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# Computational study of half-metallic behavior, optoelectronic and thermoelectric properties of new $XAlN_3$ (X = K, Rb, Cs) perovskite materials

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#### ABSTRACT

In this study, we systematically explored the properties of novel perovskite materials, XAlN<sub>3</sub> (X = K, Rb, and Cs), based on first-principles calculations and semiclassical Boltzmann transport theory. Generalized gradient approximation and HSE06 hybrid functional methods were used to investigate the electronic band structures. Our findings indicated intriguing half-metallic behavior where the spin-down state had metallic characteristics, whereas the spin-up state behaved as an insulator for all compounds, with indirect band gaps. These compounds had a significant magnetic moment of 5  $\mu_B$ , which confirmed their half-metallic nature. Analysis of the elastic constants indicated distinctive mechanical properties. Moreover, the dielectric functions indicated efficient energy absorption across a broad energy spectrum, which is particularly beneficial for ultraviolet optoelectronic applications. At 300 K with a chemical potential ( $\mu$ ) of +1.37 eV, CsAlN<sub>3</sub> had a notable thermoelectric figure of merit (ZT) of 0.99. This ZT value remained competitive at 0.97, even at a high temperature of 1000 K in the p-type region. However, the ZT and Seebeck coefficients decreased in a temperature-dependent manner to affect the thermoelectric characteristics of these materials. Overall, our findings suggest that XAlN<sub>3</sub> (X = K, Rb, and Cs) perovskite materials are promising candidates for use in various applications in spintronics, optoelectronics, and thermoelectric devices.

#### 1. Introduction

The perovskite structure represented by the chemical formula ABX<sub>3</sub> is important in materials science and condensed matter physics. This widely studied structure consists of two distinct cations (A and B) bonded to an anion (X) and it is often visualized as a cubic configuration with B atoms at the center surrounded by an octahedral arrangement of anions. Perovskite materials have great potential for use in various applications, including photovoltaics, light-emitting devices, sensors, and memory devices. Their high efficiency, low cost, and simple fabrication make them attractive for applications in renewable energy technologies [1–5]. Perovskites also have unique optical and electronic properties, which make them promising for uses in next-generation electronic devices [6–8]. Researchers have focused on ordered perovskite compounds, particularly because of their potential uses as magnetic

electrodes. For example, Rubal et al. developed new perovskite materials and proposed that their properties have many potential applications [9–13]. Perovskite structures are of significant interest in spintronics, where electron spin is harnessed for information processing. In 1983, De Groot et al. [14] conducted first-principles calculations to show that perovskites can achieve 100 % spin polarization at the Fermi level. These half-metallic ferromagnetic materials possess unique electronic structures, where one spin channel behaves metallically driven by the majority of the metallic spin electrons whereas the other exhibits semiconducting or insulating characteristics to result in 100 % spin polarization at the Fermi level. These materials have advantages, such as reduced energy consumption, higher circuit integration density, and faster data processing, thereby placing them at the forefront for applications in advanced electronics [15].

Theoretical studies by Mir et al. predicted the dynamic stability and

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Received 26 August 2023; Received in revised form 18 January 2024; Accepted 19 January 2024 Available online 30 January 2024 0022-3697/© 2024 Elsevier Ltd. All rights reserved. half-metallic characteristics of  $BaMO_3$  (M = Mg and Ca) perovskites [16]. In 2022, Abdullah et al. determined the stability and half-metallic properties of titanium-based fluoro-perovskite MTiF<sub>3</sub>, where M represents Rb and Cs. These materials exhibit metallic properties in the spin-up state and nonmetallic properties with a large indirect band gap in the spin-down state [17]. Cai et al. investigated the perovskite BiNiO<sub>3</sub> and demonstrated its half-metallic ferromagnetism due to strong p-d exchange interactions, thereby resulting in semiconducting behavior in the majority-spin electrons and metallic behavior in the minority-spin electrons [18]. Abdullah et al. demonstrated the potential uses of double perovskites K2NaMI6 and K2NaMCl6 (M: Cr, Fe), as well as  $Cs_2GeSnX_6$  (X = Cl, Br, I) for thermoelectric and spintronic applications because of their interesting optical and thermoelectric properties, with useful applications in semiconductor and optoelectronics industries [19–21]. Rahman et al. identified promising materials including halide and oxide perovskites, as well as novel inorganic cubic perovskites, for applications in solar cells, optoelectronic devices, and gas sensors [11, 22-24]. These insights into perovskite materials have contributed to their exploration and utilization in a range of technological applications.

The scientific community must address two pressing energy-related challenges comprising the ongoing energy crisis and growing environmental concerns related to conventional energy sources. Perovskite materials may provide promising solutions, particularly in thermoelectric applications [25]. The efficiency of thermoelectric materials is quantified by the dimensionless figure of merit (ZT):  $ZT = S^2 \sigma T / \kappa$ , where S represents the Seebeck coefficient,  $\sigma$  denotes the electrical conductivity, T indicates the temperature, and  $\kappa$  is the thermal conductivity [26-30]. Researchers have aimed to develop thermoelectric materials with high Seebeck coefficients, strong electrical conductivity, and low thermal conductivity to maximize the ZT values. Recent studies based on density functional theory have elucidated the thermoelectric potential of perovskite materials. In particular, RbNpO3 and RbPuO3 were found to have ZT values of 1.01 and 0.987 at 300 K, respectively, thereby indicating their suitability for use in both low- and high-temperature thermoelectric devices [31]. In addition, studies have identified CaMnO<sub>3</sub>, SrTiO<sub>3</sub>, and BaTiO<sub>3</sub> as promising alternatives to traditional thermoelectric materials, although chalcogenide thermoelectric materials currently achieve the highest ZT values [27].

Only a limited number of new nitride perovskites with potential applications have been theoretically predicted and synthesized. ThTaN<sub>3</sub> is an important example that demonstrates the potential of nitride perovskites because it has characteristics similar to those of a topological crystalline insulator [32]. Another notable nitride perovskite, LaWN<sub>3</sub>, was theoretically predicted and synthesized, and it exhibited impressive ferroelectric properties. However, its application in optoelectronics is hindered due to its status as an indirect-gap semiconductor [33]. Recently, Viet-Anh et al. identified as CeTaN<sub>3</sub> and CeNbN<sub>3</sub> promising candidates, with direct semiconducting band gaps of 1.5 eV and 1.1 eV, respectively [34].

In the present study, we comprehensively investigated the structural parameters, electronic behaviors, mechanical stability, optical properties, and thermoelectric characteristics of XAlN<sub>3</sub> perovskites, where X represents K, Rb, or Cs. Our primary aim was to identify new halfmetallic compounds with significant band gaps in the spin-up channels, with potential applications in the field of spintronics. We also investigated how these band gap variations might impact the optical properties and thermoelectric efficiency. Thus, based on computational predictions, we obtained valuable insights into the half-metallic and thermoelectric properties of these nitride perovskites. These findings are important for advancing both spintronic and thermoelectric devices.

#### 2. Computational methods

We performed first-principles calculations using the CASTEP simulation code [35] with the generalized gradient approximation (GGA) of the Perdew–Burke–Ernzerhof exchange-correlation potential [36].



Fig. 1. Crystal structure of  $XAIN_3$  (X = K, Rb, Cs), where the blue, purple, and magenta balls represent N, X, and Al atoms, respectively.

Ultrasoft pseudopotentials were employed to enhance the computational efficiency but without sacrificing accuracy [37]. The energy cutoff was 500 eV for the plane-wave basis set, and we utilized  $10 \times 10 \times 10$ k-points for geometry optimization, whereas the electronic, magnetic, elastic, optical, and thermoelectric properties were computed for  $15 \times 15 \times 15$  k-points [38]. The convergence criteria included maximum forces reaching  $10^{-5}$  eV/atom and a maximum lattice point displacement limited to  $10^{-3}$  Å, maximum ionic Hellmann–Feynman force of 0.03 eVÅ<sup>-1</sup>, and maximum stress tolerance of 0.05 GPa. We applied the Broyden–Fletcher–Goldfarb–Shanno minimization scheme with finite basis set corrections [39,40]. To calculate the electronic transport properties, we solved the semiclassical Boltzmann transport equation using the constant relaxation time approximation and implemented the BoltzTraP code [41].

### 3. Results

#### 3.1. Structural and electronic properties

The perovskite materials XAlN<sub>3</sub> (X = K, Rb, Cs) are aluminum-based nitro-perovskites with a cubic phase and pm3m space group (no. 221). The Wyckoff coordinates of the atoms in this phase are X located at (0, 0, 0), whereas Al and N atoms are located at (0.5, 0.5, 0.5) and (0, 0.5, 0.5), respectively, as shown in Fig. 1. First, we performed structural optimization and the equilibrium lattice constants obtained for these three perovskite compounds are listed in Table 1. To further confirm the stability, we employed the formation energies to obtain the lowest energies of the compounds, which were defined as:

$$E_{for} = \frac{1}{3} [E_{tot} - E_x - E_{Al} - 3E_N]$$
(1)

where  $E_{tot}$  is the total energy of XAlN<sub>3</sub> (X = K, Rb, Cs), and E denotes the energy of each (X, Al, and N) atom in the respective ground-state bulk phase. The calculated values of  $E_{for}$  are listed in Table 1. The negative values of these compounds indicate that they are thermodynamically stable and can be synthesized in the laboratory.

Half-metallic materials are highly desirable for spintronic devices. Thus, the spintronic properties of the compounds were analyzed by evaluating the electronic band using self-consistent spin-polarized calculations. The electronic band structures of  $XAIN_3$  (X = K, Rb, Cs) were investigated using the GGA method, as shown in Fig. 2. The bands in the spin-down channel crossed the Fermi level. As shown in Table 1, the spin-up channel had a high indirect energy gap, and thus all materials continued to exhibit insulating properties. It is well known that the GGA method cannot resolve the electronic band structures of solid compounds and it underestimates the band gap values. Thus, the HSE06 hybrid functional was used to accurately evaluate the features of all the

# Table 1

Optimized lattice parameters, formation energy, indirect band gaps obtained with GGA and HSE06 methods (eV), elastic constants  $C_{ij}$  (GPa); bulk (B), shear (G), and Young's (E) moduli (GPa); and Poisson's ratio  $\nu$  for XAlN<sub>3</sub> (K, Rb, Cs).

Compounds	$\mathbf{a} = \mathbf{b} = \mathbf{c}$ (Å)	E <sub>for</sub> (eV)	Eg <sub>GGA</sub> (eV)	Eg <sub>HSE06</sub> (eV)	C <sub>11</sub>	C <sub>12</sub>	C44	В	G	Е	ν
KAlN <sub>3</sub> RbAlN <sub>3</sub>	4.056 4.137	-4.707 -4.962	5.57 5.45	6.46 5.86	114.08 118.54	49.13 63.23	54.71 49.07	70.78 81.66	44.38 38.08	113.05 99.01	0.20 0.26
CsAlN <sub>3</sub>	4.200	-4.394	4.38	5.19	81.48	57.84	46.17	65.72	26.89	63.57	0.28



Fig. 2. Electronic band structures obtained for (a) KAlN<sub>3</sub>, (b) RbAlN<sub>3</sub>, and (c) CsAlN<sub>3</sub> based on the GGA and HSE06 methods.

#### Table 2

Mulliken analysis of spin magnetic moments obtained using the GGA method.

Compounds	atom	s up/ down	p up/ down	d up/ down	Total	Spin (hbar/2)
KAlN <sub>3</sub>	К	1.06/	2.77/	0.10/	3.92/	0.03
		1.08	2.74	0.07	3.90	
	Al	0.34/	0.53/	0.0/0.0	0.87/	-0.33
		0.42	0.77		1.20	
	Ν	0.96/	2.78/	0.0/0.0	3.74/	1.77
		0.91	1.06		1.97	
RbAlN <sub>3</sub>	Rb	1.04/	2.78/	0.14/	3.97/	0.06
		1.10	2.71	0.10	3.91	
	Al	0.35/	0.52/	0.0/0.0	0.87/	-0.32
		0.43	0.76		1.20	
	Ν	0.96/	2.76/	0.0/0.0	3.72/	1.75
		0.91	1.05		1.96	
CsAlN <sub>3</sub>	Cs	0.90/	2.90/	0.23/	4.04/	0.13
		0.97	2.75	0.19	3.91	
	Al	0.37/	0.50/	0.0/0.0	0.87/	-0.29
		0.44	0.72		1.16	
	Ν	0.96/	2.74/	0.0/0.0	3.70/	1.72
		0.91	1.06		1.98	

compounds. As shown in Fig. 2, the spin-down was still metallic, whereas the spin-up was an insulator for all compounds with an indirect band gap. The energy gap is a significant parameter in spintronics devices and all of the compounds were suitable. The spin polarization at the Fermi level must also be equal to 100 %. These features were confirmed for the XAlN<sub>3</sub> (X = K, Rb, Cs) compounds, thereby indicating that they are promising for use in spintronic applications.

The magnetic moment is a crucial factor for determining the properties of ferromagnetic half-metallic materials. The spin magnetic moments were calculated for all compounds using the GGA method to obtain integral values of 5  $\mu_B$ . The unexpectedly higher magnetic moment observed in these materials was due to strong hybridization effects, thereby highlighting the significant effects of orbital interactions on the magnetic properties. As shown in Table 2, the total spin magnetic moments and findings for each atom in both spin phases obtained based on Mulliken analysis confirmed the half-metallic nature of the perovskite compounds through the positive integral spin magnetic moments. These materials with high-spin magnetic moments have great promise for advanced applications in spintronics, particularly in magnetoresistive random-access memory applications where magnetic moments are utilized for data storage, where they can surpass the conventional use of electrical charges [42].



Fig. 3. Mechanical parameters: (a) bulk modulus, (b) Young's modulus (E), (c) shear modulus(G), and (d) Poisson's ratio(v) for KAIN<sub>3</sub> in the (100) direction.



Fig. 4. Mechanical parameters: (a) bulk modulus, (b) Young's modulus (E), (c) shear modulus(G), and (d) Poisson's ratio(v) for RbAlN<sub>3</sub> in the (100) direction.

## 3.1.1. elastic and mechanical properties

Calculating the elastic constants is important because they indicate fundamental properties such as the mechanical stability, stiffness, brittleness, and ductility. Elastic constants are crucial for understanding a material's response to external forces, thereby providing insights into mechanical characteristics such as the stability and toughness. Furthermore, they provide insights into the anisotropic nature of bonding. In the case of a cubic crystal, we can calculate three independent elastic constants using the Born–Huang criteria [43] as follows.

$$C_{11} - C_{12} > 0, C_{11} + 2C_{12} > 0, C_{44} > 0$$
<sup>(1)</sup>

All compounds exhibited mechanical stability according to the elastic stiffness constants,  $C_{ij}$ . In addition, the elastic constants reported in Table 1 were used to determine the essential elastic moduli for all compounds, including the bulk modulus (B), shear modulus (G), Young's modulus (E), and Poisson's ratio ( $\nu$ ), which were calculated using the following expressions:

$$B = \frac{1}{2} [B_V + B_R], G = \frac{1}{2} [G_V + G_R], E = \frac{9BG}{3B + G}, \nu = \frac{1}{2} \left[ \frac{3B - 2G}{3B + 2G} \right]$$
(2)

where B<sub>V</sub> and B<sub>R</sub> are the bulk moduli, respectively, and G<sub>V</sub> and G<sub>R</sub> are

the shear moduli calculated using Voigt and Reuss approximations [44, 45]. The bulk modulus represents the ratio of the pressure change relative to the fractional volume compression and it indicates the strength or hardness of the crystal. The shear modulus indicates the crystal's strength when exposed to significant loads in structural materials. Figs. 3–5 illustrate the following.: (i) the bulk modulus was higher for RbAlN<sub>3</sub> than the other two compounds (i.e., more able to resist the applied pressure); (ii) the shear and Young's moduli were higher for KAlN<sub>3</sub> than the other two compounds (i.e., indicating a high ability to oppose deformation and large tensile (or compressive) stiffness); and (iii) Poisson's ratio indicated that KAlN<sub>3</sub> was more compressible than RbAlN<sub>3</sub> and CsAlN<sub>3</sub> due to the low  $\nu$  values.

#### 3.1.2. Optical properties

It is important to understand the interactions between light and the materials. The dielectric function  $\varepsilon(\omega)$  describes the mechanism of interaction [46] and it can be represented as:  $\varepsilon(\omega) = \varepsilon_1(\omega) + i\varepsilon_2(\omega)$ . The real part of  $\varepsilon_1(\omega)$  explains the dispersion of photons in a material and the degree of polarization, and  $\varepsilon_2(\omega)$  represents the imaginary part. According to the Kramers–Kronig relation [47],  $\varepsilon_1(\omega)$  can be expressed as:



Fig. 5. Mechanical parameters: (a) bulk modulus, (b) Young's modulus (*E*), (c) shear modulus(*G*), and (d) Poisson's ratio(*v*) for CsAlN<sub>3</sub> in the (100) direction.

$$\varepsilon_1(\omega) = \frac{\pi}{2} P \int_0^{\infty} \frac{\omega' \varepsilon_2(\omega')}{\omega'^2 - \omega^2} d\omega'$$
(3)

where  $\omega$  denotes the light frequency and P is the principal value of the integral part. In addition,  $\varepsilon_2(\omega)$  can be calculated by employing momentum tensors derived from the occupied and unoccupied wave functions [48]:

$$\varepsilon_{2}(\omega) = \frac{2e^{2}\pi}{\Omega\varepsilon_{o}} \sum_{K,V,C} \left| \langle \varphi_{K}^{C} | \widehat{U} . \overrightarrow{r} | \varphi_{K}^{V} \rangle \right|^{2} \delta \left( E_{K}^{C} - E_{K}^{V} - E \right)$$
(4)

where the wave functions  $\phi^C_K$  and  $\phi^V_K$  represent the conduction and valence bands at a specific k-vector, respectively, e is the electronic charge,  $\Omega$  denotes the unit cell volume, U represents the incident electric field's polarization direction, energy conservation is ensured through a delta function E, and  $E^C_K$ , and  $E^V_K$  denote the energy of electrons at a certain k-vector in the conduction and valence bands.

Fig. 6 (a) and 6 (b) show the real and imaginary parts of the dielectric function, where the characteristics differ depending on the sign of the frequency  $(\pm \omega)$ . Compounds exhibit metallic properties at negative frequencies, whereas their characteristics resemble those of insulators or

semiconductors at positive frequencies depending on the value of  $\omega$ . Lower dielectric constants lead to wider band gap energies, whereas higher dielectric constants result in narrower band gap energies.

The efficiency of absorbing a substantial portion of the visible light spectrum is a crucial prerequisite for photocatalysts. The absorption coefficient ( $\alpha$ ) represents the energy absorbed by a substance per unit length when a photon transfers electrons from the valence band to the conduction band by providing the necessary energy, which can be described as follows.

$$\alpha(\omega) = \left[\sqrt{\varepsilon_1^2(\omega) + \varepsilon_2^2(\omega)} - \varepsilon_1(\omega)\right]^2$$
(5)

Fig. 6(c) clearly shows that the materials exhibited a remarkable ability to absorb energy in the energy range exceeding 7.67 eV. In addition, they had low absorption capacities within the visible spectrum (1.65–3.1 eV). These characteristics make these compounds highly suitable for effective light absorption, thereby enabling their application in optoelectronic devices. Analysis of the absorption coefficient spectra further indicated that CsAlN<sub>3</sub> exhibited superior absorption properties compared with the other compounds. Consequently, these perovskite materials are promising for use in ultraviolet (UV) applications.



**Fig. 6.** Calculated optical properties for compounds XAlN<sub>3</sub> (X = K, Rb, Cs): (a, b) real and imaginary parts of the dielectric function, (c) absorption coefficient, and (d) reflectivity.

Reflectivity is a measure of how much light a substance reflects when exposed to it. Reflection primarily occurs on the material's surface and it is calculated as follows.

$$R(\omega) = \left[\frac{\sqrt{\varepsilon(\omega)} - 1}{\sqrt{\varepsilon(\omega)} + 1}\right]$$
(6)

Fig. 6(d) shows the reflectivity spectra obtained for the compounds. All of the compounds exhibited maximum reflection in the 0 eV region. In addition, higher levels of reflectivity were observed as the wavelength increased. These characteristics are potentially important for various applications involving UV rays.

### 3.1.3. Thermoelectric properties

ZT is used to measure the performance of a thermoelectric device based on the characteristic properties of the materials used in the device. A typical thermoelectric device consists of both n-type and p-type materials, and ZT is often expressed imprecisely as:

$$Z\overline{T} = \frac{(S_p - S_n)\overline{T}}{\left[\left(\rho_p \kappa_p\right)^{1/2} + \left(\rho_n \kappa_n\right)^{1/2}\right]^2}$$
(7)

where  $\overline{T}$  represents the average temperature and  $\rho$  represents the electrical resistivity. In order to achieve maximum efficiency, n-type and p-

type thermoelectric materials should have a similar ZT. Fig. 7(a) shows the thermoelectric ZT values as a function of the chemical potential for the XAlN<sub>3</sub> (X = K, Rb, Cs) compounds at constant temperatures of 300 K and 1000 K. A positive sign ( $\pm\mu$ ) indicates the dominance of p-type carriers whereas a negative sign denotes the prevalence of n-type carriers. The maximum ZT values achieved for CsAlN<sub>3</sub>, RbAlN<sub>3</sub>, and KAlN<sub>3</sub> were 0.99, 0.98, and 0.97, respectively, at a chemical potential of  $\mu$  = +1.37 and temperature of 300 K. However, at a higher constant temperature of T = 1000 K, the ZT values decreased to 0.97, 0.94, and 0.90 for CsAlN<sub>3</sub>, RbAlN<sub>3</sub>, and KAlN<sub>3</sub>, respectively, while maintaining the same chemical potential value. Despite the decreases, the computed ZT values indicate that all compounds are still viable candidates for use in thermoelectric materials.

The Seebeck coefficient (S =  $\Delta V/\Delta T$ ) is a crucial parameter that quantifies the potential difference ( $\Delta V$ ) generated in a material due to a temperature gradient ( $\Delta T$ ). The Seebeck coefficient (S) values, which represent holes (p-type carriers), at 300 K were calculated as 3.04 mV/K ( $\mu = +1.75 \text{ eV}$ ), 2.98 mV/K ( $\mu = +1.90 \text{ eV}$ ), and 2.84 mV/K ( $\mu = +1.98 \text{ eV}$ ) for CsAlN<sub>3</sub>, RbAlN<sub>3</sub>, and KAlN<sub>3</sub>, respectively. When the temperature increased to T = 1000 K and  $\mu = +2.0 \text{ eV}$ , the S values decreased for the compounds, with values of 1.28 mV/K, 1.12 mV/K, and 0.98 mV/K for CsAlN<sub>3</sub>, RbAlN<sub>3</sub>, and KAlN<sub>3</sub>, respectively (Fig. 7(b)). The Seebeck coefficients for p-type holes in CsAlN<sub>3</sub>, RbAlN<sub>3</sub>, and KAlN<sub>3</sub> decreased as the temperature increased from 300 K to 1000 K. Determining these



**Fig. 7.** (A) Figure of merit (ZT) and (b) Seebeck coefficient values versus chemical potential  $(\pm \mu)$  at different temperatures of T = 300, 1000 K for XAlN<sub>3</sub> (X = K, Rb, Cs) compounds.

coefficients is essential for analyzing and predicting the thermoelectric properties of materials.

#### 4. Conclusion

In this study, we investigated new perovskite materials with the cubic phase  $XAlN_3$  (X = K, Rb, and Cs). The structures were optimized and shown to be thermodynamically stable based on the formation energy, where RbAlN<sub>3</sub> was the most stable compound. The GGA method was utilized to analyze the electronic band structures of the materials and to elucidate their insulating properties. We also used the HSE06 hybrid functional due to its more accurate calculation of the band gap, and the results confirmed the half-metallic nature of the materials. The compounds had a high magnetic moment of 5 µB, which indicated significant orbital interactions, and N atoms contributed greatly to this value. We also assessed the mechanical properties of the materials, where RbAlN<sub>3</sub> had a higher bulk modulus, suggesting greater volume resistance, and KAlN<sub>3</sub> had higher shear and Young's moduli. These compounds have potential applications in UV devices due to their optical properties, including the dielectric function, absorption coefficient, and reflectivity. Furthermore, the thermoelectric ZT values suggested that all compounds have potential uses as thermoelectric materials, where the highest ZT values were obtained at 300 K. The characterization of new nitride perovskites provides valuable insights into the potential applications of  $XAlN_3$  materials in spintronics, optoelectronics, and thermoelectrics, where nitrogen-based perovskites are attracting much attention. We recommend that perovskites based on nitrogen are investigated further because of their potential applications.

#### CRediT authorship contribution statement

Ahmed H. Ati: Writing – review & editing, Writing – original draft, Visualization, Validation, Supervision, Software, Resources, Project administration, Methodology, Investigation, Funding acquisition, Formal analysis, Data curation, Conceptualization. Ammar A. Kadhim: Writing – review & editing, Software, Investigation, Conceptualization. Ali A. Abdulhussain: Software, Resources, Investigation. Wed A. Abed: Software. Kadhim Fadhil Kadhim: Software. Maged Abdullah Nattiq: Software. Jabbar M. Khalaf Al-zyadi: Software, Writing – review & editing.

#### Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

#### Data availability

Data will be made available on request.

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