Ministry of Higher Education and Scientific Research
Higher Normal School of Bou Saada
Department of Science Physics and Laboratory
of Mathematics and Applied Physics

LMAP
LABORATORY OF MATHEMATICS AND APPLIED PHYSICS
المدرسة العليا للأساتذة - بوسعادة
ENS-BOUSAADA
2022

ENS Bou Saada
المجاهد الفريق أحمد قايد صالح

CERTIFICATE OF PARTICIPATION

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

Djamel ALLALİ

in recognition of his active participation in the conference with an Oral presentation entitled: “ Structural, elastic and thermodynamic characteristics of trigonal-type Zintl phases XZn2Sb2 (X = Ca or Sr) under hydrostatic pressure: Prospects for Advanced Materials in High-Pressure and Thermoelectric Devices “

Co-author: Fares ZERARGA, Abdelhak BEDJAOUI, Elhadj BENREZGUA, Missoum RADJAI, Rabie AMARI, Saber SAAD ESSAOUD, Ammar BOUKHARI

NCPA 2025
NATIONAL CONFERENCE ON PHYSICS AND IT'S APPLICATIONS
II
HIGHER SCHOOL OF TEACHERS, BOUSAADA

وزارة التعليم العالي والبحث العلمي
الملتقى الوطني الثاني للفيزياء وتطبيقاتها
المدرسة العليا للأساتذة - بوسعادة

رئيس الملتقى
د. عكه علي

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

Djamel ALLALİ[1;2,✉], Fares ZERARGA[3], Abdelhak BEDJAOUI[4], Elhadj BENREZGUA[1], Missoum RADJAI[5], Rabie AMARI[1], Saber SAAD ESSAOUD[1], Ammar BOUKHARI[1].

[1]*Laboratory of Materials and Renewable Energy, Faculty of Sciences, University Pole, Road Bordj Bou Arreridj, 28000 M'sila, Algeria,*
[2]*Department of Technology, Faculty of Technology, University Pole, Road Bordj Bou Arreridj, 28000 M'sila, Algeria,*
[3]*University Abderrahmane Mira, Department of Physics, Bejaia, 06000, Algeria,*
[4]*Department of Technology, Faculty of Technology, University of Bejaia, 6000, Bejaia, Algeria*
[5]*Laboratory of Physics of Experimental Techniques and Their Applications University of Medea, 26000 Medea, Algeria.*

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 2 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.*

✉*Corresponding Author Email : djamel.allali@univ-msila.dz*