

First principles investigation of magnesium antimonite semiconductor compound in two different phases under hydrostatic pressure

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Abstract: We investigate the electronic and the structural properties of Mg_3Sb_2 in cubic and hexagonal phases using the full potential-linearized augmented plane wave (FP-LAPW) method within the framework of density functional theory. The effects of hydrostatic pressure on band gap, bandwidths of bands under Fermi energy labeled by B1 and B2 from the top, the energy gap between B1 and B2 (anti symmetry gap) and also effective masses of electrons and holes are studied using optimized lattice parameters. We observe that the hydrostatic pressure decreases the band gap and the anti-symmetry gap while it increases the bandwidths of all bands below the Fermi energy. The effective masses of electrons and holes for the hexagonal phase depend on pressure in the G-L direction. In the cubic phase the effective mass of electrons is independent of pressure and the effective mass of holes depend on the pressure in the G-N direction.