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Entitled

FIRST-PRINCIPLES CALCULATIONS ON THE ELECTRONIC STRUCTURE, MECHANICAL, VIBRATIONAL, AND THERMAL PROPERTIES OF THE Ca_3 BiN ANTIPEROVSKITE ALLOY

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Abstract

Antiperovskites are the counterparts of perovskites. They have diverse properties that make them physically rich and technologically relevant. In the recent years, the alkaline earth based antiperovskites, especially the ones with small semiconductor bandgap, have captured tremendous attention due to their properties which make them efficient to be used in optoelectronic and thermoelectric applications. In this thesis, we are shading light on the alkaline antiperovskite Ca_3 BiN due to its narrow bandgap. Thus, it can be considered as a promising candidate for thermoelectric and optoelectronic applications. In other words, it can be used to harvest waste thermal energy into electricity at low temperature gradients. To investigate the efficiency of the Ca_3 BiN alloy as a thermoelectric material, an overall study on the various properties of this material has been done in this research. To unveil its properties, we relied on the density functional theory to do the computational work using Wien2k, VASP, and the Phonopy software. The study included the lattice dynamics, structural, elastic, electronic, thermodynamic, thermoelectric, and optical properties of the antiperovskite Ca_3 BiN alloy. The study revealed that Ca_3 BiN has a stable structure, brittle material, and resistive to plastic deformation. It has a bandgap of 0.61 eV using HSE06 exchange correlation which reveals that it is a p-type semiconductor. It has low thermal conductivity, yet high Seebeck coefficient and relatively high electric conductivity which indicates that it has high value of figure of merit. The value of figure of merit has been calculated, and it goes higher ~1 as the temperature goes toward 1000 K and the concentration of charge carries goes higher ~ 〖10〗 ^20 cm^(-3). By studying the optical properties, it is revealed that the Ca_3 BiN antiperovskite alloy is active in the visible to the ultraviolet regions of the spectrum.

Keywords: Antiperovskites, bandgap, Debye temperature, density functional theory, electron localization function, figure of merit, Grüneisen parameter, perovskites, power factor, Seebeck coefficient.