Structural and Optical Properties of GaAs$_{0.5}$Sb$_{0.5}$ and In$_{0.5}$Ga$_{0.5}$As$_{0.5}$Sb$_{0.5}$: \textit{ab initio} Calculations for Pure and Doped Materials

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Abstract:

We perform a first-principles study to evaluate the structural, electronic and optical properties of GaAs$_x$Sb$_{1-x}$ ternary and In$_y$Ga$_{1-y}$As$_x$Sb$_{1-x}$ quaternary semiconductor alloys up to $x = 0.5$, $y = 0.5$. We employ the Perdew-Burke-Ernzerhof form of the generalized gradient approximation (GGA) within the framework of density functional theory (DFT) by using a simulation program. Calculations are carried out in different configurations. For these alloys, lattice parameters and optical band gap energy are calculated. The optical band gaps vary with increasing and decreasing As and In concentrations, respectively. The optical conductivity, absorption and the real part of the dielectric function $\varepsilon_r(\omega)$ are discussed. Our results agree well with the theoretical and experimental data available in the literature.