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

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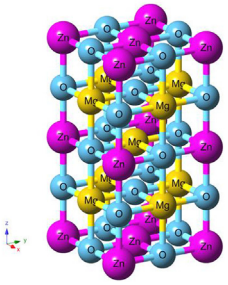
HIGHLIGHTS

- Theoretical study of optical properties of the cubic alloy $Mg_xZn_{1-x}O$.
- The lattice constants, the bulk modulus B and it's pressure derivative B′ were obtained.
- The calculated energy gaps within mBJ show good agreement with the experimental data.
- The optical properties were calculated and discussed in details.

GRAPHICAL ABSTRACT



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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 plane wave (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.

1. Introduction

In recent years, group II-VI semiconductor materials, such as ZnO, MgO and their ternary alloy $Mg_xZn_{1-x}O$, have drawn considerable attention, which have become an important part of our life.

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