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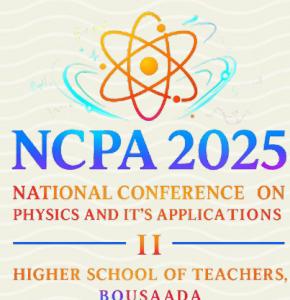
The Organizing Committee of the Second National Conference on Physics and its Applications
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Djamel ALLALI

in recognition of his active participation in the conference with an Oral presentation entitled: “
Structural, elastic and thermodynamic characteristics of trigonal-type Zintl phases $X\text{Zn}_2\text{Sb}_2$ ($X = \text{Ca}$ or Sr) under hydrostatic pressure: Prospects for Advanced Materials in High-Pressure and Ther-
moelectric Devices ”

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Structural, elastic and thermodynamic characteristics of trigonal-type Zintl phases XZn_2Sb_2 (X = Ca or Sr) under hydrostatic pressure: Prospects for Advanced Materials in High-Pressure and Thermoelectric Devices

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Abstract

We analyzed the structural, elastic, and thermodynamic attributes of the trigonal-type Zintl phases $CaZn_2Sb_2$ and $SrZn_2Sb_2$ under hydrostatic pressure through using ab initio calculations within the density functional theory framework. The predicted structural parameters agree excellently with the available experimental values, which strongly validate our method. For both of the chemicals investigated, the [001] crystal orientation exhibits a higher compressibility than the [100] direction. Both compounds predicted monocrystalline elastic constants meet the mechanical stability requirements over a pressure range of up to 20 GPa. The polycrystalline mechanical characteristics were also examined at pressures up to 20 GPa. Indicators such as Pugh's coefficient, Poisson's ratio and Cauchy pressure confirm the brittleness of the studied compounds. At constant pressures of 0, 5, 10, 15, and 20 GPa, the temperature dependence of important macroscopic physical parameters was studied using the quasiharmonic Debye approximation. These parameters include the lattice parameter, bulk modulus, volumetric thermal expansion coefficient, Debye temperature, and isobaric and isochoric heat capacities. The results are deemed trustworthy because the data acquired from the elastic constants correspond most closely to those calculated from the Debye quasiharmonic approximation.

Keywords: 122 Zintl compounds; First-principles calculations; Elastic moduli; Thermodynamic properties; Pressure and temperature effects.

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