

Electronic band structure and optical parameters of spinel SnMg_2O_4 by modified Becke - Johnson potential

Abstract

The electronic band structure and optical parameters of SnMg_2O_4 are investigated by the first-principles technique based on a new potential approximation known as modified Becke - Johnson (mBJ). The direct band gap values by LDA, GGA and EV-GGA are underestimated significantly as compared to mBJ-GGA, which generally provides the results comparable to the experimental values. Similarly, the present band gap value (4.85 eV) using mBJ-GGA is greatly enhanced to the previous value by EV-GGA (2.823 eV). The optical parametric quantities (dielectric constant, index of refraction, reflectivity, optical conductivity and absorption coefficient) relying on the band structure are presented and examined. The first critical point (optical absorption's edge) in SnMg_2O_4 occurs at about 4.85 eV. A strong absorption region is observed, extending between 5.4 eV to 25.0 eV. For SnMg_2O_4 , static dielectric constant $\epsilon(0)$, static refractive index $n(0)$, and the magnitude of the coefficient of reflectivity at zero frequency $R(0)$ are 2.296, 1.515 and 0.0419, respectively. The optoelectronic properties indicate that this material can be successfully used in optical devices.