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First principle investigation of structural, electronic and optical properties of Er-doped (ZB) ZnO using modified Becke-Johnson exchange potential.

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Abstract : In this work, we investigated the effect of Er, as a dopant element, on physical properties of ZnO. Structural, electronic and optical properties are obtained for 25% of Er doped ZnO in hypothetical zincblend structure. This study done using Density Functional Theory (DFT) with generalized gradient approximation (GGA) and modified Becke-Johnson exchange potential (mBJ). It found that, the calculated energy band gap and the lattice parameter of pure ZnO are close to the experimental ones and was in a good agreement with other theoretical calculations. It also shown that, the incorporation of Er in ZnO affects considerably the electronic and optical properties. For example, the optical energy gap has increased by 83% under Er doping. From imaginary dielectric function, we established that red shift also achieved under Er doping indicating the importance of its 4f donor occupied states.

Keywords : Er-doped ZnO, FP-LAPW, mBJ potential, Electronic structures, Optical properties.