

First-principles investigation of the optical properties for rocksalt mixed metal oxide $Mg_xZn_{1-x}O$

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Abstract: In this paper, we have presented a theoretical study of the optical properties for the cubic $Mg_xZn_{1-x}O$ ($x = 0.0, 0.125, 0.375, 0.625, 0.875$ and 1.0) alloys using the full-potential linearized augmented planewave (FP-LAPW) method based on the density functional theory (DFT). The local density approximation (LDA) was applied to calculate the structural properties. In order to explore the desired properties, the $Mg_xZn_{1-x}O$ alloys were modeled at various x compositions from 0.0 to 1.0 by step of 0.125. The recently modified semi-local Becke-Johnson potential with LDA correlation in the form of mBJ-LDA was used to predict the energy band gap, optical dielectric function, refractive index, absorption coefficient, reflectivity, optical conductivity and the electron energy loss of $Mg_xZn_{1-x}O$ alloys. The obtained results show good agreement with the experimental data, which indicate that the investigated ternary alloys are among promising material for the fabrication of electronic, optoelectronic devices and their applications.

Keywords : alloys, Electronic materials, Optical materials, Ab initio calculations, Band-structure