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First-principles investigation of the structural and electronic properties of Sr3Sb2 in hexagonal phase

M. Sedighi, M. Danesh, S. Vaji

Abstract: The electronic and structural properties of Sr3Sb2 were investigated using the Density Functional Theory (DFT). To solve the equations of Kohen-Sham the method of Full-Potential Linearized Augmented Plane Wave (FP-LAPW) was applied. The lattice parameters, volume modulus and the derivative of the volume modulus were calculated.
The band structures were also studied by two different methods of Generalized Gradient Approximation (GGA) and Engle-Vosko Generalized Gradient Approximation (EVGGA).
The results of the calculations by GGA and EV-GGA methods show that this structure is a semi-conductor and predict the energy gap of type Γ→K with a magnitude of 0.412eV and 0.977eV respectively. The effect of pressure on the band structures, the magnitude of the gap, anti-symmetric gap, and the width of the gaps were also studied. With extrapolation of the gap variation with pressure, the metallization pressure was determined which is equal to 19.984GPa. In this work, the electron and hole effective mass were investigated as well by the methods of GGA and EV-GGA.