AB INITIO INVESTIGATION OF THE PHYSICAL PROPERTIES OF PEROVSKITE RbCdBr3 STRUCTURE

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Abstract

We investigated the physical properties such as energy band structure, density of states for electrons and optical properties for RbCdBr3 compound using the density functional theory under local density approximation and the generalized gradient approximation in Abinit and Wien2k package programs. The calculated results show that the energy band structure of this crystal has an indirect band gap of value 2.693 eV from high symmetry point G to a point between T-Z high symmetry points. Besides, the real and imaginary parts of complex dielectric function, refractive index, energy-loss functions for volume and surface, coefficients of extinction, reflectivity and absorption along the crystallographic axes are investigated. The obtained results are in agreement with the experimental ones.

Keywords: DFT, electronic properties, structural properties

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