Comparative study of optical properties of $In_{0.25}Ga_{0.75}As$ and $In_{0.75}Ga_{0.25}As$ 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 $In_{0.25}Ga_{0.75}As$ and $In_{0.75}Ga_{0.25}As$ 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