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Ab initio study of topological surface states of Sb (111) surface with magnetic impurities JINHEE HAN, HYUNGJUN LEE, HYOUNG JOON CHOI , Department of Physics and IPAP, Yonsei University — We study effects of magnetic impurities on topological surface state of Sb (111) surface by using an ab-initio pseudopotential density-functional method. We have implemented the spin-orbit interaction into the SIESTA code in a form of additional fully non-local projectors. To calculate surface band structures, we use a slab of Sb using a 4x4 supercell containing 20 atomic layers. In particular, we compare Fe impurities with Mn impurities, whose atoms have larger magnetic moments, and compare interstitial impurities with substitutional impurities for each atom. To understand the impurity effects on the topological surface states, we simulate ARPES spectra and calculate projected density of states of impurity near Fermi level. This work was supported by NRF of KOREA (Grant No. 2011-0018306) and KISTI supercomputing center (Project No. KSC-2012-C2-14).

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