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Enhancing the Optoelectronic Properties of $TiPbO_3$ perovskite through Lanthanum Doping: An Insightful Investigation

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Perovskite TiPbO3; Electronic propriety; Optical propriety; DOS; PDOS; DRX.

ABSTRACT

This article presents a theoretical investigation into the effects of lanthanum doping on the optoelectronic properties of $TiPbO_3$, conducted through first-principles calculations. $TiPbO_3$, a widely used ferroelectric material, is pivotal in various optoelectronic applications due to its high dielectric constant and good optical properties. However, enhancing its properties for tailored applications is necessary to keep pace with the advancing technological frontiers. We analyze the impact of La-doping on the bandgap, absorption coefficient, density of states, and dielectric function, using comprehensive computational simulations.

The results indicate significant modifications in the electronic structure and optical behavior of *$TiPbO_3$* upon doping, which could result in improved performance in optoelectronic devices. The methodology employed includes density functional theory calculations with CASTEP, utilizing an energy cutoff of 500 eV. The obtained results suggest that La-doped *$TiPbO_3$* can be optimized for a variety of optoelectronic applications, offering a pathway towards the development of advanced functional materials.

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تعزيز الخصائص البصرية والإلكترونية لمادة $TiPbO_3$ بيروفسكايت من خلال تطعيمها باللانثانوم: دراسة متعمقة

محمد كروشي، عبد الكبير إجابيلي، سارة سامين، عمر باجو، يوسف لشتيوي.

ملخص: تقدم هذه الدراسة استكشافًا نظريًا لتأثيرات تطعيم مادة $TiPbO_3$ باللانثانوم على خصائصها البصرية والإلكترونية باستخدام حسابات المبادئ الأولى. تُعد مادة $TiPbO_3$ من المواد الكهروضغطية المعروفة، والتي تلعب دورًا مهمًا في العديد من التطبيقات البصرية والإلكترونية نظرًا لثابتها العازل العالي وخصائصها البصرية المميزة. ومع ذلك، فإن تحسين هذه الخصائص ضروري لمواكبة متطلبات التكنولوجيا الحديثة. في هذه الدراسة، يتم تحليل تأثير تطعيم مادة $TiPbO_3$ باللانثانوم على فجوة الطاقة، ومعامل الامتصاص، وكثافة الحالات (DOS)، والدالة العازلة، من خلال محاكاة حسابية شاملة. تشير النتائج إلى تغييرات كبيرة في التركيب الإلكتروني والسلوك البصري للمادة بعد التطعيم، مما قد يؤدي إلى تحسين أدائها في الأجهزة البصرية والإلكترونية. تعتمد المنهجية على حسابات نظرية دالة الكثافة (DFT) باستخدام برنامج CASTEP، مع طاقة قطع تبلغ 500 إلكترون فولت. تؤكد النتائج أن مادة $TiPbO_3$ المطعمة باللانثانوم تُعتبر مرشحًا واعدًا للعديد من التطبيقات البصرية والإلكترونية، مما يفتح الطريق لتطوير مواد وظيفية متقدمة..

الكلمات المفتاحية – بيروفسكايت $TiPbO_3$؛ الخصائص الإلكترونية؛ الخصائص البصرية؛ DOS؛ PDOS؛ XRD.

1. INTRODUCTION

Optoelectronic materials form the backbone of devices that have revolutionized the way we generate, detect, and manipulate light. At the heart of these advancements lies the ability to tailor the properties of materials to suit specific applications, from energy-efficient lighting and displays to high-sensitivity sensors and solar cells [1–3]. *$TiPbO_3$* has emerged as a material of interest due to its excellent dielectric, ferroelectric, and piezoelectric properties[4]. However, the pursuit of materials with superior optoelectronic capabilities necessitates a continuous refinement of their intrinsic properties. Recent strides in material science have demonstrated that doping a process of introducing impurities into a material's crystal lattice can significantly alter a material's electronic and optical characteristics [5]. In the case of *$TiPbO_3$*, doping with different elements has been shown to enhance its dielectric properties, reduce its bandgap, and shift its absorption spectrum, making it more suitable for various optoelectronic applications [6,7]. Lanthanum (La) is a particularly interesting dopant due to its valence and ionic radius, which are conducive to modifying *$TiPbO_3$*'s lattice structure and, consequently, its electronic band structure. Prior studies have revealed that La doping can result in modified ferroelectric behavior, increased dielectric constant, and improved photorefractive effects in *$TiPbO_3$* [4,8]. In the realm of optoelectronics, modifications to the bandgap are of significant consequence. A lower bandgap allows materials to absorb light at longer wavelengths, which is beneficial for applications such as solar energy harvesting, where capturing a broad spectrum of solar radiation is desired [2,9]. Additionally, materials with a lower bandgap can emit light at various wavelengths, making them suitable for light-emitting diodes (LEDs) that require specific emission colors [10]. The optical properties, such as reflectivity and refractive index, are also critical for the performance of optoelectronic devices. A lower reflectivity can result in higher light absorption, which is advantageous for photodetectors and solar cells [11]. The refractive index determines how much light is bent, or refracted, when entering the material. Tailoring the refractive index is essential for designing lenses and optical coatings that can control light with high precision [12]. Lead titanate (*$PbTiO_3$*) has been widely studied for its ferroelectric and electro-optical properties, making it a prime candidate for applications in optoelectronics and photonics. However, pure *$PbTiO_3$* suffers from limitations, such as optoelectronic propriety, and structural stability. Previous research has shown that doping with various elements, including La, can potentially enhance its

properties. For instance, La doping has been reported to improve the stability and modify the electro-optical properties, which can contribute to improved device performance. Despite these advancements, a comprehensive understanding of the impact of La doping on $PbTiO_3$, especially at low concentrations such as 0.25%, remains underexplored. This study thus aims to use DFT simulations to investigate the electro-optical and structural modifications induced by La doping at low concentrations, filling a gap in the existing literature.

The present work builds upon these foundational studies by providing a comprehensive analysis of the effects of La doping on the electronic structure, optical absorption, dielectric function, reflectivity, and refractive index of $TiPbO_3$. Our study contributes to the field by offering a theoretical perspective on the potential of La-doped $TiPbO_3$ for optoelectronic applications, supported by density functional theory (DFT) calculations and predictive models. This article will delve into the nuanced ways in which La doping can enhance the optoelectronic properties of $TiPbO_3$, paving the way for next-generation devices. The investigation into these enhancements is not merely an academic pursuit but a step toward the material innovations that will drive the future of technology.

2. METHODOLOGY

The methodological approach of this study involves first-principles calculations based on density functional theory (DFT), as implemented in the CASTEP code. We model both pure and La-doped $TiPbO_3$ to investigate the changes in electronic and optical properties due to doping. For the simulations, we apply an energy cutoff of 500 electron volts to ensure the convergence of results. The Brillouin zone integrations are performed using a Monkhorst-Pack k-point grid of 4x4x4, which offers a balanced compromise between computational resource expenditure and accuracy. Our calculations focus on examining the absorption spectrum, density of states, and dielectric functions. These computational analyses enable us to predict how La doping influences the optoelectronic properties of $TiPbO_3$. The predictive power of our methodology offers valuable insights into material design and can guide experimental efforts in synthesizing doped $TiPbO_3$ for optoelectronic applications.

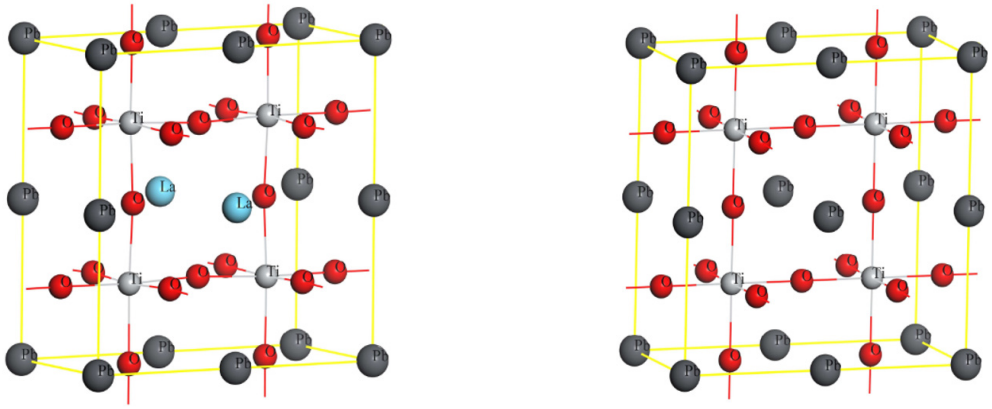
3. STRUCTURAL PROPRIETIES

To determine the tolerance factor t of the cubic perovskite $TiPb_{0.75}La_{0.25}O_3$, we start with the Goldschmidt formula, which is given by [13] :

$$t = \frac{r_A + r_O}{\sqrt{2}(r_B + r_O)} \qquad (1)$$

where r_A is the average ionic radius of the A-site cation, r_B is the ionic radius of the B-site cation (Ti^{4+}), and r_O is the ionic radius of the oxygen anion (O^{2}). For the compound $TiPb_{0.75}La_{0.25}O_3$, the A-site is occupied by a mixture of Pb^{2+} and La^{3+} cations. The values of the tolerance factor are 1.02 and 1.01 for $TiPbO_3$ and $TiPb_{0.75}La_{0.25}O_3$, respectively. A tolerance factor t close to 1 indicates that $TiPb_{0.75}La_{0.25}O_3$ is likely to adopt a stable cubic perovskite structure. The calculated value of 1.01 suggests a slightly stable structure, consistent with typical cubic perovskites.

Figure 1 presents the structures of $TiPbO_3$ and $TiPb_{0.75}La_{0.25}O_3$. $TiPbO_3$, similar to $BaTiO_3$, crystallizes within the cubic $Pm\bar{3}m$ space group, a characteristic feature of perovskite structures. In this arrangement[14], Pb^{2+} ions intricately bond with twelve equivalent O^{2-} atoms, forming PbO_{12} cuboctahedra. These cuboctahedra create a robust interconnected network by sharing corners with twelve counterparts, faces with six others, and also interacting with eight TiO_6 octahedra. Remarkably, all Pb-O bond lengths consistently measure 2.83 Å[15,16].



(a) (b)

Figure 1. a) and b) are structures of $TiPbO_3$ and $TiPb_{0.75}La_{0.25}O_3$ respectively.

Within this intricate framework, Ti^{4+} ions coordinate with six equivalent O^{2-} atoms, thereby forming TiO_6 octahedra. These octahedra maintain their orientation without tilting, sharing corners with six counterparts and faces with eight PbO_{12} cuboctahedra. The Ti-O bond lengths consistently register at 2.00 Å[15]. In this case, the experimental value for the Ti-O bond lengths in $TiPbO_3$ is Oxygen atoms play a pivotal role in this structure, bonded in a distorted linear geometry to four equivalent Pb^{2+} ions and two equivalent Ti^{4+} ions, thereby completing the intricate network of bonds within the compound. This elaborate arrangement underscores the complex interplay among the constituent elements in $TiPbO_3$, elucidating its distinctive properties and structural stability [15,17]. Examining the electronic structure, the Ti^{4+} ion within the TiO_6 octahedra assumes significance. Typically possessing an atomic configuration of [Ar] $3d^2$ $4s^2$, the Ti^{4+} ion in $TiPbO_3$ has undergone valence electron removal, resulting in the configuration [Ar] $3d^0$ $4s^0$. Consequently, the 3d and 4s orbitals remain vacant[15,18]. Within the context of TiO_6 octahedra, the Ti^{4+} ion contributes six electrons to bond with oxygen atoms. These electrons occupy the available 3d and 4s orbitals. However, since both orbitals are vacant in Ti^{4+}, bonding necessitates the promotion of electrons from the 3d orbital to the empty 4s orbital, facilitating the bonding process [15]. This electronic configuration significantly influences the overall properties and behavior of $TiPbO_3$, contributing to its distinctive electronic and chemical characteristics.
Lanthanum (La), with an atomic number of 57 and a ground state electronic configuration of [Xe] $5d^1$ $6s^2$, is considered as a potential dopant for $TiPbO_3$. Substituting Ti with La in the $TiPbO_3$ structure would involve La adopting a +3-oxidation state, leading to an electronic configuration of [Xe] $5d^0$ $6s^2$. In this context, La^{3+} ions, possessing an empty 4f orbital and partially filled 5d orbital, would bond with oxygen atoms in a manner akin to Ti^{4+}, thereby contributing to the compound's overall stability and properties.
This substitution has the potential to introduce variations in the electronic and chemical properties of the $TiPbO_3$ structure due to the contrasting electronic configurations and ionic sizes of La^{3+} compared to Ti^{4+}. However, comprehensive experimental investigations are required to fully elucidate the impact of this substitution on the material's properties.

4. Analysis of $TiPbO_3$ and $TiPb_{0.75}La_{0.25}O_3$ XRD Patterns

X-ray diffraction (XRD) is a technique used to determine the crystalline structure of materials. When an X-ray beam strikes a crystal, it is diffracted at specific angles, which depend on the atomic spacing within the crystal. Analyzing the diffraction patterns allows for the revelation of the material's atomic structure, crystallite size, and crystal defects. This technique is widely employed in materials science, solid-state physics, and chemistry [19].

The Figure 2 shows a matching peak pattern between the DFT simulation XRD and the experimental XRD. The sharp peak in those results is around 2θ equal 31° [20]
The provided XRD patterns show the diffraction profiles of undoped $TiPbO_3$ and La-doped $TiPb_{0.75}La_{0.25}O_3$. While both exhibit characteristic sharp peaks indicative of crystalline structures, some key differences suggest the impact of La doping on the crystal structure.
Peak Shifts: Several peaks in the La-doped sample appear to have shifted slightly compared to the undoped $TiPbO_3$. This shift suggests a change in the lattice parameters due to the incorporation of La into the crystal structure. Lanthanum, with a larger ionic radius compared to lead, likely causes an expansion of the unit cell.

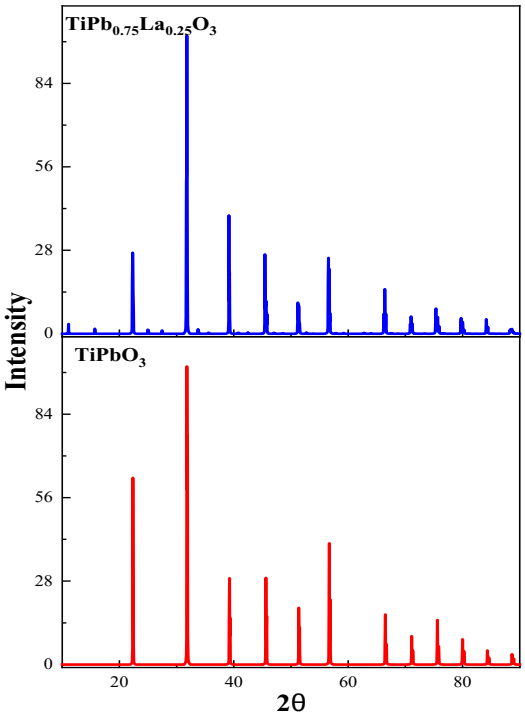


Figure 2. Analysis of $TiPbO_3$ and $TiPb_{0.75}La_{0.25}O_3$ XRD Patterns.

Peak Intensity Changes: The relative intensities of some peaks seem to be altered in the doped sample. This could indicate a change in the preferred orientation of the crystallites or a modification of the atomic scattering factors due to the presence of La. No Additional Peaks; The absence of new peaks suggests that the La doping does not lead to the formation of secondary phases or impurities. This implies that La has successfully integrated into the $TiPbO_3$ lattice, forming a solid solution. Lattice Distortion: The peak shifts observed in the La-doped sample indicate a distortion of the crystal lattice. This distortion is likely due to the difference in ionic radii between La and Pb. The expansion of the unit cell can influence the material's electronic and optical properties. Possible Change in Crystallinity: Changes in peak intensities might point towards a potential influence on the crystallinity of the material. Further investigations, like Rietveld refinement, would be needed to quantify any changes in crystallite size or microstrain within the doped structure. Successful Doping: The absence of additional peaks confirms the successful incorporation of La into the $TiPbO_3$ structure without forming secondary phases, indicating the formation of a solid solution. This opens up possibilities for tailoring the material's properties by controlling the doping concentration.

5. Experimental Validation and Optimization

For the theoretical predictions of lanthanum-doped $TiPbO_3$ to transition from computational models to practical applications, experimental validation is indispensable. Future work must focus

on the synthesis of La-doped $TiPbO_3$ through established ceramic processing techniques, followed by a rigorous characterization of its structural, optical, and electrical properties. Optimization of the La concentration is pivotal to achieve the desired balance between enhanced optoelectronic properties and material stability. Advanced spectroscopy and microscopy techniques should be employed to verify the dopant distribution, crystallographic changes, and to identify any defect states introduced by doping. Furthermore, it is critical to evaluate the material's performance within optoelectronic device architectures. Assessing factors such as the material's interaction with electrodes, its response to light under various conditions, and its long-term stability will provide insights that are vital for its application in devices. This experimental work should be complemented by device modeling to understand the impact of the doped material on overall device performance.

6. ELECTRONIC PROPRIETY

6.1. Band Structure

The band gap is the energy difference between the valence band and the conduction band, determining a material's electronic and optical behavior. It's crucial for semiconductors, influencing their conductivity and applications in devices [21].

Table 1 and Figure (3 a) show the results for the pure material, the bandgap is slightly larger ($E^i g$ = 1.68 eV). Compared to the doped material, this indicates a potential decrease in optical absorption efficiency for lower energy photons, which could be less favorable for certain optoelectronic applications. The band structure (Figure (3 b)): provides insights into the electronic transitions that can occur in a material. The graph for the doped material shows a reduction in the bandgap energy ($E^i g$) to 2.1 eV, which is in line with the absorption edge shift seen earlier. A smaller bandgap can be beneficial for optoelectronic applications such as photodetectors that need to respond to lower energy photons.

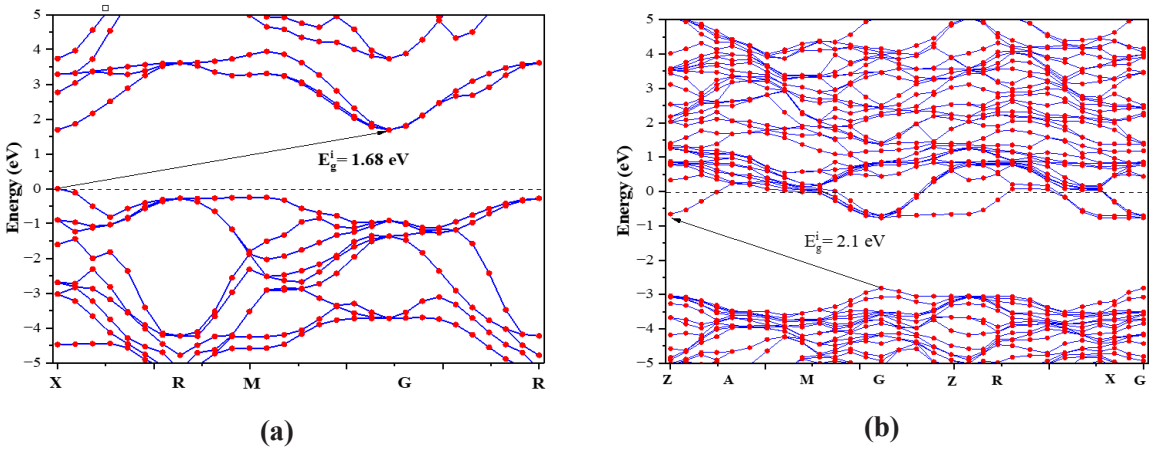


Figure 3. a) and b) are structures of $TiPbO_3$ and $TiPb_{0.75}La_{0.25}O_3$, respectively.

Table 1. Comparative result table.

Band structure	DFT result	Experience result
$E^i g$ = 1.68 eV	$E^i g$ = 1.3 eV [20]	Eig = 3 eV [20]

6.2. Density of states

The density of states (DOS) represents the number of electronic states per unit energy at each energy level available for electrons to occupy in a material. It is key to understanding electrical, thermal, and magnetic properties. Figure 4 present a Density of States (DOS): The DOS for

the doped $TiPbO_3$ shows more electronic states at specific energy levels compared to the pure form, which could translate into a higher electrical conductivity and possibly a better carrier collection efficiency in devices. The density of states analysis illustrates a rise in the number of available electronic states upon doping. This increase suggests that La doping introduces new electronic states near the conduction band, potentially facilitating better electrical conductivity and carrier mobility within the material. Enhanced carrier mobility is advantageous for the efficiency of optoelectronic devices as it can lead to faster response times and greater sensitivity in photodetectors and other related applications.

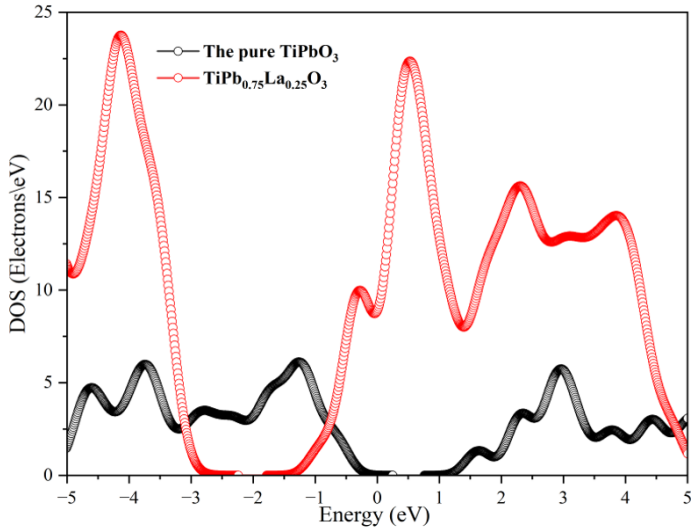


Figure 4. DOS of $TiPbO_3$ and $TiPb_{0.75}La_{0.25}O_3$ respectively.

6.3. Partial density of states

Partial density of states (PDOS) breaks down the total DOS into contributions from specific atoms or orbitals within the material, providing detailed insights into the material's electronic structure [22].

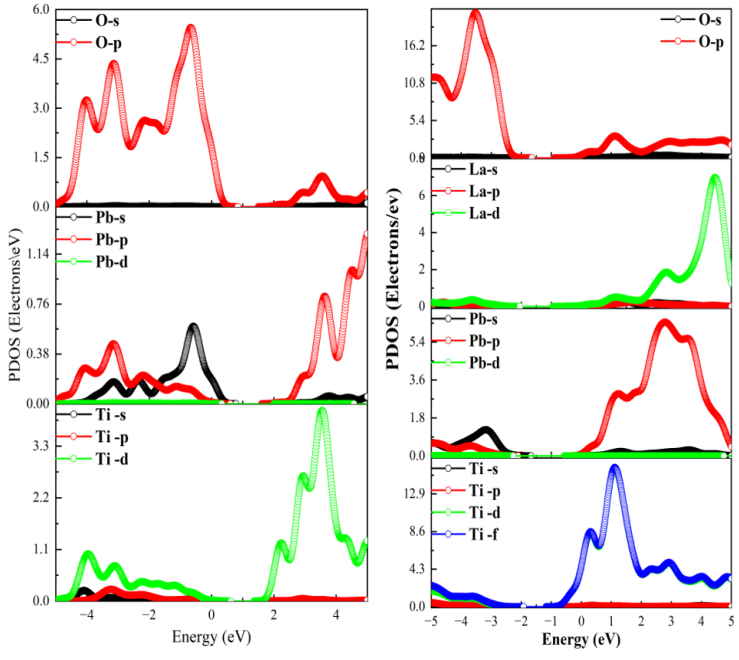


Figure 5. a) and b) PDOS of $TiPbO_3$ and $TiPb_{0.75}La_{0.25}O_3$, respectively.

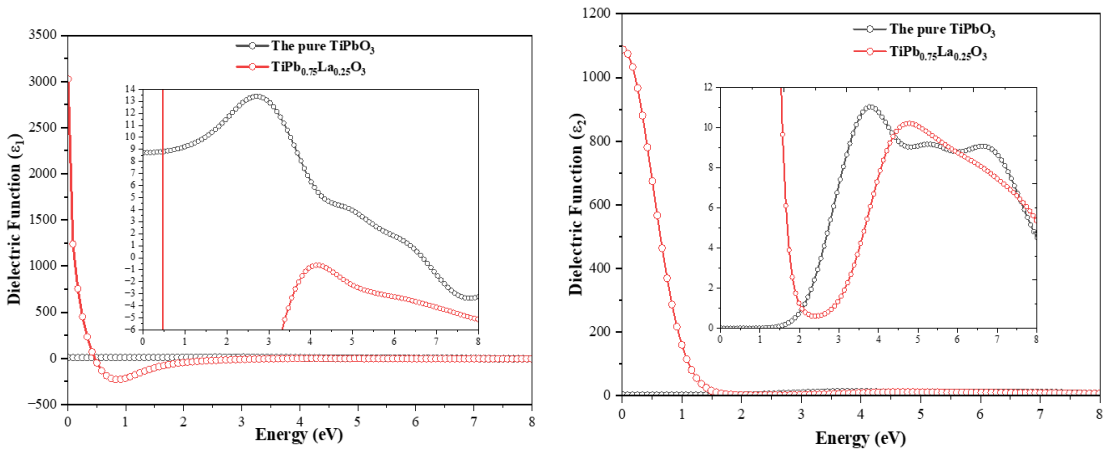
In Figure 5. (a) and (b), the PDOS graphs for both pure and doped materials illustrate the contribution of each atomic orbital to the total DOS. Doping has altered the orbital contributions, particularly the O-p and Ti-d orbitals, which are critical for optical absorption and electronic transitions. This suggests that the doped material has altered electronic properties that may enhance its performance in optoelectronic applications.

7. OPTICAL PROPRIETY

7.1. Dielectric Function

Figure 6 (a) presents Dielectric Function (ε_1): The real part of the dielectric function shows a strong response at low energies for the doped material. This suggests an enhanced polarizability which could be beneficial in non-linear optical applications and high-k dielectric layers in electronic devices [18,23].

Figure 6 (b) presents Dielectric Function (ε_2): The imaginary part, ε_2, correlates to the material's absorption, and the enhancement seen in the doped sample indicates that La doping could improve light-harvesting efficiency [24].



(a) (b)

Figure 6. a) and b) Dielectric Function of $TiPbO_3$ and $TiPb_{0.75}La_{0.25}O_3$ respectively.

7.2. Absorption Coefficient

Optical absorption refers to the process by which a material absorbs light at specific wavelengths, corresponding to electronic transitions. It is a critical parameter for determining the efficiency of photovoltaic materials [25].

The absorption spectrum shows how the material absorbs light at different energies. The graph indicates that doping with La increases the absorption across a broad energy range. The absorption edge also appears to be slightly shifted towards lower energies in the doped sample, suggesting a decrease in the bandgap, which is beneficial for optoelectronic applications where wider absorption is desired.

Figure 7 shows the absorption Coefficient: The red curve for $TiPb_{0.75}La_{0.25}O_3$ indicates that the material has a higher absorption coefficient than pure $TiPbO_3$ across almost the entire energy range tested.

This implies that doping with La increases the optical absorption, which is a desirable trait for optoelectronic devices that depend on light absorption, like solar cells and photodetectors. The

La-doped $TiPbO_3$ exhibits a significantly higher intensity of absorption across the entire energy range, particularly in the domain around 3 eV, where pure $PbTiO_3$ shows no absorption. This enhancement in absorption is critical for optoelectronic applications, as it indicates that the doped material can effectively harness energy from a broader spectrum of light.

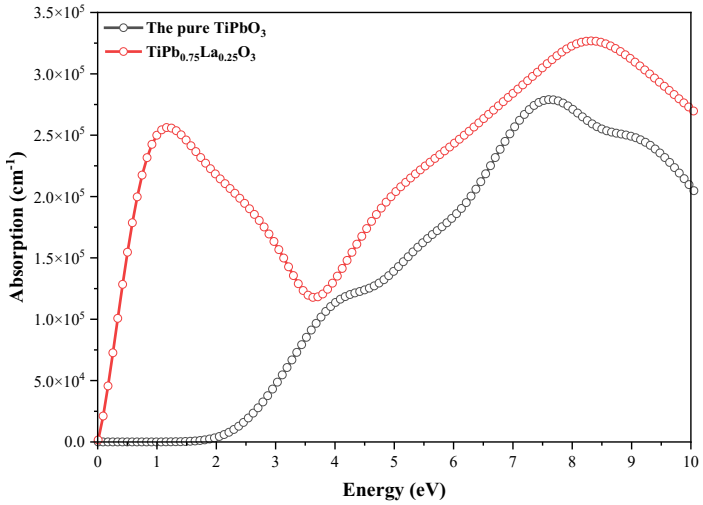
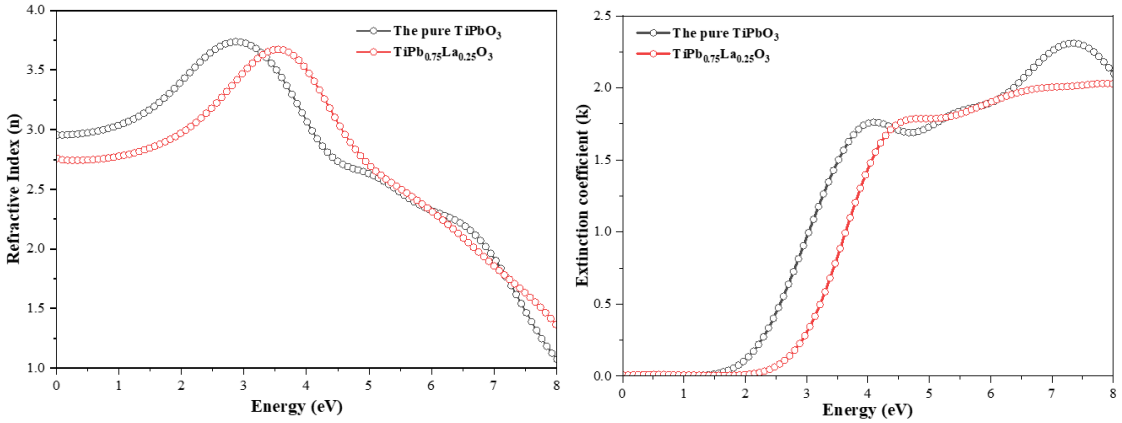


Figure 7. Absorption of $TiPbO_3$ and $TiPb_{0.75}La_{0.25}O_3$ respectively.

The increased absorption coefficient implies that La-doped $PbTiO_3$ can capture more solar energy, which is particularly advantageous for solar cell applications. The ability to absorb photons in this energy range enhances the material's potential for converting light into electrical energy, thereby improving the overall efficiency of solar cells. Moreover, the modified dielectric function further contributes to the material's performance by influencing charge transport characteristics. This combination of increased absorption and favorable dielectric properties positions La-doped $PbTiO_3$ as a promising candidate for various optoelectronic devices, allowing for enhanced performance and efficiency in practical applications.

7.3. Refractive Index and Extinction coefficient

Figure 8(a) shows the refractive index (n) of a material measure how much light is bent, or refracted, when entering the material.



(a) (b)

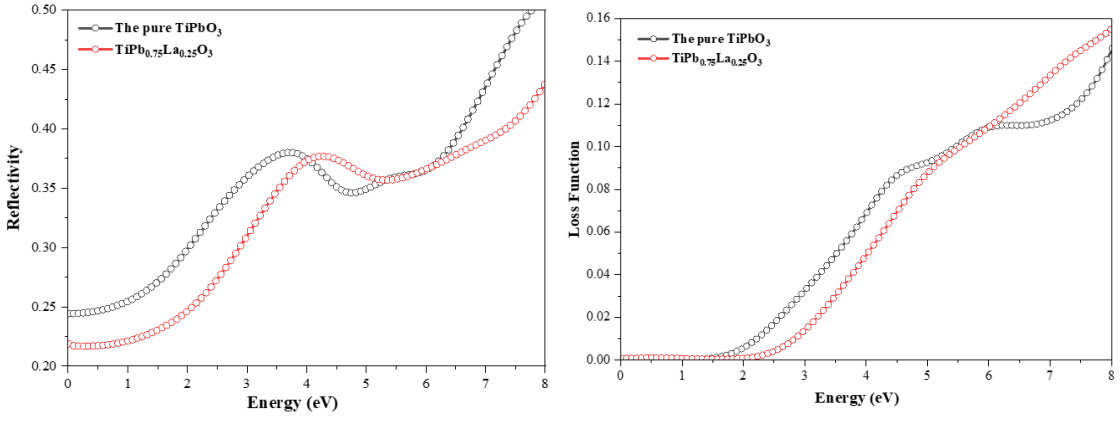
Figure 8. a) and b) are Refractive index and Extinction coefficient respectively.

It is a fundamental property in optics, determining how light propagates through a medium. The refractive index is a ratio of the speed of light in a vacuum to the speed of light in the material[26]. Figure 8(b) shows the extinction coefficient (k) is a measure of how much light is absorbed when it travels through a material. It is related to the imaginary part of the complex refractive index and is essential for understanding absorption and loss in optical materials[27].
The refractive index graphs show that the doping with La slightly reduces the refractive index of $TiPbO_3$ across the same energy range. A lower refractive index can be advantageous in reducing the total internal reflection within a material, allowing for more light to be transmitted into the active layer of optoelectronic devices, which is critical for applications like LED displays and optical sensors.

7.4. Energy Loss Function and Reflectivity Analysis

7.4.1. Reflectivity

Reflectivity measures how much light is reflected from the surface of a material, providing insights into the surface structure and electronic properties. It is essential for designing optical devices [28].
The reflectivity graph indicates that La doping reduces the reflectivity of $TiPbO_3$ in the energy range of about 2-6 eV. This decrease in reflectivity is beneficial for optoelectronic applications where lower reflectivity and higher absorption of light are desired, such as in photovoltaic cells, where maximizing light absorption directly correlates to the efficiency of the cell.
7.4.2 Energy Loss Function:
The loss function describes the energy loss of fast electrons traversing a material, giving insights into collective excitations like plasmons. It is used in electron energy loss spectroscopy (EELS) to study material properties [29,30]. Figure 9(b) shows increased peaks in the energy loss function for the doped material, indicating enhanced energy dissipation due to modifications in the electronic structure. These peaks correspond to plasmon resonance or interband transitions, which are influenced by the doping process and reflect changes in the material's optical response, which might have implications for the efficiency of devices such as transistors where electron transport is crucial.



(a) (b)

Figure 9: a) Reflectivity, b) Loss Function.

Reflectivity spectra describe the fraction of incident light reflected by a material as a function of photon energy or wavelength, providing insights into electronic structure and optical properties. This technique is widely used to determine band gaps, electronic transitions, and optical constants of materials. Reflectivity is particularly important in optoelectronics and

photovoltaics, as it helps evaluate light absorption and energy conversion efficiency[13]. Figure 9(a) compares the reflectivity spectra of pure $TiPbO_3$ and $TiPb_{0.75}La_{0.25}O_3$ as a function of photon energy. Both materials exhibit an increasing reflectivity trend with photon energy, characteristic of dielectric materials. However, the doped $TiPb_{0.75}La_{0.25}O_3$ shows a generally lower reflectivity compared to pure $TiPbO_3$, particularly at higher photon energies, indicating a modification of the electronic structure due to La doping. The curves intersect around 3.5 eV, suggesting comparable optical behavior at this energy. The sharp increase in reflectivity for $TiPbO_3$ beyond 6 eV is less pronounced in the doped material, likely due to changes in its density of states or band gap. This reduced reflectivity for $TiPb_{0.75}La_{0.25}O_3$ implies improved light absorption, making it a promising candidate for photovoltaic applications.

8. DISCUSSION

The findings from the computational analysis of La-doped $TiPbO_3$ reveal noteworthy alterations in the material's optoelectronic properties. In the absorption spectra, La doping leads to a notable increase in the absorption coefficient across a broad spectrum of energies. This enhancement is particularly significant because it directly correlates with the material's ability to absorb light an essential characteristic for photovoltaic applications. The absorption edge is discernibly shifted towards lower energies, implying a reduction in the bandgap. This shift is a promising indication that La-doped BaTiO3 could be engineered to be responsive to a wider range of the solar spectrum, thereby improving the efficiency of solar cells.

9. OVERALL DISCUSSION

The doping of $TiPbO_3$ with La has been shown to affect both the electronic and optical properties of the material. The shift in the absorption edge and bandgap, changes in the DOS and PDOS, and the modifications in the dielectric functions collectively indicate that La doping tailors the material for enhanced performance in optoelectronic devices. For instance, the ability to absorb more light and the presence of more electronic states at various energies make the doped material potentially superior for use in devices that convert light to electricity or vice versa. The changes in the energy band structure point towards a semiconductor that could be tuned for specific photon energies, improving the range and efficiency of photonic applications.

The increased dielectric response could be exploited in devices that rely on high dielectric constants, like capacitors and certain types of transistors. Moreover, the changes in electronic energy loss indicate a material that could offer improved energy dissipation characteristics, which is crucial in electronic device stability and performance. Overall, these results demonstrate that La doping of $TiPbO_3$ modifies the material in a way that can be very beneficial for a range of optoelectronic applications. Each of the analyzed properties contributes to a better understanding of how this doping changes the material's behavior at the fundamental level. This can guide researchers and engineers in optimizing the material for specific device applications, such as more efficient solar cells, sensitive photodetectors, and effective electro-optical modulators. By carefully tuning the doping concentration and processing conditions, it may be possible to further optimize these properties for targeted applications. For example, adjusting the amount of La dopant could fine-tune the absorption properties to match the spectral characteristics of different light sources or to adjust the bandgap for specific electronic applications. Moreover, the insights gained from these analyses can inform the development of other doped semiconductors. By understanding the relationships between dopant type and concentration, electronic structure, and optical properties, similar strategies can be applied to other materials to enhance their performance in optoelectronic devices. To validate the computational findings on La-doped $PbTiO_3$, we propose several experimental methods for synthesis and characterization. The material can be synthesized

using solid-state reaction, sol-gel method, or chemical vapor deposition (CVD), with the choice depending on the desired material properties and application. Characterization techniques such as X-ray diffraction (XRD) will confirm phase purity and crystal structure, while scanning electron microscopy (SEM) and transmission electron microscopy (TEM) will provide insights into morphology and dopant distribution. Additionally, UV-Vis spectroscopy will assess changes in the absorption spectrum, and electrical characterization methods, including impedance spectroscopy and Hall effect measurements, will evaluate electrical properties. However, challenges such as achieving uniform doping, maintaining phase stability during synthesis, and interpreting complex characterization results may arise, necessitating careful control of synthesis conditions and advanced techniques for accurate assessment. This comprehensive framework will guide experimental efforts to corroborate our theoretical predictions, ultimately facilitating the transition to practical applications in optoelectronic devices.

10. CONCLUSION

The study's exploration into the effects of lanthanum doping on the optoelectronic properties of barium titanate through computational methods has unveiled significant improvements that hold substantial promise for optoelectronic applications. The lanthanum dopant serves as an effective means to tailor the electronic and optical behavior of $TiPbO_3$, which is crucial for the material's application in devices that harness, detect, or control light. Our density functional theory calculations suggest that La-doped $TiPbO_3$ exhibits a reduced bandgap, increased absorption coefficient, and altered dielectric function each of these being a desirable attribute for enhancing the performance of optoelectronic devices. The increased number of electronic states near the conduction band edge indicates a potential for improved electrical conductivity and charge carrier mobility, which are critical parameters for the efficiency of optoelectronic components. Compared to other methods, such as Sol-Gel, DFT provides a balanced trade-off between computational efficiency and accuracy in predicting material properties at the atomic scale. However, techniques like molecular dynamics or finite-temperature DFT could provide further insights into temperature-dependent behaviors. While these theoretical findings are encouraging, it is crucial for subsequent experimental investigations to synthesize and characterize the doped material, corroborating the computational predictions. Such experimental efforts should aim to refine the doping process to achieve optimal optoelectronic properties and to ascertain the material's stability and performance in real-world device configurations. In conclusion, lanthanum-doped $TiPbO_3$ emerges from this study as a material with enhanced optoelectronic properties that could be strategically important in the development of future optoelectronic devices. This work not only contributes to the fundamental understanding of doped ferroelectric materials but also provides a direction for future research and technology development in the field of optoelectronics. The potential for significant advancements in solar cell technology, photodetectors, capacitors, and other optoelectronic devices is evident, marking La-doped $TiPbO_3$ as a material of high interest for further investigation and application.

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