Adıyaman University Journal of Science
https://dergipark.org.tr/en/pub/adyujsci
DergiPark AKADEMİK
ISSN 2147-1630
e-ISSN 2146-586X

Elucidating The Semiconducting Nature of $SrThO_3$ for Electronic Structure Engineering Using Density Functional Theory Method

Merve ÖZCAN[1,*]

[1]*Toros University, Faculty of Engineering, Department of Electric Electronic Engineering, 33210, Mersin, Türkiye*
merve.ozcan@toros.edu.tr, ORCID: 0000-0003-3772-2229

Received: 18.08.2025 **Accepted:** 10.06.2026 **Published:** 30.06.2026

Abstract

In this study, the ground-state structural and electronic band structure of cubic $SrThO_3$ (*space group* $P_m\bar{3}m$*, No. 221*) were comprehensively investigated using first-principles calculations within the framework of density functional theory (DFT) at ambient conditions, as implemented in the Quantum Espresso software and code. The structural and electronic characteristics of pristine $SrThO_3$ were calculated using the Generalized Gradient Approximation (GGA) within the Perdew Burke Ernzerhof (PBE) exchange–correlation functional. The structural parameters show good agreement with previously reported theoretical data, validating the reliability of the adopted methodology. The electronic band gap was calculated as 1.986 eV with direct band characterization. This paper focused on the investigation of the structural model and electronic behavior of pristine $SrThO_3$ to understand its potential use in optoelectronics devices.

Keywords: $SrThO_3$; Modelling; Structural; Electronic structure; Density functional theory.

* Corresponding Author DOI: 10.37094/adyujsci.1767897

Yoğunluk Fonksiyonel Teorisi Yöntemi Kullanılarak $SrThO_3$'ün Yarı İletken Doğasının Elektronik Yapı Mühendisliği için Aydınlatılması

Öz

Bu çalışmada, kübik $SrThO_3$'ün (uzay grubu $Pm\bar{3}m$, No. 221) temel durum yapısal ve elektronik bant yapısı, yoğunluk fonksiyonel teorisi (DFT) çerçevesinde ilk prensip hesaplamaları yoluyla kapsamlı bir şekilde Quantum Espresso yazılımı ve kodu kullanılarak ortam koşullarında incelenmiştir. $SrThO_3$'ün yapısal ve elektronik özellikleri, Perdew Burke Ernzerhof (PBE) değişim-korelasyon fonksiyoneli içinde Genelleştirilmiş Gradyan Yaklaşımı (GGA) kullanılarak hesaplanmıştır. Yapısal parametreler, daha önce bildirilen teorik verilerle iyi bir uyum göstermektedir ve benimsenen metodolojinin güvenilirliğini doğrulamaktadır. Elektronik bant aralığı, doğrudan bant karakteristiği ile 1.986 eV olarak hesaplanmıştır. Bu makale, optoelektronik cihazlarda potansiyel kullanımını anlamak için $SrThO_3$'ün yapısal modelinin ve elektronik davranışının araştırılmasına odaklanmıştır.

Anahtar Kelimeler: $SrThO_3$; Modelleme; Yapısal; Elektronik yapı; Yoğunluk fonksiyonel teorisi.

1. Introduction

Recently, perovskite structures have attracted significant attention in the field of materials science due to their outstanding electrical and magnetic properties, making them promising candidates for a wide range of technological applications. In addition to their tunable band gaps and high carrier mobilities, these materials exhibit remarkable functionalities such as ferroelectricity, superconductivity, and piezoelectricity, which have been extensively explored in both experimental and theoretical studies. Among perovskite structures, $SrThO_3$ has become increasingly interesting recent decades. While $SrSiO_3$ has been investigated in detail, the physical properties of $SrTbO_3$ and $SrThO_3$ have not been thoroughly reported [1]. $SrThO_3$ was first synthesized in 1947 by Mary-Szabo using the solid-state method [2]. In addition, $SrThO_3$ has been synthesised using the sol-gel approach [3, 4]. The thermodynamic stability of $SrThO_3$ has also been discussed and reported [4, 5]. Notably, comprehensive investigations focusing on the prediction of electronic characteristics and the nature of chemical bonding in $SrThO_3$ remain largely unexplored [2, 4]. Shein et al. reported the electronic and thermal properties of $SrThO_3$ perovskite with cubic symmetry FPLAPW method within GGA [2]. Enhancing crystal stability is a critical parameter for the accurate prediction of electronic properties in solid-state materials. In perovskite compounds, the Goldschmidt tolerance factor (τ) is a widely adopted descriptor for

understanding structural stability. The Goldschmidt tolerance factor (τ) equal to 1 indicates the stability of perovskite structure. One method of calculating the tolerance factor is by using bond lengths, as given in Eqn. (1) [6].

$$\tau = \frac{0.707(L_{A-X})}{L_{B-X}} \quad (1)$$

L_A and L_B denote the bond lengths between the A-site and X-site, and the B-site and X-site, respectively, where A and B are cations, X is a halogen site. A positive formation energy of +1.440 eV was obtained for $SrThO_3$ from total energy difference analysis, suggesting that the compound is thermodynamically unfavorable and structurally unstable [2]. Mechanical stability of $SrThO_3$ was reported by Jamila et al [1], as it satisfies the born stability criteria. Band gap tuning can be effectively achieved through various approaches, such as chemical modifications [7], substitution of halogen elements [8, 9], and incorporation of metal dopants [9], all of which are widely recognized strategies in material design. Tuning band gaps by these method improves optoelectronic properties. This paper aims to calculate and predict the electronic properties of pristine $SrThO_3$ structure through first-principles calculations based on DFT calculations. As a quantum-mechanical approach, DFT provides a robust theoretical basis for the study of many-electron systems, enabling accurate predictions of their fundamental characteristics. Due to its efficiency and versatility, DFT has become an indispensable tool across multiple disciplines, including physics, chemistry, materials science, and geoscience, for exploring the electronic, structural, mechanical, dynamical, and optical properties of complex condensed matter systems. Although hybrid functionals offer improved accuracy in predicting the electronic band gap, the PBE functional remains widely employed and well accepted for predicting the electronic properties of solids due to its computational efficiency and reasonable agreement with experimental data [9].

2. Materials and Methods

2.1. Simulation Method

The first-principles calculations based on DFT were conducted to evaluate the ground state structural parameters of cubic $SrThO_3$ (space group $Pm\bar{3}m$, No. 221) at ambient conditions using the Quantum Espresso software and code [10]. The equilibrium atomic positions of the $SrThO_3$ unit cell were obtained through full structural optimization calculations. To achieve an optimized geometry, the lattice constants and optimized atomic positions were determined. Using the unit cell structure, the electronic gap and energy states distribution were investigated within the generalized gradient approximation (GGA) using the Perdew–Burke–Ernzerhof (PBE) functional

[11]. Convergence tests were systematically performed to identify suitable parameters for the plane-wave basis set and Brillouin zone sampling. A kinetic energy cutoff of 60 Ry was selected based on total energy convergence, while Monkhorst–Pack grids of 16×16×16 were adopted for both unit cell and supercell calculations, to ensure accurate reciprocal space integration.

In this study, systematic optimization of the computational approach was performed with a detailed demonstration of how these parameters sensitively influence the results. While Shein et al. [2] employed the full-potential linearized augmented plane wave (FP-LAPW) method using the Wien2k code, and Jamila et al. [1] used projector augmented-wave (PAW) potentials with the VASP software, this work utilizes PAW potentials within the Quantum ESPRESSO software package. In particular, comprehensive convergence tests were performed to determine the kinetic energy cutoff at 60 Ry. Such details of cutoff energy optimization are rarely reported in the literature for this examined compound. Regarding Brillouin zone sampling density, the 16×16×16 Monkhorst-Pack grid employed in this work is denser than those used in most previous studies, which may enable more accurate calculation of the density of states (DOS) and may explain why the obtained band gap value of 1.986 eV is lower than other PBE calculations in the literatüre, such as 2.186 eV [1] and 2.25 eV [2]. Consequently, this study presents a high-precision computational method that can serve as a reference for $SrThO_3$ and clarifies the source of variability among different DFT implementations at the parameter level such as cutoff energy value and Monkhorst-Pack grid. The 16×16×16 k-grid and 10^{-6} Ry energy tolerance employed in this study provide higher precision compared to previous investigations, leading to more accurate determination of band extrema.

The methodological distinction of the approach used, particularly in terms of exchange-correlation functional selection and convergence criteria, offers a valuable benchmark for future computational studies. Thus, this contribution establishes a methodological reference point that enables meaningful cross-comparison with both prior $SrThO_3$ calculations and the broader perovskite literature, underscoring the significance of the findings within this narrowly defined but strategically important research domain.

3. Results and Discussion

3.1. Modelling of Perovskite Structure

In the general formula for oxide perovskite structures, ABO3, A and B refer to ions of different sizes. $SrThO_3$ has a cubic symmetry (space group $Pm\bar{3}m$, No. 221). The Wyckoff positions of Sr, Th and O atoms are 1a (0.5, 0.5,0.5), 1b (0.0, 0.0, 0.0) and 3d (0.0.,0.0, 0.5), respectively. In the unit cell structure, Sr atoms are located at the body center, while Th and O are

positioned at the corners and edge centers, respectively [1], as shown in Fig. 1. The calculated structural parameters are given in Table 1. The calculated bond lengths refer to the nearest bond lengths of different phase compositions.

Table 1: The structural parameters samples and electronic band gap of $SrThO_3$

Phase composition	**a (Å)**	**V_0 (Å^3)**	**Sr-O (Å)**	**Th-O (Å)**	**E_g (eV)**
$SrThO_3$ unit cell	4.46	93.641	3.153	2.230	1.986

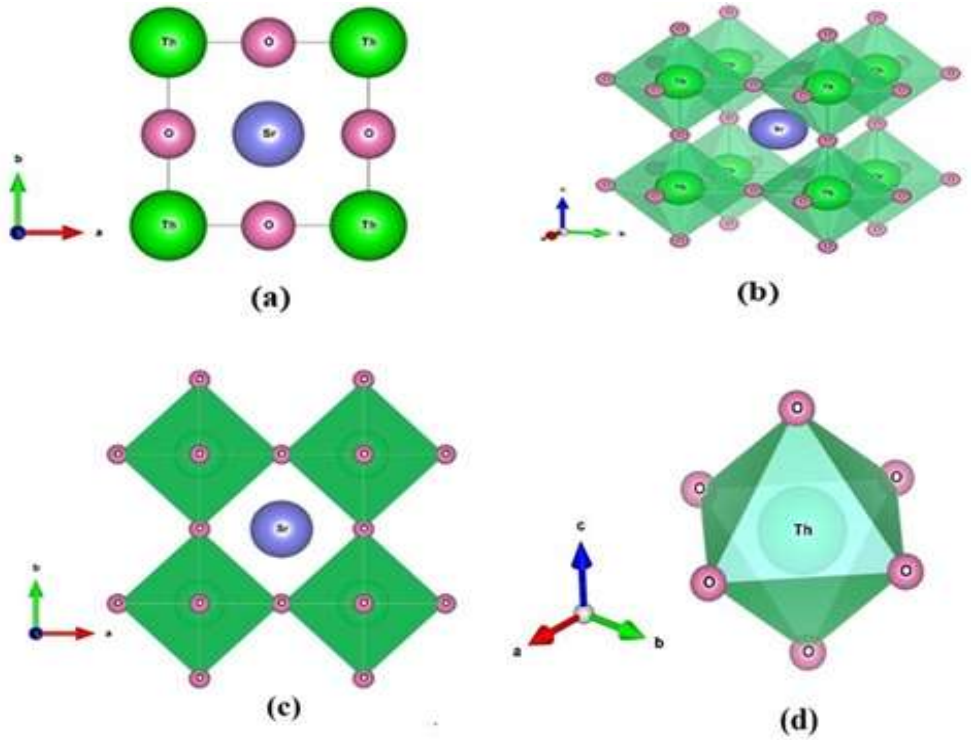

Figure 1: $SrThO_3$ perovskite: (a) unit cell structure view along the c-axis, (b) crystal orientation with Th-centered ThO_6 polyhedra, (c) c-axis view of ThO_6 polyhedra, and (d) bonding diagram of ThO_6.entered polyhedral form of ThO_6

Regarding the calculated values in Table 1, the Goldschmidt tolerance factor was determined to be 0.9996 using Eqn. (1) for $SrThO_3$ with a cubic structure. This value indicates that the perovskite has ideal cubic symmetry, meaning it is perfectly stable. Theoretically, Jamila et al. calculated the lattice constant, a (Å), as a 4.551 [1]. Tezuka et al. reported the lattice constant, a (Å), as a 4.542 [12]. Mehta et al. also reported this parameter experimentally as 4.430 (Å) [13]. According to theoretical calculations by Jamila et al. [1] and Tezuka et al. [12], the unit cell volume was found to be 94.258 Å^3 and 94.215 Å^3, respectively. In contrast, Metha et al. [13] experimentally measured the volume as 86.938 Å^3, indicating a slight underestimation by theoretical methods. When the calculated structural parameters of $SrThO_3$ oxide perovskite are compared with the literature values, the obtained error ratios for the lattice constants are 1.99%

[1], 1.80% [12], 0.67 [13]. Similarly, the comparative analysis for the cell volume yields the following ratios: 0.65% [1], 0.61% [12], 7.15 [13] for unit cell volumes calculated at ambient conditions. The computed structural parameters in this study are in good agreement with previously reported literature values. Cherif et al. employed first-principles methods to calculate the lattice constant, reporting values of 4.53 Å and 4.52 Å using LDA and GGA [14], respectively, which are in good agreement with the reported experimental values of 4.542 Å [15] and 4.42 Å [16].

3.2. Compute Electronic Band Gap, Density of States and Partial Density of States

Predicting the nature of solids requires a detailed understanding of their electronic properties. A comprehensive understanding of the nature of solids is required to analyse their electronic properties in detail. The physical properties of solid-state materials are significantly influenced by the characteristics of their electronic structure, especially the energy states located near the Fermi energy (E_f). The band gap value and the nature of the band gap play a key role in their potential use in electronic and optical applications. The band structures were calculated using the PBE functional within GGA for the unit cell of the $SrThO_3$ compound along the (R- Γ -X- M- Γ) K-points path. While it is well established that the utilization of hybrid functionals significantly enhances the band gap and brings it closer to experimental values, PBE functionals are also frequently employed, particularly in investigations of the electronic nature of semiconductors. In other words, they generally provide sufficient accuracy for the topological characteristics of the band structure (direct or near-indirect band gap character, and the orbital character of valence and conduction bands). The electronic band structure illustrates the dispersion of energy levels throughout k-space, whereas the density of states (DOS) quantifies the number of available states at each energy level. Consequently, the band gap revealed along the energy levels of the band structure directly corresponds to the gap evident along the energy axis of the DOS plots for the investigated compound.

Owing to the non-magnetic nature of the investigated oxide perovskite, spin-polarized states were not considered in the present study. Huang et al. underscored the necessity of incorporating spin-orbit coupling (SOC) effects in compounds containing elements such as U, Np, and Pu. They described these actinide-based materials as exhibiting complex magnetic behavior, noting that the 5f electrons of these elements result in substantial band dispersions and broad bandwidths, making SOC inclusion indispensable. Therefore, in actinide-based compounds, the main challenges and research interest are concentrated on elements beyond thorium-particularly from uranium onward [17]. DOS analysis of $SrThO_3$ calculated by Jamila et al. [1], which incorporated spin-orbit coupling, highlighted that the dominant contribution to the

valence band originates from O-*p* orbitals, whereas Sr-*p* states were observed to contribute to both the valence and conduction bands. These findings demonstrate general consistency with the results of the present study where spin-orbit interaction was neglected. Consequently, it can be argued that these results provide evidence for predicting the overall topological characteristics of the electronic structure. The electronic band gap value was calculated as 1.986 eV with direct band characterization as depicted in Fig. 2(a).

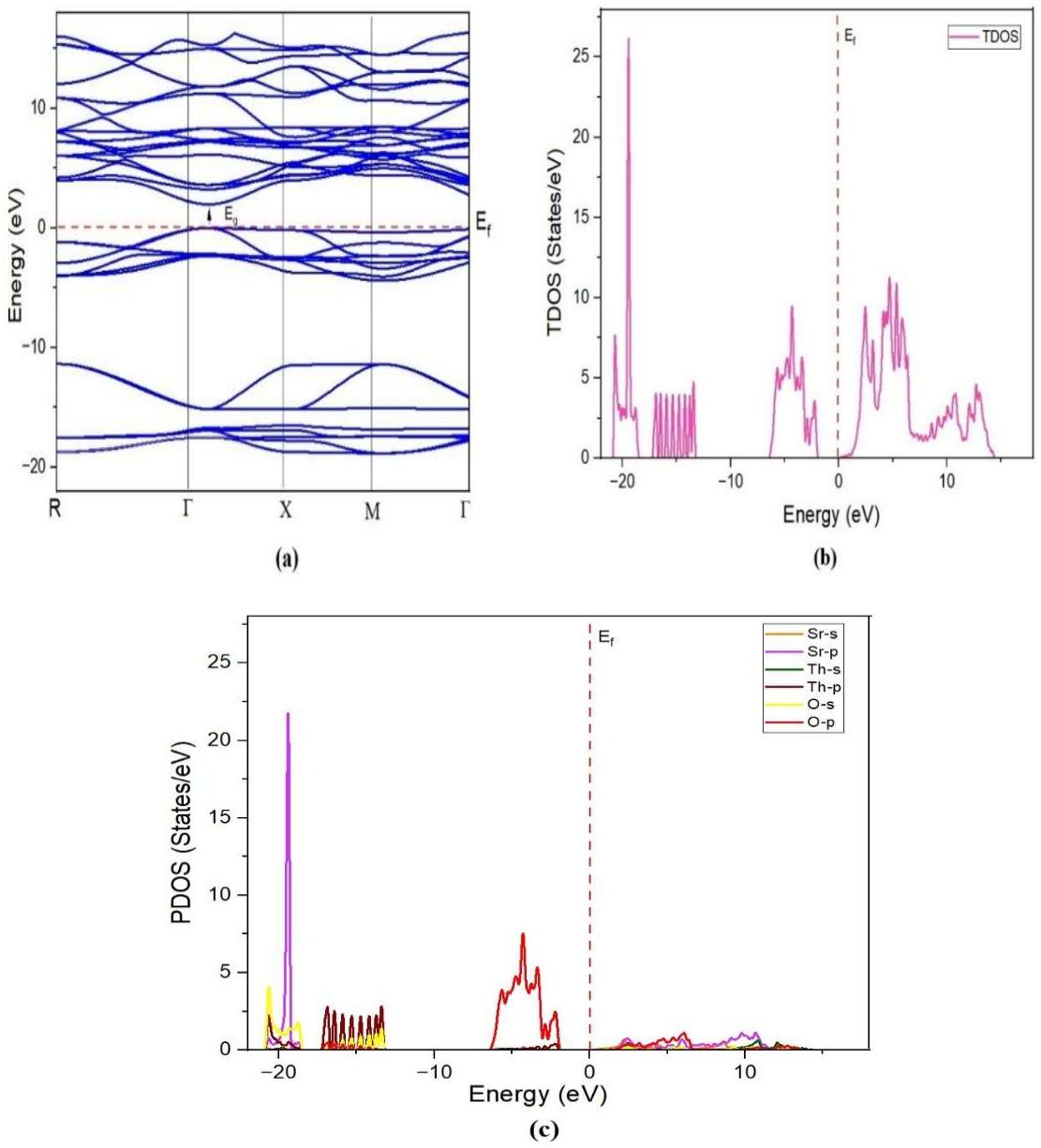

Figure 2: a) Electronic band gap b) TDOS c) PDOS of $SrThO_3$

In optoelectronic device applications, the electronic band gap value and the nature of band gap in compounds are key factors. The direct nature of the band gap at the Γ point (k=0) implies that optical transitions will possess high oscillator strength due to momentum conservation. This

suggests that $SrThO_3$ will exhibit a high absorption coefficient, making it promising for photovoltaic and photodetector applications. It is well known that a narrow band gap enables electrons to be easily excited from the valence band to the conduction band, resulting in higher light absorption. The TDOS and PDOS graphs help in understanding the nature of the chemical bonds between atoms. The hybridization implies a covalent nature of the chemical bonds between orbitals in the relevant energy regions. Increased hybridization may be concluded to increase the elastic modulus, resulting in enhanced mechanical properties of solids. The hybridization between *O-p*, *O-s* and *Th-p* states was revealed in the region between –12.5 eV and –17.5 eV. Another hybridization between *Sr-p*, *Sr-s,* and *Th-p* states occurs around –20 eV. TDOS and PDOS show two regions denoted by energy levels from 0 to –10 eV and from –10 to –20 eV in the valence band at ambient conditions. The *Sr-p* states are more dominant at energy levels around –20 eV as depicted in Fig. 2. Sharp peaks caused by *Sr-p* states were observed in the valence band in this region. The remaining energy levels of the valence band primarily consist of *O-p* states. The contributions of the *Th-p* and *O-s* states are slightly weaker than those of the *O-p* states throughout the valence band. Nevertheless, examination of the orbital projections reveals that contributions from O-*p*, O-*s*, and Sr-*p* states, albeit at low densities, are particularly notable near the Fermi level in the conduction band. Consequently, it can be inferred that these orbital contributions may play a significant role in determining the conductive and optical properties. Shein et al. computed band gap of $SrThO_3$ as a 2.25 eV using the direct band gap FLAPW method. This electronic band gap was also calculated as 3 eV using the local density approximation (LDA). The valence band can be categorized into three distinct regions: the first valence band energy states range from –18.1 eV to –16.1 eV, the second part between –14.9 eV and –11.8 eV, and the upper valence band from –3.85 eV up to O eV (E_f). The valence band is composed of three parts: –18.1 eV and –16.1 eV, –14.9 eV and –11.8 eV and the highest valence band from–3.85 eV to O eV (E_f). The highest valence band is composed of O-*2p* orbitals. Th-*5f* orbitals are more dominant at the bottom of the conduction band. The second higher contribution arises from Th-*6d* in the bottom of conduction band. From DOS calculations, the covalent bond arises from hybridization between O-*2p* and Th-*6d* and *5f* orbitals [2]. Jamila et al. focused on the electronic band nature of $SrXO_3$ (X=Si, Tb and Th) using the PBE functional within the GGA approximation. The electronic band gap reveals at 2.695 eV, 3.622 eV and 2.186 eV for X=Si, Tb and Th, respectively. In electronic properties, the contributions of Sr-*4p* and O-*2p* states are dominant [1]. Ghebouli et al. [18] reported that the electronic band gap as a 2.23 eV with direct band nature. They also emphasized that the lower energy region of the valence band consists of Sr-*p* and O-*s* states. The greater contribution in the valence band comes from O-*p* states [17], which agrees with the results reported in this study. Cherif et al. calculated the electronic band gap using LDA and GGA approximation. It revealed

1.912 eV and 2.058 eV, respectively with direct band gap nature. (problematic sentence structure) In reported study by Cherif et al., the electronic band structure comprises four distinct regions. The lowest energy region lies from −18.30 eV to −16 eV and is characterized by contributions from O-*s* and Sr-*p* orbitals. This is followed by the second region situated between −14.80 eV and −11.30 eV, where Th-*p* orbitals are predominant. The third region, located from −3.90 eV to 0 eV within the valence band, is primarily composed of O-*p* orbitals. Finally, the fourth region extends from 2.25 eV to 8 eV in the conduction band [14], which is in good agreement with the results reported in this study.

4. Conclusion

In summary, the structural properties of pristine $SrThO_3$ were comprehensively evaluated using DFT. Crystal stability was assessed by computing the Goldschmidt tolerance factor, which confirmed the structural feasibility of the perovskite lattice. The electronic properties were further examined by calculating the electronic band gap and mapping the electronic band structure to elucidate the semiconducting behavior of $SrThO_3$. The results revealed a direct band gap of 1.986 eV, indicating potential suitability for optoelectronic applications. The combination of favorable structural stability and a relatively narrow direct band gap highlights $SrThO_3$ as a promising candidate for advanced semiconductor and optoelectronic devices. These findings provide valuable theoretical insights that may guide future experimental synthesis and device engineering efforts involving $SrThO_3$ oxide perovskites.

References

[1] Jamila, N., Farah, I.J., Modak, J.K., Hasan, W., Rahman, Md.A., Hossain, Md.M. et al., *DFT based computational investigations of the physical properties of perovskites-structure $SrXO_3$ (X=Si, Tb, Th) for optoelectronic and thermomechanical applications,* Materials Today Communications, 38, 107650, 2024.

[2] Shein, I.R., Shein, K.I., Ivanovskii, A.L., *Elastic and electronic properties and stability of $SrThO_3$, $SrZrO_3$, and ThO_2 from first principles*, Journal of Nuclear Materials, 361, 69–77, 2007.

[3] Ali, M., Mishra, R., Bharadwaj, S.R., Kerkar, A.S., Dharwadkar, S.D., Das, D., *Thermodynamic stability of solid $SrThO_3$*, Journal of Nuclear Materials, 299(2), 165–170, 2001.

[4] Prasad, R., Dash, S., Parida, S.C., Singh, Z., Venugopal, V., *Thermodynamic studies on $SrThO_3(s)$*, Journal of Nuclear Materials, 312(1), 1–9, 2003.

[5] Dash, S., Singh, Z., Parida, S.C, Venugopal, V., *Thermodynamic studies on $Rb_2ThO_3(s)$*, Journal of Alloys and Compounds, 398(1–2), 219–227, 2005.

[6] Jellil, Z., Ez-Zahraouy, H., *Pressure-induced band gap engineering and enhanced optoelectronic properties of non-toxic Ca-based perovskite $CsCaCl_3$: insights from density functional theory*, Computational Condensed Matter, 38, e00879, 2024.

[7] Roknuzzaman, Md., Ostrikov, K., Wang, H., Du, A., *Tesfamichael T. Towards lead-free perovskite photovoltaics and optoelectronics by ab-initio simulations*, Scientific Reports, 7, 14025, 2017.

[8] Hayatullah, Murtaza, G., Muhammad, S., Naeem, S., Khalid, M.N., Manzar, A., *Physical Properties of $CsSnM_3$ (M=Cl, Br, I): a first principle study,* Acta Physica Polonica A, 124, 102–107, 2013.

[9] Kholil, Md.I., Bhuiyan, T.H., *Effects of Cr-and Mn-alloying on the band gap tuning, and optical and electronic properties of lead-free $CsSnBr_3$ perovskites for optoelectronic applications*, RSC Advances, 10, 43660–43669, 2020.

[10] Giannozzi, P. et al., *Quantum Espresso: a modular and open-source software project for quantum simulations of materials*, Journal of Physics: Condensed Matter, 21(39), 395502, 2009.

[11] Perdew, J. P., *Density functional theory and the band gap problem*, International Journal of Quantum Chemistry, 28, 497–523, 1985.

[12] Tezuka, K., Itoh, M., Haga, M., Hinatsu, Y., *Crystal and magnetic structures of $SrTbO_3$ and $BaTbO_3$ by powder neutron diffraction*, Materials Science Forum, 315–317, 578–585, 1999.

[13] Mehta, R.J., *Pyridine nucleotide-linked oxidation of methanol in methanolassimilating yeasts*, Journal of Bacteriology, 124(3), 1165–1167, 1975.

[14] Cherif, Y.B., Rouaighia, M., Zaoui, A., Boukortt, A., *Optoelectronic, elastic and thermal properties of cubic perovskite-type $SrThO_3$*, Acta Physica Polonica A, 131(3), 406–414, 2017.

[15] Moreira, R.L., Dias, A., *Comment on prediction of lattice constants in cubic perovskites*, Journal of Physics and Chemistry of Solids, 68(8), 1617–1622, 2007.

[16] Blanco, M.A., Francisco, R., Luana,V., *Gibbs: istothermal-isobaric thermodynamics of solids from energy curves using a quasi-harmonic debye model,* Computer Physics Communications, 158(1), 57–72, 2004.

[17] Huang, Li, Chen, R., Lu, H., *Reexaming the ground state and magnetic properties of curium dioxide*, Physical Review B, 102, 085127, 2020.

[18] Ghebouli, M.A., Chihi, T., Dahmane, F., Ghebouli, B., Fatmi, M., Seddik, T., Abdiche, A., Khenata, R., *Structural, elastic and optoelectronic properties of Sr-based perovskite-type oxides $SrXO_3$ (M = Th, Zr) via first-principles calculations*, Chinese Journal of Physics, 54(4), 625–638, 2016.