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The Organizing Committee of the Second National Conference on Physics and its Applications (20 Novembre 2025) is pleased to award this certificate to :

Fares ZERARGA

in recognition of his active participation in the conference with an Poster presentation entitled: “ First principales studies of pressure dependence of structural, elastic andthermodynamic properties of trigonal-type Zintl phases SrCd2Sb2 and BaZn2Sb2 “

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First principales studies of pressure dependence of structural, elastic and thermodynamic properties of trigonal-type Zintl phases $SrCd_2Sb_2$ and $BaZn_2Sb_2$.

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Abstract

We report ab initio density functional theory calculations of the structural, elastic and thermodynamic properties of the trigonal-type Zintl phases $SrCd_2Sb_2$ and $BaZn_2Sb_2$ under hydrostatic pressure. The predicted structural parameters are in good agreement with the available experimental values, which strongly validate our method. For both of the compounds 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 2 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: *Zintl compounds; First-principles calculations, Elastic moduli; Thermodynamic properties; Pressure and temperature effects.*

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