

Structural and electronic properties of zinc blende $B_xAl_{1-x}N_yP_{1-y}$ quaternary alloys via rst-principle calculations

Abstract

The structural and electronic properties of cubic zinc blende BN, BP, AlN and AlP compounds and their $B_xAl_{1-x}N_yP_{1-y}$ quaternary alloys, have been calculated using the non relativistic full-potential linearized-augmented plane wave FP-LAPW method. The exchange-correlation potential is treated with the local density approximation of Perdew and Wang (LDA-PW) as well as the generalized gradient approximation (GGA) of PerdewBurke and Ernzerhof (GGA-PBE). The calculated structural properties of BN, BP, AlN and AlP compounds are in good agreement with the available experimental and theoretical data. A nonlinear variation of compositions x and y with the lattice constants, bulk modulus, direct and indirect band gaps is found. The calculated bowing of the fundamental band gaps is in good agreement with the available experimental and theoretical value. To our knowledge this is the first quantitative theoretical investigation on $B_xAl_{1-x}N_yP_{1-y}$ quaternary alloy and still awaits experimental confirmations.