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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 InxGa1?xAs for 0?x?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 ofthe 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.

**Keywords :** Ab inition, DFT, Cubic, InxGa1-xAs alloys, structural parameters, Optoelectronic properties