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Electronic structure of Mn and Fe impurities in Bi-Sb-Te
BYUNGKI RYU, KYUNGHAN AHN, SANG MOCK LEE, KYU HYOUNG LEE, Samsung Advanced Institute of Technology — Bi_2Te_3-based thermoelectric materials are well known room temperature thermoelectric materials. Here we present a density-functional study of the electronic structure of Mn and Fe doped p-type Bi-Sb-Te (p-BST) to investigate the effect of metal impurities on the thermoelectronic properties. Our calculations show that, for both Mn and Fe, the substitutional impurity at the Bi/Sb-site is the most stable geometry. Mn is a single acceptor, whereas Fe is an isovalent defect. The metal d bands are located within the host bands, not in the band gap. Due to the octahedral symmetry of the Bi/Sb-site, the metal d bands of Mn and Fe are split into three t_{2g} and two e_g^* states in the high spin configuration. The electronic charge distribution analysis reveals that occupied e_g^* states are well resonant with the host valence bands. As the e_g^* states are located near the valence band maximum, Mn and Fe impurities are expected to enhance the p-type Seebeck coefficient of BST.

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