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First principles calculations of structural, electronic and opticalproperties of $Zn_{1-x}Be_xSe_yTe_{1-y}$ quaternary alloys

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Abstract: The structural, electronic and optical properties of $Zn_{1-x}Be_xSe_yTe_{1-y}$ quaternary alloys are investigatedusing the full potential-linearized augmented plane wave (FP-LAPW) method within density functionaltheory (DFT). We used both the Wu–Cohen and the Engel–Vosko generalized gradient approximationsof the exchange-correlation energy that are based on the optimization of the total energy and the corre-sponding potential, respectively. Some basic physical properties, such as lattice constant, bulk modulus,electronic band structures, and optical properties (dielectric constant and refractive index) are calculated,nonlinear dependence on the compositions x and y are found. In addition, the energy band gap of zinc-blende $Zn_{1-x}Be_xSe_yTe_{1-y}$ quaternary alloys lattice matched to GaAs substrate is investigated. To ourknowledge this is the ?rst quantitative theoretical investigation on $Zn_{1-x}Be_xSe_yTe_{1-y}$ quaternary alloysand still awaits experimental con?rmations

Keywords : alloys, Ab initio calculations, Electronic structure, optical properties