Nanocomposites and Nanomaterials

First-Principles Calculations on Structural and Electronic Properties of InNP Alloys

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We have reported the structural and electronic properties of high mobility ternary $InN_{1-x}P$ alloys with various P and N concentration. We have obtained minimum 3,125 % of guest atom in the lattice with using 2x2x1 supercell. The results of studied ternary alloy structures are presented by means of density functional theory. For all studied alloy structure, we have implemented geometric optimization before the volume optimization calculation. The obtained equilibrium lattice constants of studied binary compounds are more compatible with experimental data compared to standard semilocal (LDA-PBE) calculations. Electronic band structures of the studied alloys were obtained using the calculated lattice constants at the equilibrium. We found the effects of guest phosphate to host InN band structure, and nitrate to host InP band structure. We have identified the effective mass of electron in ternary InNP alloy with various P and N concentration. All of the calculated materials are characterized by direct band gap along the Γ direction. Our calculated structural and electronic results are in good agreement with other theoretical and experimental values