

Density functional approach to study structural and electronic properties of III-Sb semi-conductors by modified Becke-Johnson Potential

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Abstract : In this work, we present the structure and electronic properties of the semiconductors III-Sb binaries, using a first principles calculations have been performed, using the FullPotential Linearized Augmented Plane Wave (FP-LAPW) calculations based on Density Functional Theory (DFT) [1-2]. The local density approximation (LDA) and the revised Perdew-Burke-Ernzerhof generalized gradient approximation (GGA-PBEsol) were used only in calculating structural properties, the modified Becke-Johnson (mBJ-GGA) approach were used to calculate the electronic properties. Our calculations are in good agreement with the theoretical works and experimental data, deducing the possibility of these materials to be used in the optoelectronics devices.

Keywords : FP-LAPW, mBJ-GGA, wien2k, structural parameters, electronic properties