A Study of the structural and electronic properties of LaX (X=Se, Te) in two phases B1, B2 ander high pressure

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Abstract

The objective of this work is a study of the structural properties (lattice parameters, total energy, bulk modulus) and electronic properties (band structure, density of states) of rare earth monochalcogenides LaX (X=Se, Te) under ambient and high pressure in two phases : the face centred cubic structure type B1(NaCl) and the simple cubic structure type B2 (CsCl) were investigated(1) with the full potential linearized plane wave (FP-LAPW) methode implemented in Wien2K code, based on density functional theory (DFT)(2).

The exchange-correlation term is calculated with generalized gradient approximation(3) and local density approximation(4). The equilibrium lattice parameters, bulk modulus B and the minimal energy are investigated and compared with the previous theoretical and experimental data, we have also determined the band structure, total density of states and the electron charge density.

Our results are in reasonable agreement with the available theoretical and experimental data in the litterature.

Keywords: Band structure ; Density of state ; Generalized Gradient Approximation ; Local Density Approximation ; Face centred cubic structure.

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