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First-Principles Study of Topological Insulators with Defects

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Using first-principles density-functional calculations, we study atomic and electronic structures of topological insulator Bi_2Se_3 with defects and Sb (111) surface with magnetic impurities. The spin-orbit interaction is implemented into the SIESTA code in a form of additional fully non-local projectors, and supercells are used to calculate surface band structures. As for Bi_2Se_3, we consider Bi vacancy, Se vacancy, and Bi substitutional defects on Se sites, and Se substitutional defects on Bi sites. We examine effects of these defects on atomic structures, local densities of states, and the energy-band dispersion of the topological surface states. As for Sb (111) surface, we consider interstitial Fe impurities and substitutional Mn impurities, and we obtain their effects on electronic structures by simulating ARPES spectra and calculating local densities of states near the Fermi level as well as band dispersions and projected densities of states near the impurities. We discuss different characteristics of defects in Bi_2Se_3 and effects of magnetic impurities on surface electronic structures in Sb. This work was supported by the NRF of Korea (Grant No. 2011-0018306) and KISTI Supercomputing Center (Project No. KSC-2012-C2-14).