Structural and Electronic Properties of $ZnSiAs_2$, $ZnSnAs_2$, and Their Mixed Crystals $ZnSi_{1x}Sn_xAs_2$

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In this work, the structural and electronic properties of the ternary chalcopyrite semiconductors $ZnSiAs_2$ and $ZnSnAs_2$ and their related $ZnSi_{1-x}Sn_xAs_2$ quaternary alloys are presented. The density functional theory (DFT) within full-potential linearized augmented plane wave is employed. To treat the exchange–correlation potential for the total energy calculations, the generalized gradient approximation by Wu−Cohen is used. Additionally, the modified Becke–Johnson potential approximation has also been used to improve the underestimated band gap. For the ternary compounds, the optimized equilibrium structural parameters (a, c, and u) are in good agreement with available theoretical and experimental data. $ZnSi_{1-x}Sn_xAs_2$ alloys are direct band gap semiconductors. The effects of the composition x on lattice parameters, bulk modulus, and band gaps are investigated. A quadratic fit of the lattice parameter, bulk modulus, and band gap is performed, where a non-linear variation with the composition is found. A decrease in the band gap is observed with an increasing Sn content.

Keywords: DFT, alloys, chalcopyrite, band gap.

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