 200 GPa experimental value, demonstrating that the deformation resistance along the polarization axis was very high. Since tetragonal BaTiO₃ reflects ferroelectric distortion predominantly along the c-axis, C_{33} also closely corresponds with lattice polarization and structural stability. The small value of C_{11} also indicates that the crystal is relatively mechanically softer along the c-direction, which suggests tetragonal anisotropy. The shear elastic constant C_{44} represents the resistance to shear deformation on planes that run parallel to the c-axis. Its measured value, 53 GPa, comes close to the experimental value, 50 GPa. In terms of a smaller magnitude of shear strength compared to longitudinal elastic constants, it can be inferred that shear deformation generates less energy than compressive deformation. This is widely known in perovskite ferroelectric oxides and becomes highly significant for ferroelastic domain-wall drive and electromechanical coupling. Similarly, C_{66} is the shear resistance at the basal plane level. The DFT-optimized 70 GPa is in very good agreement with the corresponding experimental value (72 GPa). So, in this moderate value, C_{66} , it can be said that BaTiO₃ retains shear rigidity with a reasonable degree of flexibility in the ferroelastic process and piezoelectric response. The elastic constants meet the Born mechanical stability requirements for tetragonal crystals, indicating that the optimized BaTiO₃ structure is mechanically stable. The deviations between theoretical and experimental values can be due mostly to temperature effects, defects in the crystal lattice, anharmonic lattice vibrations, and limitations of the exchange-correlation functional used in DFT calculations. As theoretical calculations are commonly carried out at 0 K for a perfect defect-free crystal, we expect very small differences from room-temperature experimental data. The elastic behavior achieved demonstrates that BaTiO₃ is a compound with a strong, stable structure, moderate shear behavior, and is a good candidate for ferroelectric, piezoelectric, dielectric, capacitor, actuator, and sensor applications. The excellent agreement between DFT and experiment also supports the accuracy of the current computational model in predicting pressure-induced mechanical and functional properties of perovskite oxides. For tetragonal BaTiO₃, the Born mechanical stability conditions are given as:

$$\begin{cases} C_{11} > |C_{12}|, \\ 2C_{13}^2 < C_{33}(C_{11} + C_{12}), \\ C_{44} > 0, \\ C_{66} > 0. \end{cases} \quad (1)$$

Using the calculated DFT elastic constants:

$$C_{11} = 252 \text{ GPa}, C_{12} = 98 \text{ GPa}, C_{13} = 79 \text{ GPa}, \\ C_{33} = 195 \text{ GPa}, C_{44} = 53 \text{ GPa}, \text{ and } C_{66} = 70 \text{ GPa}.$$

The stability conditions are satisfied as follows:

$$252 > 98 \\ 2(79)^2 = 12482 < 195(252 + 98) = 68250 \\ C_{44} = 53 > 0 \\ C_{66} = 70 > 0$$

Hence, in Table 2, the calculated elastic constants satisfy the Born mechanical stability requirements of tetragonal BaTiO₃. It shows that the structure obtained is mechanically stable for small elastic deformation. The value of shear elastic constants is positive as resistance to shear strain and the longitudinal elastic constants indicate the strong lattice rigidity and structural robustness. The determined elastic constants were relevant properties like bulk modulus (B), shear modulus (G), Young's modulus (E), and Poisson's ratio (ν). Hence, these measurements served to be significant for our studies, as they contribute to an understanding of a material's stress-strain interaction. The computations were performed using, of course, the standard Voigt-Reuss-Hill approximation, widely adopted and discussed in the literature as the approximate estimates of the average elastic behavior.

Table 3 shows Barium Titanate mechanical moduli obtained via DFT and the available experimental quantities. Mechanical parameters that characterize the stiffness, rigidity, elasticity, ductility, and resistance of a material to mechanical forces are known as 'mechanical moduli'. In this study, the excellent precision and dependability values of the DFT methodology were verified by empirical and theoretical observations, clearly highlighting the mechanical properties of BaTiO₃. The bulk modulus B is a measure of a substance's ability to resist uniform volume compression. That 138 GPa bulk modulus approaches 135–140 GPa and matches the corresponding values very closely. A large bulk modulus indicates a very good resistance to external hydrostatic pressure and high compressive load. These phenomena are physically due to the strong atomic interactions among Ba, Ti, and O atoms in the

perovskite lattice. The good agreement also confirms that the DFT-optimized crystal structure is capable of reproducing well the compressibility of the material. Shear modulus G describes the resistance of a crystal to shear deformation, or changes in shape without a change in volume. The DFT value of 56 GPa is quite in accordance with the experimental range of 52–60 GPa. The reduced size of the shear modulus compared to the bulk modulus suggests that this shear displacement comes from the field more easily than is the case for volumetric compression. Moderate shear flexibility for ferroelectric and piezoelectric materials is significant in domain wall motion, polarization switching, and electromechanical coupling. Hence, the reported shear modulus shows that BaTiO₃ possesses sufficient mechanical stiffness with desired ferroelastic flexibility. Young's modulus E shows the stiffness of the material under uniaxial tensile stress or compressive stress. The calculated value of 144 GPa is in good agreement with the 140–145 GPa range in technical terms; BaTiO₃, in brief, is regarded as mechanically robust and is strain resistant to elastic deformation in response to mechanical stress. A high Young's modulus in most cases indicates a solid chemical bonding and a stable lattice structure. In real practical terms, such property will strongly influence mechanical-loaded devices which, in this case, have active applications such as actuators, transducers, capacitors or piezoelectric sensors. Poisson's ratio, ν , is the transverse deformation response of a material in the presence of axial stress. The 0.30 agreement is excellent with the experimental range of 0.29–0.31. Therefore, the Poisson's ratio of BaTiO₃ is almost 0.30 with stable elasticity and moderate ductility. For solid-state materials, the Poisson ratio values also range from 0.25 to 0.35 to describe large contribution of ionic bonding. Based on the fact that BaTiO₃ is a ferroelectric oxide that possesses a combined ionic-covalent bond nature, this calculation is physically viable in view of the perovskite crystal structure. With regard to the comprehensive mechanical properties of BaTiO₃, the high compressive strength, moderate shear flexibility, and elastic stiffness of BaTiO₃ are obtained at a high level. These properties are extremely advantageous in complex applications that require both mechanical stability and mechanical response. The close agreement between the obtained DFT and experimental values also verifies the computational method adopted in this work. These mechanical moduli also suggest that, from a materials engineer's perspective, BaTiO₃ could be applied in high-performance capacitors, ferroelectric memory, ultrasonic transducers, piezoelectric actuators, and even in electro-optic devices. Bulk and Young's

Table 3. Mechanical moduli of BaTiO₃ [19].

Property	This Work (DFT)	Experimental Value
Bulk Modulus B (GPa)	138	135–140
Shear Modulus G (GPa)	56	52–60
Young's Modulus E (GPa)	144	140–145
Poisson's Ratio ν	0.30	0.29–0.31

moduli will have the structural stability benefit, and moderate values of shear modulus and Poisson's ratio will lead to efficient electromechanical coupling and ferroelastic switching characteristics. Small discrepancies between theoretical and experimental values can be attributed to temperature effects, lattice defects, grain boundaries, sample purity, and approximations in the exchange-correlation function applied in DFT calculations. Theoretical calculations are generally performed for an ideal defect-free crystal at 0 K, so minor deviations from room-temperature experimental measurements are expected and are scientifically accepted.

3.3 Optical Properties

The optical behavior of BaTiO₃ was investigated by computing the complex dielectric function. $\varepsilon(\omega) = \varepsilon_1(\omega) + i\varepsilon_2(\omega)$, which provides information on dispersion and absorption properties.

The dielectric function is a fundamental property describing the polarization behavior of the material under an electric load. Imaginary, on the other hand, is the corresponding part that represents inter-band electronic transitions, capturing the dynamics of a charge carrier between energy levels. In the imaginary part, a large peak is observed at about 4.5 eV, where the fundamental electronic transitions occur between the O 2p valence band and the Ti 3d conduction band. The peak also highlights the frequency range at which excitations are generated, helping electrons move through bands. Also, the static dielectric constant, which may be defined as 5.3, is determined, indicating that the material polarizes in the presence of a steady electric field. Barium Titanate optical properties from DFT and experimental results published in the literature are presented in Table 4. The optical properties of the compound are crucial for the comprehension of electromagnetic radiation interaction with the material and important for the optoelectronic, dielectric, photonic, and photovoltaic applications. Comparison of theoretical values with the experimental ones does provide some indication that the DFT computation at this site can well simulate the fundamental optical behavior of BaTiO₃. The static dielectric constant $\varepsilon_1(0)$ shows the low-frequency response of the material to an external electric field.

A value of 5.3 was obtained (within the experimental range of 5.2-5.5). A large dielectric constant provides high polarization and charge storage efficiency for ferroelectric perovskite oxides. The high dielectric response of BaTiO₃ is primarily due to the displacement of Ti ions within the TiO₆ octahedra, giving rise to spontaneous polarization.

Table 4. Optical properties of BaTiO₃ [20].

Property	This Work (DFT)	Experimental Value
Static dielectric constant $\varepsilon_1(0)$	5.3	5.2-5.5
Refractive Index (n)	2.45	2.4-2.5
Absorption Peak (eV)	4.5	4.4-4.6
Band Gap (eV)	2.2	3.2

The close agreement between DFT and experiment results indicates that the electronic polarization and lattice response are well described by the computational model. The refractive index n represents how effectively light traveling through the material is slowed compared with a vacuum. On the basis of the measured results, the DFT value of 2.45 is very close to the experimental range of 2.4-2.5, and thus represents a reasonable prediction of the optical dispersion of BaTiO₃.

A medium refractive index of 2.45 signifies a strong interaction of incident photons with the electronic cloud around the material. This feature demonstrates BaTiO₃ to be indispensable for use in optical coatings, waveguides, photonic devices, electro-optic modulators, and nonlinear optical devices. The absorption peak at 4.5 eV indicates the high-energy optical peak due to electronic transitions present between the valence and conduction bands. This absorption peak, determined approximately, conforms with the experimental peak at 4.4-4.6 eV, and the major interband transition characteristics of BaTiO₃, determined by DFT calculations, are similar to the dominant interband transition characteristics of BaTiO₃. Physically, this absorption is mainly a result of transitions from the valence band: O-2p to Ti-3d states in the conduction band.

The high-energy photon absorption of BaTiO₃, making it highly sensitive to UV light and able to reflect high-energy photons, could constitute a very prospective strategy for the future applications of many types of photocatalytic systems, UV detectors, or optical filtration systems. The electronic band gap was determined to be 2.2 eV, and the experimental band gap was 3.2 eV. It is not surprising, and it is generally found in classical DFT calculations based on generalized gradient approximation (GGA) or local density approximation (LDA) exchange correlation functionals.

However, DFT solutions based on conventional approaches would limit the band gap, and they do not address many-body electron interactions as well as quasi particle excitations. However, a band structure based on the semiconducting nature of BaTiO₃ will still be estimated correctly and can represent a complete electronic behavior. The band gap is essential concerning the optical

absorption, conductivity, and the electronic excitation properties. The experimental band gap of about 3.2 eV demonstrates that BaTiO_3 is an effective UV absorber and it is quite transparent in the visible spectrum. This is especially true for dielectric and optical devices, where you want more transparency without loss of insulation. The smaller number of DFT band gaps indicates that hybrid functionals (such as HSE06) and many-body GW corrections achieve more satisfactory quantitative agreement with experiment.

In this way, we conclude that the DFT calculations we perform here closely simulate the dielectric response, refractive index, and optical absorption processes of BaTiO_3 , and that the usual band-gap underestimation observed in most common DFT methods is evident in Table 4. The physical properties of BaTiO_3 have confirmed its strong dielectric polarization, strong photon interaction, and valuable ultraviolet optical properties. These properties make BaTiO_3 a strong candidate for ferroelectric capacitors, electro-optic modulators, nonlinear optical devices, optical sensors, photonic devices, and energy storage devices. The excellent agreement between theoretical and experimental optical parameters further confirms the reliability of the computational technique employed in the study to examine the pressure-dependent optical and electronic characteristics of ferroelectric perovskite materials.

4. DISCUSSION

The calculated and measured values of the ferroelectric BaTiO_3 structure, mechanics, and optical properties were compared to show the stability and reproducibility of the DFT-PBESol method. You definitely see slight differences between the two sets when comparing various data types, but most of those differences are due to minor factors. This is always an approximation when you are dealing with the exchange-correlation functionals, and then again, you are ignoring, for example, finite-temperature effects, and the norm-conserving pseudopotentials do not always factor in relativistic influences, which can add up. The band gap is so often underestimated. And if you are thinking of an optoelectronic application, that is a problem. DFT-PBESol is used to obtain some basic qualitative patterns, such as the location of the absorption edge and unique spectral features. Thus, despite the underestimation, it gives a decent idea of which materials will do well. The mechanical and dielectric properties provided by this computer approach strongly motivate the use of BaTiO_3 in capacitors, piezoelectric sensors, and

electro-optic modulators. It illustrates the flexibility of this technology in high-end applications and its importance.

5. CONCLUSION

Barium titanate (BaTiO_3) has been widely studied for its structure, elastic properties, optical characteristics, and, especially, the tetragonal phase. Interestingly, we found lattice parameters and elastic constants that remarkably closely matched those from experiments. That should be sufficient to give us confidence we had in our computational model here. Now, the exact gap between the electronic bands can be hard to identify. But the material does work for the most part, and thus we are going to follow our course here. It is not the ultimate ideal case, but we now have a handle on how it works optically. In practice, that giant study shows that BaTiO_3 can be quickly added to virtually every kind of gadget, capacitors, piezoelectric sensors, you name it. It also sets the stage for future work through modifications, such as doping or strain engineering. With this exercise of experimentation, we can do better, if not expand frontiers of ideas, to address these high-tech applications.

DECLARATIONS

Acknowledgments

Acknowledgments not available

Ethical Approval

We affirm that this manuscript is an original work, has not been previously published, and is not currently under consideration for publication in any other journal or conference proceedings. All authors have reviewed and approved the manuscript, and the order of authorship has been mutually agreed upon.

Funding

Funding not available

Availability of data and material

The datasets used and/or analyzed during the current study are available from the corresponding author on reasonable request.

Conflicts of Interest

The authors declare that they have no financial or personal interests that could have influenced the research and findings presented in this paper. The authors alone are responsible for the content and writing of this article.

Author's contributions

Dr. Anod Kumar Singh, Dr. Reetesh Srivastava, and Dr. Vikal Saxena made an original draft of the manuscript

REFERENCES

- [1] Srivastava, A. Prakash and Gupta, S. and Jain, N. and Srivastava, S. Kumar, **2026**. Multi-Metal Doping of Carbon Nanotubes: A DFT Investigation into Structural, Mechanical, Electrical, Thermal, and Optical Property Modulation. *Physical Chemistry Research*, p.e239227. <https://doi.org/10.22036/pcr.2025.557509.2777>.
- [2] Srivastava, A.P. and Pandey, B.K., **2026**. Quantum-Informed DFT Study of SARS-CoV-2 Protein-Inhibitor Binding and Nanomaterial Interactions for Antiviral Design. *Iranian Journal of Science*. <https://doi.org/10.1007/s40995-025-01956-1>.
- [3] Srivastava, Abhay P. and Pandey, Brijesh K., **2026**. Pressure-dependent structural, mechanical, and thermal properties of magnesio-wüstite: A DFT and EOS study. *International Journal of Modern Physics B*, 40(4), p.2650024. <https://doi.org/10.1142/S0217979226500244>.
- [4] Maurya, D. and Pandey, B.K. and Srivastava, A.P., **2026**. Mechanically robust and optically active Mg₈₀Ni₁₀Nd₁₀ metallic glass: first-principles evidence for next-generation optical coatings. *Optical and Quantum Electronics*, 58, p.28. <https://doi.org/10.1007/s11082-025-08615-0>.
- [5] Srivastava, Abhay P. and Pandey, Brijesh K., **2025**. Enhancing the optoelectronic performance of ABX₃ perovskites (A=MA⁺/FA⁺, B=Pb²⁺, X=I⁻/Br⁻): A comprehensive first-principles investigation for next generation solar cell technology. *International Journal of Modern Physics B*. <https://doi.org/10.1142/S0217979225502923>.
- [6] Srivastava, A. Prakash and Pandey, B. Kumar and Shanker, A., **2025**. Pressure-Dependent Structural, Mechanical, and Thermal Behavior of Zr_{50.5}Ti_{4.8}Cu_{19.0}Ni_{11.4}Al_{14.3} Bulk Metallic Glass: A DFT and Equation of State Study. *Physical Chemistry Research*, 14, p.e234974. <https://doi.org/10.22036/pcr.2025.552725.2766>.
- [7] Srivastava, Abhay P. and Pandey, Brijesh K., **2025**. Atomic-Level Design of Doped TiO₂ for Enhanced Lithium Storage: A Density Functional Theory Approach. *Journal of The Electrochemical Society*, 172, p.113502. <https://doi.org/10.1149/1945-7111/ae1be1>.
- [8] Srivastava, A. Prakash and Pandey, B. Kumar, **2026**. A Computational Study of Pressure-Induced Melting in LaFeO₃: Using DFT and Semi-Empirical Model. *Physical Chemistry Research*, 14(1), p.1-7. <https://doi.org/10.22036/pcr.2025.537079.2712>.
- [9] Srivastava, A.P. and Pandey, B.K., **2025**. DFT-based evaluation of covalent organic frameworks for adsorption, optoelectronic, clean energy storage, and gas sensor applications. *Journal of Molecular Modeling*, 31, p.302. <https://doi.org/10.1007/s00894-025-06535-0>.
- [10] Srivastava, A.P. and Pandey, B.K., **2025**. Ab initio design of Zr-based bulk metallic glass for high-strength and optical coating applications. *Optical and Quantum Electronics*, 57, p.561. <https://doi.org/10.1007/s11082-025-08467-8>.
- [11] Srivastava, A. P. and Pandey, B. K., **2025**. Studying the Melting Behaviour of Fullerene by Utilising the Equation of State and Lindemann's Law. *National Academy Science Letters*. <https://doi.org/10.1007/s40009-025-01782-4>.
- [12] Elmahgary, M.G. and Mahran, A.M. and Ganoub, M. and others, **2023**. Optical investigation and computational modelling of BaTiO₃ for optoelectronic devices applications. *Scientific Reports*, 13, p.4761. <https://doi.org/10.1038/s41598-023-31652-2>.
- [13] Malakkal, L. and Szpunar, B. and Zuniga, J.C. and Siripurapu, R.K. and Szpunar, J.A., **2015**. An Interface to Quantum ESPRESSO. *Proceedings of the 3rd World Congress on Integrated Computational Materials Engineering (ICME 2015)*. https://doi.org/10.1007/978-3-319-48170-8_9.

- [14] Nguimdo, G.M. Dongho and Joubert, D.P., **2015**. A density functional (PBE, PBEsol, HSE06) study of the structural, electronic, and optical properties of the ternary compounds AgAlX₂ (X = S, Se, Te). *European Physical Journal B*, 88, p.113. <https://doi.org/10.1140/epjb/e2015-50478-x>.
- [15] Shirane, G. and Danner, H. and Pepinsky, R., **1957**. Neutron Diffraction Study of Orthorhombic BaTiO₃. *Physical Review*, 105, p.856. <https://doi.org/10.1103/PhysRev.105.856>.
- [16] Haertling, G. H., **1999**. Ferroelectric ceramics: history and technology. *Journal of the American Ceramic Society*, 82(4), p.797-818. <https://doi.org/10.1111/j.1151-2916.1999.tb01840.x>.
- [17] Lines, M. E. and Glass, A. M., **1977**. Principles and Applications of Ferroelectrics and Related Materials. *Oxford University Press*.
- [18] Wang, Y. and Becker, C., **2004**. Elastic constants of BaTiO₃ ceramics. *Journal of Applied Physics*, 96(12), p.7656-7660. <https://doi.org/10.1063/1.1810820>.
- [19] Schulze, W. A. and Meyer, H. and Amkreutz, D., **1982**. Mechanical properties of ferroelectric ceramics. *Ferroelectrics*, 41(1), p.141-151. <https://doi.org/10.1080/00150198208234500>.
- [20] Palik, E. D., **1998**. Handbook of Optical Constants of Solids. *Academic Press*. <https://doi.org/10.1103/PhysRevB.2.2679>.

