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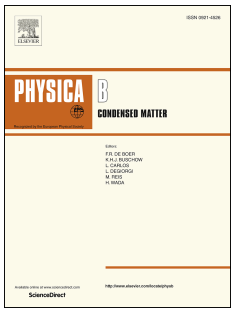

Structural, electronic and thermoelectric properties of bulk and monolayer of Sb_2Se_3 under high pressure: By GGA and mBJ approaches

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Structural, electronic and thermoelectric properties of bulk and monolayer of Sb_2Se_3 under high pressure: by GGA and mBJ approaches

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Abstract

The effects of high pressure on the structural, electronic and thermoelectric properties of Sb_2Se_3 have been studied by using FP-LAPW method combined with Boltzmann transport theory. The variation of lattice constants, band structure, density of states, seebeck coefficient, electrical conductivity, electronic part of thermal conductivity and figure of merit (*ZT*) with pressure (up to 45.2 GPa) are calculated. Our results show that Sb_2Se_3 has a direct band gap of 1.43 eV in the bulk structure and it has an indirect band gap of 0.4 eV in the monolayer structure, at zero pressure. Increasing pressure led to a decrease in the band gap value and the nature of the band gap shifts from direct to the indirect. With the increase in pressure, the seebeck coefficient, electrical conductivity and electronic part of thermal conductivity increase and *ZT* decreases. The maximum *ZT* of 1.12 was achieved at 800 K, $n=10^{19}$ per cm^{-3} for *n* -type doping. Hence, Sb_2Se_3 is a good candidate for thermoelectric applications. The obtained results are in close agreement with the experimental results.

Keywords: Electronic; thermoelectric; pressure; bulk and monolayer; Sb_2Se_3

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