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The Role of d-Orbitals in the Rashba Splitting on Au(111) and Ag(111) HYUNGJUN LEE, HYOUNG JOON CHOI, Department of Physics and IPAP, Yonsei University — We investigate the Rashba-type spin splitting in sp-derived Shockley surface states on (111) surfaces of noble metals, such as Au(111) and Ag(111), based on first-principles calculations including the spin-orbit interaction. By turning on and off l-dependent spin-orbit coupling one by one, we find that although the surface states on Au(111) have predominantly p-orbital character, the spin splitting in energy originates mainly from d-orbital character of the surface states. We also demonstrate that the spin splitting in surface states of both metallic surfaces of Au(111) and Ag(111) can be controlled by varying the sizes of d-orbital parts of the surface-state wave functions. These results show that in addition to difference in the atomic spin-orbit strength in Au and Ag, difference in d-orbital contributions to the surface states makes substantial difference in the sizes of the Rashba-type spin splitting in their surface electronic structures. 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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