Differential equations to calculate the ionicity factor of hexagonal structure semiconductors

Abstract

New mathematical models based on analytical expression and differential equations are established. The work aims to model ionicity factor based on energy gap of hexagonal structure semiconductors using density functional theory (DFT) of full-potential linear augmented plane wave (FP-LAPW) within Engel Vosko-General Gradient Approximation (EV-GGA). Our calculated values are in agreement with experimental and theoretical results.