

Modeling of structural properties of hexagonal semi conductors

Abstract

Bulk modulus of hexagonal structure semiconductors are calculated by using density functional theory (DFT) of full-potential linear augmented plane wave (FP-LAPW) within general gradient approximation (GGA). In this work, a new mathematical model based on analytical expression and differential equation is established. Our calculated values are in accordance with the experimental one.

Keyword

Structure semiconductors; Mathematical model; Density functional theory (DFT)