Electronic, structural, and magnetic properties of TbO under pressure: FP-LAPW study

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Abstract

Using the framework of the density functional theory (DFT), we have calculated the electronic, magnetic and structural properties of TbO in rocksalt (RS), cesium chloride (CsCl), and zincblende (ZB). Full potential linearized augmented plane wave (FP-LAPW) method within the local spin density approximation (LSDA) and generalized gradient (PBE-GGA) approximations are used. Magnetic and nonmagnetic (NM) calculations are performed and a modified version of Becke and Johnson (mBJ) exchange potential has been used to calculate the band gaps. We found that though TbO is stable in a ferromagnetic (FM) state, it is stable in rocksalt phase at ambient condition. Both LSDA and PBE-GGA calculations revealed that the three structures are metallic. However, using the mBJ calculation, it is clear that RS and CsCl phases of TbO compound are metallic, while ZB phase is found to be an insulator in the spin up case and a semiconductor in the spin down case at ambient pressure.