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Structural, elastic, thermal, electronic and optical properties of Ag_2O under pressure

Abstract

In present paper, the structural, elastic, thermal, electronic, optical properties at ambient and high-pressure study of Ag_2O are performed using the full-potential linearized augmented plane wave (FP-LAPW) method within the framework of Density functional theory (DFT) as implemented in Wien2k Code. We have used the local density approximation (LDA), Generalized Gradient approximation (GGA) and Engel–Vosko generalized gradient approximation (EV–GGA) for calculating structural properties at 0.0–20.0 GPa pressure. The lattice constant obtained at 0.0 GPa using GGA method, is in good agreement with available experimental results. Decrease in lattice constant is observed with increase in pressure from 0.0 to 20.0 GPa. The electronic, optical and band structure calculations are also carried out using modified Becke–Johnson exchange correlation potential plus generalized gradient approximation (mBJ–GGA). At zero pressure, the calculated band gap using mBJ potential is found to be narrow, direct and comparatively better than calculated through LDA, GGA and EV–GGA. Also, the band gap increases with increase in pressure from 0.0 to 20.0 GPa. From elastic calculations, it is noted that Ag_2O is elastically stable and have ductile nature. Moreover, it is revealed that Ag_2O is suitable for optoelectronic devices.

Keywords; Structural, Elastic, Thermal, Electronic, Optical properties, Under-pressure