STRUSCTURAL, ELASTIC AND ELECTRONIC PROPERTIES OF BiTeI CRYSTAL

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Abstract

The geometric structural optimization, elastic constants and related properties, electronic density of states and energy band structure of hexagonal BiTeI crystal have been investigated by linearized augmented plane wave method using the density functional theory under the generalized gradient and local density approximations in this study. Calculated lattice parameters, ground state properties and experimental results are consistent. Elastic constants and related properties were calculated. No experimental data we could find in literature to be able to compare elastic properties.

Keywords: Structural properties, elastic properties, electronic properties

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