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First-principle calculations of the structural, electronic, thermodynamic and thermal properties of $ZnS_xSe_{1?x}$ ternary alloys

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Abstract: First-principle calculations were performed to study the structural, electronic, thermodynamic and thermal properties of $ZnS_xSe_{1?x}$ ternary alloys using the full potential-linearized augmented plane wave method (FP-LAPW) within the density functional theory (DFT). In this approach the Wu–Cohen generalized gradient approximation (WC-GGA) and Perdew–Wang local density approximation (LDA) were used for the exchange–correlation potential. For band structure calculations, in addition to WC-GGA approximation, both Engel–Vosko (EV-GGA) generalized gradient approximation and recently proposed modified Becke–Johnson (mBJ) potential approximation have been used. Our investigation on the effect of composition on lattice constant, bulk modulus and band gap for ternary alloys shows a linear dependence on alloy composition with a small deviation. The microscopic origins of the gap bowing were explained using the approach of Zunger and co-workers. Besides, a regular-solution model was used to investigate the thermodynamic stability of the alloys which mainly indicates a phase miscibility gap. Finally, the quasi-harmonic Debye model was applied to see how the thermal properties vary with temperature at different pressures

Keywords : FP-LAPW, DFT, energy band structure, Thermal Properties, Debye model, critical temperature