Digest Journal of Nanomaterials and Biostructures

Volume 18, Issue 1, 2023, Pages 11-19

# Theoretical study of structural and optical properties of ZnO in wurtzite phase

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**Abstract:** Our calculations are done with the help of density functional theory (DFT). Actually, we could find the structural and optical properties of the wurtzite-type ZnO compound. The pseudo-potential linearised augmented plane wave (PP-LAPW) method is applied to solve the Kuhn-Sham equations. The results are obtained using Both Generalized Gradient Approximation according to the scheme described by Perdew-Burke-Ernzerhof(GGA-PBE) and Local Density Approximation according to the scheme described by Ceperly-Alder (LDA-CA) approximations as two types of exchange-correlation. The convergence of energy and charge has been checked. This is in order to study the properties of the ground state. It was found that the primary cell constants calculated in the equilibrium state are very close to the previous theoretical works. The general results of optical properties including the imaginary part of the dielectric constant, reflectivity, absorption coefficient, refractive index, optical conductivity, and extinction coefficient of wurtzite-phase ZnO under the imposed conditions are discussed and compared with previous works. Our results show new and important optical properties. Besides, we predicted the behavior of transparent conductive oxides in the direction of light.

**Keywords :** ZnO, Structural properties, reflectivity, absorption, Refractive index, Optical conductivity