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A first-principles study of magnetic phase transitions in Fe-doped Bi_2Se_3 JEONGWOO KIM, SEUNG-HOON JHI, Pohang Univ of Sci & Tech — Magnetic impurities perturb helical surface states of topological insulators because they act as the spin-flipping scattering centers. Counter-intuitively, the energy gap of the surface states, presumably opened by such scattering, decreases with Fe concentration in Fe-doped topological insulating Bi2Te3 [1]. In addition, the ground magnetic phase of the compound is changed as Fe concentration is increased, which is atypical in dilute magnetic semiconductors. We study the magnetic phase transition and the behavior of surface states in Fe-doped Bi2Se3 using first-principles calculations. We find that the localized spin states of Fe atoms are aligned via hybridization with conduction electrons at dilute doping regimes (<1.7 %) but, at dense impurity levels (>1.7%), are ordered mainly via the super-exchange interaction. We show that topological surfaces states are sensitive to the type of magnetic ordering of adjacent Fe impurities and that the ground magnetic phase barely perturbs the linear band dispersion and the helical nature of the surface states. This finding explains the observation of the band gap of the surface-states in the presence of magnetic impurities.

[1] H.-J. Kim et al., Phys. Rev. Lett. 110, 136601 (2013).

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