

STRUCCTURAL, DYNAMIC AND OPTICAL PROPERTIES OF
DOUBLE-LAYER HEXAGONAL BiTeCl CRYSTAL

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Abstract

The geometric structural optimization, density of states for phonons, phonon band structure and optical features of double-layer hexagonal BiTeCl crystal have been investigated by linearized augmented plane wave method using the density functional theory under the generalized gradient and the local density approximations in this study. Ground state properties of new-type ferroelectric BiTeCl structure were studied. Calculated lattice parameters, ground state properties and experimental results are consistent. Linear dielectric functions and related properties were calculated. The frequency dependent phonon spectrum of hexagonal BiTeCl crystal was calculated using the harmonic approximation model.

Keywords: Structural properties, dynamic properties, optic properties

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