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# INVESTIGATION OF THE OPTOELECTRONIC PROPERTIES OF ZNO BY DENSITY FUNCTIONAL THEORY

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**ABSTRACT**

This paper presents ab-initio study of electronic band structure and some important optical parameters of ZnO using density functional theory (DFT) based on full-potential linear augmented plane wave (FP-LAPW) method. The exchange-correlation (XC) potential was measured using well known generalized gradient approximation (GGA) for the computation. The structural parameters like lattice constant, bulk modulus, pressure derivative of bulk modulus and electronic band structure are calculated and analyzed for both zinc-blende and high pressure rock-salt structure. Furthermore, some optical properties like dielectric constant, static refractive index and eloss function have also been calculated and explained in details for the energy ranges 14 eV. The obtained results have been found to be in well agreement with earlier observed data in the literature.

**Keywords**: Lattice constant, GGA, LAPW, density functional theory, band structure, ZnO.

 ISBN: 978-81-947843-2-6; DOI: 10.21467/abstracts.108