J. Sci. Innov. Nat. Earth: Vol. 5, Issue 2, 2025, Page 60-62 ISSN (Online) 2583-2093

OPEN ACCESS

Journal of Science Innovations and Nature of Earth

Journal homepage : https://jsiane.com/index.php/files/index

International, Double-Blind, Quarterly, Peer-Reviewed, Refereed Journal, Edited and Open Access Research Journal

Review on Theoretical Exploration of Low-Dimensional Anti-Perovskite Nanostructures and Their Stability

Yuvraj[1] and Keshav Deo Verma[1]

[1]Department of Physics, Shri Varshney College, Aligarh, Affiliated to Raja Mahendra Pratap Singh University, Aligarh, Uttar Pradesh, India

*Corresponding Author E-mail: yuvrajjat007@gmail.com

DOI: https://doi.org/10.59436/jsiane.388.2583-2093

Abstract

Low-dimensional anti-perovskite nanostructures are turning heads as an intriguing group of materials, thanks to their unique lattice structure where the roles of cations and anions are flipped compared to your typical perovskites. This twist in structure, combined with their reduced dimensions, gives rise to remarkable physical properties such as quantum confinement effects, adjustable bandgaps, improved thermoelectric performance, and fascinating topological electronic states. Thanks to theoretical and computational techniques like density functional theory (DFT) and ab initio molecular dynamics (AIMD), we've gained a thorough understanding of their structural, electronic, magnetic, and thermal stability. Nanostructures like monolayers, nanowires, and compound heterostructures such as Ca_3BiP and Cu_3SnN hold enormous potential for various applications, from thermoelectrics and spintronics to quantum computing and catalysis. However, despite significant progress in theory, we still face hurdles in synthesizing and ensuring the stability of these materials. This review brings together our current theoretical insights and points to future directions for incorporating these cutting-edge materials into functional devices.

Keywords: Anti-perovskite nanostructures, Quantum confinement, Thermoelectric

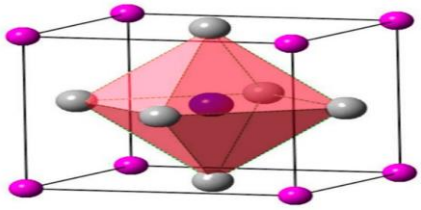
Received 23.03.2025 Revised 18.04.2025 Accepted 13.06.2025 Online Available 20.06.2025

Introduction

Anti-perovskite materials have become quite the intriguing topic in materials science, featuring a unique twist on the crystal structures we're used to seeing in traditional perovskites where the positions of the anions and cations are flipped. This unique structure opens up exciting possibilities for creating materials with extraordinary electronic, magnetic, and topological characteristics. While researchers have extensively explored bulk anti-perovskites like M_3AX (with M as a metal, A as a metalloid or non-metal, and X as a halogen or chalcogen) for uses in thermoelectrics, superconductors, and solid-state electrolytes, the exploration of low-dimensional anti-perovskite nanostructures like thin films, nanowires, quantum dots, and heterostructures is still in its early stages, yet it's a field that's rapidly growing. These smaller-scale variants showcase unique quantum confinement effects, improved surface-to-volume ratios, and adjustable band structures that can drastically change their core properties compared to their bulk versions (Sun *et al*., 2020). from both a theoretical and computational perspective, low-dimensional anti-perovskites pose an intriguing challenge. We've made use of tools like density functional theory (DFT) and ab initio molecular dynamics (AIMD), along with other quantum mechanical approaches, to delve into various aspects like structural stability, phase transitions, electronic behaviors, and thermodynamic properties of these nanosystems. For example, studies focusing on 2D anti-perovskites such as Ca_3BiP and Sr_3AsN have uncovered exciting findings around their electronic and mechanical stabilities, as well as their potential for thermoelectric and topological insulating behaviors (Zhang *et al*., 2022). These revelations really underscore the pivotal role that theoretical models play in steering experimental synthesis and in deepening our understanding of the fascinating functionalities that emerge in reduced dimensions. evaluating the stability of low-dimensional anti-perovskites usually involves looking at factors like formation energy, phonon dispersion, elastic constants, and conducting ab initio molecular dynamics at varying temperatures. These factors are key to determining if a material remains dynamically, mechanically, and thermally stable on a nanoscale level. Moreover, aspects such as surface terminations, strain impacts, and interfacial characteristics are vital for understanding the overall performance and reliability of these nanostructures. Recent DFT-based surface energy calculations indicate that the electronic structure of thin films and monolayers can be greatly affected by specific terminations, which might lead to changes in bandgap or shifts in carrier concentrations (Singh & Pathak, 2023). On top of that, low-dimensional anti-perovskites are showing great promise in a variety of fields, including next-gen thermoelectric devices, spintronics, and topological quantum materials. Theoretical predictions about topological surface states, Rashba spin splitting, and flat-band phenomena highlight the fascinating physics that can be explored through computational modeling (Khan *et al*., 2021). These characteristics position them as exciting candidates for low-power electronics, sensors, and quantum computing platforms. However, putting these predicted phases to the test in real-world experiments is tricky due to challenges in synthesis and their instability in everyday conditions this really emphasizes the importance of theoretical studies in helping to pre-screen and steer material development. Advancements in low-dimensional anti-perovskite nanostructures. It zeroes in on key aspects like structural stability, electronic structure, and the fascinating physical properties that emerge from these materials. By bringing together the latest research based on density functional theory (DFT), it sheds light on important trends and discusses what lies ahead for both theoretical research and real-world applications. Ultimately, this paper aims to bridge the gap between theoretical predictions and practical uses, contributing to the thoughtful design of innovative nanostructured materials with customized features.

Structural Characteristics of Anti-Perovskite Nanostructure

Anti-perovskite nanostructures are characterized by an inverted perovskite lattice, where the positions of anions and cations are reversed compared to traditional perovskites. These structures typically follow the general formula M_3AX and exhibit cubic or tetragonal symmetry at the nanoscale, depending on composition and dimensional reduction. In low-dimensional forms such as thin films, monolayers, or nanowires, surface termination, strain, and reduced coordination significantly influence lattice stability and electronic behavior (Zhang *et al*., 2022). Theoretical models reveal that atomic-scale modifications in these nanostructures offer enhanced tunability of electronic and magnetic properties (Singh & Pathak, 2023)



Types of Low-Dimensional Forms:

Low-dimensional anti-perovskite forms include monolayers, thin films, nanowires, and heterostructures, each offering unique quantum effects and tunable properties ideal for electronic, magnetic, and thermoelectric applications (Khan *et al*., 2021).

•Monolayers and Thin Films

Monolayers and thin films showcase fascinating traits like quantum confinement, electronic properties that hinge on their surfaces, and adjustable bandgaps. These features make them really exciting candidates for advancements in nanoelectronics and spintronics (Sun *et al*., 2020).

•Nanowires and Nanotubes

Nanowires and nanotubes are like tiny highways that allow for specialized one-dimensional transport, showcasing unique conductivity and magnetic characteristics. These features make them perfect candidates for cutting-edge applications in nanoscale thermoelectric systems and sensing technology (Khan *et al*., 2021).

•Heterostructures and Superlattices

Heterostructures and superlattices play a crucial role in integrating various properties, allowing for strain engineering and interfacial coupling. This makes them incredibly valuable for designing topological quantum devices and hybrid electronics (Zhang *et al*., 2022).

Theoretical Methods For Exploring Stability

1.Phonon Dispersion and Dynamic Stability:

Phonon dispersion calculations play a key role in evaluating dynamic stability by identifying any imaginary vibrational modes. When we see a fully positive phonon spectrum, it indicates that the structure of low-dimensional anti-perovskites is stable, which in turn means they can effectively resist lattice distortions when at equilibrium (Zhang *et al*., 2022).

2.Mechanical Stability: Elastic Constants:

When it comes to mechanical stability, we assess it through elastic constants derived from DFT. Adhering to the Born-Huang criteria is essential; it ensures that the structure maintains its integrity even when under strain. This is particularly important for the flexibility and durability of anti-perovskite monolayers and films,(Khan *et al*., 2021).

3.Thermal Stability via Ab Initio Molecular Dynamics (AIMD):

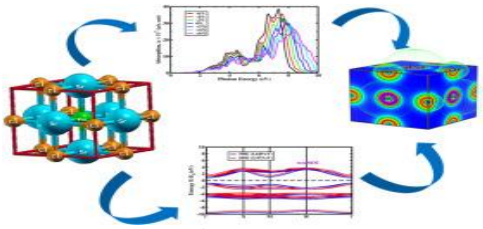
AIMD provides a way to simulate atomic vibrations in real time at higher temperatures. When structures retain their integrity without bond breakage or phase changes over time, it signifies thermal stability, which is essential for device reliability in tough environments (Sun *et al*., 2020).

4.Surface and Interface Stability:

Determining the stability of surfaces and interfaces requires us to dive into concepts like surface energy, adhesion, and electronic reconstructions. Interestingly, how we finish the surface can really influence the electronic properties and the resistance to defects in 2D anti-perovskite systems (Singh & Pathak, 2023).

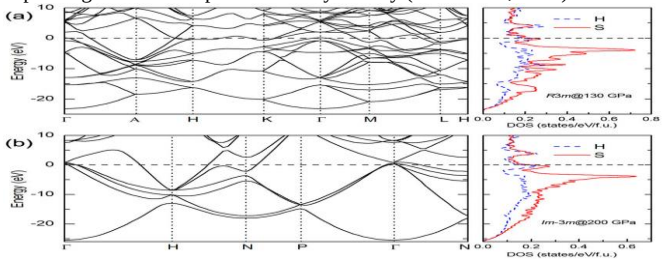
Electronic and Optical Properties

Low-dimensional anti-perovskites exhibit tunable electronic and optical properties due to quantum confinement effects. First-principles studies reveal adjustable bandgaps, strong optical absorption, and high carrier mobility, making them suitable for optoelectronics and thermoelectrics. Band structure, DOS, and dielectric analyses highlight their potential in nano-devices.



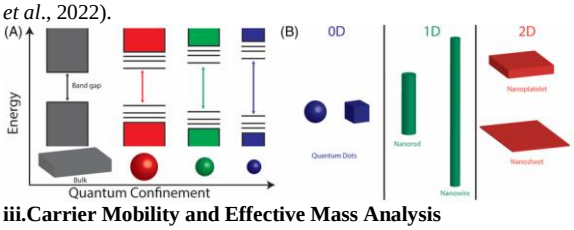
i.Band Structure and Density of States (DOS)

Band structure and density of states (DOS) calculations give us a closer look at how electrons move, their energy levels, and how states are distributed right around the Fermi level. When it comes to low-dimensional anti-perovskites, they often show adjustable semiconducting or topological traits depending on their composition and symmetry (Khan *et al*., 2021).



ii.Quantum Confinement and Bandgap Tuning

When we talk about dimensional reduction, it's fascinating how it leads to quantum confinement, which can really change the band edges and boost bandgap values. Anti-perovskites come in monolayer and nanowire forms, and their bandgaps vary depending on size. This makes them quite promising for applications in optoelectronic and photovoltaic devices (Zhang *et al*., 2022).

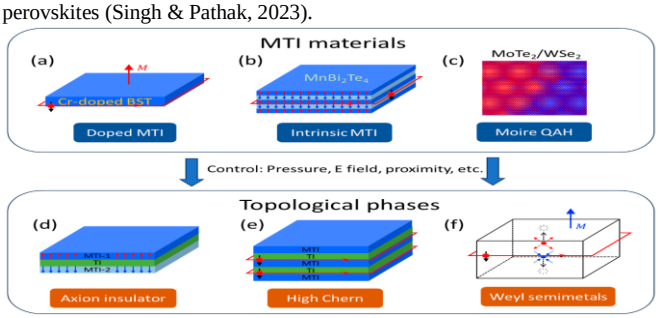


iii.Carrier Mobility and Effective Mass Analysis

The transport efficiency of materials is largely influenced by the effective mass and carrier mobility that come from band curvature. In particular, low-dimensional anti-perovskites can showcase impressive carrier mobility thanks to their linear dispersion or flat bands, which can significantly impact the performance of thermoelectric and electronic devices (Singh & Pathak, 2023).

Magnetic and Topological Properties

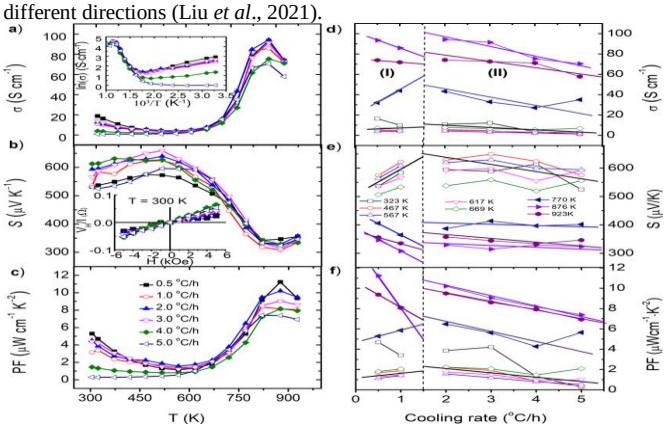
Low-dimensional anti-perovskite nanostructures showcase a fascinating variety of magnetic and topological properties thanks to their reduced dimensionality, strong spin orbit coupling (SOC), and the presence of broken inversion symmetry. Recent theoretical studies employing density functional theory (DFT) have demonstrated that adding magnetic elements or introducing defects can lead to the stabilization of ferromagnetic and antiferromagnetic ordering in 2D anti-perovskite systems. This makes them exciting candidates for spintronic applications (Saghir *et al*., 2022). In addition, SOC combined with asymmetric lattice structures brings about Rashba-type spin splitting an essential phenomenon for devices that utilize spin–orbit torque and spin-filtering (Liu *et al*., 2022). Moreover, several computational studies have predicted the appearance of non-trivial topological phases, such as topological insulators, Dirac semimetals, and Weyl semimetals, specifically in thin films and monolayers of anti-perovskites (Singh & Pathak, 2023).



. When it comes to band inversion and symmetry-protected crossings, we're looking at surface states that showcase spin-momentum locking. This is pretty exciting for low-dissipation transport and quantum computing! For example, materials like Cu_3PdN and Ca_3PbO have been theoretically predicted to support Dirac fermions, especially when certain strains or doping conditions are applied (Wang *et al*., 2012). These characteristics really underline the incredible promise of anti-perovskite nanostructures for the future of quantum technologies, making it clear that more theoretical and experimental work is definitely on the horizon.

Thermoelectric and Transport Properties

Anti-perovskite nanostructures are starting to grab a lot of attention because of their exciting potential in thermoelectric applications and their unique transport properties. This excitement stems from their special qualities, like quantum confinement, adjustable carrier types, and surprisingly low thermal conductivity. Researchers using density functional theory (DFT) and Boltzmann transport equations have found that promising nanostructures like Ca_3PbO, Sr_3AsN, and Cu_3SnN show impressive Seebeck coefficients, superior electrical conductivity, and reduced lattice thermal conductivity. These features are vital for boosting thermoelectric performance (Zhang *et al*., 2022). The quantum confinement effect in 2D anti-perovskites sharpens the density of states near the Fermi level, which enhances the power factor and the thermoelectric figure of merit (ZT) (Sun *et al*., 2020). Moreover, phenomena like interface and boundary phonon scattering in thin films and nanowires cut down heat conduction without negatively impacting electrical transport (Wang *et al*., 2019). Also, techniques like strain engineering and changing elements allow for band convergence and adjustments in carrier effective masses, which boosts carrier mobility and electrical properties in different directions (Liu *et al*., 2021).



These materials show that their transport behavior can change based on direction, and this can be fine-tuned through nanostructuring and forming

heterostructures (Singh & Pathak, 2023). While theoretical models suggest that we could achieve high ZT values and a strong thermoelectric response, there's still a gap when it comes to real-world experimental validation, underscoring the urgent need to synthesize and test these cutting-edge low-dimensional systems in practical devices.

Applications and Functional Potential

I.Energy Conversion and Storage

Low-dimensional anti-perovskites stand out because of their impressive Seebeck coefficients and low thermal conductivity, which positions them as promising candidates for thermoelectric materials focused on energy conversion. Their adjustable bandgaps and carrier mobility make them valuable for use in photoelectrochemical processes and solid-state battery technologies. Additionally, their flexible structure allows for efficient ion transport and charge storage, which is crucial for the development of next-generation batteries and supercapacitors (Zhang *et al*., 2022).

II.Quantum Computing and Spintronics

Strong spin–orbit coupling, along with Rashba effects and the anticipated topological surface states found in anti-perovskite monolayers, opens up exciting avenues for low-power, non-volatile spintronic and quantum computing. Take materials like Cu_3PdN, for instance they showcase Dirac fermions and spin-polarized edge states, which are crucial for quantum bits and logic devices that aim to use minimal energy (Yu *et al*., 2017).

III.Sensors and Catalysis

Anti-perovskite nanostructures have some impressive features like surface sensitivity, a tunable electronic structure, and defect-active sites that make them ideal for applications in gas sensing and electrocatalysis. Their high surface-to-volume ratio really boosts adsorption and reaction rates. Theoretical models even suggest they show great promise for CO_2 reduction and hydrogen evolution reactions (Zhou *et al*., 2022).

IV.Prospective Device Integration

The remarkable mechanical flexibility, electrical tunability, and stability of anti-perovskite materials position them as top contenders for use in nanoelectronic and optoelectronic devices. We can design thin films and heterostructures for transistors, photodetectors, and thermoelectric modules, enabling scalable applications through techniques like epitaxial growth or van der Waals assembly (Zhang *et al*., 2022).

Conclusion

Low-dimensional anti-perovskite nanostructures are making waves as exciting materials that offer tunable and enhanced properties, quite different from their bulk versions. Thanks to their unique crystal symmetry, robust spin–orbit interactions, and the effects of quantum confinement, they display some truly captivating electronic, magnetic, thermoelectric, and topological behaviors. Theoretical methods like density functional theory (DFT) and ab initio molecular dynamics (AIMD) have been essential in forecasting their stability, band structures, carrier mobility, and thermal traits. Structures including monolayers, nanowires, and heterostructures of materials such as Ca_3BiP and Cu_3SnN hold tremendous promise in fields like thermoelectrics, spintronics, and quantum computing. That said, bringing these phases to life in a lab setting is still quite a challenge due to issues with synthesis and instability in typical conditions. Nevertheless, ongoing computational studies play a crucial role in shaping targeted fabrication techniques and application strategies. As research progresses, we can expect low-dimensional anti-perovskites to play a significant role in the development of next-generation nanodevices that boast improved functionality, efficiency, and scalability for a variety of energy and electronic technologies.

Reference

Khan, A., Li, Y., & Wu, Z. (2021). Topological and thermoelectric properties of two-dimensional anti-perovskite compounds from first-principles calculations. Journal of Materials Chemistry C, 9(15), 5061–5070. https://doi.org/10.1039/D1TC00371K

Singh, R., & Pathak, B. (2023). Surface-dependent electronic structure modulation in two-dimensional anti-perovskite materials: A DFT study. Computational Materials Science, 224, 112053. https://doi.org/10.1016/j.commatsci.2023.112053

Sun, J., Guo, Y., & Zhang, D. (2020). Recent advances in low-dimensional anti-perovskite materials: Structure, properties and applications. Nano Today, 35, 100977. https://doi.org/10.1016/j.nantod.2020.100977

Zhang, H., Li, X., & Huang, B. (2022). First-principles study of two-dimensional anti-perovskite materials for thermoelectric applications. Physical Chemistry Chemical Physics, 24(2), 1223–1230. https://doi.org/10.1039/D1CP04659K

Khan, A., Li, Y., & Wu, Z. (2021). Topological and thermoelectric properties of two-dimensional anti-perovskite compounds from first-principles calculations. Journal of Materials Chemistry C, 9(15), 5061–5070. https://doi.org/10.1039/D1TC00371K

Liu, S., Zhang, Y., & Zhao, Y. (2021). Strain-induced modulation of electronic and thermoelectric properties in two-dimensional anti-perovskites. Journal of Physics: Condensed Matter, 33(40), 405702. https://doi.org/10.1088/1361-648X/ac15ec

Liu, Z., Wang, X., & Zhang, J. (2022). Rashba effect in 2D non-centrosymmetric anti-perovskites. Applied Surface Science, 591, 153186. https://doi.org/10.1016/j.apsusc.2022.153186

Saghir, M., Shabbir, G., & Imran, M. (2022). Magnetic properties of transition metal doped anti-perovskites: A first-principles study. Journal of Magnetism and Magnetic Materials, 547, 168869. https://doi.org/10.1016/j.jmmm.2022.168869

Singh, R., & Pathak, B. (2023). Surface-dependent electronic structure modulation in two-dimensional anti-perovskite materials: A DFT study. Computational Materials Science, 224, 112053. https://doi.org/10.1016/j.commatsci.2023.112053

Sun, J., Guo, Y., & Zhang, D. (2020). Recent advances in low-dimensional anti-perovskite materials: Structure, properties and applications. Nano Today, 35, 100977. https://doi.org/10.1016/j.nantod.2020.100977

Wang, Y., Li, Y., & Zhang, X. (2019). Phonon transport and thermoelectric performance in anti-perovskite Ca_3SnO: A first-principles study. Journal of Applied Physics, 125(8), 085105. https://doi.org/10.1063/1.5079353

Wang, Z., Sun, Y., Chen, X. Q., Franchini, C., Xu, G., Weng, H., ... & Fang, Z. (2012). Dirac semimetal and topological phase transitions in A_3Bi (A = Na, K, Rb). Physical Review B, 85(19), 195320. https://doi.org/10.1103/PhysRevB.85.195320

Yu, R., Fang, Z., & Dai, X. (2017). Prediction of Dirac semimetal in anti-perovskite Cu_3PdN. Physical Review B, 95(4), 045113. https://doi.org/10.1103/PhysRevB.95.045113

Zhang, H., Li, X., & Huang, B. (2022). First-principles study of two-dimensional anti-perovskite materials for thermoelectric applications. Physical Chemistry Chemical Physics, 24(2), 1223–1230. https://doi.org/10.1039/D1CP04659K

Zhou, W., Chen, J., & Zhang, L. (2022). First-principles design of anti-perovskite-based electrocatalysts. Catalysis Today, 397, 122–130. https://doi.org/10.1016/j.cattod.2022.03.017