World Academy of Science, Engineering and Technology
International Journal of Physical and Mathematical Sciences
Vol:8, No:12, 2014

Theoretical Prediction of the Structural, Elastic, Electronic, Optical, and Thermal Properties of Cubic Perovskites CsXF3 (X = Ca, Sr, and Hg) under Pressure Effect

Authors : M. A. Ghebouli, A. Bouhemadou, H. Choutri, L. Louaila

Abstract : Some physical properties of the cubic perovskites CsXF3 (X = Sr, Ca, and Hg) have been investigated using pseudopotential plane–wave (PP-PW) method based on the density functional theory (DFT). The calculated lattice constants within GGA (PBE) and LDA (CA-PZ) agree reasonably with the available experiment data. The elastic constants and their pressure derivatives are predicted using the static finite strain technique. We derived the bulk and shear moduli, Young's modulus, Poisson's ratio and Lamé's constants for ideal polycrystalline aggregates. The analysis of B/G ratio indicates that CsXF3 (X = Ca, Sr, and Hg) are ductile materials. The thermal effect on the volume, bulk modulus, heat capacities CV, CP, and Debye temperature was predicted.

Keywords : perovskite, PP-PW method, elastic constants, electronic band structure
Conference Title : ICP 2014 : International Conference on Physics
Conference Location : Istanbul, Türkiye
Conference Dates : December 05-06, 2014