

Theoretical investigations of structural, electronic and thermal properties of various phases of ZnO

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Abstract

We present the results of a theoretical study of the structural, electronic and optical properties of all possible phases (rocksalt, zinc blende and wurtzite) of ZnO, using the full-potential linearized augmented plane wave (FP-LAPW) method. The exchange-correlation potential is treated by local density approximation (LDA) and GGA (PBE), a more accurate nonempirical density functional generalized gradient approximation (GGA), as proposed by Wu and Cohen [Phys. Rev. B 73, 235116 (2006)]. Quantities such as, equilibrium lattice constants, bulk modulus, band structures, density of states and optical properties have been calculated for all the phases and the results have been discussed and compared with the existing experimental data. Furthermore, the quasi-harmonic Debye model is applied to determine the thermal properties at room temperature.

Keywords: FP-LAPW; ZnO, Electronic properties, Optical properties.