Theoretical investigations of structural, electronic and thermal properties of CdO and ZnO

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First-principles calculations are performed to investigate the structural, electronic and thermal properties of CdO and ZnO in Rocksalt structure using the full-potential linearized augmented plane wave method. In this approach, the generalized gradient approximation (GGA) of Perdew et al. was used for exchange correlation potentials. Moreover, the alternative form of GGA proposed by Engel and Vosko (GGA-EV) and modified Becke-Johnson exchange correlation potential (MBJ) are also used for band structure calculations. Results are given for lattice constant, bulk modulus and electronic properties are in agreement with experimental and theoretical data. The quasi-harmonic Debye model, using a set of total energy versus volume calculations obtained with the FP-LAPW method which is applied to study the thermal and vibrational effects. Temperature effects on the structural parameters, band gap, thermal expansions, heat capacities and Debye temperatures are determined from the non-equilibrium Gibbs functions.

References

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