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Mechanism for asymmetric charge distribution in Rashba-type surface states and the origin of the energy splitting scale[1] BEOMYOUNG KIM, WONSIG JUNG, YEONGKWAN KIM, YOONYOUNG KOH, WONSHIK KYUNG, CHANGYOUNG KIM, Yonsei University, PANJIN KIM, JUNG HOON HAN, Sungkyunkwan University, JOONBUM PARK, JUN SUNG KIM, Pohang University of Science and Technology, MASAHARU MATSUNAMI, SHIN-ICHI KIMURA, UVSOR Facility, Institute for Molecular Science and Graduate University for Advanced Studies — The mechanism for Rashba-type band splitting is examined in detail. We show how an asymmetric charge distribution is formed when the local orbital angular momentum (OAM) and crystal momentum get interlocked due to surface effects. An electrostatic energy term in the Hamiltonian appears when such an OAM- and crystal-momentum-dependent asymmetric charge distribution is placed in an electric field produced by inversion-symmetry breaking. Analysis by using an effective Hamiltonian shows that, as the atomic spin-orbit coupling (SOC) strength increases from weak to strong, the originally OAM-quenched states evolve into well-defined chiral OAM states and then to states of total angular momentum J. In addition, the energy scale of the band splitting changes from the atomic SOC energy to electrostatic energy. To confirm the validity of the model, we performed circular dichroism angle-resolved photoemission spectroscopy experiments as well as first-principles calculations. We find that the effective model can explain various aspects of the spin and OAM structures of the system.

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