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(Research Article)
Investigation of thermodynamic and phononic properties of HgTe in Zinc Blende phase using pseudopotential method

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Abstract

In this paper, the phononic and thermodynamic properties of mercury telluride (HgTe) in Zinc Blende phase have been studied. The calculations have been performed with the pseudopotantial method by using Quntume Espresso package that is based on density functional theory. The result of the band structure indicates that the bottom of the conduction band touches the top of the valence band at Γ point, this giving rise to zero bandgaps. The phonon spectrum shows that this compound has a frequancy gap between 80 cm^{-1} and 127 cm^{-1}. Also, the study of thermal properties shows that the heat capacity of this compound in the Zinc Blende phase in low temperatures according to experience is proportional to the third power of temperature and high temperatures reach a value of saturation that is not temperature-dependent, which is consistent with experimental facts.

Keywords: Mercury telluride, Phononic properties, Thermodynamic properties.

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