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Full-potential calculations of structural and optoelectronic properties of cubic indium gallium arsenide semiconductor alloys

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ABSTRACT

In this work, the first-principle calculations have been performed to predict the structural, electronic and optical properties of cubic $In_xGa_{1-x}As$ for $0 \leq x \leq 1$, using 16-atom within the Full Potential Linearized Augmented Plane Wave (FP-LAPW) method based on Density Functional Theory (DFT) as implemented in WIEN2k computational code. The Local Density Approximation (LDA) and Wu–Cohen Generalized Gradient Approximation (WC–GGA) were employed as the exchange–correlation term to calculate the structural and electronic properties. Moreover, the Engel–Vosko GGA (EV-GGA) and the recently modified semi–local Becke–Johnson (mBJ) functional were also used to compute the electronic and optical properties in order to get some better degree of precision. The real and the imaginary parts of the dielectric function, refractive index, extinction coefficient, reflectivity, absorption coefficient and optical conductivity were calculated to discuss the linear optical properties of $In_xGa_{1-x}As$ alloys. The achieved results show a great potential utilization in optoelectronic devices especially in infrared applications.

1. Introduction

Currently, the III–V Semiconductors materials based on GaAs, InAs and their ternary alloys $In_xGa_{1-x}As$ are promising materials in vast scientific and technological usefulness because of their potential use in photonic, electronic and optoelectronic devices, such as, Blue and Green Light-Emitting Diode [1], Metal Insulator Semiconductor Photodetectors, [2], thin films solar cells [3,4], diode lasers [5,6], Electrooptic Waveguide Modulators [7,8], High-Electron-Mobility-Transistor (HEMT) [9] and metal–oxide–semiconductor capacitor (MOSCAP) [10]. In recent years, some experimental and theoretical works have been published about the physical properties of these compounds. Kumar et al. [11] have investigated some of these

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