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Iron impurities on Sb (111) surface and their effects on topological surface state JINHEE HAN, HYUNGJUN LEE, HY-OUNG JOON CHOI, Department of Physics and IPAP, Yonsei University — We study iron impurities on Sb (111) surface and their effects on topological surface state by using an *ab-initio* pseudopotential densityfunctional method. We implemented the spin-orbit interaction into the SIESTA in a form of additional fully non-local projectors. To calculate electronic structure of topological surface states, we consider a slab of Sb using a supercell containing 20 atomic layers with experimental bulk Sb lattice parameters. We determine atomic positions of Fe impurities on Sb (111) surface by minimizing the total energy, and calculate surface band structures near the Fermi level. To find effects of the impurity on the surface states of Sb (111) surface, we simulate ARPES spectra as a function of impurity density on the surface. From the results, we find that Fe impurity states are present near Fermi level and they strongly interact with the surface states. This work was supported by the NRF of Korea (Grant Nos. 2009-0081204 and 2011-0018306) and KISTI Supercomputing Center (Project No. KSC-2011-C2-04).

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