

Comparative study of optical properties of $\text{In}_{0.25}\text{Ga}_{0.75}\text{As}$ and $\text{In}_{0.75}\text{Ga}_{0.25}\text{As}$ in zinc-blende phase by first-principles calculations

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Abstract : The full-potential linearized augmented plane wave method (FP-LAPW) within Density Functional Theory (DFT) framework as implemented in the WIEN2K computational code is used in order to study the structural, electronic and optical properties of $\text{In}_{0.25}\text{Ga}_{0.75}\text{As}$ and $\text{In}_{0.75}\text{Ga}_{0.25}\text{As}$ ternaries alloys. The structural parameters such as lattice parameters, bulk modulus, and its pressure derivative were extracted using the Local Density Approximation (LDA)³, and the one of Wu and Cohen (GGA-WC) for the exchange-correlation (XC) functional. In addition, the electronic and the optical properties of our compounds were obtained by using the new semi-local modified Becke–Johnson potential (TB-mBJ) developed by Tran and Blaha. The performed results were compared with experimental data and other computational works. Consequently, our computations of the equilibrium lattice parameter and bulk modulus generally give a good agreement with the experimental measurements. For electronic and optical properties, we deduced that the TB-mBJ approach is relatively more suitable for the properties of our both ternaries alloys.

Keywords : DFT, FP-LAPW, InGaAs, Optical parameters