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Ab- initio investigation of physical properties of KTP and RTP

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Abstract
In this work, some physical properties of KTP and RTP single-crystals have been investigated by performing accurate total energy calculations in the framework of density functional theory, using the full-potential linearized augmented plane wave method. Effects of Rb substitution on structural, electronic and optical properties are discussed for KTP single crystal. The structural properties have been calculated using different exchange correlation including LDA, PBE, WC and PBEsol. In addition, PBEsol approximation with more accurate mBJ is employed to calculate values of energy gap. The Pseudo inversion values of both crystals have been calculated by using Pseudo Symmetry software .The Rb substitution effects on pseudosymmetry of KTP and its relation between second-order susceptibility of crystals and the Pseudoinversion values are discussed. Optical constants such as refractive index, birefringence values and absorption coefficients are calculated using the dielectric function. The anisotropy in the linear optical properties of KTP and RTP crystals have been demonstrated

Keywords: DFT, KTP, RTP, structural properties pseudoinversion, dielectric function, anisotropy, birefringence

For full article, refer to the Persian section