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ADVANCEMENTS IN ANTIPEROVSKITE STRUCTURED SOLIDS: A COMPREHENSIVE REVIEW

Shrawan Kumar[1], Sushil Kumar Pathak[2], Deepak Sharma[3], Peeyush Kumar Kamlesh[4], Ajay Singh Verma[5]*
[1]Department of Physics, G.L.A. College, Medininagar (Daltonganj), Palamau, Nilamber Pitamber University, Jharkhand 822101, India
[2]Department of Physics, Chandrapur, Pombhurna, Chandrapur, Maharashtra-442918, India
[3]Department of Applied Sciences & Humanities, IIMT College of Engineering, Greater Noida, 201310, India
[4]Department of Physics, Poornima University, Jaipur – 303905, Rajasthan, India
[5]Department of Physics, Anand School of Engineering & Technology, Sharda University Agra, Keetham, Agra – 282007, India
**Corresponding author e-mail: ajay_phy@rediffmail.com*

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Antiperovskite-structured solids are attracting growing attention as a new class of multifunctional materials. Unlike conventional perovskites, their inverted cubic framework gives rise to unusual and highly tunable properties, from fast-ion conduction and giant magnetoresistance to superconductivity and negative thermal expansion. These different behaviors indicate promise for applications in areas such as solid-state batteries, energy-harvesting refrigeration, superconducting electronics, and thermal management. This review collates recent work in both experimental and theoretical research, emphasizing how a single simple cubic lattice can provide such a wide range of functionality. We argue that the structural versatility of antiperovskites is the common link between ionic transport, spin–lattice coupling, superconductivity, and thermal expansion. Recent advancements in Li- and Na-based solid electrolytes with high conductivity, giant magneto- and barocaloric responses, non-oxide superconductivity, and isotropic negative thermal expansion demonstrate that antiperovskites retain scientific importance and are increasingly viable competitors with the best of today's functional materials.

Keywords: *Antiperovskites; Magnetism; Superconductivity; Renewable energy; Battery materials*
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1. INTRODUCTION

Energy is the convertible commodity of technology, and modern society collapses quickly without it. This dependency has motivated researchers to seek renewable sources due to the gradual decline and environmental burden of non-renewables. Renewable sources (sun, wind, water) can be replenished naturally, while non-renewables such as coal and oil exist in finite amounts. Rising energy demand and CO_2 emissions have forced governments to invest in renewables, yet fossil fuels still account for over 80% of global use **[1]**. Although fossil fuels remain abundant in the short term, their continued use accelerates climate change. To mitigate shortages and climate change, solar cells and other renewables are being developed. Global warming is evident, with a ~0.6 °C rise in average temperature (Figure 1) **[2]**.

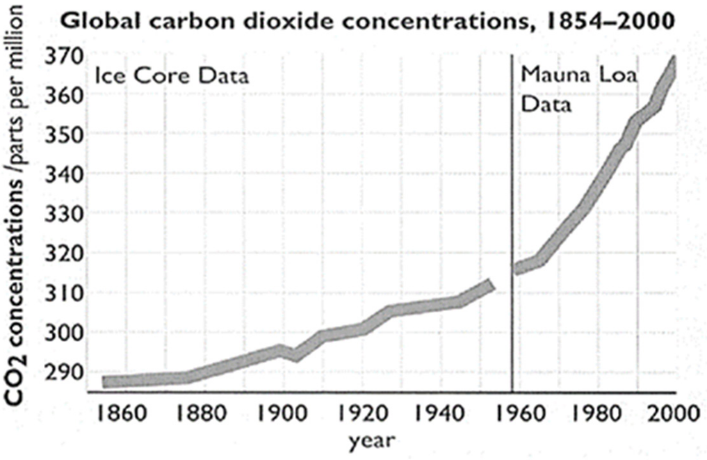

Figure 1. Atmospheric concentration of CO_2 gas **[2]**

Additionally, the improvement of the sun's energy utilization is necessary for an environmentally friendly and cleaner world. Devices like space photovoltaic cell technology were also mentioned; this subject is continuing to advance. Perovskite is one of the most affordable and abundant materials for environmental sustainability solutions **[3]**. Antiperovskites (ANX_3) are structural inverses of the conventional perovskite (ABX_3) framework. In this structure, the

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X-site cations (e.g., Ca, Sr, Ba, Mg) occupy the face-centered positions of the cube, while the A-site anion (commonly N, C, or O) resides at the cube corners. The B-site element (e.g., Bi, Sb, As) sits at the octahedral center, surrounded by six X cations.

The electronic band gap is a key parameter governing the physical behavior of antiperovskites. It determines whether a compound is metallic, semiconducting, or insulating, and thereby influences its potential applications. For example, Li_3OCl and related antiperovskites exhibit wide band gaps (>5 eV), making them good solid electrolytes but electronically insulating. In contrast, Mn_3AN (A = Ga, Zn, Cu) antiperovskites are metallic with negligible gaps, enabling strong spin-lattice coupling and giant magnetoresistance. Tunable narrow band gaps have also been predicted in Sb- and Bi-based antiperovskites (e.g., Ca_3BiN, Ca_3SbN), making them promising for thermoelectrics and optoelectronic devices. The ability to shift from insulating to metallic behavior by chemical substitution, pressure, or doping underscores the central role of band gap engineering in this materials family.

As compared to classical perovskites, the ionic reversal leads to unusual bonding, tunable band structures, and multifunctional physical properties (Figure 3). Due to their reduced band gap and figure of merit, the antiperovskite compounds are potential candidates in thermoelectric devices that have the potential of recycling waste heat to reduce greenhouse gas emissions. When choosing semiconducting components for thermoelectric generators, care must be taken. Since the band gap affects thermoelectric properties greatly, accurate band gap computation is required. As a result, narrow band gap semiconductor alkaline earth-based antiperovskites are potential prospects for optoelectronics and thermoelectric purposes **[4]**. Perovskites come in a variety of forms, including double perovskites $(CH_3NH_3)_2AgInBr_6$ **[5]**. Double antiperovskites X_6SOA_2 (X= Na, K and A= Cl, Br, I) **[6]**, simple perovskites $EASnCl_3$ **[7]** and $RbPbBr_{3-x}I_x$ (x= 0 to 3) **[8]**, anti-perovskites ANX_3 (A= P, As, Sb, Bi; X= Sr, Ca, Mg) **[9]** and $AsPX_3$ (X= Mg, Ca, and Sr) **[10]**.

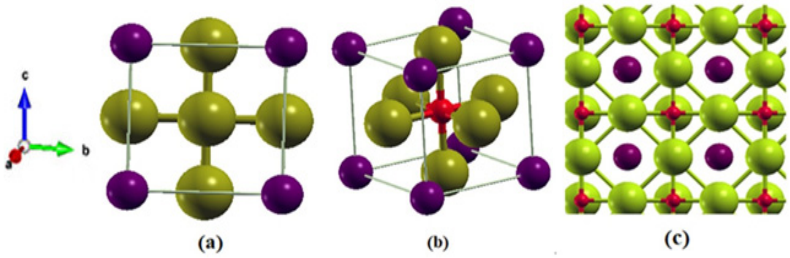

Figure 2. Crystal structure of a cubic antiperovskite ANX_3. Here, X (green atom) cations occupy the face-centered positions, the A (purple atom) anion resides at the cube corners, and the B-site element (e.g., N, P, AS, Sb, Bi – red atom) sits at the octahedral center

Antiperovskites have received plenty of research focused on due to their usefulness in various industrial applications **[11]**. Due to their favorable thermoelectric (TE) properties, antiperovskites have a significant potential to alleviate the energy crisis **[12]**. To achieve high efficiency, researchers are looking for appropriate materials for thermoelectric generators. Good thermoelectric materials often feature band gaps that are also broad enough to have an enormous Seebeck value and narrow enough to have a suitable conductivity for electrical use **[13]**. Solids with super ionic conductivity are regarded to be preferable to organic liquid electrolytes in batteries; hence, lithium-based antiperovskites can be employed as solid electrolytes **[14]**. These materials also have remarkable physical properties, such as magnetostriction **[15]**, virtually zero temperature coefficients of resistivity **[16]**, and gigantic magnetoresistance (GMR) **[17]**.

Beyond conventional antiperovskites, new classes of antiperovskite-derived or 'reverse perovskite' structures have been recently reported. Tang et al. **[18]** developed a family of antiperovskite derivatives in which the A-site anion of the cubic framework is split into three edge-centered positions while preserving the corner-sharing octahedral network. Screening several compounds, they identified nine promising candidates such as Ba_3BiI_3, Ba_3SbI_3, and Ba_3BiBr_3, achieving predicted photovoltaic efficiencies above 24.5%, comparable to classical $CH_3NH_3PbI_3$ solar cells. Complementary to this, Hu et al. **[19]** studied X_3AsCl_3 (X = Mg, Ca, Sr, Ba) under hydrostatic pressure, showing that band gaps and lattice constants evolve linearly with pressure, and that Ba_3AsCl_3 can reach conversion efficiencies above 30% under moderate compression. These studies illustrate how derivative antiperovskite structures behave to atomic rearrangements or an applied external stress thereby widening the design space for optoelectronic applications.

Antiperovskites are especially well-suited for industrial applications related to biosensors, magnetic field sensors, biosensors, micro-electromechanical systems, giant magnetoresistance, and other gadgets that read data from hard discs given these properties. Likewise, antiperovskites are ideal building blocks in any climate because of their zero-temperature coefficient of resistivity. Antiperovskites also display excellent mechanical properties **[20-22]**, and could be of use in the automotive and space industries, which both require materials that are lightweight and also mechanically strong. Additionally, antiperovskites display superconductivity. $MgCNi_3$ is particularly interesting because it is one of the few (yet) known non-oxide/perovskite-derived superconductors with a relatively high Tc of ~8 K **[23]**. Additionally, its electronic structure comprises mainly Ni 3d states near the Fermi level which makes this compound a prototype for investigating unconventional superconductivity in antiperovskites. The discovery of $MgCNi_3$ lead to increased investigation into other related compounds including ZnNNi3 and $CdCNi_3$ **[24]**, emphasizing the structural tunability of this family. The goal of this review paper is to evaluate, the theoretical studies focused on the properties of antiperovskite-type materials.

2. PREVIOUS STUDIES AND RESULTS

In first-principles studies of antiperovskites, the choice of exchange–correlation functional strongly influences the predicted electronic structure. The Local Density Approximation (LDA) often underestimates lattice constants and band gaps due to its assumption of uniform electron density. The Generalized Gradient Approximation (GGA) improves on this by incorporating density gradients, yielding more accurate structural parameters but still typically underestimating band gaps. To address this, the Engel–Vosko GGA (EV-GGA) modifies the exchange potential to give better agreement with experimental band gaps. Moakafi et al. **[25]** have investigated the electronic, optical, and elastic characteristics of the cubic antiperovskite $SbNCa_3$ and $BiNCa_3$ and found their band gaps to be 0.65 and 0.36 eV, respectively. The authors used LDA, GGA, and EV-GGA potentials to examine the electronic characteristics of these compounds. Despite the fact that the investigators used EV-GGA to attain bigger band gaps, the valence bands of these materials pass through the Fermi level and demonstrate metallic behavior, which is contrary to the data from experiments. Bilal et al. **[26]** presented an analysis of the previously discussed systems to examine the impact of different computational schemes for predicting the electronic structures of $BiNCa_3$ and $SbNCa_3$ antiperovskites. The authors found that LDA and GGA underestimated the band gap, while the mBJ potential gave band gap values of 1.09 and 1.1 eV for $BiNCa_3$ and $SbNCa_3$, respectively, which were much closer to the experimental values. The study demonstrates the sensitivity of antiperovskite band structures to the choice of functional and shows that these systems are compact gap semiconducting materials that can find relevance in thermoelectric and optoelectronic applications.

We see that the reported physical properties of antiperovskites depend strongly on the chosen method. For instance, $SbNCa_3$ and $BiNCa_3$ show band gaps of only 0.36–0.65 eV when studied using LDA and GGA, while EV-GGA increases these values slightly but still underestimates them. In contrast, the modified Becke–Johnson (mBJ) potential produces more reliable results, giving direct band gaps close to 1.0–1.1 eV, in much better agreement with experiments. In several cases, GGA predicts metallic behavior, whereas mBJ or hybrid functionals reveal semiconducting nature. These variations highlight the importance of method selection when evaluating the electronic structure of antiperovskites, as also discussed in recent literature **[27]**.

The chemical bonds and electronic band structure in the compounds $SbNMg_3$ and $AsNMg_3$ were investigated by Shein and Ivanovskii using GGA **[28]**. Small band gap and both compounds display ionic semiconducting properties. $AsNMg_3$ has a direct band gap, in contrast to $SbNMg_3$, which has an indirect band gap. The GGA technique was used to examine these materials' Electronic and Optical properties. These compounds' optical properties have never been investigated previously. The author of this study confirmed the earlier findings and showed that $AsNMg_3$ has a direct band gap and $SbNMg_3$ has an indirect band gap, both compounds having low band gaps **[29]**. This writer asserts that the computed optical spectrum positions can be lower than the values obtained from experiments because DFT typically underestimates band gaps.

The dielectric function's hypothetical component, as presented in their work, supports the materials' semiconducting properties. Using the pseudo-potential plane waves approach within the GGA, Bouhemadou and colleagues **[30]** studied the structural, optical, elastic, and electronic properties of $AsNMg_3$ and $SbNMg_3$ compounds. $AsNMg_3$ has a fundamental direct band gap that in the beginning boosts up to 4 GPa, then gradually reduces as a function of pressure, whereas simultaneously maintaining its direct band gap nature throughout the whole pressure range executed, in opposition to $SbNMg_3$, which transitions from a fundamental indirect band gap to a fundamental direct band gap as pressure attains 6.85 GPa. Since these were the initial theoretical investigations on the elastic characteristics of these compounds, Belaroussi et al. **[31]** have examined the Elastic and Structural characteristics of $SbNMg_3$ theoretically and contrasted their research with this study. Amara et al. **[32]** have studied the structural, elastic, and electronic characteristics of $BiNMg_3$, $SbNMg_3$, $AsNMg_3$, and $PNMg_3$ via the full-potential augmented plane waves plus local orbital within the GGA to improve results by addressing the exchange and correlation effects by the Tran-Blaha mBJ potential for the charge density, density of states, and band structure. These scientists reported on the magnetic, electrical, optical, and bonding characteristics of these sorts of compounds. These materials are semiconductors, according to studies on electrical resistivity. By using the diffuse reflectivity method, the optical band gaps for $BiNSr_3$ and $SbNSr_3$ are 0.89 eV and 1.15 eV, respectively.

Haddadi et al. **[33]** have examined the electronic, elastic, and structural characteristics of $ANSr_3$ (A = Bi, Sb, and As) compounds in 2009 using the plane waves pseudo potential total energy approach in the CASTEP code. The optical, electronic, and elastic characteristics of $ANSr_3$ (A = Bi, Sb, and As) antiperovskite compounds were studied by Hichour et al. **[34]** in 2010. The investigators used the EVGGA potential to increase the band gaps of these compounds, yielding values of 0.36, 0.55, and 0.84eV for $BiNSr_3$, $SbNSr_3$, and $AsNSr_3$, correspondingly. All compounds' band gap values decrease with increasing pressure. The charge density charts show that these materials have a combination of covalent and ionic bonds. Their work's depiction of the imaginary component of the dielectric function also illustrates how $SbNSr_3$ behaves semiconducting material.

What makes antiperovskites especially intriguing is that their diverse applications, from batteries and ionic conductors to magnetoresistive devices, superconductors, and thermal expansion compensators, all originate from the same structural motif. The cubic lattice allows a high degree of tunability, enabling properties as distinct as superconductivity and solid-state ionic conduction to coexist in the same materials family. This unifying theme forms the focus of the present review, which not only summarizes individual applications but also highlights the common structural and electronic factors connecting them.

3. APPLICATIONS

The diverse applications of antiperovskites arise from a few unifying material characteristics. Their cubic framework, with interchangeable cation/anion positions, provides structural flexibility. Strong spin–lattice–charge coupling enables multifunctional responses, such as magnetoresistance, negative thermal expansion, and magnetocaloric effects. At the same time, tunable band gaps and ionic transport pathways make them attractive for electrochemical and superconducting applications. The following subsections discuss batteries, magneto-electronics, superconductivity, and thermal expansion versatility of the antiperovskite lattice.

3.1 Antiperovskite as Modern Battery Materials:

In particular, lightweight Lithium or sodium ion batteries with an elevated energy density have attracted a lot of research interest due to the urgent energy needs of the modern industrialized world **[35]**. The primary strategy for attaining this objective is the development of improved electrode materials with excellent capacity and a wide voltage window. Both their exceptionally large theoretical considerations, specific capacity, as well as their extremely low electrochemical potential, set Lithium metal anode materials apart from other materials. Therefore, it is envisaged that a battery or cell that has a Lithium metal anode will result in long-lasting, lightweight power to electronic devices. The conventional electrolyte's flammability and ease of leakage must first be eliminated in order to realize this vision. A secure, solid-state electrolyte has therefore been recommended as an alternative. Particularly enticing aspect of it is that, since it achieves an ultrathin dimension, it will not just resolve risks brought on by inflammability but additionally improve energy density. Batteries endorsed by solid-state electrolytes have been on the verge of becoming a common commercial technology **[36]**. SSEs still have to overcome significant obstacles, such as ionic conductivity, stability, Li dendrite growth, surface contact, etc. **[37]**. In this section, we primarily discuss the ionic conductivity of the antiperovskite group. Few among these SSEs can match an ionic liquid's room-temperature ionic conductivity. However, without material engineering optimization, few of these electrolytes can achieve this high level. The literature has focused considerable amounts of interest on several groups of inorganic solid-state electrolytes, such as Lithium halides, Garnets, Lithium nitrides **[38-41]**. The intrinsic high ionic conductivity of Li^+/Na^+ antiperovskite is generally very promising, and through the use of chemical doping and structural design, it could improve even more. Their high stability and minimal surface resistance as they come into touch with Lithium metal anodes are two further advantages for commercial use. They must also address their elevated susceptibility to moisture and a small potential window, which are two problems. There must be more research towards cheap, massive industrial fabrication. Figure 3 illustrates lithium-ion conduction in Li_3OCl-type antiperovskites. Recent studies have reported room-temperature conductivities as high as ~10^{-3} S/cm in doped $Li_{3-2x}Sr_xOCl$ antiperovskites, making them competitive with NASICON and garnet-type electrolytes **[14, 42]**. Na-based analogues such as Na_3OCl have also achieved ~10^{-4} S/cm, offering a potential pathway for cost-effective sodium-ion batteries **[43]**. These values (Table 1) demonstrate that antiperovskite solid electrolytes are approaching the performance of state-of-the-art oxide and sulfide systems, while offering superior mechanical processability.

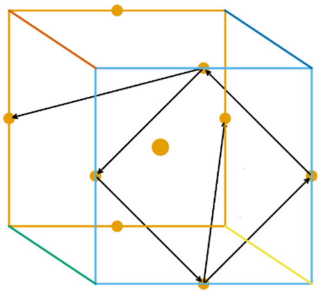

Figure 3: Schematic of Li^+ migration pathways in Li_3OCl-type antiperovskite solid electrolytes, highlighting face-centered and edge-sharing conduction channels **[13, 14]**

Table 1: Ionic Conductivity of Antiperovskite Solid Electrolytes

Compound	Temperature (°C)	Ionic Conductivity (S/cm)	Remarks
Li_3OCl **[13]**	25 °C	~10^{-5}	Good solid electrolyte; moisture sensitive
Li_3OBr **[44]**	25 °C	~10^{-6}	Similar to Li_3OCl, lower conductivity
Na_3OCl **[43]**	25 °C	~10^{-4}	Promising Na-based analogue
$Li_{3-2x}Sr_xOCl$ (doped) **[42]**	25 °C	~10^{-3}	Enhanced by Sr doping (defect engineering)

These ionic conduction studies are important because they show how antiperovskites can work as solid electrolytes. But other types of antiperovskites show metallic behavior, which opens the door to magnetic and magnetoresistive applications, discussed in the next section.

3.2 Antiperovskite as electronics and Magnetoresistive devices

ABO_3 perovskites are widely used in contemporary electronics, including storage, magneto-caloric, and magnetoresistive devices **[45-49]**. Magnetic antiperovskites $M_3M'X$ (M = Mn, Fe, etc.; M′ = Ga, Al, Zn, In, Sn, etc.; X =

N, C) were additionally thoroughly explored as an innovative family of potential magnetic compounds. Mn-based magnetic antiperovskites are perhaps the most intriguing among these compounds because of their newly identified Giant magnetoresistance (GMR) **[21]**, massive Magneto-caloric effect (MCE) **[50]**, and giant Magnetostriction **[51]**. Additionally, the metallic nature of these $Mn_3M'X$ antiperovskites suggests that they have strong Mechanical, Electrical, and Thermal conductivities **[26]**. Three magnetic changes occur as the test sample of giant magnetoresistance compound Mn_3GaC cools: a paramagnetic to ferromagnetic transition at 246 K, an FM intermediate magnetic phase transition at 160 K, as well as an intermediate phase to antiferromagnetic transition at 158 K. While the hybridization of the Mn-X p-d orbitals widens the conduction band over the Fermi level and produces a significantly high conductivity, the Mn 3d orbitals in $Mn_3M'X$ antiperovskites offer to the DOS at the Fermi level. Both magnetic exchange interactions & conduction behavior include these Mn 3d electrons. As a result, the magnetic coupling interactions between these third-dimensional electrons and the Mn-X-Mn atoms will be competitive.

Due to the tight couplings between the various degrees of freedom & the conflicting magnetic interactions, $Mn_3M'A$ is highly responsive to every minor alteration in the external magnetic field, chemical composition, temperature & pressure **[52]**. From 135 to 165 K, Mn_3GaC (Figure 4) displays GMR curves that resemble plateaus, with a maximum MR of 50% at 5 T **[53]**.

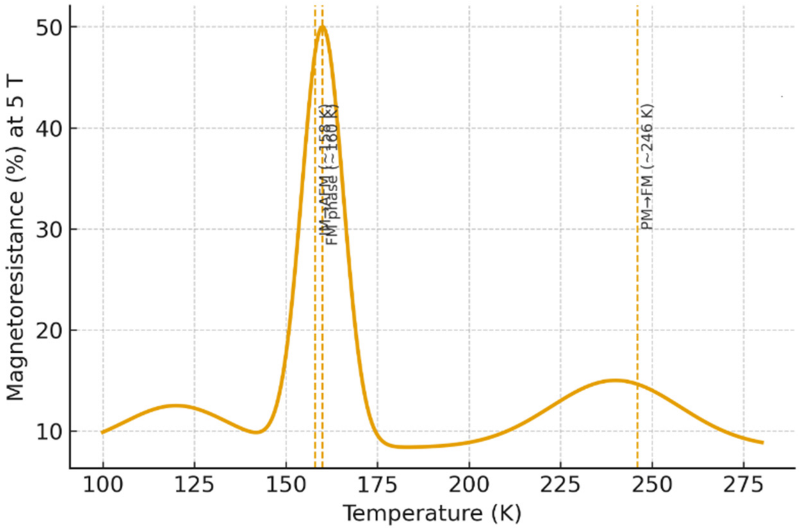

Figure 4. Temperature-dependent magnetoresistance in Mn_3GaC, showing strong MR effects linked to successive phase transitions [53]

The giant magnetoresistance is connected to the field-induced ferromagnetic, antiferromagnetic, or intermediate magnetic phase transition, where there is a strong correlation between the lattice, spin, and charge. The possibility of a giant magnetoresistance with a larger temperature range exists if an external magnetic field can efficiently reduce the antiferromagnetic ground state. The antiperovskite $Mn_3M'A$ compounds offer benefits in the role of refrigerant substance because of their adjustable broad working temperature, as well as their availability, affordable and harmless raw materials, stable behavior, ease of manufacturing and design, strong conductivity, and excellent mechanical characteristics. These materials present an intriguing alternative material platform to investigate novel big Magneto-caloric effect compounds at room temperature. This close relation between spin, lattice, and electronic states also creates conditions that are favorable for superconductivity. Therefore, in the following section, we describe the discovery of superconductivity in $MgCNi_3$ and other antiperovskites.

3.3 Evolution of superconductivity in Antiperovskites

Ni_3MgC, which was found in 2001, was the first antiperovskite to exhibit superconductivity **[27]**. When examining the superconducting mechanism, the cubic Ni_3MgC serves as a special illustration of an s-wave Bardeen–Cooper–Schrieffer type-2 superconductor similar to that of the noncuprate superconductor $Ba_{12x}K_xBiO_3$. As a result, in-depth experimental and theoretical research was done on superconductors related to Ni_3MgC, including Ni_3CuN, Ni_3ZnN, Cr_3GaN, and K_2NiF_4-type layered A_2CNi_4 (A = Al, Ga, Sn) **[54, 55]**. The crystal structure's high Ni content suggests that magnetic interactions may be crucial to the development of superconductivity. T_c experimentally decreased whenever the nickel site was enriched via additional transition metals, such as Mn, Fe, Co, and Cu, but might be marginally enhanced by raising the value of x in Ni_3MgC_x. The family of ternary platinum phosphides Pt_3AP, where A = Ca, Sr, La **[56]**, is another intriguing example of an antiperovskite-based structure closely connected to the heavy fermion superconductor Pt_3CeSi. The so-called antipost-perovskites V_3PnN_x (Pn = P, As) have superconductivity **[57]**. In comparison to the post-perovskite structure, the cation and anion positions are interchanged. When these compounds crystallize, they give rise to the filled Re_3B structure. The antipost-perovskites V_3PnN_x have NV_6 octahedral layers and Pn layers alternately stacked, resulting in a quasi-2D electronic state. The first antiperovskite oxide that is superconducting (T_c = 5 K) is $Sr_{3x}SnO$ **[58]**. Table 2 summarizes superconducting transition temperatures across representative compounds.

Table 2. Superconducting Transition Temperatures (T_c) in Antiperovskites

Compound	Structure Type	T_c (K)	Notes/Reference
$MgCNi_3$	Cubic antiperovskite	~8	First discovered non-oxide antiperovskite superconductor **[23]**
$ZnNNi_3$	Cubic antiperovskite	~3	Ni-rich, lower Tc compared to $MgCNi_3$
$CdCNi_3$	Cubic antiperovskite	~3	Similar to $ZnNNi_3$, sensitive to Ni substitution
$Sr_{3-x}SnO$	Antiperovskite oxide	~5	Dirac metal-based superconductor **[58]**
Pt_3SrP (family)	Antiperovskite phosphide	~8.4	Strong coupling superconductor **[56]**

All of the findings above encourage additional research into novel superconductors with extended antiperovskite structures. Improving T_c and knowing more about the fundamental relationship between the electronic and structure of crystals will be the top targets for researchers. It is observed that, besides electronic effects like superconductivity, antiperovskites also show unusual structural effects such as negative thermal expansion, which is presented in the next section.

3.4 Antiperovskites with Variable Thermal Expansion Behavior:

The complex interplay between the lattice, electrons, and phonons of solids leads to the intriguing & uncommon thermal expansion behavior known as negative thermal expansion **[59]**. Since Sleight and colleagues discovered isotropic NTE in ZrW_2O_8 in 1996, the emergence of various oxides as well as fluorides due to their ReO_3-like structure and negative thermal expansion behavior has since made up for the positive thermal expansion of other materials. These materials have been used as separate components or in expansion-controlled composites. In addition to ZrW_2O_8, a number of open-framework material systems, including the sodium zirconate phosphate family **[60]**. Fluorides formed by ScF_3 and $M_{1x}[M_2(CN)_6]$, where M_1 is Ag, Fe, and M_2 is Fe, Co **[61]**, display negative thermal expansion behavior. In such materials, it is thought that the corner-sharing polyhedra's correlated motion causes low-frequency vibrations that give rise to the negative thermal expansion. When compared to ceramic negative thermal expansion materials, a characteristic metal-based negative thermal expansion family exhibiting high electric & thermal conductivity, isotropic negative thermal expansion, along with excellent mechanical characteristics, is the manganese antiperovskites Mn_3BA, where B = Zn, Cu, Ni, Ge, Sn, and A = N, C **[62]**. In conclusion, negative thermal expansion materials have advanced significantly over the past 20 years, and antiperovskites have been convincingly established as distinct negative thermal expansion family members. One can anticipate that additional structural design initiatives, theoretical predictions, and particularly magneto-structural coupling will modulate the negative thermal expansion in antiperovskite materials.

3.5 Other New emerging properties of Antiperovskites

Other recently discovered characteristics of antiperovskites include giant Magnetostriction in some manganese nitride antiperovskites and ferromagnetic shape memory effects **[63]**. Based on first-principles calculations, a fresh class of antiperovskite-structured three-dimensional topological insulators was recently developed **[64]**. The antiperovskite $Mn_3Ni_{1x}Cu_xN$ showed a temperature coefficient of resistivity that was almost zero **[65]**. The AE_3NBi group (where AE is Ca, Sr, and Ba) provides a foundation for straightforward integration with electronic gadgets due to its chemical inertness as well as a compatible lattice to significant semiconductors.

Additionally, recently created organic-inorganic hybrid antiperovskite-type materials that can function as new ferroelectrics enrich the antiperovskite family and broaden the antiperovskite family's range of applications. When exposed to external fields like pressure and temperature, antiperovskites also exhibit intriguing properties. It has frequently been claimed that $Mn_3Ga_{0.95}N_{0.94}$ exhibits a significant "Baromagnetic effect" **[66]**. Piezomagnetism was studied both through experimentation in Mn_3NiN as well as in several types of magnetically frustrated Mn-based antiperovskite nitrides. Boldrin et al. **[67]** studied the multisite exchange-enhanced barocaloric response in Mn_3NiN through the Néel transition temperature.

3.6 Phase Change Phenomena in Antiperovskites

Phase transitions play a central role in defining the multifunctional behavior of antiperovskite solids. Several Mn-based antiperovskites, such as Mn_3GaC and Mn_3SnC, exhibit a sequence of temperature-dependent magnetic phase transitions including paramagnetic → ferromagnetic → antiferromagnetic states. Volume changes often accompany these transitions and result in giant magnetoresistance (GMR), magnetocaloric effect (MCE), and large Magnetostriction. For example, Mn_3GaC shows a ferromagnetic to antiferromagnetic transition near 160 K, directly linked to its observed GMR of ~50% at 5 T. Similarly, pressure-induced phase transitions have been observed in $SbNMg_3$ and $AsNMg_3$, where the indirect band gap changes into a direct one above 6–7 GPa, significantly altering their optical response.

Another important area is superconductivity in $MgCNi_3$ and related systems, where the superconducting phase emerges below ~8 K, indicating a structural/electronic phase change in relation to the density of states at the Fermi level. Thermal expansion anomalies are also phase-transition driven: manganese antiperovskites (Mn_3BA; B = Zn, Cu, Ni, Ge, Sn; A = N, C) display negative thermal expansion due to strong magneto-structural coupling near magnetic ordering temperatures. Recent reports also highlight barocaloric and piezomagnetic effects in Mn_3NiN and $Mn_3Ga_{0.95}N_{0.94}$, where applied pressure drives phase changes with promising caloric responses.

A collection of evidence suggests that antiperovskites represent extremely phase-tunable materials where structural, magnetic, or electronic transitions can be tuned by temperature, pressure, or chemical doping to develop interesting new functionalities. This strong coupling between phase change and physical properties, in addition to a promise of relatively low-cost synthesis, makes antiperovskites highly exciting for potential next-generation applications in solid-state cooling, sensing, and energy devices.

4. SUMMARY AND CONCLUSION

Antiperovskites are fascinating because a simple reversal of ionic positions unlocks a whole range of properties, from fast-ion conduction to superconductivity, magnetoresistance, and negative thermal expansion. This versatility makes them one of the few material families that can genuinely impact several technologies at once. The field, however, is still young. Many predicted compounds have not been synthesized, and even the known ones face hurdles such as stability and phase purity. Theory has advanced quickly, but experiments lag; closing this gap is essential for real applications. From the literature, some points are clear: Li- and Na-based antiperovskites are improving as solid electrolytes, Mn-based systems show striking magnetoresistive and caloric effects but need better control of transitions, Ni-based compounds are rare non-oxide superconductors, and doped Mn nitrides demonstrate useful negative thermal expansion. These examples confirm the structural flexibility of the antiperovskite lattice, even if progress is uneven across applications. Looking ahead, progress will depend on smarter synthesis routes, computational and machine learning tools to guide discovery, interface engineering for batteries, and careful tuning of magnetic and structural properties. If these challenges are met, antiperovskites could move from being mainly of academic interest to becoming a versatile platform with real impact on energy, electronics, and thermal technologies.

Conflict of Interest: This manuscript does not include a conflict of interest.

ORCID

Deepak Sharma, https://orcid.org/0000-0001-9163-9050; **Peeyush Kumar Kamlesh,** https://orcid.org/0000-0001-7361-3519
Ajay Singh Verma, https://orcid.org/0000-0001-8223-7658

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ДОСЯГНЕННЯ В ВИВЧЕННІ ТВЕРДИХ ТІЛ ІЗ СТРУКТУРОЮ АНТИПЕРІВСКІТУ: КОМПЛЕКСНИЙ ОГЛЯД

Шраван Кумар[1], Сушил Кумар Патхак[2], Діпак Шарма[3], Піюш Кумар Камлеш[4],
Аджай Сінгх Верма[5]
[1]Кафедра фізики, G.L.A. Коледж, Медінінагар (Далтонгандж), Паламау, Університет Ніламбер Пітамбер, Джаркханд 822101, Індія
[2]Кафедра фізики, Чандрапур, Помбхурна, Чандрапур, Махараштра-442918, Індія
[3]Кафедра прикладних та гуманітарних наук, інженерний коледж IIMT, Велика Нойда, 201310, Індія
[4]Кафедра фізики, Університет Пурніма, Джайпур – 303905, Раджастхан, Індія
[5]Кафедра фізики, школа інженерії та технологій Ананда, Університет Шарда, Агра, Кітхам, Агра – 282007, Індія

Тверді тіла зі структурою антиперовскіту привертають все більшу увагу як новий клас функціональних матеріалів. На відміну від звичайних перовскітів, їх перевернута кубічна структура обумовлює незвичайні властивості, що легко налаштовуються: від провідності швидких іонів і гігантського магнітоопору до надпровідності та негативного теплового розширення. Ці різні характеристики вказують на перспективність їх застосування в таких областях, як твердотільні акумулятори, енергозберігаюче охолодження, надпровідна електроніка та терморегулювання. У цьому огляді узагальнені недавні роботи, як експериментальні, і теоретичні, і підкреслюється, як прості кубічні грати може забезпечити настільки широкий спектр функціональних можливостей. Ми стверджуємо, що структурна універсальність антиперовскітів є сполучною ланкою між іонним транспортом, спін-решітковим зв'язком, надпровідністю та тепловим розширенням. Нещодавні досягнення в галузі твердих електролітів на основі Li і Na з високою провідністю, гігантськими магніто- і барокалоричними відгуками, неоксидною надпровідністю та ізотропним негативним тепловим розширенням демонструють, що антиперовскіти зберігають наукову значущість і стають все більш життєздатними конкурентами кращим матеріалом.

Ключові слова: *антиперовскіти; магнетизм; надпровідність; відновлювана енергія; матеріали для акумуляторів*