2nd World Congress and Expo on
Nanotechnology and Material Science
April 04-06, 2016 at Dubai, UAE

Theory study of structural, electronic and elastic properties of ternary borides MgBPd3

A. Benamer, A. Roumili and Y. Medkour
Laboratoire d'Etudes des Surfaces et Interfaces des Matériaux Solides (LESIMS), Université de Sétif1, Algéria

We have applied the pseudopotential linearized augmented plane wave (P-W) method to study the structural, elastic and electronic properties of the ternary borides MgBPd3. We have employed the local density approximation (LDA) and the generalized gradient approximation (GGA) for the exchange and correlation potential. The equilibrium lattice constants and the bulk modulus and its pressure derivative are calculated and compared with available experiment and theoretical results. we have also predicted the elastic constants, Young's modulus (E), Poisson ratio (υ), shear modulus (G). The contribution of the different bands was analysed from total and partial density of states curves.