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

Ahmed H. Ati [a], Ammar A. Kadhim [a], Ali A. Abdulhussain [b], Wed A. Abed [c], Kadhim Fadhil Kadhim [d], Maged Abdullah Nattiq [e], Jabbar M. Khalaf Al-zyadi [f,*]

[a] Department of Chemistry, College of Education/Qurna, University of Basrah, Basrah, 61004, Iraq
[b] Department of Physics, College of Science, University of Basrah, Basrah, 61004, Iraq
[c] Department of Pharmacognosy and Medicinal Plants, College of Pharmacy, University of Basrah, Basrah, 61004, Iraq
[d] Department of Biology, College of Education/Qurna, University of Basrah, Basrah, 61004, Iraq
[e] Department of Physics, College of Education for Pure Sciences, University of Basrah, Basrah, 61004, Iraq

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ABSTRACT

In this study, we systematically explored the properties of novel perovskite materials, $XAlN_3$ (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 μ_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 (μ) of −1.37 eV, $CsAlN_3$ 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 $XAlN_3$ (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_3 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, Ruhal 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

* Corresponding author.
E-mail address: jabbar.khalaf@uobasrah.edu.iq (J.M. Khalaf Al-zyadi).

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