

## **ELECTRONIC STRUCTURE CALCULATION OF BULK SEMICONDUCTORS USING THE $sp^3s^*$ EMPIRICAL TIGHT BINDING METHOD**

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### **ABSTRACT**

The  $sp^3s^*$  empirical tight binding method with fitted input parameters from the literature is used to calculate the band structure of the bulk semiconductor compounds of GaAs and AlAs. Two sets of calculations are performed, namely with and without spin orbit coupling, resulting in 10 and 20 band Hamiltonians, respectively. From these band structures, we then calculate the energy gaps, effective mass of electrons and holes using the curvature method and the corresponding Luttinger parameters. It is found that the energy gaps and effective masses for the spin orbit coupling case are in excellent agreement with their established experimental values. This is as expected as the fitted  $sp^3s^*$  input parameters are optimised for the band gaps and effective masses. However, the corresponding Luttinger parameters are poorly estimated by the fitted parameters available in the literature.

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