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The effect of hydrostatic pressure on the physical properties of magnesium arsenide in cubic and hexagonal phases

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Abstract: Full potential-linearized augmented plane wave (FP-LAPW) method within density functional theory (DFT) was applied to study the structural and electronic properties of the magnesium arsenide in both cubic and hexagonal phases. The exchange–correlation functional was approximated as a generalized gradient functional introduced by Perdew–Burke–Ernzerhof (GGA96) and Engel–Vosko (EV–GGA). The lattice parameters, bulk modulus and its pressure derivative, cohesive energy, band structures and effective mass of electrons and holes (EME and EMH) were obtained and compared to the available experimental and theoretical results. A phase transition was predicted at pressure of about 1.63 GPa from the cubic to the hexagonal phase. The effect of hydrostatic pressure on the behavior of the electronic properties such as band gap, valence bandwidths, anti-symmetry gap (the energy gap between two parts of the valence bands), EME and EMH were investigated using both GGA96 and EV–GGA methods. High applied pressure can decrease (increase) the holes mobility of cubic (hexagonal) phase of this compound.