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# Calculation of the structural and electronic properties of III-V semiconductor compounds using advanced functionals of density functional theory

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**Abstract**

In this study, the structural and electronic properties of III-V semiconductor compounds are studied using Density Functional Theory computations within the Full Potential Linearized Augmented Plane Wave (FP-LAPW) method. After considering several exchange-correlation functionals, it is determined that the SOGGA and GGA-WC functionals are suitable alternatives for calculating the structural properties of the desired compounds. For the calculation of electronic properties, particularly the energy band gap, the GGA-EV functional and the TB-mBJ exchange potential with spin-orbit correction are approved. The results show that the exchange potential TB-mBJ + SOC accurately calculates the band gap of these compounds. In the case of materials such as TlAs, which have negative band gaps, it is found that the exchange potential TB-mBJ is not able to predict this gap; in fact, the gap is set to zero. For the calculation of the effective mass, several methods are used; after comparing with experimental data, it is found that the GGA-PBE and GGA-EV functionals calculate this quantity for small band gap and large band gap materials, respectively; this is done with proper accuracy and of course, the best effective mass results are obtained with the method of hybrid functional $HSE_{bgfit}$. It is also found that the spin-orbit correction makes the calculated effective mass results closer to the experimental values.

**Keywords:** III-V materials, lattice parameter, energy gap, effective mass, DFT

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