First principles study on electronic structure and optical properties of ternary semiconductor $In_xAl_{1-x}P$ alloys

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The elastic, electronic and optical properties of the indium doped AlP, have been investigated by the first-principle calculations within the framework of the density functional theory (DFT). Our calculated lattice constants and bulk moduli for AlP and InP are in good agreement with the available theoretical and experimental data. The lattice constants increase while the bulk modulus decreases with In concentration increasing. The elastic constants C_{ij} of $In_xAl_{1-x}P$ alloys have been calculated for the first time. Result shows that with the increase of indium concentration, the band gap of $In_xAl_{1-x}P$ decreases and varies from indirect band gap to direct band gap; the absorption band edge and the absorption peak move to low energy side; the static reflectivity increases. With the increasing of the incident photon energy, $In_xAl_{1-x}P$ shows metal reflective properties in certain energy range. With the increasing of Indium concentration, static dielectric constant increases and the intersection of dielectric function and the x-axis move towards low energy side; the peak of energy loss function move to high energy side and the peak value reduces.

Keywords: In doped AlP, DFT, elastic properties, optical constants.

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