

Review Article

Electronic Properties of Antiperovskite Materials from State-of-the-Art Density Functional Theory

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We present a review on the research developments on the theoretical electronic properties of the antiperovskite materials. The antiperovskite materials have perovskite type structure with the positions of cations and anions interchanged. The electronic structures are used to explain different physical properties of materials; therefore it is crucial to understand band structures and densities of states of materials for their effective use in technology. The theoretical results of the electronic structure of antiperovskites were discussed and compared with the available experimental results to measure the accuracy of the research done so far on these materials. The important physical properties of these compounds like magnetic properties and superconductivity are also highlighted. Nevertheless the thermoelectric properties of these materials are still unexplored except for a few reports which suggest that antiperovskite materials may be potential candidates for thermoelectric generators.

1. Introduction

Many materials adopt perovskite type structure with formula ABX_3 , where A and B are cations while X is anion. The X atoms make twelfold symmetry being at the center of the edges of the unit cell, A atom at the center and B atoms at the corners of the unit cell. Generally, X atoms make octahedral coordination being at the face centers of the unit cell, A atoms at the corners and B atom at the center [1]. The first perovskite material $CaTiO_3$ was discovered by Gustav Rose [2] and he named it after a Russian mineralogist Lev Perovski. Perovskites have different types like simple perovskites ($KMnF_3$ [3] and $SrTiO_3$ [4]), antiperovskites ($SbNCa_3$ and $BiNCa_3$ [1]), inverse perovskites ($(Eu_3O)In$ and $(Eu_3O)Sn$ [5]), double perovskites ($SrLaVMoO_6$ [6]), and double antiperovskites ($Na_6FeCl(SO_4)_2$ [7]) depending on composition and chemistry of the constituent elements of the material. Different structures are found in all these types like cubic [8], orthorhombic [9], tetragonal [10], rhombohedral [11], and hexagonal [12].

Antiperovskite materials are inorganic compounds, having perovskite type structure with the positions of anions

and cations interchanged [13]. Figure 1 presents the simplest cubic antiperovskites structure, with space group $Pm\bar{3}m$ (221) [14]. For having utility in different industrial applications, antiperovskites have attracted significant attention of the researchers in the past decade [15]. Wide range of band gaps in these materials is one of the important reasons for their industrial utility [16, 17]. Antiperovskites have immense potential to solve energy crisis as these materials have good thermoelectric (TE) properties [18]. In thermoelectrics, waste heat is directly converted to electrical energy. Researchers seek suitable materials for thermoelectric generators to achieve high efficiency. Good thermoelectric materials typically have band gaps large enough to have a large Seebeck coefficient, but small enough to have a sufficiently high electrical conductivity [19].

The family of antiperovskite materials has all kind of compounds including metals, semiconductors, insulators, and superconductors which make them applicable in various technologies. In batteries, solids having super ionic conductance are considered better than the organic liquid electrolytes [20] and hence lithium-based antiperovskites can

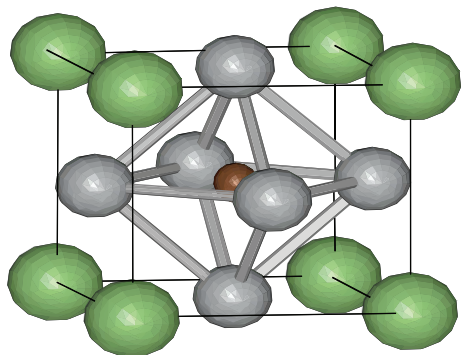


FIGURE 1: Unit cell of cubic antiperovskite with space group $Pm\bar{3}m$ (221), where green atoms at corner and brown atom at body center are anions while face centered grey atoms are cations. Figure reproduced with permission from Sieberer et al. [14].

be used as solid electrolytes in batteries [21]. Furthermore, these materials have interesting physical properties like giant magnetoresistance (GMR) [22], nearly zero temperature coefficients of resistivity [23], and magnetostriction [24]. These properties make antiperovskites very useful in industrial applications as GMR, used in magnetic field sensors, which are used to read data in hard disk drives, biosensors, microelectromechanical systems (MEMS), and other devices. Similarly, zero temperature coefficient of resistivity makes antiperovskites suitable materials in all weathers. Along with these applications, antiperovskites also show excellent mechanical properties [25–27], which make their possible utility in automobile and space technology, as we need materials with lightweight on one hand and large mechanical strength on the other hand in this industry. Superconductivity is also found in antiperovskites. In 2001, first antiperovskite material $MgCNi_3$ was reported to have superconductivity below 8 K temperature [28]. This finding opened new avenues in research, regarding antiperovskite family. Literature reveals that other materials like $CdCNi_3$ and $ZnNNi_3$ also show superconductivity [29]. Furthermore, magnetism is one of the most important properties found in antiperovskites with diverse magnetic structures and different transition temperatures [25, 30]. Due to strong magnetic effects, these materials are very attractive for applications in memory devices and sensors and appropriate for spintronics. Moreover, the presence of small band gaps in many antiperovskites makes them good candidates for optical devices. The available literature on these compounds shows that researchers around the globe are taking keen interest in the optical properties of antiperovskites [17, 31, 32].

Different physical properties like thermoelectric, optical, magnetic, and mechanical properties are strongly dependent upon the electronic properties of a material. Small variation in the electronic structure causes large changes in these properties. Therefore, it is very important to have a deep understanding of band structures and density of states of materials for their effective use in optical, memory storage, and thermoelectric devices. The aim of this review article is to present a comprehensive discussion on the theoretical studies of the electronic properties of antiperovskite type materials.

This work presents deep insight into the development of research on the subject and we hope that this review will benefit the researchers working in this field.

2. Group II-A Based Antiperovskites Materials

Group II-A elements are very important due to their diverse applications in electronics [33], mechanics [34], and military [35]. These elements have two electrons in their outermost shell and easily lose them to make ionic bonds in general. There are many antiperovskite materials which have a group II-A element at face center of the unit cell making octahedral coordination. Chern et al. synthesized calcium based antiperovskite material $BiNCa_3$, by mixing and pressing powders of Ca_3N_2 and Bi into a pellet and afterwards heating the pellet at 1000°C in flowing, dry N_2 gas [1]. The authors substituted Bi with other trivalent elements, P, As, Sb, Ge, Sn, and Pb, and found the same result as expected. The authors report that all these materials are found in cubic structure except $PNCa_3$ and $AsNCa_3$ which have distorted orthorhombic structure due to small P^{-3} and As^{-3} atomic size. Resistivity measurements show that $PbNCa_3$, $SnNCa_3$, and $GeNCa_3$ materials are metallic in nature, $BiNCa_3$ and $SbNCa_3$ are semiconductors with small band gaps, while $AsNCa_3$ and $PNCa_3$ show insulating behavior with structural phase transitions.

Consequently, different researchers theoretically investigated the electronic properties like band structures and densities of states of these materials for the deep understanding of their relevant behavior in other physical properties. Papaconstantopoulos and Pickett [36] studied the electronic properties of $BiNCa_3$ and $PbNCa_3$ using local density approximation (LDA) which generally underestimates band gaps. The authors show that $BiNCa_3$ is a narrow band gap semiconductor and $PbNCa_3$ is a metallic material confirming the experimental results as presented in Figures 2(a) and 2(b). Pb has one electron less than Bi and $BiNCa_3$ has a very small band gap; therefore $PbNCa_3$ was expected to be a metal. The valences of the constituent elements in $BiNCa_3$ give an ionic picture of the compound; however, authors argue that at the same time strong covalent mixing is present due to p-states of Bi and N.

Vansant et al. [37] studied pressure dependent structural and electronic properties of $PNCa_3$, $AsNCa_3$, and $BiNCa_3$ using LDA. The atomic positions of the orthorhombic $AsNCa_3$ are presented in Table 1, reproduced from [38]. Vansant et al. verified that at ambient temperature and pressures $AsNCa_3$ and $PNCa_3$ adopt orthorhombic structure with $Pbnm$ space group while $BiNCa_3$ is a simple cube with $Pm\bar{3}m$ space group. It is also worth noting that the orthorhombic $AsNCa_3$ structure turns out to be more stable than the cubic SC5 structure with increasing pressure whereas band gap decreases with pressure for this material. At 59 GPa pressure, $AsNCa_3$ shows a phase transition to cubic SC15 with 15 atoms per unit cell.

Moakafi et al. studied elastic, electronic, and optical properties of cubic antiperovskites $SbNCa_3$ and $BiNCa_3$ [31]. The authors used three different potentials, that is, LDA, generalized gradient approximation (GGA), and Engel Vosko (EV-GGA), to investigate the electronic properties of these

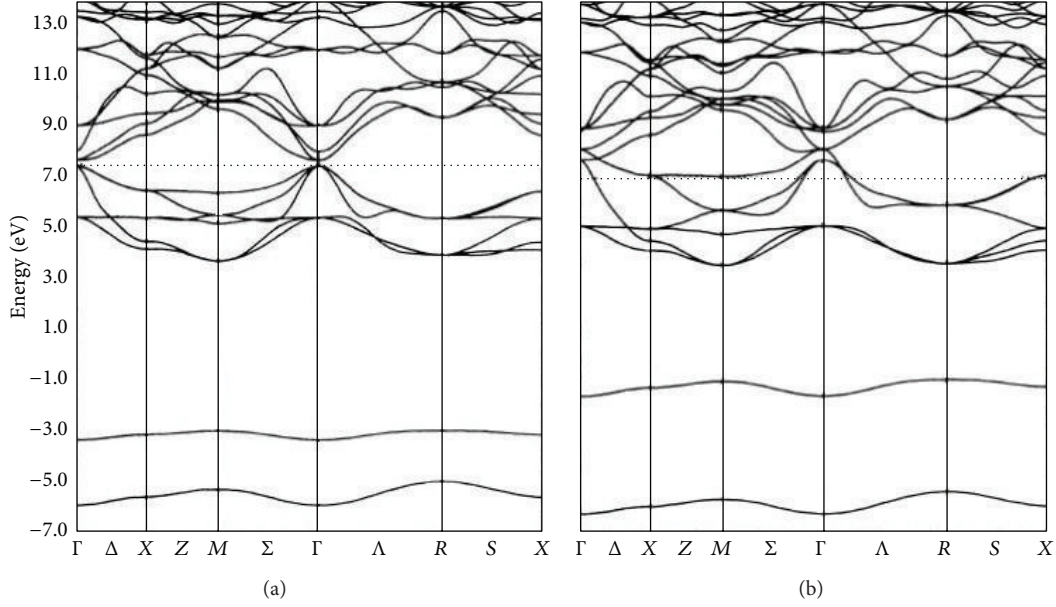


FIGURE 2: Band structures of (a) BiNCa₃ and (b) PbNCa₃ reproduced with permission from [36].

TABLE 1: Atomic positions of orthorhombic AsNCa₃ with space group Pbnm reproduced with permission of [38].

Ca (1)	$\pm(3/4 - \Delta_1, 1/4 + \Delta_2, \delta);$ $\pm(3/4 + \Delta_1, 3/4 + \Delta_2, \delta);$	$\pm(3/4 - \Delta_1, 1/4 + \Delta_2, 1/2 - \delta);$ $\pm(3/4 + \Delta_1, 3/4 + \Delta_2, 1/2 - \delta);$
Ca (2)	$\pm(\gamma_1, 1/2 - \gamma_2, 1/4);$	$\pm(1/2 - \gamma_1, -\gamma_2, 1/4);$
N	$1/2, 0, 0;$ $0, 1/2, 0;$	$1/2, 0, 1/2;$ $0, 1/2, 1/2;$
As	$\pm(-\lambda_1, \lambda_2, 1/4);$	$\pm(1/2 - \lambda_1, 1/2 - \lambda_2, 3/4);$

materials, and obtained band gaps of 0.65 and 0.36 eV for SbNCa₃ and BiNCa₃, respectively. Their work shows that EV-GGA is a better technique than LDA and GGA for the calculation of the band structures of these materials. However, the authors got wider band gaps using EV-GGA but the valence bands crossing the Fermi level show metallic behavior of these materials which is in contradiction to the experimental results.

This work was revisited by Bilal et al. [39] and they presented a comprehensive study on the band profiles and structural and optical properties of SbNCa₃ and BiNCa₃ antiperovskites. Along with LDA, GGA, and EV-GGA potentials, they also used modified Becke-Johnson (mBJ) potential to calculate accurate electronic properties of these materials. They achieved direct band gap values of 1.1 and 1.09 eV for SbNCa₃ and BiNCa₃, respectively, from mBJ potential. The band structures calculated by all potentials mentioned above are presented in Figure 3. It is clear from the figure that both materials show semiconducting behavior, verifying the experimental results with mBJ, giving the largest values of band gaps.

Chi et al. synthesized magnesium-based antiperovskites, AsNMg₃ and SbNMg₃, by the reaction of pnictogen with Mg₃N₂ at 800°C and investigated structural, transport, and magnetic properties of these materials [40]. The authors

report cubic structures for both materials with no distortion. Both materials show ionic bonding with negative 3 valence of As, Sb, and N. The authors classified both materials semiconductors based on resistivity data. Paramagnetic behavior is observed according to low-field magnetization data obtained at 50 G.

Shein and Ivanovskii studied the electronic band structure and chemical bonding in AsNMg₃ and SbNMg₃ antiperovskite materials using GGA [41]. Figures 4(a) and 4(b) present band structures of the materials achieved by the authors. Both materials show narrow band gap ionic semiconducting behavior. AsNMg₃ has direct band gap while SbNMg₃ shows indirect band gap nature.

Okoye discussed structural, electronic, and optical properties of AsNMg₃ and SbNMg₃ using full potential augmented plane waves plus local orbital (APW + lo) method [17]. GGA scheme was used for the electronic and optical properties of these materials. This was the first study on the optical properties of these materials. In this work the author verified the previous results [17] and confirmed that both materials have narrow band gaps with AsNMg₃ possessing direct band gap whereas SbNMg₃ reveals indirect band gap nature. The author argues that as DFT usually underestimates band gaps, therefore the calculated positions of the optical spectrum may be smaller than the experimental values.

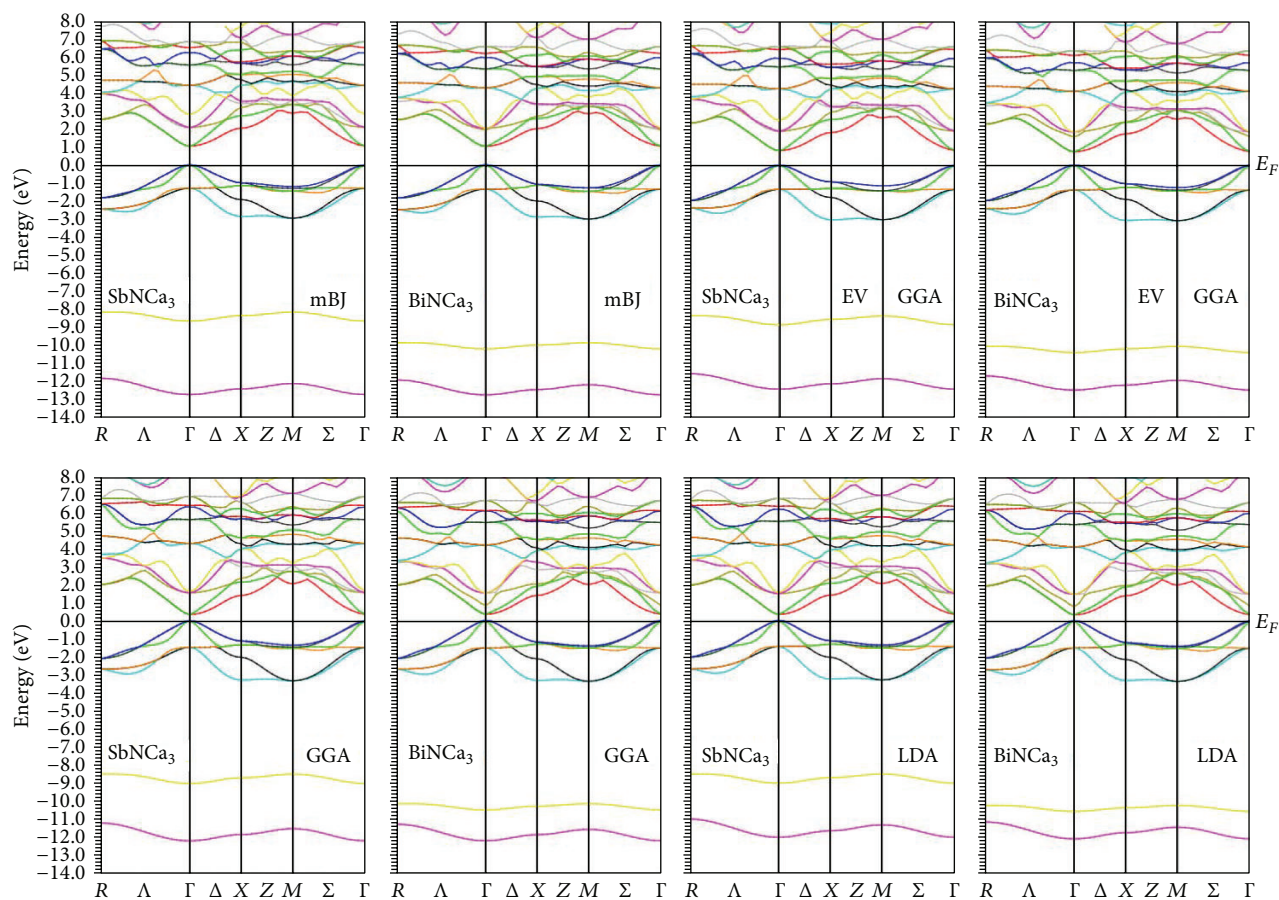


FIGURE 3: Band structures of SbNCa_3 and BiNCa_3 from LDA, GGA, EV-GGA, and mBJ reproduced from our previous work [39].

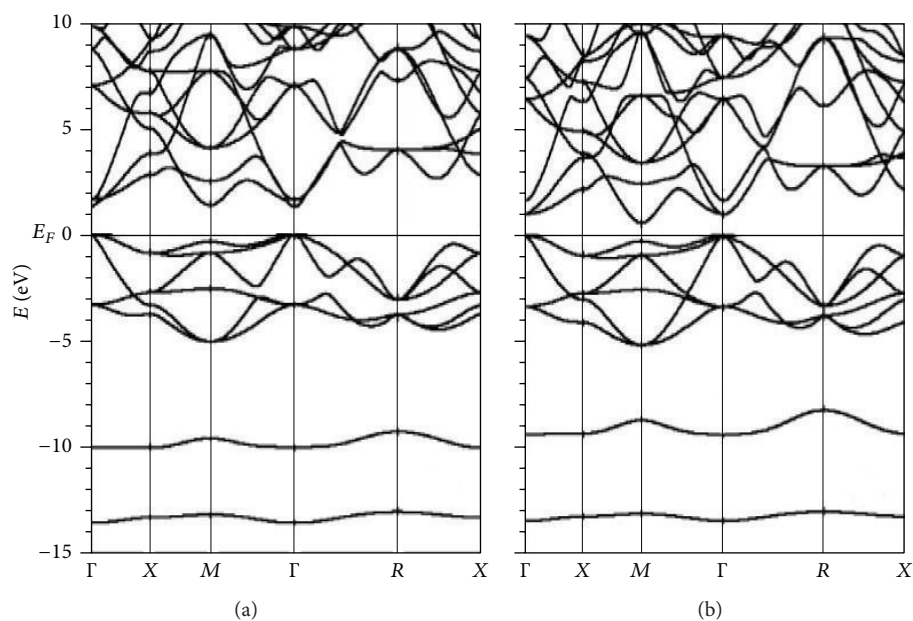


FIGURE 4: Band structures of (a) AsNMg_3 and (b) SbNMg_3 reproduced with permission from [41].

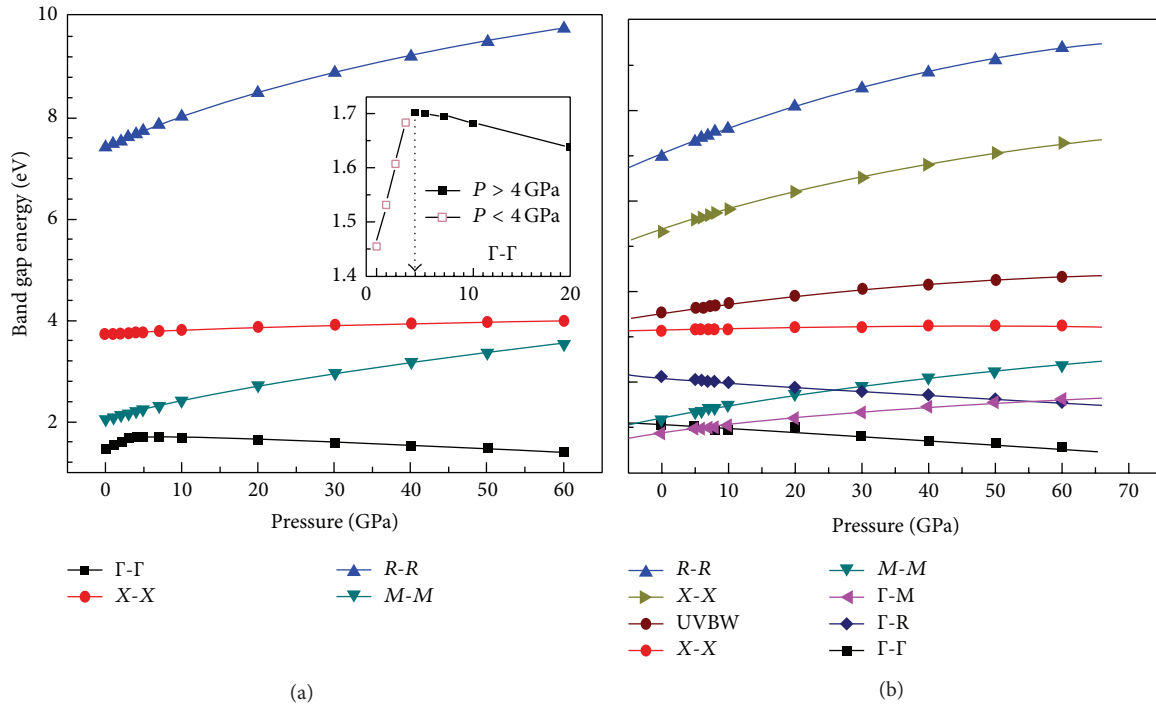


FIGURE 5: Direct and indirect band gap energies and upper valence bandwidth versus pressure for (a) AsNMg₃ and (b) SbNMg₃ reproduced with permission from [42] and [16], respectively.

The imaginary part of dielectric function, presented in their work, also confirms the semiconducting behavior of the materials.

Bouhemadou and coauthors investigated the structural electronic, elastic, and optical properties of AsNMg₃ [42] and SbNMg₃ [16] materials using pseudopotential plane waves method (PP-PW) within the generalized gradient approximation (GGA). For AsNMg₃ the fundamental direct band gap initially increases up to 4 GPa and then decreases as a function of pressure, concurrently retaining its direct band gap nature in entire pressure range applied, while SbNMg₃ shows transition from fundamental indirect band gap to direct band gap nature as pressure reaches 6.85 GPa as shown in Figures 5(a) and 5(b). These were the first theoretical studies on elastic properties of these materials; consequently Belaroussi et al. [43] studied the structural and elastic properties of SbNMg₃ theoretically and compared their studies with this work.

Amara et al. investigated the structural, elastic, and electronic properties of PNMg₃, AsNMg₃, SbNMg₃, and BiNMg₃ using the full-potential augmented plane waves plus local orbital (FP-LAPW + lo) within the GGA, while treating the exchange and correlation effects by the Tran-Blaha mBJ potential for the band structure, density of states, and charge density to achieve better results [44]. This is the first study on PNMg₃ and BiNMg₃ antiperovskite materials. All materials show semiconducting behavior. Table 2 reproduced from [44] shows that PNMg₃ and AsNMg₃ are direct band gap materials while SbNMg₃ and BiNMg₃ are indirect band gap materials. The authors achieved largest values of band gaps as compared to previous studies due to the use of mBJ potential. The elastic

TABLE 2: Band gap type and energy gap for XNMg₃ (X = P, As, Sb, and Bi), reproduced with permission from [44].

Compound	Band gap type	Energy gap (eV)
PNMg ₃	Direct band gap	2.60
AsNMg ₃	Direct band gap	2.41
SbNMg ₃	Indirect band gap	1.48
BiNMg ₃	Indirect band gap	1.42

properties show that PNMg₃ is the hardest while BiNMg₃ is the softest material out of all. Increase in covalent nature is observed in these materials in moving from BiNMg₃ to PNMg₃.

Beznosikov worked on nitrides with antiperovskites structure and analytically calculated lattice parameters of AsNSr₃, SbNSr₃, and BiNSr₃ materials [45]. Gäbler et al. synthesized SbNX₃ and BiNX₃ (X = Sr and Ba) antiperovskite materials in 2004 for the first time [46]. The compositions were derived from chemical analyses and supported by Rietveld refinements based on powder X-ray diffraction patterns. SbNSr₃ and BiNSr₃ are found in cubic (Pm3m) while SbNBa₃ and BiNBa₃ are found in hexagonal (P63/mmc) structure. The authors reported magnetic, electronic, optical, and bonding properties of these materials. The electrical resistivity studies show that these materials are semiconductors. The optical band gaps of 1.15 eV for SbNSr₃ and 0.89 eV for BiNSr₃ are measured by diffuse reflectivity method. The authors also calculated the electronic band gaps

TABLE 3: Experimental and theoretical band gap values (in eV) of antiperovskite materials.

Material	Experimental band gap	LDA	GGA	EVGGA	mBJ
SbNCa ₃	Semiconductor [1]	0.13 [31], 0.4 [39],	0.33 [31], 0.42 [39],	0.65 [31], 0.84 [39],	1.1 [39],
BiNCa ₃	Semiconductor [1]	0.1 [36], 0.28 [37], 0.11 [31], 0.38 [39],	0.08 [31], 0.4 [39],	0.36 [31], 0.8 [39],	1.09 [39],
AsNCa ₃	Insulator [1]	0.87 [37]			
PNCa ₃	Insulator [1]	1.1 [37]			
AsNMg ₃	Semiconductor [40]		1.332 [17, 41], 1.455 [42],		2.41 [44],
SbNMg ₃	Semiconductor [40]		0.623 [41], 0.866 [16], 0.726 [17],		1.48 [44],
PNMg ₃					2.6 [44],
BiNMg ₃					1.42 [44],
SbNSr ₃	Semiconductor 1.15 [46]		0.31 [47]	0.55 [32]	
BiNSr ₃	Semiconductor 0.89 [46]		0.26 [47]	0.36 [32]	
AsNSr ₃			0.49 [47]	0.84 [32]	
SbNBa ₃	Semiconductor [46]		0.529 [48], metallic [50]		
BiNBa ₃	Semiconductor [46]		0.529 [48], metallic [50]		

by DFT-based employing LDA and received small values arguing that LDA severely underestimated band gaps of crystalline materials. The susceptibility measurements show that the materials are diamagnetic.

Haddadi et al. [47] worked on the structural, elastic, and electronic properties of ANSr₃ (A = As, Sb, and Bi) materials in 2009 using CASTEP code, in which the plane waves pseudopotential total energy method is employed. The authors used theoretical lattice parameters from [45] instead of using experimental lattice parameters from [46] for optimization. Surprisingly, the lattice parameters achieved by the authors exactly match the experimental data. The band gap values of 0.49, 0.31, and 0.26 eV are calculated for AsNSr₃, SbNSr₃, and BiNSr₃ materials, respectively, which are underestimated from their experimental optical band gaps [46] (see Table 3).

Hichour et al., in 2010, studied pressure dependent elastic, electronic, and optical properties of ANSr₃ (A = As, Sb, and Bi) antiperovskites materials [32]. The authors used EV-GGA potential to improve the band gaps of these materials and achieved 0.84, 0.55, and 0.36 eV for AsNSr₃, SbNSr₃, and BiNSr₃, respectively. The band gap values decrease for all materials as pressure increases. The charge density plots show that these materials have mixed covalent and ionic bonding nature. The semiconducting behavior for SbNSr₃ is also evident from the imaginary part of the dielectric function as presented in their work.

Haddadi et al. [48] investigated structural, elastic, and electronic properties of the hexagonal antiperovskites SbNBa₃ and BiNBa₃ using Wu-Cohen generalized gradient approximation (GGA-WC). The authors achieved the band gap of 0.529 eV for both of these materials which is consistent

with the previous theoretical work [46]. Both materials show direct band gap semiconducting nature on ambient pressure. Figure 6 presents the pressure dependence on the band gaps of these materials. The band gap decreases with pressure and pressure-induced metallization is predicted at 7.95 and 8.02 GPa pressure for SbNBa₃ and BiNBa₃, respectively.

Hichour et al. [49] studied the structural and elastic properties of cubic SbNBa₃ and BiNBa₃ materials (while these materials are hexagonal experimentally [46]) comparing structural results with theoretical data from [45]. Jha and Gupta [50] also worked on the lattice dynamic study of antiperovskite compounds AsNBa₃ and SbNBa₃ in cubic structure. The authors presented metallic band structures of these materials which are in contradiction with the experimental work [46].

3. Transition Metals Based Antiperovskite Materials

Since 1960s, extensive research has been carried out on the different physical properties of manganese based antiperovskites materials with general formula AXMn₃ (A is a metal or semiconducting elements and X is C or N) [25]. In the last decade, after the discovery of superconductivity in MgCNi₃ [28], Mn based antiperovskites gained huge attention of researchers all around the globe. Different properties like giant magnetoresistance and magnetocaloric effect (GMR) of GaCMn₃ [22, 51], negative or zero thermal expansion (NTE or ZTE) of Cu (Ge) NMn₃ [52], nearly zero temperature coefficient of resistance (TCR) of Ag_{1-x}Cu_xNMn₃ [53], and giant magnetostriction (MS) of CuNMn₃ [24] are reported. Generally, these materials show metallic behavior. The 3d

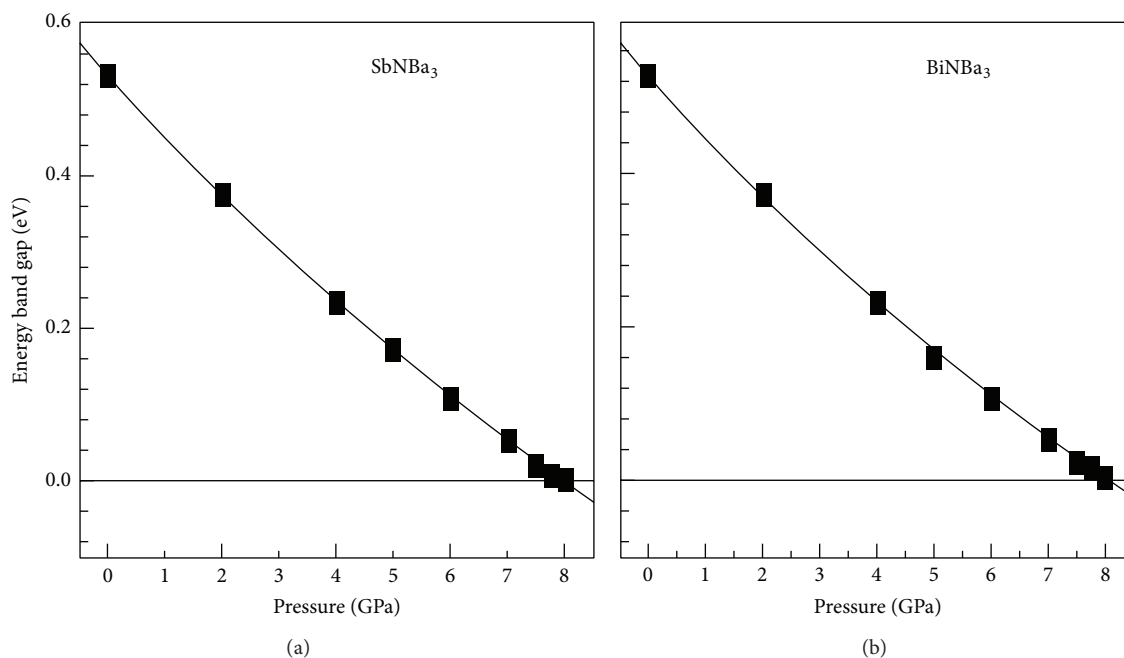


FIGURE 6: Band gap energies versus pressure for (a) SbNSr₃ and (b) BiNSr₃ reproduced with permission from [48].

orbitals of Mn have high density of states at Fermi level (E_F) while hybridization between X-p states and Mn-d states is the main cause of wide conduction band crossing over the Fermi level [54]. Sun et al. [15] reported unusual phase separation and irregularity in the electronic transport properties of ZnNMn₃. The authors further presented [55] the thermodynamic, electromagnetic, and structural properties of antiperovskite SbNMn₃. The authors found that at room temperature the materials exist in tetragonal structure with lattice parameters $a = b = 4.17994 \text{ \AA}$ and $c = 4.27718 \text{ \AA}$. Wang et al. [56] studied the structural, magnetic, electrical transport properties, and reversible room-temperature magnetocaloric effect in antiperovskite compound AlCMn₃. The material shows good metallic behavior with ferromagnetic-paramagnetic phase transition at $T_C = 287 \text{ K}$. GaCMn₃ is a widely studied antiperovskites material [22, 57, 58]. It is a metallic material with antiferromagnetic (AFM) behavior at ambient temperature. GaCMn₃ shows transition and becomes ferromagnet (FM) at 163.9 K and paramagnet (PM) at 245.8 K [22]. Shim et al. [59] studied the electronic properties of GaCMn₃, ZnCMn₃, SnCMn₃, and ZnNMn₃ using linearized muffin-tin orbital (LMTO) method in the local spin density approximation (LSDA). The electronic properties are calculated in paramagnetic state for these materials. The density of states for GaCMn₃ show strong hybridization between Mn-3d and C-2p states which increases bonding states between -3 eV and -7 eV whereas the nonbonding states Mn-3d are at the Fermi level.

After the discovery of superconductivity in MgCNi₃ [28], Ni based isostructural antiperovskites materials have gained enormous attention among the researchers [29]. Uehara et al. [60, 61] reported superconductivity in CdCNi₃ and ZnNNi₃ antiperovskites with transition temperatures of 3.2 and 3 K,

respectively. Shim et al. [62] studied the electronic properties of MgXNi₃ ($X = \text{B, C, and N}$). Ni-3d and C-2p states form the antibonding subband near Fermi level in MgCNi₃ with Ni-3d dominant character. The DOS for MgXNi₃ reveals that changing X changes the density of states near the Fermi level with B-2p state in MgBNi₃ located higher in energy than the C-2p state of MgCNi₃, and so the hybridization with Ni-3d is stronger.

Johannes and Pickett [63] studied the electronic structure of ZnCNi₃ and showed that no superconductivity is found in this material down to 2 K. According to the authors the absence of superconductivity in ZnCNi₃ as compared to MgCNi₃ can only be explained by assuming Mg deficient in this material. Wu et al. [64] investigated the structure, electronic, and magnetic state of InCNi₃ antiperovskite material using LDA and GGA. The authors reported that the material is paramagnetic with strong hybridization between Ni-3d and C-2p states. Hou studied the elastic properties and electronic structures of InNCo₃ and InNNi₃ antiperovskite materials [65]. Due to the different strength of 2p-3d hybridization for the N-Co atoms in InNCo₃ and the N-Ni atoms in InNNi₃, InNCo₃ is ferromagnetic while the ground state of InNNi₃ is nonmagnetic. Li et al. [66] investigated the mechanical and electronic properties of MNi₃ ($M = \text{Zn, Mg, or Cd}$). The maximum states are occupied by Ni-3d and N-2p hybridization near the Fermi level while M elements have very small contribution here. However, this small contribution of M elements may cause a small shift in the bands near the Fermi level, resulting in superconductivity in ZnNNi₃ at $T_C \approx 3 \text{ K}$ while the other two compounds do not show superconductivity.

Grandjeant and Gerard [67] synthesized and studied the structural and magnetic properties of ACFe₃ ($A = \text{Al,}$

Zn, Ga, Sn, and Ge) antiperovskites materials. Fe based antiperovskites materials have been investigated by different researchers [68–72]. Ivanovskii et al. [73–75] reported the electronic properties of these materials, while the electronic band structure of the cubic antiperovskites $M_3M'C$ ($M = \text{Mn, Fe; } M' = \text{Zn, Al, Ga, Sn}$) in ferromagnetic state is calculated by using LMTO-ASA nonempirical self-consistent method [73]. All materials have high density of states at Fermi level mainly due to Fe-3d states and show metallic behavior. Furthermore, the authors show that these materials are ferromagnetic in nature.

Tian and Nemoto [76] performed transmission electron microscopy on AlTi_3 . Subsequently different researchers investigated the physical properties like electronic, mechanical, and thermal properties of this material using different techniques [77–81]. Yu-Lei [78] studied the electronic properties of this material using GGA potential. The band structure presented by the author shows that this is a metallic material. The density of states is also discussed for the understanding of the different states at Fermi level. The strong hybridization between Ti-3d and Al-3p states and between Ti-3d and C-2p states stabilizes the structure of Ti_3AlC . Medkour et al. [81] studied the structural, elastic, and electronic properties of ACTi_3 ($A = \text{Al, In, and Tl}$) antiperovskites materials using first principle calculations. All of these materials show metallic character with strong ionic covalent bonds between Ti and C atoms, and ionic bonds along A and Ti atoms. The authors suggest that the stiffness decreases with an increase in the antibonding state between Ti and A atoms.

Brady et al. [82, 83] worked on the synthesis of chromium based nitride antiperovskites PtNCr_3 . Wiendlocha et al. [84] studied the electronic properties, superconductivity, and magnetism in GaNCr_3 and RhNCr_3 materials. The band structures of these materials presented in the paper show that both materials are metallic in nature. The spin-polarized calculations show nonferromagnetic ground state for both compounds. The authors are of the opinion that there may be superconductivity in these materials because of the high values of electronic part of electron-phonon coupling constant. Tütüncü and Srivastava [85] theoretically investigated structural, electronic, vibrational, and superconducting properties of the cubic antiperovskite RhNCr_3 . The authors claim that this material is metallic with superconducting nature below 17 K.

Shao et al. [86] studied the structural, elastic, and electronic properties of ACCr_3 ($A = \text{Al and Ga}$) antiperovskites materials using first principles methods. The analysis of formation energies shows that both materials can be synthesized at ambient pressure and are nonmagnetic in nature. The band structures show that the materials are metallic in nature. Shao et al. [87] investigated the electronic structure, magnetic properties, and lattice dynamics of the AXCr_3 ($X = \text{C or N, } A = \text{Zn, Al, Ga, Sn, Ag, Cd, Mg, and In}$) using ABINIT code. The authors claim that among the nitride materials only ZnNCr_3 , AlNCr_3 , GaNCr_3 , and SnNCr_3 can be synthesized for having negative formation energies. Furthermore, all materials show metallic nature with AlCCr_3 , GaCCr_3 , and ZnNCr_3 being the potential candidates of superconductivity.

4. Summary

We present the research progress on theoretical electronic properties of carbon and nitrogen based antiperovskite materials comparing with the available experimental data. In a nutshell, we can classify antiperovskite materials into two groups: materials having an element of group-IIA of the periodic table and the materials having a transition metal at the face centers of the unit cell of these materials. The former are mostly semiconductors while the latter are generally metals. Literature reveals that enormous research is being carried out on the different physical properties of antiperovskites. Superconductivity is found in some metallic materials though there is still room for research in this aspect. Similarly magnetism is one of the most important features of antiperovskites and properties like giant magnetoresistance, magnetocaloric effect, and temperature coefficient of resistivity are important industrial utilities. Thermoelectric properties of these materials have been less explored. There are many semiconducting materials which can be potential candidates for thermoelectric properties as these materials have suitable band gaps and dense electronic states near Fermi level. It is also clear from these studies that despite vast studies on the electronic properties of these materials still there are some ambiguities which need to be addressed. On one hand, exact band gaps of some materials are not known, while on the other hand the experimentally known band gaps have not been reproduced theoretically. As the electronic properties are very important in determining different physical properties of materials, therefore, we hope that this work will benefit the researchers working in this field.

Conflict of Interests

The authors declare that there is no conflict of interests regarding the publication of this paper.

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