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Trends of electronic and magnetic properties of transition-metal impurities in Sb₂Te₃ topological insulator. CARLO M. CANALI, Department of Physics and Electrical Engineering, Linnaeus University, 391 82 Kalmar, Sweden, ANNA PERTSOVA, Nordita, KTH Royal Institute of Technology and Stockholm University, FHOKRUL ISLAM, Department of Physics and Electrical Engineering, Linnaeus University, 391 82 Kalmar, Sweden, ALEXANDER BALATSKY, Nordita, KTH Royal Institute of Technology and Stockholm University; Institute for Materials Science, Los Alamos National Laboratory — The interaction between topological insulator (TI) surface states and magnetic order is crucial for future applications in spintronics and for the realization of novel quantum phenomena such as the quantum anomalous Hall effect (QAHE). Despite experimental progress in measuring the signatures of the QAHE in thin films of magnetically-doped TIs, the fate of the topological surface states, i.e. the presence or absence of a gap upon magnetic doping [1] as well as the nature of magnetic interactions in these systems [2] are under debate. Motivated by on-going experiments, we have systematically investigated the electronic structure and the magnetic anisotropy of transition-metal doped Sb₂Te₃ for both bulk and surface doping, using first-principles calculations based on density functional theory. In addition to magnetization-dependent gap, magnetic dopants introduce impurity states in the gap, whose detailed electronic and magnetic structure depends on the specific character of the dopant. We use these results to identify the conditions for the realization of a robust QAHE. [1] Sessi et al., Nat. Comm. 7, 12027 (2016); [2] Grauer et al., Phys. Rev. B 92, 201304 (2015).

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