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Spatial characters of metallic surface states of topological insulators JINHEE HAN, HYUNGJUN LEE, HYOUNG JOON CHOI, Department of Physics and IPAP, Yonsei University — We study the electronic structure of metallic surface states in Bi_2Se_3, Bi_2Te_3, and Sb_2Te_3 using an ab-initio pseudopotential density-functional method. We implemented the spin-orbit interaction into the SIESTA in a form of additional fully non-local projectors. For surface states on (001) surface, we used a supercell containing 10 quintuple layers. We obtained bulk and surface electronic structures of topological insulators Bi_2Se_3, Bi_2Te_3, and Sb_2Te_3, which are close to previous theoretical results and consistent with Dirac-cone band dispersions measured by angle-resolved photoemission spectroscopy. Then, we analyzed the wavefunctions of the metallic surface states near the Fermi level to find out spatial distributions of the surface-state wavefunctions, which turn out to be localized in the surface region with a typical spread of about 2 quintuple layers, and the shapes of the wavefunctions around Bi (or Sb) atoms close to the surface. This work was supported by the NRF of Korea (Grant No. 2009-0081204) and KISTI Supercomputing Center (Project No. KSC-2008-S02-0004).

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