

Electronic structure and x-ray magnetic circular dichroism in Sm-Doped Bi_2Se_3

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One of the most striking discoveries in recent years which has emerged from research into spin-orbit coupling (SOC) is a new state of matter known as a topological insulator (TI). The electronic structure of Sm-doped TI Bi_2Se_3 has been investigated in the generalized gradient approximation (GGA) and GGA+ U approximations using the fully relativistic spin-polarized Dirac LMTO method. The effects of the subtle interplay among the SOC and electron correlations on the electronic structure of the Sm-doped Bi_2Se_3 has been studied. The x-ray absorption spectra (XAS) and x-ray magnetic circular dichroism at the Sm $M_{4,5}$ edges were investigated theoretically from first principles. The calculated results are in good agreement with experimental data (T. Chen *et al.* Adv. Mater. 2015, **27**, 4823–4829). The complex fine structure of the Sm $M_{4,5}$ XAS in Sm-doped Bi_2Se_3 was found to be not compatible with a pure Sm^{3+} valency state. The interpretation demands mixed valent states.