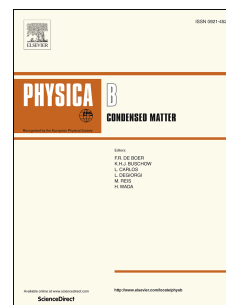


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First-principles investigation of the structural, electronic and optical properties of Ge-doped MgSiAs_2

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Abstract

We report the results of studies on the structural, electronic and optical properties of $\text{MgSi}_{1-x}\text{Ge}_x\text{As}_2$ ($x = 0, 0.25, 0.5, 0.75$ and 1) using density functional theory (DFT) based on the full-potential linear augmented plane wave (FP-LAPW) method. To treat the exchange-correlation potential for the total energy calculations, the generalized gradient approximation (WC-GGA) by Wu-Cohen was used. Additionally, the modified Becke Johnson (mBJ) potential approximation, which successfully corrects the band-gap problem, was used for the band structure calculations. The calculated lattice constants and band-gap values for these alloys are in good agreement with the available theoretical and experimental data. A decrease in the band gap is observed with an increasing Ge content. The dielectric function and absorption coefficient are calculated to investigate the optical properties. Electronic and optical properties reveal that these alloys should be very useful for applications in photonics, optoelectronics and optics.

Keywords: Chalcopyrite; Semiconductors; Band structure; ab initio; DFT; Optoelectronics.

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