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Ab initio study of novel III–V nitride alloys $B_{1-x}Tl_xN$ for optoelectronic applications

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Abstract:

In this study, we propose the cubic $B_{1-x}Tl_xN$ ternary alloy as a promising infrared material. We used the full potential-linearized augmented plane wave (FP-LAPW) method within the Density Functional Theory (DFT) to predict the structural, electronic and optical properties of the $B_{1-x}Tl_xN$ ternary alloys. The structural properties such as the equilibrium lattice parameter, bulk modulus and its pressure derivative are investigated with the effect of the concentration variation of Tl atom, x ($x=0, 0.25, 0.50, 0.75, \text{ and } 1$). We note that, because of existence of heavy elements in our alloys, spin-orbit coupling (SOC) is incorporated for electronic and optical calculations in order to test the effect of spin-orbit interaction on these properties. Our results show the direct nature of the energy band gap of the ternary $B_{1-x}Tl_xN$ alloy for all composition of Tl-substitution. Furthermore, investigation of the dielectric function and refractive index shows that our materials are active in infrared and visible energy regions. We found that the spin-orbit effects open up a very small gap at concentrations $x = (0.75 \text{ and } 1)$, resulting in a nearly metallic behavior of its optical response (imaginary part of dielectric function).

Keywords: III-nitrides; III-V; FP-LAPW; GGA-PBEsol, TB-mBJ, Spin-Orbit Coupling; electronic structure; optical properties;

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