Fundamental properties of the rocksalt ZnO and MgO: an ab-initio prediction

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Abstract : The one of the most accurate first-principales methods is the Full Potential Linearized Augmented Plane Wave (FP-LAPW) formalism, based on Density Functional Theory (DFT), has been exploited to study theatrically, the fundamental properties of the both ZnO and MgO rocksalt binary compound using 16 atoms rocksalt supercell which corresponds to (1×1×2) conventional cell. The Local Density Approximation (LDA) was used only for the structural properties, to treat the exchange-correlation terms. In order to explore the wanted properties. The recently modified semi-local Becke-Johnson potential within LDA correlation in the form of (mBJ) was used to predict the optoelectronic properties of ZnO and MgO binary materials. As results, our computed lattices parameters equal to: 4.22 Å and 4.16 Å respectively, showed satisfactory agreements with experimental values (4.27 Å and 4.2 Å) for ZnO and MgO respectively again. in order to understand the changeability between relaxed and un-relaxed of the electronic structures, The calculated band structures reveal that ZnO posses indirect band gap (?-M) while for MgO have an indirect band gap (?-?) which agree well with the experiment and other theoretical calculations. Optical dielectric function, refractive index, absorption coefficient and optical conductivity, are well described in a wide range of the incident photon energy. The acquired results are used to give an significant guideline to the material's design for optoelectronic applications.

Keywords : ZnO, MgO, FP-LAPW, Electronic materials, Optical parameters, ab initio calculations.