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The Pressure Effect and First-Principles Study of Strontium Chalcogenides SrS

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Abstract : The study of the pressure effect on the materials, their functionality and their properties is very important, insofar as it provides the opportunity to identify others applications such the optical properties in the alkaline earth chalcogenides, as like the SrS. Here we present the first-principles calculations which have been performed using the full potential linearized augmented plane wave method (FP-LAPW) within the Generalized Gradient Approximation developed by Perdew–Burke–Ernzerhor for solids (PBEsol). The calculated structural parameters like the lattice parameters, the bulk modulus B and their pressure derivative B' are in reasonable agreement with the available experimental and theoretical data. In addition, the elastic properties such as elastic constants (C11, C12, and C44), the shear modulus G, the Young modulus E, the Poisson's ratio ν and the B/G ratio are also given. The treatments of exchange and correlation effects were done by the Tran-Blaha modified Becke-Johnson (TB-mBJ) potential for the electronic. The pressure effect on the electronic properties was visualized by calculating the variations of the gap as a function of pressure. The obtained results are compared to available experimental data and to other theoretical calculations

Keywords : SrS, GGA-PBEsol+TB-MBJ, density functional, Perdew–Burke–Ernzerhor, FP-LAPW, pressure effect
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