**Composition dependence on the optical and electrical properties of the wurtzite ZnS1-*x*O*x*: a first principle study**

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**ABSTACT :**

The present contribution aims to give further insights as concerns the structural, electronic and optical properties of ZnS1-*x*O*x* in the zinc-wurtzite phase for *x* vary between 0 and 1, using ab-initio calculations based on the full-potential linearized augmented plane waves (FP-LAPW) method in the framework of the density functional theory (DFT). The structural properties (Lattice constant, Bulk modulus and its pressure derivative) were treated by the Generalized Gradient Approximation (GGA) parameterized by Perdew Burke Ernzerhof (PBE-GGA) formalism. While for the electronic and optical properties calculations, the modified semi-local Becke-Johnson exchange potential has been included with the PBE-GGA formalism to overcome under estimation of band-gap by (PBE). The agreement between our calculated results and available experimental and theoretical data is generally good.

**Keywords:** Structural properties; Optical and electronic properties; DFT; Band-Gap Engineering; mBJ-GGA.