Uluslararası İleri Doğa Bilimleri ve Mühendislik Araştırmaları Dergisi
Sayı 8, S. 418-425, 7, 2024

Araştırma Makalesi

IJANSER

International Journal of Advanced Natural Sciences and Engineering Researches
Volume 8, pp. 418-425, 7, 2024

Research Article

https://as-proceeding.com/index.php/ijanser
ISSN: 2980-0811

Electronic and Optical Properties of $BaNb_2O_6$ Compounds: Theoretical Study

Mohanad ASAFI[*] and Murat AYCİBİN [2]

[1]*Department of Physics/ Faculty of Science, Van Yuzuncu Yil University, Van, Turkey*
[2] *Vocational School of Technical Sciences/Opticianry /mersin-university Turkey*

[*]*mohanadasafi@gmail.com*

(Received: 21 July 2024, Accepted: 31 August 2024)

(4th International Conference on Scientific and Academic Research ICSAR 2024, July 19 - 20, 2024)

ATIF/REFERENCE: Asafi, M. & Aycibin, M. (2024). Electronic and Optical Properties of BaNb2O6 Compounds: Theoretical Study. *International Journal of Advanced Natural Sciences and Engineering Researches*, 8(7), 418-425.

Abstract – In this study, we utilize WIEN2k and density functional theory (DFT) to investigate $BaNb_2O_6$ (BNO) compounds. Our results, which closely align with experimental data, identify the optimal lattice constants using the PBE-GGA method. We reveal that BNO possesses an indirect bandgap, with significant contributions from oxygen and niobium atoms. Furthermore, our analysis of the anisotropic optical properties, particularly in UV light reflection, highlights BNO's potential for various applications. This research not only uncovers the unique characteristics of BNO but also paves the way for similar analyses in other compounds, promising advancements in materials science.

Keywords – $BaNb_2O_6$ (BNO), Density Functional Theory (DFT), PBE-GGA Method, Indirect Bandgap, Optical Properties

I. INTRODUCTION

Solid-state compounds with the formula AB2O6, encompassing diverse main group and transition metal cations denoted as A and B, have been extensively studied. Researchers have unveiled their complex structures and physical properties. [1]

Niobate crystals, like $BaNb_2O_6$, are renowned ferroelectric materials prized for their remarkable pyroelectric coefficients, and electro-optic capabilities [2]

Layden (1967, 1968) identified temperature-dependent structural variations in BaNb2O6 (BNO) [3]. Chemical solution precipitation was used to produce (Sr, Ba)(Nb, Ta)2O6 (SBNT) thin films in 2001 [4] Scientists created tungsten bronze crystal systems by combining BaNb2O6 (BNO) with various chemicals and studying their characteristics [5–9] Yamaguchi et al. achieved pure hexagonal BNO utilizing simultaneous barium and niobium hydrolysis in 1985 [10]. Various techniques have been used to make pure or doped Strontium barium niobate ferroelectric films, and numerous features of this material have been studied [11–16]. Kim et al. used the solid state reaction technique in 2002 to generate BNO in orthorhombic and hexagonal structures. The electrical characteristics of the compounds were studied [17]. In 2005, BNO was produced utilizing sol-gel or urea techniques, and an X-ray analysis of the final product was performed [18,19]. The photoluminescence characteristics of Eu and Sm doped BNO compounds were studied [20–23].

While experimental studies on $BaNb_2O_6$ abound, theoretical investigations are limited. Our research utilizes WIEN2k to delve into the compound's electrical, structural, and optical characteristics, offering

valuable insights into its future technological applications and expanding scientific comprehension of this compound.

II. Materials and Method

The investigation into the physical properties of the BNO system involved numerical computation using the Wien2k package [24],This software facilitated the implementation of Density Functional Theory (DFT) within the framework of the local spin density approximation (LSDA), specifically designed to address exchange-correlation effects.

III. Results and Discussion

BaNb2O6 exhibits a hexagonal crystal structure (see Figure 1), featuring a unique arrangement of barium, niobium, and oxygen ions. Niobium ions form distorted octahedra within this structure, sharing edges with adjacent octahedra and creating channels along specific crystallographic directions. These channels play a crucial role in dictating the material's electrical properties and contributing to its ferroelectric behavior. A comprehensive understanding of BaNb2O6's hexagonal structure is imperative for unlocking its technological applications and predicting potential phase transitions.

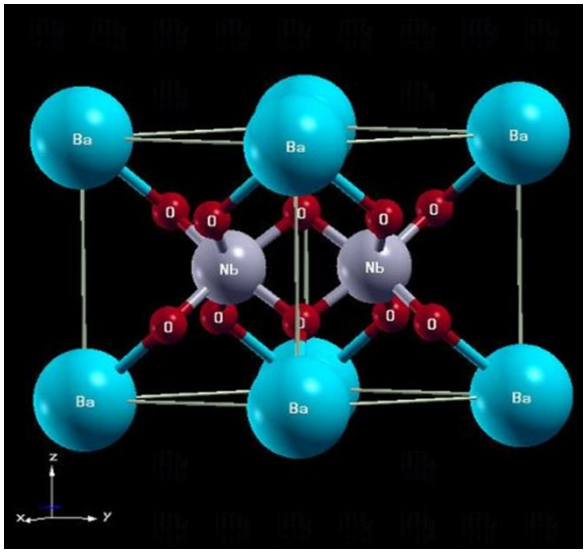


Fig. 1 BNO structure view

A. Volume Optimization

To attain the lowest total energy, reflecting the most stable crystal structure, volume optimization was performed. This process, depicted in Figure 1, was executed using four embedded potentials: Perdew–Burke–Ernzerhof (PBE), Local Spin Density Approximation (LSDA), Wu-Cohen Generalized Gradients Approximation (WC-GGA), and PBEsol-GGA, chosen for the exchange-correlation potential. The theoretical lattice constants obtained from this optimization are presented in Table 1 [25]

Table 1. The experimental and calculated lattice constants according to chosen exchange-correlation potential.

Lattice parameter	Experimental	PBE-GGA	LSDA	WC-GGA	PBEsol-GGA
a (Å)	5.3760001	5.3760023	5.3033446	5.3399208	5.3399208
b (Å)	5.3760001	5.3760023	5.3033446	5.3399208	5.3399208
c (Å)	5.6130000	5.6130075	5.5371415	5.5753301	5.5753301

The theoretical lattice constant obtained using the(PBE-GGA) potential closely matches the experimental findings.

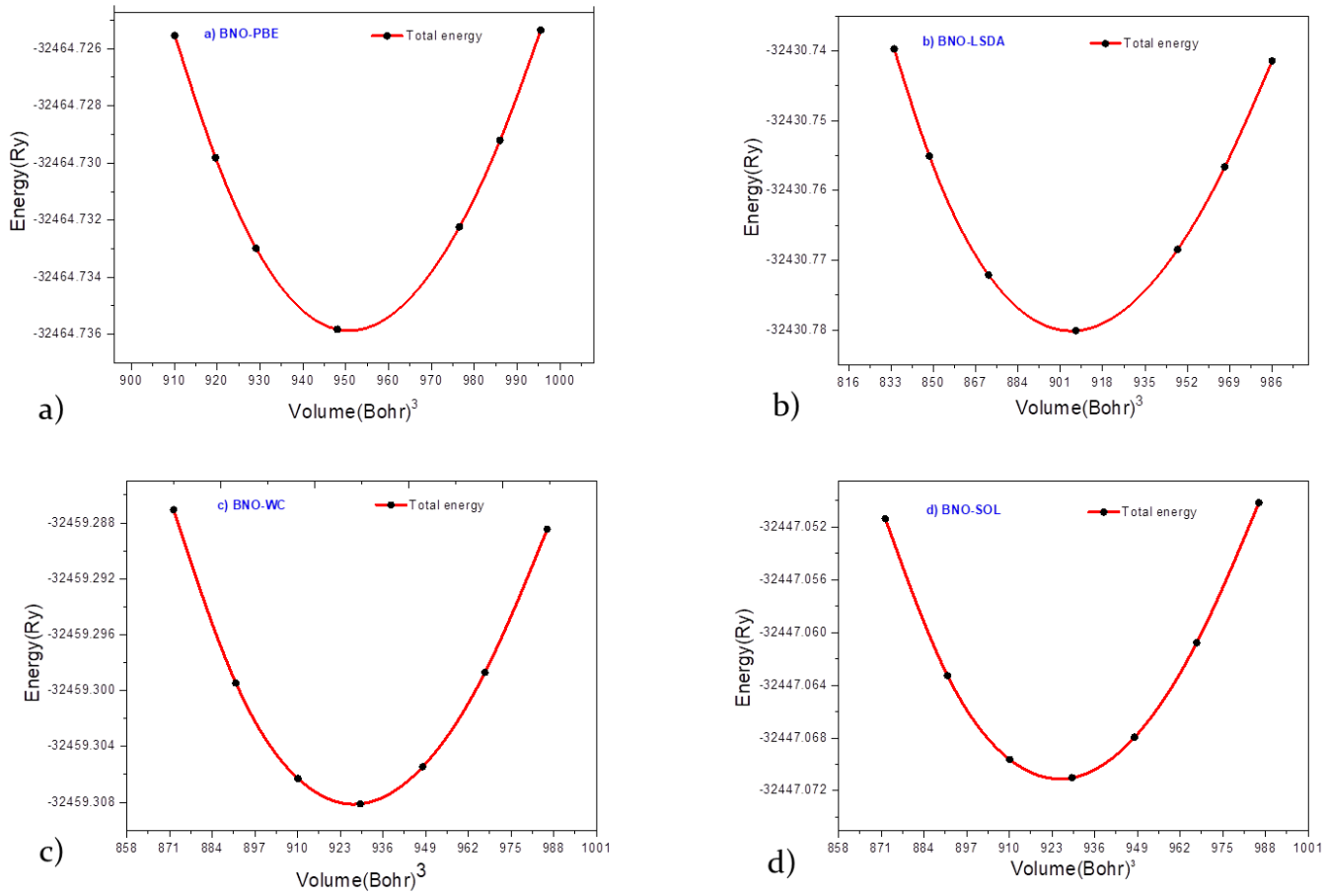


Fig. 2 Energy (eV) vs Volume . plots of BaNb2O6 under
(a) LSDA, (b) WC-GGA, (c) PBE-GGA, (d) PBEsol-GGA .

Fig. 2 Theoretical lattice constants for four potentials determined via WIEN2k, compared with experimental values for BaNb2O6 (Table 1). Evaluates agreement between theory and experiment."

B. Electronic Band Structure

Figure 3 showcases our electronic band structure analysis, revealing crucial energy levels and bandgap information for the crystal.

The VBtop (valence band top, in black) and CBbottom (conduction band bottom, in blue) span from Γ to K points in the high-symmetry Brillouin zone, outlining critical energy levels. The Y-axis denotes the forbidden energy bandgap, indicating where electronic transitions are restricted. Theoretical prediction sets the energy band gap at 4.1 eV, while experimental data (Jana, 2020) reports 3.76 eV[26]. This gap showcases an indirect transition mechanism.

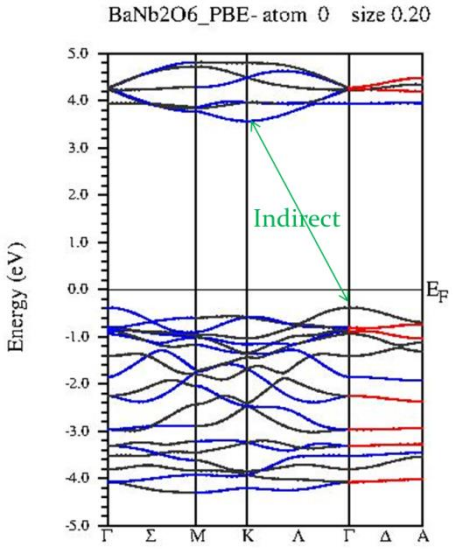


Fig. 3 Electronic band structure of $BaNb_2O_6$

C. Electronic Density of States

The total and partial density of states were calculated to understand the band structure. From (Fig 4.) Total density is ranging from -5eV to 7 eV**,**

The valence bands, ranging from -4 to 0 eV, exhibit strong electronic interaction between Nb and O atoms. According to the Fig 4. O_2 corresponds to the valence band, while Nb represents the conduction band, with Ba being negligible in this context.

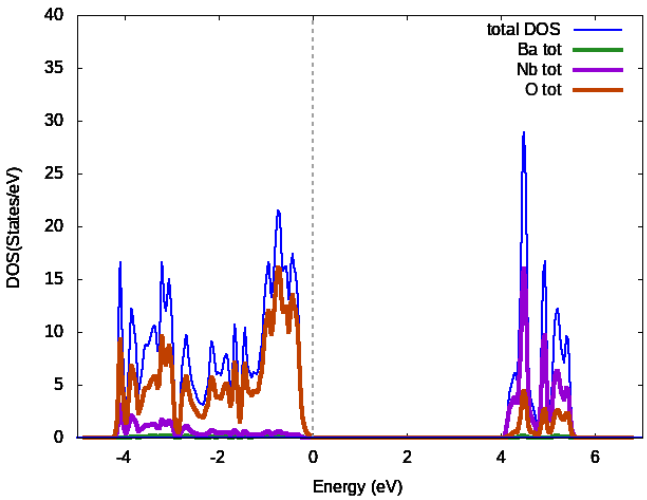


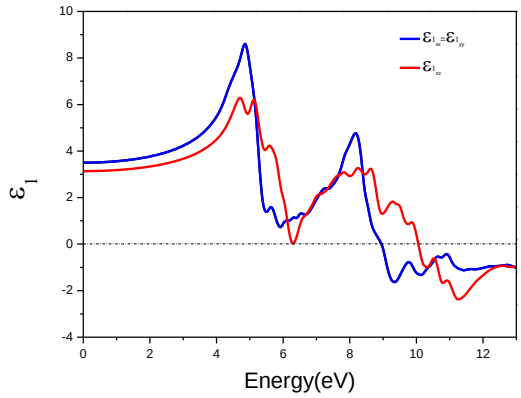
Fig. 4 Electronic density of BaNb2O6

D. Optical Properties

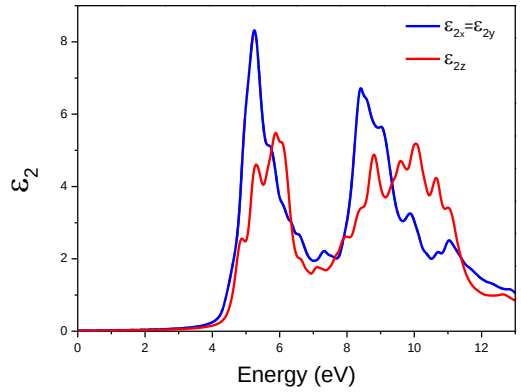
We analyze BNO's optical properties, considering its structure and orientation. Utilizing the dielectric tensor, we examine its interaction with electromagnetic radiation. Figure 5a shows the real part of the frequency-dependent dielectric function, providing insights into optical behavior and transition probabilities."

In addition, we delve into the imaginary part (Fig. 5.b) of the dielectric function to elucidate the energy band structure of BNO.

In the range of 3.7 to 7.0 eV, we observe transitions from the highest valence band to the lowest conduction band. This transition is particularly significant in materials exhibiting anisotropy. Notably, at 5.2 eV, we observe a prominent maximum peak indicative of specific electronic transition



a)



b)

Fig. **5** a) Real and b) imaginary part of the dielectric constant

The absorption coefficient versus energy is shown in Fig 6. there is no photon absorbance before 4eV . The wide absorption band is observed after 4 eV where the transition occurs.

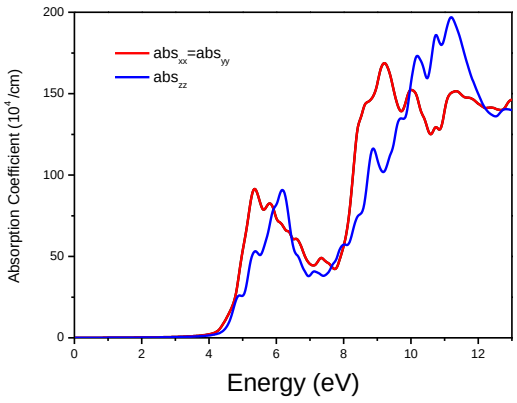


Fig. 6 Absorption coefficient of BNO

The energy loss function describes in fig 7, The energy loss of a very fast electron penetrating through the material

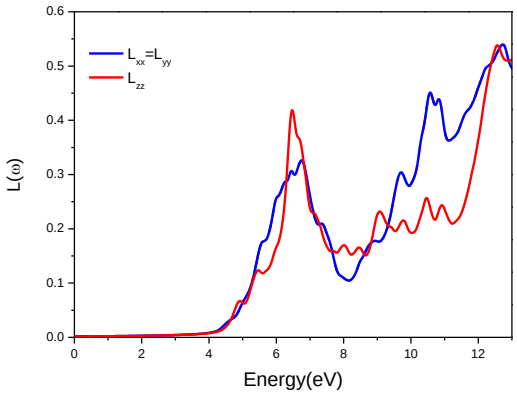


Fig. 7 Energy loss function coefficient of BNO

In Figure 8. showed that 35% of the incoming electromagnetic light are Reflected in UV region, and After 300 nm, 15% of electromagnetic wave was reflected.

It is noteworthy that the peaks are consistent with the energy in the electron energy loss function .

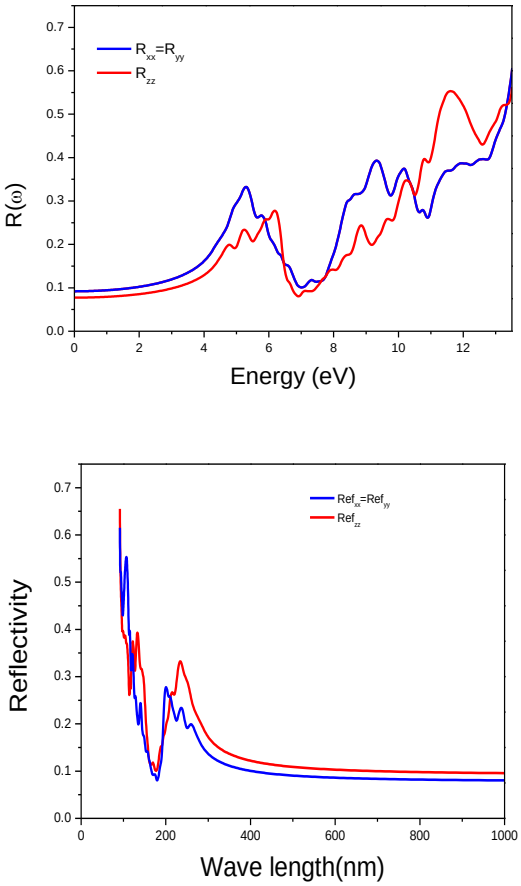


Fig. 8 Reflectivity of BNO

In Fig9. Materials with a high refractive index are sought in photovoltaic applications. The values of the static refractive index (1.7 , 1.8)

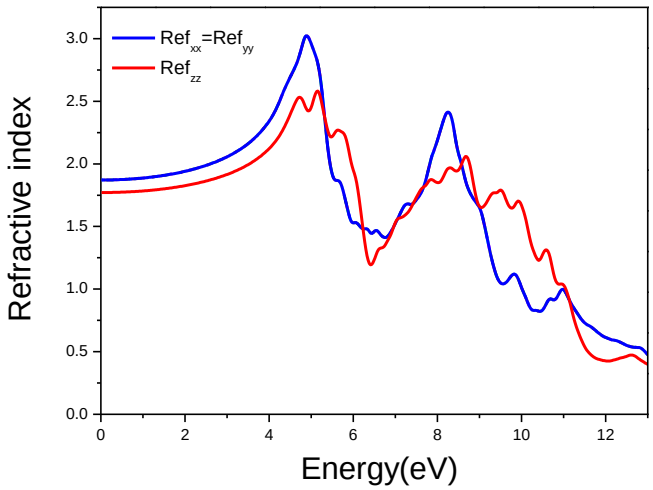


Fig. 9 Refractive index of BNO

In figure 10, Values Material's conductivity and interaction with light at different energy levels

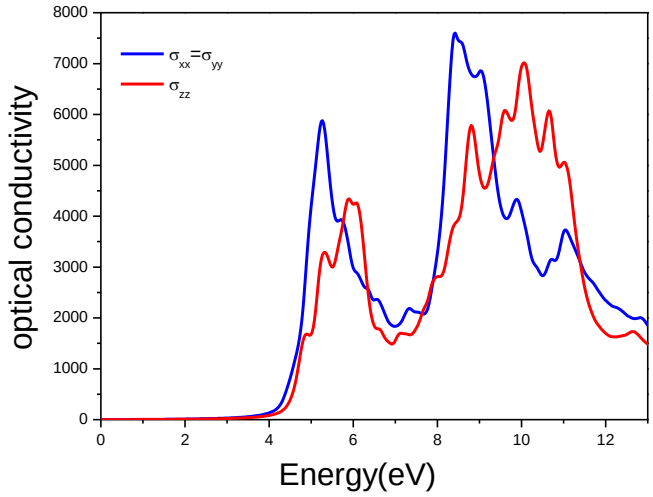


Fig. 10 Optical conductivity

should be clear and concise. The most important features and trends in the results should be described but should not interpreted in detail.

IV. CONCLUSION

WIEN2k, based on density functional theory, was used to analyze the electronic, structural, and optical properties of BNO.

PBE-GGA provided the best lattice constant . BNO displayed indirect bandgap

Energy bandgap 4.1 eV and is good with expriment 3.76 eV . Nb and O are Influenced the conduction band.

Optical properties, including absorption coefficient, refractive index, and reflectivity, showed anisotropy. The compound reflected UV light predominantly.

REFERENCES

[1] H. P. Beck, "A study on AB2O6 compounds, Part II: The branches of the hcp family," *Zeitschrift für Kristallographie-Crystalline Materials*, vol. 227, pp. 843-858, 2012.

[2] M. H. Francombe, "The relation between structure and ferroelectricity in lead barium and barium strontium niobates, " *Acta Crystallographica*, vol. 13, pp. 131-140, 1960.

[3] G. K. Layden, "Polymorphism of BaTa2O6," *Materials Research Bulletin*, vol. **2**, pp. 533-539, May.1967.

[4] W. Sakamoto, Y. Horie, T.Yogo, and S. Hirano, Synthesis and Properties of Highly Oriented (Sr, Ba)(Nb, Ta)2O6 Thin Films by Chemical Solution Deposition," *Japanese Journal of Applied Physics*, vol. 40, pp. 5599-5604, 2001.

[5] B. A. SCOTT, E. A. GIESS, D. F. O'KANE, and G. BURNS, "Phase Equilibria in the KNbO3-SrNb2O6 and KNbO3-BaNb2O6 Systems," *J Am Ceram Soc*., vol, 53, pp. 106–109, 1970.

[6] Y. Itoh, and H. Iwasaki, "Tungsten bronze field in the pseudo-ternary system NaNbO3□BaTiO3□BaNb2O6," *Mater Res Bull*., vol. 7, pp. 663–672, 1972.

[7] B. A. SCOTT, E. A. GIESS, and D. F. O'KANE , "Phase equilibria in the NaNbO3□BaNb2O6 system," *Mater Res Bull.*, vol. 4, pp.107-117, 1969.

[8] R. Lane, D. L. Mack , and K. R. Brown," Dielectric, piezoelectric and pyroelectric properties of PbNb2O6-BaNb2O6 system," *Trans J Br Ceram Soc.*, vol. 71, pp. 11-17. 1972.

[9] A. N. Salak, A. D. Shilin, N.P. Vyshatko, and & D.D. Khalyavin, "Structural characteristics of metastable solid solutions in the PbZrO3-BaNb2O6 and PbTiO3-BaNb2O6 systems synthesized under high pressure," *Crystallography Reports*, vol. 43, pp. 995-998, 1998.

[10] O. YAMAGUCHI, K. MATSUI, and K. SHIMIZU , " Crystallization of Hexagonal BaNb2O6," *J Am Ceram Soc*., vol. 68, pp. 173-175, 1985.

[11] R. G. Mendes, E. B. Araújo, H. Klein, and J.A, Eiras , " Synthesis of strontium barium niobate ferroelectric thin films by an alternative chemical method," *J Mater Sci Lett.,* vol. 18, pp. 1941–1943, 1999.

[12] X. Wang, "Phase transformation in Sr1− xBaxNb2O6 ceramics," *J Mater Res*., vol. 12 , pp. 600-603, 1997.

[13] A. V. Rao, D.S. Paik, and S. Komarneni , " Barium Sodium Niobate Powders and Thin Films: Preparation and Ferroelectric Behavior," *J Sol-Gel Sci Technol*., vol. 10, pp. 221-229, 1997.

[14] W. Sakamoto, T. Yogo, A, Kawase, and S. Hirano , "Chemical Processing of Potassium-Substituted Strontium Barium Niobate Thin Films through Metallo-organics,". *J Am Ceram Soc*., vol. 81, pp. 2692-2698, 1998.

[15] Y. Jiang, R. Guo, and A. S. Bhalla, "Single crystal growth and ferroelectric properties of α (Ba1−xSrx) Nb_2O_6: β (Na1−yKy) NbO3 solid solutions," *J. Appl. Phys*., vol. 84, pp. 5140–5146, 1998.

[16] A. G. Abubakarov, I. A. Verbenko, A. V. Pavlenko, G. N. Tolmachev, L. A. Reznichenko, L. A. Shilkina, et al., "Optimizing conditions of fabrication and the properties of $BaNb_2O_6$-$SrNb_2O_6$ binary ceramics," *Bull. Russ. Acad. Sci. Phys.*, vol. 78, pp. 716–718, 2014.

[17] D. W. Kim, H. B. Hong, K. S. Hong, C. K. Kim, and D. J. Kim, "The reversible phase transition and dielectric properties of BaNb2O6 polymorphs," *Jpn. J. Appl. Phys.*, vol. 41, pp. 6045, 2002.

[18] S. P. Gaikwad, V. Samuel, R. Pasricha, and V. Ravi, "Preparation of nanocrystalline ferroelectric BaNb2O6 by citrate gel method," *Bull. Mater. Sci.*, vol. 28, pp. 121–123, 2005.

[19] S. R. Dhage, R. Pasricha, and V. Ravi, "Preparation of ferroelectric $BaNb_2O_6$ by the urea method," *Mater. Lett.*, vol. 59, pp. 1929–1931, 2005.

[20] A. K. Vishwakarma, K. Jha, M. Jayasimhadri, A. S. Rao, K. Jang, B. Sivaiah, et al., "Red light emitting $BaNb_2O_6$: Eu3+ phosphor for solid state lighting applications," *J. Alloys Compd.*, vol. 622, pp. 97–101, 2015.

[21] A. K. Vishwakarma and M. Jayasimhadri, "Pure orange color emitting Sm3+ doped $BaNb_2O_6$ phosphor for solid-state lighting applications," *J. Lumin.*, vol. 176, pp. 112–117, 2016.

[22] A. K. Vishwakarma and M. Jayasimhadri, "Significant enhancement in photoluminescent properties via flux assisted Eu3+ doped $BaNb_2O_6$ phosphor for white LEDs," *J. Alloys Compd.*, vol. 683, pp. 379–386, 2016.

[23] A. K. Vishwakarma, K. Jha, and M. Jayasimhadri, "Enhancement of luminescent properties in Eu3+ doped $BaNb_2O_6$ nanophosphor synthesized by facile metal citrate gel method," *Opt. Mater. (Amst).*, vol. 96, pp. 109301, 2019.

[24] P. Blaha, K. Schwarz, F. Tran, R. Laskowski, G. K. H. Madsen, and L. D. Marks, "WIEN2k: An APW+lo program for calculating the properties of solids," J. Chem. Phys., vol. 152, pp. 74101, 2020.

[25] S. Kirklin, J. E. Saal, B. Meredig, A. Thompson, J. W. Doak, M. Aykol, S. Rühl, and C. Wolverton, "Computational Materials," *npj Comput. Mater.*, vol. 1, pp. 15010, Dec. 2015.

[26] S. Jana, A. Mondal, J. Manam, and S. Das, "Pr3+ doped BaNb2O6 reddish orange emitting phosphor for solid state lighting and optical thermometry applications," *J. Alloys Compd.*, vol. 821, 153342, Apr. 2020.