Structural, Electronic and Thermodynamic Behaviours of Full Heusler Alloy Ac2AgPb

Sitanshu Pradhan, Rakesh Kumar Ahirwar and Madhu Sarwan

Department of Physics, Barkatullah University, Bhopal (M.P.) India-462026

corresponding author's e-mail: contactsitanshu.bls@gmail.com

**Abstract**. A theoretical investigation has been conducted on structural, electronic and thermodynamic behaviours of full Heusler compound Ac2AgPb. The compound crystallizes in the L2₁ cubic structure, characterized by the arrangement of actinide, silver, and lead atoms in distinct interstitial sites. Structural properties have been studied in terms of lattice parameter, bulk modulus and pressure derivative of bulk modulus. Optimized lattice parameter is found to be good agreement with available data. The electronic structure reveals metallic behavior, influenced by the hybridization of d-orbitals of the transition metal and s-p orbitals of the heavier elements. Thermodynamic properties, including Debye temperature also explored. This work provides a comprehensive understanding of Ac₂AgPb as a promising candidate for advanced materials in various technological applications.