Structural, electronic and optical properties of spinel MgAl₂O₄ oxide

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Abstract

The structural, the band structure, the total density of states, the dielectric function, the reflectivity, the refractive index and the loss function have been calculated for spinel MgAl₂O₄ oxide using density functional theory (DFT). The full potential linearized augmented plane wave (FL-LAPW) method was used with the generalized gradient approximation (GGA). The calculated results show a 5.2eV direct band gap along Γ-Γ direction for this structure. Calculations of the optical spectra have been performed for the energy range 0-40eV. The high frequency dielectric constant, ε(ω), of spinel MgAl₂O₄ oxide is equal to 3.112 and close to experimental value of 2.89. The excitonic transition associated with the fundamental absorption edge increases in the series from 6.27 to 10.19eV. It is shown that the material is transparent in the visible wavelengths and dispersion curve of refractive index is fairly flat in the long wavelength region and rises rapidly towards shorter wavelengths. The refractive index value is 1.774 at 800 nm near the visible region. The energy of volume plasmon, hωₚ, is assigned to the energy of the maximum peak of Im[-ε'(ω)] is 27.66eV.
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