First-principles study on optoelectronic properties for caswellsilverite mixed metal oxide MgZnO

In this work, we investigated the optoelectronic properties of MgZnO using density functional theory based on linear augmented plane wave (FP-LAPW) method. To deal with the exchange-correlation potential for total energy calculations, the LDA and GGA approximations were used. In addition, the modified Becke Johnson (TB-mBJ) approach, which successfully corrects the band gap problem, was used for the band structure calculations. The calculated lattice constants and band gap values for this compound are in good agreement with available theoretical data. As well as the dielectric function and the absorption coefficient are calculated to get the optical parameters. The achieved results indicate that this material is particularly interesting for photovoltaic conversion applications.