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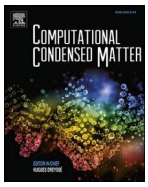

Enhanced thermoelectric performance of double perovskites Ba_2NbBiS_6 and Ba_2TaSbS_6 via carrier engineering and chemical potential tuning

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ABSTRACT

The elastic and thermoelectric properties of Ba_2NbBiS_6 and Ba_2TaSbS_6 were investigated to assess their mechanical stability and thermoelectric efficiency. Elastic property calculations confirmed that both compounds satisfy the mechanical stability criteria. Ba_2TaSbS_6 exhibits a higher bulk modulus (127.34 GPa), shear modulus (54.92 GPa), and Young's modulus (139.83 GPa), indicating superior stiffness and hardness, while Ba_2NbBiS_6, with a lower bulk modulus (112.51 GPa) and shear modulus (48.76 GPa), demonstrates greater ductility, making it more adaptable for flexible applications.

Thermoelectric transport properties were analyzed as functions of temperature, carrier concentration, and chemical potential. At 900 K, Ba_2NbBiS_6 exhibited an initial ZT of 0.6090 at a carrier concentration of $n_0 = -3.2920 \times 10^{19}$ cm^{-3} and chemical potential $\mu_0 = 0.5411$ Ryd, while Ba_2TaSbS_6 had a ZT of 0.4968 at $n_0 = 0.9666 \times 10^{19}$ cm^{-3} and $\mu_0 = 0.62138$ Ryd. An increase in ZT was observed with temperature, attributed to enhanced charge carrier mobility and reduced lattice thermal conductivity. A systematic optimization of carrier concentration through controlled doping led to significant enhancements in ZT, reaching 0.9209 for Ba_2NbBiS_6 at $n = -23.6592 \times 10^{21}$ cm^{-3} and $\mu = \mu_0 + 0.1782$ Ryd, and 0.8646 for Ba_2TaSbS_6 at $n = -1.6144 \times 10^{21}$ cm^{-3} with $\mu = \mu_0 + 0.1073$ Ryd, representing increases of 51.2 % and 74.1 %, respectively. These findings highlight the potential of Ba_2NbBiS_6 and Ba_2TaSbS_6 for high-temperature thermoelectric applications, where a balance between mechanical stability and energy efficiency is crucial. Ba_2TaSbS_6 stands out as a mechanically robust material suitable for high-strength applications, while Ba_2NbBiS_6, with its enhanced ductility, is promising for flexible thermoelectric devices. Future studies should explore doping strategies and nanostructuring techniques to further enhance their thermoelectric properties for practical energy conversion applications.

1. Introduction

Perovskite-based materials, particularly double perovskites, have emerged as a highly versatile class of compounds due to their diverse structural, electronic, and functional properties. These materials are widely explored for applications in optoelectronics, photovoltaics, and thermoelectrics [1,2]. Among them, chalcogenide-based double perovskites have gained significant attention owing to their enhanced stability, strong spin-orbit coupling, and tunable bandgap properties, which are critical for high-performance semiconductor and thermoelectric applications [3,4]. The ability to tailor these materials through chemical substitution and structural modifications has opened new avenues for optimizing their electronic and transport properties, making them promising candidates for next-generation technologies [5,6].

Double perovskites, with the general formula $A_2BB'X_6$ (where A is an alkaline-earth or rare-earth metal, B and B′ are transition metals or main-group elements, and X is a chalcogen or halogen), exhibit unique structural characteristics that distinguish them from conventional perovskites. The ordered arrangement of B and B′ cations within the octahedral framework introduces strong electronic correlations, spin-orbit coupling effects, and tailored bandgap engineering, making them ideal for optoelectronic and thermoelectric applications [7,8]. Furthermore, the flexibility in cation selection allows for fine-tuning of physical properties such as charge transport, phonon dynamics, and mechanical stability, which are essential for energy harvesting and storage technologies [9,10].

Recent studies have identified Ba_2NbBiS_6 and Ba_2TaSbS_6 as promising semiconducting chalcogenide-based double perovskites. First-

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