

Structural, electronic properties of compounds AlAs, BAs and AlP, BP

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Abstract : We determine the structural, electronic properties of AlAs, BAs and AlP BP alloys using the full potential-linearized augmented plane wave method (FP-LAPW) within the density functional theory (DFT). The exchange-correlation potential is treated by the generalized gradient approximation (WC-GGA). The investigation on the effect of composition on lattice constant, bulk modulus and band gap shows not linear dependence on the composition. The ground state properties such as lattice constant, bulk modulus, pressure derivative of the bulk modulus are in good agreement with numerous experimental and theoretical data. For the electronic properties, we used the mBJ-LDA approximation. The bowing of the fundamental gap versus composition predicted on the composition is in a good agreement with experiment.

Keywords : FP-LAPW, DFT, Ternary alloys, bands structure, bowing gap and thermodynamic propertie