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STRUCTURAL AND ELECTRONIC PROPERTIES OF BaTe AND SrTe: A FIRST PRINCIPLES STUDY

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ABSTRACT:

First principles calculations have been used to investigate the structural and electronic properties of Alkaline earth (AE) telluride (AE = Ba, Sr) at an equilibrium volume. These compounds form a closed-shell ionic system crystallized in the NaCl-type (B1) structure at an ambient condition. We have considered the pressure induced B1-B2 phase transition of BaTe and SrTe compounds. MT potential method within Density functional theory (DFT) have been adapted to perform the comparative study of Barium Telluride and Strontium Telluride. Exchange correlation energy optimization is used to compute the total energy with the Local density approximation (LDA). The total energy of the system completely depends on the volume. Equilibrium lattice parameter and Bulk modulus of AETe (AE = Ba, Sr) compounds are calculated by using Murnaghan equation of state studies and the results were found to be in satisfactory agreement with the available literature.

Keywords: *Ab-initio calculations; Bulk modulus; Density of states; Semiconducting II-VI materials; Alkaline earth chalcogenides; Optical device.*