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First principles calculations of structural, electronic and opticalproperties of Zn_{1-x}Be_xSe_y Te_{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 investigated using the full potential-linearized augmented plane wave (FP-LAPW) method within density functional theory (DFT). We used both the Wu–Cohen and the Engel–Vosko generalized gradient approximations of 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 $Zn_{1-x}Be_x$ SeyTe_{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 alloys and still awaits experimental con?rmations

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