First Principle Study of Rock Salt, Cesium Chloride and Zincblende for EuTe Compound

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Abstract:

We present first-principle calculations of the structural and electronic properties of rock salt, cesium chloride and zincblende of EuTe compound. The computational method is based on the full potential linearized augmented plane wave method (FP-LAPW). The exchange and correlation energy is described in the generalized gradient approximation (GGA) and the local density approximation (LDA). We have investigated the lattice parameter, bulk modulus, pressure derivative, band gap and the transition pressure for EuTe . The results obtained are in good agreement with theoretical and experimental values.

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