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Interplay between Mn-acceptor state and Dirac surface states in Mn-doped Bi_2Se_3 topological insulator M.R. MAHANI, A. PERTSOVA, Linnaeus University, Norra Vgen 49, 39182 Kalmar, Sweden, F. ISLAM, Virginia Commonwealth University, Richmond, Virginia 23284, USA, C.M. CANALI, Linnaeus University, Norra Vgen 49, 39182 Kalmar, Sweden — Bi_2Se_3 is a 3D topological insulator (TI) exhibiting a single Dirac cone of surface states localized on the (111) surface. Magnetic impurities embedded in the surface of a TI may cause a breaking of time-reversal symmetry, opening a gap at the Dirac point that changes the topological character of the surface states. Substitutional Mn also introduces acceptor states in the bulk gap of the host material. These acceptor levels can be directly probed by scanning tunneling spectroscopy. However, the nature of these states and their interplay with the Dirac surface states has not been analyzed theoretically. Here we present results of DFT calculations investigating the properties of a single substitutional Mn and its associated acceptor state in Bi_2Se_3TI. In agreement with experiment we find that Mn impurities are in Mn^{2+} valence state, with a magnetic moment close to 5 μ_B. The Mn-acceptor is predominantly of p character and is localized mainly on the Mn and the nearest-neighbor Se atoms. Its electronic structure and spin-polarization are determined by the hybridization with the Mn d levels, which is strongly affected by lattice relaxation and electronic correlations at the Mn site. We argue that magnetism and the topological character of Mn-doped Bi_2Se_3 is the result of this non-trivial interplay between acceptor and Dirac electron spins, and their coupling with the localized Mn magnetic moment.

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