Optik

Volume 166, Issue 1, 2018, Pages 169-176

Optical study of cubic, and orthorhombic structures of XCaCl3 (X = K, Rb) compounds: Comparative Ab initio calculations

A.HADJ LARBI, S. Hiadsi, M. HADJAB, M. A. SAEED

Abstract: The study predicts the optical properties of cubic and orthorhombic structures of XCaCl3 (X = K, Rb) perovskite compounds through electronic band structure computation within the framework of density functional theory (DFT). The ground state functions are computed employing full potential linearized augmented plane wave (FP-LAPW) method. Improved band gap values and the electronic as well as optical properties were calculated by Tran and Blaha modified Becke–Johnson (mBJ) functional. The studied compounds' density of states reveals that Cl-p states dominate the valence band. To understand the optical properties, and predicting the optically isotropic nature of these materials, the real and imaginary parts of dielectric function, refractive index, absorption coefficient, and energy loss spectra are plotted. The present study shows a great potential utilization in ceramic scintillators.

Keywords : DFT, FP-LAPW, Perovskites, Optical parameters, Scintillators