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GGA-PBEsol+TB-MBJ Studies of SrxPb1-xS Ternary Semiconductor Alloys

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Abstract : In this paper, we report a density functional study of the structural, electronic and elastic properties of the ordered phases of SrxPb1-xS ternary semiconductor alloys namely rocksalt compounds: PbS and SrS and the rocksalt-based compounds: SrPb3S4, SrPbS2, and Sr3PbS4. These First-principles calculations 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. For the electronic properties calculations, the exchange and correlation effects were treated by the Tran-Blaha modified Becke-Johnson (TB-mBJ) potential to prevent the shortcoming of the underestimation of the energy gaps in both LDA and GGA approximations. The obtained results are compared to available experimental data and to other theoretical calculations.

Keywords : SrxPb1-xS, GGA-PBEsol+TB-MBJ, density functional, Perdew–Burke–Ernzerhor, FP-LAPW
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