Electronic, Magnetic and Optical Properties of Mn doped SnO2 using Tran-Blaha's modified Becke-Johnson exchange potential

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Abstract

Theoretical study was carried out in Mn doped rutile SnO_2 using recently implemented Tran and Blaha's modified Becke-Johnson exchange potential model (TB-mBJ). The routine density functional theory calculations based on local density approximation (LDA) and generalized gradient approximation (GGA) underestimated the band gap of strongly correlated systems whereas TB-mBJ exchange potential model was found to predict band structures and properties accurately. The electronic, magnetic, dielectric and optical properties have been calculated by full-potential linearized-augmented-plane-wave method (FP-LAPW) by WIEN2k code. The calculated values of magnetic moment, dielectric constant and refractive index of doped and undoped compounds agree well with the literature values. The effect of Mn doping with SnO2 resulted ferromagnetic behaviour, reduction in bandgap and improvement in optical properties in lower energy region.

Keywords: Local density approximation, TB-mBJ, SnO_2, spintronics, FP-LAPW

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