Rachana Gaur¹, Ruby Jindal¹*, Archana Tripathi², Harleen Kaur³, Aparna Shekhar⁴

- ¹School of Basic and Applied Sciences, K.R. Mangalam University, Gurugram, Haryana, India,
- ²Department of Physics, Deshbandhu College (University of Delhi), New Delhi, India,
- ³Department of Applied Sciences, Baba Banda Singh Bahadur Engineering College, Fatehgarh Sahib, Punjab, India,
- ⁴Department of Chemistry, Deshbandhu College (University of Delhi), New Delhi, India

Scientific paper

ISSN 0351-9465, E-ISSN 2466-2585 https://doi.org/10.62638/ZasMat1452



ZastitaMaterijala 66 () (2025)

Columbite-structured AB₂O₆oxides: Understanding their structure, synthesis, and potential for future technologies

ABSTRACT

AB2O6Oxides have recently attracted significant attention these days due to their exclusive properties. These compounds exhibit a variety of structural forms with diverse characteristics. Among them, Columbite-type Oxides possess an orthorhombic structure, belong to Pbcn space group and exhibit D_{2h}^{14} symmetry. The structureof thesematerialsconsists of AO₆ and BO₆ octahedra which are arranged in zig zag manner and have a powerful impact on the characteristics of these materials. These materials play a vital role in different applications such as microwave technology, catalysis, energy storage, electronic sensors and optical materials. From a comprehensive literature survey, this review has covered the detailed study of the structure, physical properties, synthesis techniques, and the applications of these Oxides. Subsequently, we discuss the future potential of the Columbite Oxides, with an emphasis on strategies and computational modelingto enhancetheir properties and performance for the future technologies.

Keywords: Columbite, microwave technology, computational modelling

1. INTRODUCTION

1.1. Theneed of Columbite AB₂O₆ oxides

The global demand for eco-friendly and sustainable energy alternatives continues to grow, largely driven by concerns over global warming linked to fossil fuel consumption, which poses a serious threat to our environment and long-term survival. Among the promising renewable energy technologies, thermoelectric (TE) modules are gaining attention. Thermoelectricdevicecan convert waste heat originated from various sources, such as power plants, industrial processes, vehicles, and electronic devicesinto electricity via See-beck effect. However, present TE materials have low efficiency, which limits their broad commercial use. Also, a large number of these materials are unstable at high temperatures. On the other hand, oxide materials have become gradually attractive due to their abundance, cost-effectiveness, and reduced environmental impact.

*Corresponding author: Ruby Jindal

E-mail: ruby.jindal@krmangalam.edu.in(RJ)

Paper received: 06.05.2025. Paper corrected: 17.06.2025. Paper accepted: 23.06.2025.

Besides, certain oxides exhibit spin-related properties that offer fascinating possibilities for optimizing their behavior for multiple applications. Among them, AB₂O₆-type oxides are notably significant due to their distinct compositions and structural variations. Exploring the impact of the structure on the properties may expand the possibilities for thermoelectric applications at high temperatures[1].

More than 50% of the input energy is wasted heat in almost half of the industrial processes[2,3]. This energy loss occurs in many systems extended from household items like kitchen kettles to large-scale manufacturing and power generation facilities. In the same way, gasoline-powered vehicles utilize only about 25% of the fuel's energy into actual motion and associated functions, while the rest is wasted as heat through exhaust gases, engine cooling systems, friction, and other parasitic effects.A sustainable energy solution involves taking this waste heat and converting it into electricity using specific devices. These devices work thermoelectric principles, where heat is converted directly into electrical power through See-beck effect, a phenomenon in which a voltage is induced across a material due to a temperature difference, causing an electric current to flow. Thermoelectric (TE) modules produce electricity without any mechanical component and without releasing greenhouse gases. Power generation devices are known as thermoelectric generators (TEGs) [3].Current TE materials face challenges such as poor thermal stability, insufficiency, deadliness, which has prompted the search for alternatives that are abundant, environment-friendly, and thermally stable at higher temperatures. Manythermoelectric (TE) materials contain elements that are limited and toxic. For instance, lead (Pb) gives rise to serious health hazards, which includes brain damage, seizures, and coma. Materials that containLead and Antimony, are particularly harmful emphasizing the urgent need of environmentally friendly alternatives, such as TE oxides, for thermoelectric applications [1].TE oxides offer greater thermal stability compared to current TE materials, making them strong candidates for hightemperature applications [3].

As 5G technology has become everyday technology, scientists are already working on the next advancement, 6G. This upcoming technology provide incredibly speeds, potentially in terabits per second, while supporting the growing number of connected devices in the Internet of Things (IoT). To achieve these goals, 6G will work in terahertz frequency spectrum, which will require advanced electronic components [4,5].Mie theoryexplains electromagnetic waves interact with tiny particles, especially how certain resonances occur in materials like dielectric spheres and how the wave behave at high temeratures[6]. In the terahertz range, wave propagate differently, they're more likely to scatter or reflect from the surfaces, especially when there's no direct line of sight between the transmitter and receiver [7,8]. To tackle these challenges, scientists are exploring special materials called dielectric metamaterials. These don't rely on electric currents like traditional materials but instead use the movement of electric charges within the material itself. performance, however, depends a lot on how much energy they lose in the process, so understanding these losses is key for 6G development [9-12].

A group of materials called ColumbiteNiobates (with the formula ANb₂O₆, where A can be Zn, Co, Mn, Ni, etc.) is gaining attention because they have useful features due to their unique structure and the different properties of the metals involved [13–17]. Among them, ZnNb₂O₆ and MgNb₂O₆ stand out for their very low energy losses at microwave frequencies (with Qxf values above 80,000 GHz), making them strong candidates for next-generation

electronic components. Interestingly, even though some of these materials look and behave similarly, they still show big differences in performance, for example, between ZnNb₂O₆ and NiNb₂O₆—and scientists are still figuring out why [18,19].

2. STRUCTURE

Columbite-type compounds with the general formula AB2O6 exhibit a well-defined crystal structure that belongs to the orthorhombic crystal system, specifically categorized under the space group Pbcn (No. 60). In this structural framework, the A and B represent two different metal cations, each coordinated by six oxygen atoms to form AO₆ and BO₆ octahedra, respectively. These octahedra are not randomly distributed; instead, they are systematically arranged in layers, forming a unique zigzag stacking sequence that follows an -A-B-B-A pattern along the crystallographic [100] direction [20].AO₆ and BO₆ octahedra are connected to one another via edge-sharing, i.e. by sharing two common oxygen atoms along their edges resulting in the formation of distinct one-dimensional chains. each made up of of alternating A and B octahedra. These chains repeat in a particular ABBABB sequence, and are not confined but again interconnected via corner-sharing, where they share single oxygen atoms at the corners of octahedra. This connectivity between the chains results intoa strong and continuous threedimensional structure, giving rise to a stable patternidentified by $AO_6-BO_6-BO_6$ chains [21-27]. The spatial distribution of A and B cations within the structure is majorly determined by their ionic radii and oxidation states. Generally, the A-site cation is a divalent transition metal ion such as Mn2+, Fe2+, Co2+, or Ni2+, whereas the Bsite is accommodated by pentavalent metal ion like Nb5+ or Ta5+ [20,28]. This unique combination of cation sizes and charges supports the systematic filling of the octahedral voids in the oxygen lattice. contributing to the structural stability. Structurally the Columbite-type framework is derived from the α-PbO₂ structure, where oxygen atoms are arranged in a slightly distorted hexagonal closepacked (HCP) configuration. In this derivative structure, only half of the octahedral voids created by the oxygen packing are occupied by metal cations. This partial filling gives rise to two crystallo-graphically distinct octahedral referred to as the 4c and 8d positions [29,30], which are key in determining the cation coordination and overall symmetry.

In summary, the $AB_2O_6Columbite$ structure is characterized by a well-organized three-dimensional network composed of zigzag chains of edge-sharing AO_6 and BO_6 octahedra,

interconnected through corner-sharing. This combination of geometric ordering and cation size-dependent occupancy leads to a structurally versatile and chemically robust material class,

making Columbite-type oxides particularly significant in solid-state chemistry and materials science [31–33].

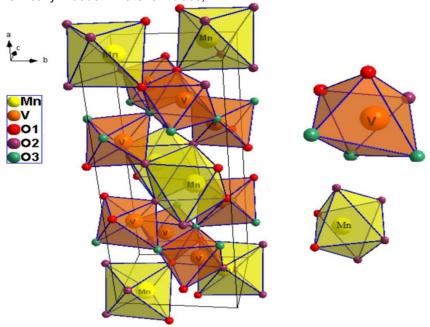


Figure 1: Structure of Columbite MnV₂0₆ Oxides using DIAMOND

3. METHODS OF SYNTHESIS OF COLUMBITE-TYPE AB_2O_6 OXIDES

From previous research, various synthesis techniques have been employed to produce Columbite-type AB_2O_6 oxides. These methods include conventional solid-state reactions [34,35], hydrothermal synthesis [36,37], pulsed laser deposition [38], the molten salt method [39], polymeric precursor methods [40], ceramic flux techniques [41,42], precipitation [43], and molten salt synthesis [44,45]. A selection of these methods is discussed in detail below:

• High-Pressure Synthesis:

Polycrystalline MV_2O_6 (M = Mn, Co, Ni, Zn) samples were synthesized from phase-pure precursors under pressures ranging from 5.5 to 6.7 GPa at temperatures of 700–900 °C using Belt and Conac presses, with a holding time of 60 minutes followed by rapid cooling. Room-temperature X-ray diffraction (XRD) was conducted using Cu-K $\alpha_{1,2}$ radiation, and structures were refined using the Rietveld method with FULLPROF, while VESTA was used for visualization [46].

Hydrothermal Method:

 $MnNb_2O_6$ and Ca-substituted derivatives were synthesized hydrothermally by reacting $NH_4(NbO(C_2O_4)_2)\cdot (H_2O)_2\cdot xH_2O$ with $MnSO_4\cdot H_2O$ in a 2:1 molar ratio, followed by alkali addition

(LiOH, NaOH, or KOH), stirring, and heating at 240 °C for 18 hours. Products were treated with 0.5 M acetic acid to eliminate $MnCO_3$ impurities, then sintered at 1000 °C [47].

Sol-Gel and Solid-State Methods:

 $ZnNb_2O_6$, $NiNb_2O_6$, and $CoNb_2O_6$ were synthesized via both sol-gel and solid-state methods. ZnO and Nb_2O_5 were calcined at 1000°C, and NiO nanoparticles were derived from nickel nitrate hexahydrate and ethylene glycol before calcination at 800°C. The final Columbite phases were obtained after solid-state reactions [48].

Polymeric Precursor Route:

 $MgNb_2O_6$ was synthesized using $Nb_2O_5, NaOH,$ and glacial acetic acid to form hydrated niobic acid, followed by complexation with citric acid. A viscous liquid formed was evaporated and annealed at varying temperatures to obtain the crystalline ceramic phase [49].

Ammonia-Assisted Synthesis:

 $ZnNb_2O_6$ was also synthesized using $ZnCl_2$ in strongly alkaline conditions (pH 14) with ammonia as a mineralizer. Alternatively, $ZnNb_2O_6$ powders were prepared by calcining a suspension of $K_8Nb_6O_{19}$ and $ZnCl_2$ in the presence of H_3BO_3 catalyst at $500\,^{\circ}C$ [50].

Solid-State with CuO Doping and Sol-Gel:

NiNb₂O₆ ceramics were produced by solidstate reaction and CuO doping, enabling sintering at lower temperatures while maintaining high densification and dielectric performance. The solgel method also produced fine NiNb₂O₆ nanoparticles at 700 °C, which demonstrated excellent properties upon further sintering [51].

Mechanochemical Synthesis:

Pure-phase $MgNb_2O_6$ was synthesized at 800 °C after 15 hours of high-energy ball milling, which reduced the necessary synthesis temperature by 100 °C compared to conventional methods [52].

Doped Solid-State Reaction:

 Mn^{2+} -doped $Mg_{1-x}Mn_xTa_2O_6$ (x=0.02-0.12) ceramics were synthesized via a solid-state method, with the influence of Mn substitution on structural and dielectric properties thoroughly examined [53].

Conventional Solid-State Synthesis:

Polycrystalline BaNb₂O₆ was synthesized at temperatures above 1100 °C using the conventional solid-state reaction method. Increasing sintering time led to enhanced grain growth, higher density, and improved energy storage efficiency [54].

4. PROPERTIES OF AB₂O₆COLUMBITE-TYPE OXIDES

The $AB_2O_6Columbite$ -type oxides, particularly those based on vanadium and niobium, exhibit a wide range of intriguing electronic, optical, and thermoelectric properties, making them valuable candidates for various technological applications. Akhlaq Ahmed et al. (2024) have studied the thermoelectric properties of di-vanadate oxides such as MgV_2O_6 , CaV_2O_6 , and BaV_2O_6 , reporting band gaps of $3.20\,eV$, $2.14\,eV$, and $1.76\,eV$, respectively. The results obtained demonstrate the potential of these materials for thermoelectric power generation and their use in renewable energy systems[55].

Likely, Niobate-based oxides also exhibit semiconducting behavior, making them well suited for high-voltage and high-temperature applications [56]. In this context, Kieran B. Spooner et al. (2021) explored the optical and thermoelectric properties of BaBi₂O₆, a Columbite-type oxide, revealing a band gap of 2.6 eV and emphasizing its potential for thermoelectric applications due to its PbSb₂O₆-type crystal structure [57]. Similarly, Basavaraju et al. (2021) investigated MgNb₂O₆ nanoparticles and found a comparatively large band gap of 4.4 eV, indicating the material's use for photocatalytic and sensor applications [58].

The optical properties of these compounds also attract significant attention. In 2023, José Fábio de Lima Nascimento et al. synthesized CaNb2O6and obtained an optical band gap of 3.18 eV, further confirming the potential of Niobium-based Columbite-type oxides for optical photocatalytic applications [59,60]. The Raman and infrared vibrational modes of Columbite-type compounds have been predicted using correlation methods [61] and further analyzed through theoretical calculations employing the Wilson GF matrix method [62]. The electronic and optical properties of these materials has also been studied theoretically by using density functional theory (DFT). DFT calculations using the Wien2k package were utilized to improving the lattice constants and atomic positions in CaNb₂O₆, giving a direct band gap of 3.5 eV, making it suitable for photovoltaic applications. The calculations indicated that the valence band is mainly determined by Oxygen orbitals, while the conduction band isnotably influenced by both Calcium and Niobium, further increasing the material's electronic properties [63]. Furthermore, ab initio DFT simulations have been applied to MgV₂O₆exploring its mechanical, structural, optical, electronic, and thermodynamic properties[64].

So we can conclude, the AB₂O₆Columbite-type oxides, especially Vanadates and Niobates, demonstrate magnificent integration а semiconducting, optical, thermoelectric properties, placing them as promising materials for many applications. Their capacity to conduct electricity under specific conditions, stability in high-temperature and high-voltage environments, makes them right choice for thermoelectric devices, photovoltaic cells, light-emitting diodes, and photocatalysts.

5. USES AND APPLICATIONS

Ternary metal oxides (TMOs), particularly ABO₄ and AB₂O₆ crystal structures, have recently gained significant attention in the field of gas sensing. These materials have a wide range of advantages including sensing capabilities, ease of synthesis, cost-effectiveness, and environmental friendliness. They offer considerable advantages in terms of material design adaptability and surface sensitivity also, being the crucial parameters in enhancing the selectivity and sensitivity of gas sensors, consequently TMOs play key role into sensors next-generation designed for environmental monitoring and industrial safety applications [65].

 In the energy storage sector, Niobium-based ternary oxides have potential as anode

- materials for lithium-ion batteries. These materials, such as MgNb₂O₆, CaNb₂O₆, and structural strength and show BaNb₂O₆, outstanding electrochemical stability under high charge-discharge rates. Theyunder-go, extended cycling without significant destruction. making them substitute traditional graphite-based anodes, specifically for high-power applications such as electric vehicles and portable electronic devices [48].
- There is rise in the use of cadmium-based phosphor materials, for optoelectronic devices particularly due to their efficiency and efficient photoluminescence. These materials investigated in applications including solar cells, light-emitting diodes (LEDs), biosensors, biomedical imaging. Considerably, cadmium selenide/zinc sulfide (CdSe/ZnS) core/shell quantum dots (QDs) are being researched for their role in cancer diagnostics and therapy. Although the inherent toxicity of cadmium imposes constraints for industrial and biomedical adoption, these QDs offer high brightness, reducing the X-ray dosage needed in medical imaging, thus reducing related health risks. Research by Guleryuz et.alfocuses on modification surface and encapsulation techniques to lessen their cytotoxic and genotoxic effects [66].
- In the realm of photocatalysis and $MgNb_2O_6$ environmental remediation. nanoparticles have demonstrated exceptional photocatalytic activity under UV irradiation. nanoparticles effectively These degrade organic dyes such as Acid Red 88 (AR-88) and Fast Orange Red (FOR), indicating their potential for wastewater treatment applications. Additionally, MgNb₂O₆ nanoparticles show high sensitivity and electrochemical response in detecting paracetamol (acetaminophen), a commonly used pharmaceutical compound. Their responsive behavior over a wide potential range (-1.5 V to +0.3 V) positions them as strong candidates for chemical sensing applications in pharmaceutical and environmental fields [57].
- Microwave dielectric materials play a foundational role in the advancement of modern communication systems. ZnNb₂O₆ ceramics stand out as one of the most promising materials in this category, owing to their impressive dielectric constant (ε ~ 25), high quality factor (Qxf = 83.7 GHz), and a low temperature coefficient of resonant frequency (τ_f = -56 ppm/°C). These properties make ZnNb₂O₆ an ideal material for the fabrication of dielectric resonators, filters, and antennas used

- in microwave communication devices. Furthermore, its relatively low sintering temperature (~1200 °C) makes it compatible with conventional ceramic processing techniques, thereby reducing manufacturing costs [67].
- Cadmium-based quantum dots, especially CdSe/ZnSQDs, are extensively researched for a wide range of high-performance applications, such as biomedical screening, solar energy harvesting, and LEDs. While cadmium's cytotoxic effects pose a challenge, particularly in clinical and therapeutic contexts—the remarkable optical properties of these QDs, including their tunable emission wavelengths and photostability, remain unmatched. The high brightness of cadmium-based phosphors enables reduced exposure times and lower doses in X-ray-based diagnostics, thereby offering a balance between performance and safety when used judiciously [68].
- In photoelectrochemical (PEC) water splitting applications, NiV₂O₆ thin films have emerged as effective photoanode materials. Their synthesis and evaluation have revealed favorable electronic properties for solar-driven Hydrogen production, a clean and sustainable alternative energy source. The efficient light absorption and charge transport characteristics of NiV₂O₆ make it a valuable component in PEC devices aimed at large-scale hydrogen generation [69].
- ZnTa₂O₆ (ZTO) is a lead-free piezoelectric material that offers a combination of high thermal stability and excellent piezoelectric response. It crystallizes in the orthorhombic Pbcn space group and exhibits strong Raman activity. The material's dielectric constant (7.05), low loss tangent, moderate piezoelectric coefficient ($d_{33} = 20 \text{ pC/N}$), and energy storage efficiency of 43% make it an attractive option for applications in energy harvesting, electronic actuators, and environmentally friendly transducers that operate under temperature conditions [70].
- A novel electrocatalyst with the Columbite— Tantalite structure, Fe_{0.79}Mn_{0.21}Nb_{0.16}Ta_{0.84}O₆, has been developed for water splitting, demonstrating efficient hydrogen evolution reaction (HER) and oxygen evolution reaction (OER) performance. The material delivers low overpotentials (190.2 mV for HER and 284.8 mV for OER) and exhibits fast reaction kinetics and long-term stability. Density functional theory (DFT) calculations support its outstanding catalytic activity by revealing low Gibbs free energy for intermediate reaction

- steps and minimal OER overpotential, confirming its suitability for renewable hydrogen production [71].
- Finally, an advanced electrochemical gas sensor based on a stabilized zirconia platform and using MnNb₂O₆ as the sensing electrode (SE) is fabricated to detect trace levels of Sulfur dioxide (SO₂) at elevated temperatures. Among various electrode sintering conditions, the MnNb₂O₆-SE calcined at 1000 °C delivered the best performance, offering a strong voltage

response (-27 mV to 5 ppm SO₂), a notably low detection limit (50 ppb), and a swift response time (37 seconds for 1 ppm SO₂ at 700 °C). This sensor also displayed outstanding linearity, stability, and selectivity against interfering gases, proving it a reliable tool for real-time gas monitoring in extreme environments. The detection mechanism was linked to a mixed potential model, where both ionic and electronic contributions govern sensor output [72].

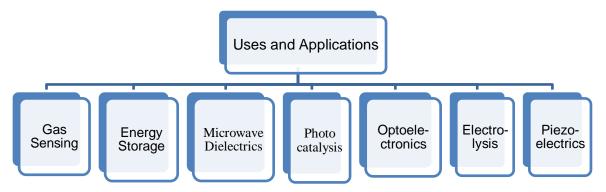


Figure 2. Uses and Applications of Columbite-type oxides

Future potentials

The future potential of Columbite Oxides and related ternary oxides is immense, spanning numerous high-impact fields such as energy storage, optoelectronics, photocatalysis, and biological applications.NiV₂O₆ is one of the important Columbite Oxides with immense future potential given as below:

- NiV2O₆, with its direct band gap of 0.172 eV, has the potential as a semiconductor that could be employed for thermal shielding and optoelectronic devices. The versatility of its electronic properties could open the door for its incorporation into advanced optoelectronic devices, such as photodetectors, modulators, and lasers, offering efficient performance in energy conversion technologies [73].
- Furthermore, NiV_2O_6 has demonstrated exceptional photocatalytic activity, particularly when integrated into nanostructures like the Eu³⁺-doped MgNb₂O₆nanophosphors. These materials exhibited significant photocatalytic degradation of organic dyes like AR-88, as evidenced by the Langmuir-Hinshelwood great model, showing potential environmental remediation applications, such elevating wastewater treatment, and photocatalytic processes for energy harvesting. As such, NiV₂O₆ could be investigated for use in sustainable energy applications, particularly in the field of photocatalysis, where it could

- promote both the degradation of pollutants and the synthesis of renewable energy sources [74,75].
- The potential of NiV₂O₆ in the field of biological applications also promising. is nanoengineeredNiV2O6nanoflowers exhibited oxidase-like enhanced activity, boosting fluorescence by a remarkable 8-fold. This increase in fluorescence was attributed to the unique properties of the nanostructures, suggesting their application in biosensing. Through radical scavenger studies, insights underlying mechanism of into the enhancement were gathered, and the material's sensitivity was demonstrated in detecting low concentrations of glutathione (0.05-12.5 µM) in serum and cancer cells. This highlights its potential as a powerful bioanalytical tool, especially in diagnostic applications and cancer therapy monitoring
- The integration of NiV₂O₆ into energy storage technologies also holds significant promise. The graphene/MnV₂O₆nanocomposite demonstrated excellent electrochemical performance, making it a strong contender for high-efficiency electrode materials in supercapacitor applications. The composite's enhanced charge storage capabilities could contribute to the development of advanced energy storage devices with higher energy

- density and faster charge-discharge cycles, essential for next-generation electronics, electric vehicles, and portable devices [77].
- Additionally. the DFT-based analysis of MgV₂O₆ confirmed its mechanical stability and semiconducting nature, with a band gap of 2.195 eV. The material's optical properties suggest its suitability for solar heat shielding applications, where it could play a role in passive energy management systems for buildings and solar energy devices, contributing to both energy conservation and efficiency improvements [60].
- The future applications of NiV₂O₆ and related ternary metal oxides extend across a wide range of high-tech domains, from energy storage to environmental sustainability and medical diagnostics. The material's unique properties, such as its band gap, fluorescence enhancement, and photocatalytic capabilities, position it as a versatile material for advanced technologies, offering vast potential for innovation in both industrial and biomedical fields. As research progresses, it is expected that these materials will undergo further optimization to unlock even more applications, driving the development of more efficient,

- sustainable, and high-performance technologies [54,60,73-77].
- In recent years, AB₂O₆oxides based phosphor materials with Columbite type structure have attracted increasing attention due to their promising photoluminescence properties as well as potential forensic applications. In this context, a recent study focusing on CdNb2O6 [78] investigated both the luminescence and latent fingerprint detection behavior capabilities of this host material. The results demonstrated strong visible emission, indicating that CdNb₂O₆ can serve as an efficient phosphor when doped with appropriate activator ions. Moreover, its morphology and optical characteristics enabled high-contrast visualization of latent fingerprints under UV excitation, emphasizing its suitability for forensic imaging. This work highlights the dual-functional nature of Columbite-type hosts like CdNb₂O₆, which are not only viable for lighting and display technologies but also hold significant promise in the field of forensic science, particularly in advanced latent fingerprint visualization techniques.

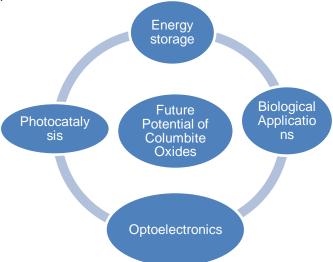


Figure 3. Future Potential of Columbite Oxides

6. CONCLUSION

Columbite-type AB₂O₆ oxides hold great promise for future technology. Their distinctive crystal structures and highly flexible synthesis approaches enable scientists to improve their properties to suit diverse applications. The materials are being used for various uses like converting heat into electricity, purifying pollution with light, battery storage, enhancing and upgrading electronic devices. However, implementing large-scale applications is not simple.

They usually need extremely high temperatures to synthesize, are poor absorbers of sunlight, are poor conductors of electricity, and rely on expensive or hard-to-get rare elements. To get past these issues, scientists have to continue to develop new methods for enhancing them, like chemical adjustments or computational simulations to forecast how they will act. In the future, through the improvement of their synthesis and use, these oxides may be used as an integral component of greener, smarter, and more efficient technologies.

They have the potential to drive everything from environmentally friendly electronics to clean energy solutions.

7. REFERENCES

- [1] H. J. Goldsmid (2010) Introduction to thermoelectricity, book (Vol. 121). Springer. https://doi.org/10.1007/978-3-642-00716-3
- [2] G.S.Nolas, J.Sharp, H.J.Goldsmid (2013) Thermoelectrics: Basic principles and new materials developments, book (Vol. 45). Springer Science & Business Media. https://doi.org/10.1007/978-3-662-04569-5
- [3] E. Tetsi (2017) AB₂O₆ oxides: potential thermoelectric and magnetic materials. The University of Liverpool.
- [4] P.Sen, J. Siles, N. Thawdar, et al. (2023) Multikilometre and multi-gigabit-per-second subterahertz communications for wireless backhaul applications. *Nature Electronics*, 6, 164–175.
- [5] R.Jia, S.Kumar, T.Tan, et al. (2023) Valleyconserved topological integrated antenna for 100-Gbps THz 6G wireless. Science Advances, 9, eadi8500.
- [6] K.Bi, D. Yang, J. Chen, et al. (2019) Experimental demonstration of ultralarge-scale terahertz alldielectric metamaterials. *Photonics Research*, 7, 457–463.
- [7] Q.L. Yang, S. Kruk, Y.H. Xu, et al. (2020) Mieresonant membrane Huygens' metasurfaces. Advanced Functional Materials, 30, 1906851.
- [8] A. Maleki, A. Singh, A. Jaber, et al. (2023) Metamaterial-based octave-wide terahertz bandpass filters. *Photonics Research*, 11, 526–532.
- [9] Y.D. Sırmacı, A. Barreda Gomez, T. Pertsch, et al. (2023) All-dielectric Huygens' meta-waveguides for resonant integrated photonics. *Laser & Photonics Reviews*, 17, 2200860.
- [10] T. Nagatsuma, G. Ducournau, C.C. Renaud (2016) Advances in terahertz communications accelerated by photonics. *Nature Photonics*, 10, 371–379.
- [11] Q. Xia, J.M. Jornet (2019) Expedited neighbor discovery in directional terahertz communication networks enhanced by antenna side-lobe information. *IEEE Transactions on Vehicular Technology*, 68, 7804–7814.
- [12] J.H. Yan, X.Z. Yang, X.Y. Liu, et al. (2023) Van der Waals heterostructures with built-in Mie resonances for polarization-sensitive photodetection. *Advanced Science*, 10, 2207022.
- [13] Y.Q. Lu, C.H. Jiang, Y. Bai, et al. (2024) Enhancing the lithium storage properties of SiO@NC anode by MnNb₂O₆ decoration. *Journal of Energy Storage*, 89, 111699.
- [14] A.W. Kinross, M. Fu, T.J. Munsie, et al. (2014) Evolution of quantum fluctuations near the quantum critical point of the transverse field Ising chain system CoNb₂O₆. *Physical Review X*, 4, 031008.
- [15] R. Coldea, D.A. Tennant, E.M. Wheeler, et al. (2010) Quantum criticality in an Ising chain:

- Experimental evidence for emergent E8 symmetry. *Science*, 327, 177–180.
- [16] F.M. Liu, X. Yang, B. Wang, et al. (2016) High performance mixed potential type acetone sensor based on stabilized zirconia and NiNb₂O₆ sensing electrode. Sensors and Actuators B: Chemical, 229, 200–208.
- [17] S. Zhao, T. Chen, H.P. Li, et al. (2023) An advanced CoNb₂O₆ anode material with in situ interstitial doping for high-rate lithium-ion batteries. *Chemical Engineering Journal*, 472, 145115.
- [18] R.C. Pullar, J.D. Breeze, N.M. Alford (2005) Characterization and microwave dielectric properties of M²⁺Nb₂O₆ ceramics. *Journal of the American Ceramic Society*, 88, 2466–2471.
- [19] H.Y. Yang, S.R. Zhang, H.C. Yang, et al. (2019) Intrinsic dielectric properties of ColumbiteZnNb₂O₆ ceramics studied by P–V–L bond theory and infrared spectroscopy. *Journal of the American Ceramic Society*, 102, 5365–5374.
- [20] H.P. Beck (2012) A study on AB₂O₆ compounds, part II: The branches of the hcp family. *ZeitschriftfürKristallographie-Crystalline Materials*, 227(12), 843–858. https://doi.org/10.1524/zkri.2012.1550
- [21] M.K. Ekmekçi, M. İlhan, L.F. Güleryüz, A. Mergen (2017) Study on molten salt synthesis, microstructural determination and white light emitting properties of CoNb₂O₆:Dy³⁺ phosphor. *Optik*, 128, 26–33. https://doi.org/10.1016/j.ijleo.2016.10.012
- [22] M. İlhan, M.K. Ekmekçi, İ.Ç. Keskin (2021) Judd– Ofelt parameters and X-ray irradiation results of MNb₂O₆:Eu³⁺ (M = Sr, Cd, Ni) phosphors synthesized via a molten salt method. *RSC Advances*, 11, 10451–10458. https://doi.org/10.1039/d0ra10834k
- [23] M. İlhan, M.K. Ekmekçi (2015) Synthesis and photoluminescence properties of Dy³⁺ doped white light emitting CdTa₂O₆ phosphors. *Journal of Solid State Chemistry*, 226, 243–249. https://doi.org/10.1016/j.jssc.2015.02.023
- [24] M. İlhan, İ.Ç. Keskin (2018) Photoluminescence, radioluminescence and thermoluminescence properties of Eu³⁺ doped cadmium tantalate phosphor. *Dalton Transactions*, 47, 13939–13948. https://doi.org/10.1039/c8dt02395f
- [25] R. Erdem, M. İlhan, M.K. Ekmekçi, Ö. Erdem (2017) Electrospinning, preparation and photoluminescence properties of CoNb₂O₆:Dy³⁺ incorporated polyamide 6 composite fibers. *Applied Surface Science*, 421, 240–246. https://doi.org/10.1016/j.apsusc.2016.11.134
- [26] A.S. Başak, M.K. Ekmekçi, M. Erdem, M. İlhan, A. Mergen (2016) Investigation of boron-doping effect on photoluminescence properties of CdNb₂O₆:Eu³⁺ phosphors. *Journal of Fluorescence*, 26, 719–724. https://doi.org/10.1007/s10895-015-1759-y
- [27] M. İlhan, İ.Ç. Keskin (2020) Analysis of Judd–Ofelt parameters and radioluminescence results of

- SrNb₂O₆:Dy³⁺ phosphors synthesized via molten salt method. *Physical Chemistry Chemical Physics*, 22, 19769–19777. https://doi.org/10.1039/d0cp02256j
- [28] S. Karmakar, A.B. Garg, M. Sahu, A. Tripathi, G.D. Mukherjee, R. Thapa, D. Behera (2020) Pressure-
- Mukherjee, R. Thapa, D. Behera (2020) Pressure-induced octahedral tilting distortion and structural phase transition in Columbite structured NiNb₂O₆. *Journal of Applied Physics*, 128, 215902. https://doi.org/10.1063/5.0026096
- [29] S.C. Tarantino, M. Zema (2005) Mixing and ordering behavior in manganoColumbiteferroColumbite solid solution: A single-crystal X-ray diffraction study. *American Mineralogist*, 90(8–9), 1291–1300.
- [30] P. Bordet, A. McHale, A. Santoro, R.S. Roth (1986) Powder neutron diffraction study of ZrTiO₄, Zr₅Ti₇O₂₄, and FeNb₂O₆. Journal of Solid State Chemistry, 64, 30–46.
- [31] M. İlhan, M.K. Ekmekçi, L.F. Güleryüz (2023) Effect of boron incorporation on the structural, morphological, and spectral properties of CdNb₂O₆:Dy³⁺ phosphor synthesized by molten salt process. *Materials Science & Engineering B*, 298, 116858.
 - https://doi.org/10.1016/j.mseb.2023.116858
- [32] M. İlhan, M.K. Ekmekçi, K. Esmer (2024) Structural and dielectric properties of Eu³⁺, B³⁺ co-doped CoNb₂O₆ ceramic. *Journal of The Turkish Chemical Society Section A: Chemistry*, 11, 765–774. https://doi.org/10.18596/jotcsa.1397311
- [33] M.K. Ekmekçi, M. Erdem, A.S. Başak, M. İlhan, A. Mergen (2016) Molten salt synthesis and optical properties of Eu³⁺, Dy³⁺ or Nd³⁺ doped NiNb₂O₆Columbite-type phosphors. *Ceramics International*, 41, 9680–9685. http://dx.doi.org/10.1016/j.ceramint.2015.04.036
- [34] T.A. Vanderah, R.S. Roth, T. Siegrist, W. Febo, J.M. Loezos, W. Wong-Ng (2003) Subsolidus phase equilibria and crystal chemistry in the system BaO– TiO₂–Ta₂O₅. Solid State Sciences, 5(1), 149–164.
- [35] M. İlhan (2022) Heat capacities and thermodynamic functions of CdNb₂O₆ and CdTa₂O₆. Journal of Thermal Analysis and Calorimetry, 147, 12383– 12389. https://doi.org/10.1007/s10973-022-11490-6
- [36] [36] M. Nyman, M.A. Rodriguez, L.E. Rohwer, J.E. Martin, M. Waller, F.E. Osterloh (2009) Unique LaTaO₄ polymorph for multiple energy applications. *Chemistry of Materials*, 21(19), 4731–4737.
- [37] M. Nyman, M.A. Rodriguez, L.E. Shea-Rohwer, J.E. Martin, P.P. Provencio (2009) Highly versatile rare earth tantalate pyrochlore nanophosphors. *Journal* of the American Chemical Society, 131(33), 11652– 11653.
- [38] J. Narkilahti, M. Tyunina (2012) The structure of strained perovskiteKTaO₃ thin films prepared by pulsed laser deposition. *Journal of Physics:* Condensed Matter, 24(32), 325901.
- [39] A.K. Ganguli, S. Nangia, M. Thirumal, P.L. Gai (2006) A new form of $MgTa_2O_6$ obtained by the

- molten salt method. *Journal of Chemical Sciences*, 118, 37–42.
- [40] C.G. Almeida, H.M.C. Andrade, A.J.S. Mascarenhas, L.A. Silva (2010) Synthesis of nanosized β-BiTaO₄by the polymeric precursor method. *Materials Letters*, 64(9), 1088–1090.
- [41] G.K. Layden (1967) Polymorphism of BaTa₂O₆. *Materials Research Bulletin*, 2(5), 533–539.
- [42] W.G. Mumme, I.E. Grey, R.S. Roth, T.A. Vanderah (2007) Contrasting oxide crystal chemistry of Nb and Ta: The structures of the hexagonal bronzes BaTa₂O₆ and Ba_{0.93}Nb_{2.3}O₆. *Journal of Solid State Chemistry*, 180(9), 2429–2436.
- [43] S.C. Navale, V. Samuel, A.B. Gaikwad, V. Ravi (2007) A co-precipitation technique to prepare BaTa₂O₆. Ceramics International, 33(2), 297–299.
- [44] M.K. Ekmekçi, M. Erdem, M. İlhan, A.S. Başak, A. Mergen (2016) Synthesis, characterization and photoluminescence properties of Eu³⁺ doped ColumbiteCdNb₂O₆. *Optik*, 127, 1918–1921. http://dx.doi.org/10.1016/j.ijleo.2015.11.031
- [45] M.K. Ekmekçi, M. İlhan, A. Ege, M. Ayvacıklı (2017) Microstructural and radioluminescence characteristics of Nd³+ doped Columbite-type SrNb₂O₆ phosphor. *Journal of Fluorescence*, 27, 973–979. http://dx.doi.org/10.1007/s10895-017-2032-3
- [46] J.P. Peña, P. Bouvier, M. Hneda, C. Goujon, O. Isnard (2021) Raman spectra of vanadatesMV₂O₆ (M = Mn, Co, Ni, Zn) crystallized in the non-usual Columbite-type structure. *Journal of Physics and Chemistry of Solids*, 154, 110034.
- [47] W. Lima da Silva, M. Walker, R.M. Ribas, R.S. Monteiro, E. Kendrick, R.I. Walton (2023) Morphological control of Ca_xMn₁-_xNb₂O₆Columbites for use as lithium hosts in batteries. *Materials Chemistry Frontiers*, 7(23), 5941-5956
- [48] P. Kumar, B. Mishra, M. Pastor (2020) Preparation and synthesis of ColumbiteMNb₂O₆ ceramics by chemical reaction (M = Zn, Ni, Co). *International Journal of Scientific Research and Engineering Development*, 3(5), 521–525.
- [49] K. Sarkar, S. Mukherjee (2016) Characterization and evaluation of property of Columbite–MgNb₂O₆ synthesized by chemical route. *Journal of The Institution of Engineers (India): Series E.*
- [50] S.Y. Wu, X.Q. Liu, X.M. Chen (2009) Low temperature synthesis of ZnNb₂O₆ fine powders by wet-chemical processes. *Ferroelectrics*, 388(1), 114–119.
- [51] C.Y. You, Y.C. Zhang (2016) Effects of CuO additives and sol-gel technique on NiNb₂O₆ dielectric ceramics for LTCC application. *Journal of Materials Science: Materials in Electronics*, 27, 6606–6613.
- [52] Z.F. Fu, J.L. Ma, P. Liu, Y.X. Tang (2013) Microwave dielectric properties of MgNb₂O₆ ceramics prepared via high energy ball milling method. Advanced Materials Research, 631, 499– 503.

- [53] L. Shi, X. Wang, R. Peng, Y. Lu, C. Liu, D. Zhang, H. Zhang (2022) Effect of Mn²⁺ doping on the lattice and the microwave dielectric properties of MgTa₂O₆ ceramics. Ceramics International, 48(14), 20096https://doi.org/10.1016/j.ceramint.2022.03.287
- [54] D.K. Tiwari, S.K. Rout (2020) Enhancement of electrical energy storage ability by controlling grain
- size of polycrystalline BaNb2O6 for high density capacitor application. Journal of Alloys and Compounds, 829, 154573.
- [55] A. Ahmed, M. Ghulam, M. Irfan, A. Ahmad, A. Hind (2024) Investigating the novel thermoelectric properties of magnesium, calcium, and barium divanadate oxides (XV_2O_6) where X = Mg, Ca, and Ba) for waste heat recovery applications in energy harvesting devices. Applied Physics A, 130(1),1–13. https://doi.org/10.1007/s00339-023-07235-3
- [56] A. Ahmed, G. Murtaza, A. Ayyaz, M. Shafiq, H. Albalawi (2024) Synthesis, characterization, and novel thermoelectric properties of Nb-based metal oxides XNb_2O_6 (X = Mg, Ca, Ba) for energy harvesting applications: Experimental and DFT insight. Journal of Materials Research, 39(12), 1727-1740.
 - https://doi.org/10.1557/s43578-024-01341-5
- [57] K.B. Spooner, A.M. Ganose, W.W.W. Leung, J. Buckeridge, B.A.D. Williamson, R.G. Palgrave, D.O. Scanlon, R.G. Palgrave (2021) BaBi₂O₆: A promising n-type thermoelectric oxide with the PbSb₂O₆ crystal structure. Chemistry of Materials, 33(18), 7441-7456.
 - https://doi.org/10.1021/acs.chemmater.1c02164
- [58] N. Basavaraju, S.C. Prashantha, B.S. Surendra, T.R. Shekhar, M.R. Anil Kumar, C.R. Ravikumar, N. Raghavendra, T.S. Shashidhara (2021) Structural and optical properties of MgNb₂O₆ nanoparticles: Its potential application in photocatalytic pharmaceutical industries as а sensor. Environmental Nanotechnology, Monitoring Management, 16, 100581.
 - https://doi.org/10.1016/j.enmm.2021.100581
- [59] J.F. de Lima Nascimento, F.X. Nobre, F.M.C. Batista, A. Cabot, X. Vendrell, L. Mestres, O. da Cunha Mendes, R.D. Ferreira, Y.L. Ruiz, J.N. Nonato Quaresma, O. da Cunha Mendes (2023) Synthesis of CaNb₂O₆ with a rynersonite-like structure: Morphology, Rietveld refinement, optical, and vibrational properties. Inorganic Chemistry, 62(40), 16323-16328.
 - https://doi.org/10.1021/acs.inorgchem.3c01311
- [60] M.A. Rahman, M.Z. Rahaman, M.A.R. Sarker (2017) Ab-initio study of structural, elastic, electronic, optical, and thermodynamic properties of MgV₂O₆. arXiv Preprint, arXiv:1709.08208.
- [61] R. Gaur, R. Jindal, A. Tripathi (2025) Identification of optically active vibrational modes of Columbite correlation method. using the ZastitaMaterijala, 66(1), 126–132. https://doi.org/10.62638/ZasMat1214

- [62] R. Gaur, R. Jindal, A. Tripathi (2025) Study of vibrational properties of thermoelectric ColumbiteMnV₂O₆. *Indian Journal of Physics*, 1–9. https://doi.org/10.1007/s12648-025-03586-0
- [63] U. Duman, M. Aycibin, Ö.F. Özdemir (2021) The electronic, structural, and optical properties of $CaNb_2O_6$ compound: Theoretical study. *Physica* Status Solidi (B), 258(12), 2100416. https://doi.org/10.1002/pssb.202100416
- [64] M.A. Rahman, M.Z. Rahaman, M.S. Ali, M.A.R. Sarker (2018) Theoretical investigation on MgV₂O₆: ab-initio study. Philosophical Magazine, 98(22), 2077-2093. https://doi.org/10.1080/14786435.2018.1468094
- [65] N. Saxena, P. Kumar (2024) ABO₄ and AB₂O₆ structured metal oxide-based gas sensors. In: Complex and Composite Metal Oxides for Gas, VOC and Humidity Sensors, Volume 2, pp. 385-404. Elsevier.
- [66] L.F. Güleryüz (2023) Effect of Nd3+ doping on structural, near-infrared, and cathodoluminescent properties for cadmium tantalate phosphors. Journal of the Turkish Chemical Society Section A: Chemistry, 10(1), 77-88. https://doi.org/10.18596/jotcsa.1202284
- [67] E.İ. Şahin (2022) Microwave electromagnetic shielding effectiveness of ZnNb₂O₆-chopped strands composites for radar and wideband (6.5-18 GHz) applications. Lithuanian Journal of Physics, 62(3). https://doi.org/10.3952/physics.v62i3.4799
- [68] L.F. Güleryüz (2022) Assessing of photoluminescence and structural properties of Dy3+ doped cadmium tantalate phosphor. Hacettepe Journal of Chemistry, Biology and 50(3), 247-254. https://doi.org/10.15671/hjbc.1056363
- [69] H.X. Dang, A.J. Rettie, C.B. Mullins (2015) Visiblelight-active NiV2O6 films for photoelectrochemical water oxidation. The Journal of Physical Chemistry C, 119(26), 14524-14531. https://doi.org/10.1021/jp508349g
- [70] R. Mitra, A. Ramadoss, S. Anwar, U. Manju (2023) ZnTa₂O₆—holistic insights into a potential hightemperature piezoelectric candidate with tri-α-PbO₂ structure. Materials Research Bulletin, 157, 112038. https://doi.org/10.1016/j.materresbull.2022.112038
- [71] P. Bacirhonde, N. Dzade, C. Chalony, J. Park, E. Afranie, S. Lee, C.S. Kim, C.S. Kim (2021) Extraction of non-noble metal Columbite-tantalite as a highly efficient electrocatalyst for water splitting. Nature Communications, 12(1), 1-10. https://doi.org/10.21203/rs.3.rs-199656/v1
- [72] F. Liu, Y. Wang, B. Wang, X. Yang, Q. Wang, X. Liang, P. Sun, X. Chuai, Y. Wang, G. Lu (2017) Stabilized zirconia-based mixed potential type sensors utilizing MnNb2O6 sensing electrode for detection of low-concentration SO2. Sensors and Actuators B: Chemical, 238, 1024-1031. https://doi.org/10.1016/j.snb.2016.07.145
- [73] M.A. Rahman, M.Z. Rahaman, M.A. Khatun, M.A.R. Sarker (2018) First principles investigation of

- structural, electronic and optical properties of NiV_2O_6 . Computational Condensed Matter, 15, 95–99. https://doi.org/10.1016/j.cocom.2017.10.004
- [74] N. Basavaraju, S.C. Prashantha, H. Nagabhushana, M. Chandrasekhar, A.N. Kumar, T.S. Shekhar, K.S. Anantharaju (2021) A benign approach for novel synthesis of Eu³⁺ doped MgNb₂O₆: Its photoluminescence and photocatalytic studies. *Ceramics International*, 47(10), 14899–14906. https://doi.org/10.1016/j.ceramint.2020.07.242
- [75] N. Basavaraju, S.C. Prashantha, H. Nagabhushana, C. Pratapkumar, C.R. Ravikumar, M.A. Kumar, H.P. Nagaswarupa (2021) MgNb₂O₆:Dy³⁺nanophosphor: A facile preparation, down conversion photoluminescence and UV-driven photocatalytic properties. *Ceramics International*, 47(7), 10370– 10380.

https://doi.org/10.1016/j.ceramint.2020.10.186

- [76] N. Khanehsari, M. Amjadi, T. Hallaj, V. Shafiei-Irannejad (2024) NiV₂O₀nanoflowers as an oxidase-mimic nanozyme for sensitive fluorimetric assay of glutathione. *Microchemical Journal*, 199, 110160. https://doi.org/10.1016/j.microc.2024.110160
- [77] W.H. Low, S.S. Lim, C.W. Siong, C.H. Chia, P.S. Khiew (2021) One-dimensional MnV₂O₆nanobelts on graphene as outstanding electrode material for high energy density symmetric supercapacitor. *Ceramics International*, 47(7), 9560–9568. https://doi.org/10.1016/j.ceramint.2020.12.090
- [78] M. İlhan, L.F. Güleryüz, M.K. Ekmekçi, M. Erdem (2025) Multicolor emission of CdNb₂O₆:Eu³⁺, Er³⁺ and CdNb₂O₆:Eu³⁺, Er³⁺, Yb³⁺ phosphors with dual excitation and dual emission in UV to IR for latent fingerprint applications. *Optical Materials*, 166, 117178.

https://doi.org/10.1016/j.optmat.2025.117178

IZVOD

OKSIDI AB₂O₆ SA STRUKTUROM KOLUMBITA: RAZUMEVANJE NJIHOVE STRUKTURE, SINTEZE I POTENCIJALA ZA BUDUĆE TEHNOLOGIJE

Oksidi AB_2O_6 su nedavno privukli značajnu pažnju zbog svojih ekskluzivnih svojstava. Ova jedinjenja pokazuju raznovrsne strukturne oblike sa različitim karakteristikama. Među njima, oksidi tipa Kolumbita poseduju ortorombičnu strukturu, pripadaju prostornoj grupi Pbcn i pokazuju simetriju D_2h^14 . Struktura ovih materijala sastoji se od oktaedara AO_2 i BO_2 koji su raspoređeni cik-cak i imaju snažan uticaj na karakteristike ovih materijala. Ovi materijali igraju vitalnu ulogu u različitim primenama kao što su mikrotalasna tehnologija, kataliza, skladištenje energije, elektronski senzori i optički materijali. Na osnovu sveobuhvatnog pregleda literature, ovaj pregled je obuhvatio detaljnu studiju strukture, fizičkih svojstava, tehnika sinteze i primene ovih oksida. Nakon toga, razmatramo budući potencijal oksida Kolumbita, sa naglaskom na strategije i računarsko modeliranje za poboljšanje njihovih svojstava i performansi za buduće tehnologije. **Ključne reči:** Kolumbajt, mikrotalasna tehnologija, računarsko modeliranje

Naučni rad

Rad primljen: 06.05.2025. Rad korigovan: 17.06.2025. Rad prihvaćen: 23.06.2025.

^{© 2025} Authors. Published by Engineering Society for Corrosion. This article is an open access article distributed under the terms and conditions of the Creative Commons Attribution 4.0 International license (https://creativecommons.org/licenses/by/4.0/)