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Structural, optoelectronic and thermoelectric properties of Ca-based antiperovskites Ca3BN (B=As, Bi, P and Sb) compounds: Insights from DFT

Hadjer Bendjilali, Chahed Abbes, Rozale Habib
University of Sidi Bel-Abbes, Algeria

Recently, alkaline-earth based antiperovskites compounds have been proven to be promising candidate for optoelectronic and thermoelectric applications. In this work a theoretical study structural, electronic, optical and thermoelectric properties of Ca3BN (B=As, Bi, P and Sb) compounds using first-principles calculation with the full-potential linearized augmented plane wave (FP-LAPW) method based on the density functional theory (DFT) as embodied in the Wien2k package. The computed lattice constant was found to be in agreement with the available experimental and theoretical results. Electronic properties shows that the nature of materials is semiconducting with small band gaps (Ca3SbN and Ca3BiN) also semiconducting with large band gaps (~insulating : Ca3AsN and Ca3PN) .Important optical responses of studied antiperovskites are found in the visible and ultraviolet energy range .Finally the thermoelectric properties such as Seebeck coefficient and thermal/chemical coefficients, power factor and figure of merit are calculated .Very interesting results shows that the four antiperovskites compounds could be candidate for thermoelectric devices and alternative energy sources.

hadjer.bendjilali@yahoo.com