Effect of cation substitution on electronic band structure of $ZnGeAs_2$ pnictides: A mBJLDA approach

Abstract

The electronic properties of $ABAs_2$ (A = Zn, Cd; B = Ge, Sn) compounds have been investigated using WIEN2k implementation of full potential linearized augmented plane wave (FPLAPW) method with an aim to study the effect of changing local environment by substituting cation(s) with corresponding next group element in reference compound ($ZnGeAs_2$) on these properties. The exchange and correlation (XC) effects are taken into account by an orbital independent modified Becke-Johnson (mBJ) potential as coupled with Local Density Approximation (LDA) for these calculations. We predict a direct band gap in all these compounds and observe that the band gap decreases with the change of either one or both cations. The calculated band gaps are in better agreement with corresponding experimental ones as compared to other calculations. The electronic band structure is analyzed in terms of contributions from various electrons and the covalency of two bonds, ZnAs and GeAs has been discussed with respect to substitutions.