A mechanism for orbital angular momentum and giant spin-splitting in solids and nanostructures

Sehoon Oh and Hyoung Joon Choi*
Department of Physics and IPAP, Yonsei University, Seoul 03722, Korea

Giant spin-splitting of electronic bands, which is several orders of magnitude greater than Rashba splitting, has been observed in noble-metal surfaces, thin films of transition-metal dichalcogenides, etc. Here, we study structural and orbital conditions for emergence of a giant spin-splitting by using tight-binding and first-principles calculations. We find that broken mirror symmetry of local atomic structure around an atom can produce non-zero orbital angular momentum (OAM) at the atom. This OAM results in a giant spin-splitting if the atom is a high-atomic number element. We demonstrate these structural and orbital conditions in the cases of simple atomic chains, WSe_2 monolayer, Au(111) surface, and bulk HgTe. Based on this mechanism of the spin-splitting, we suggest methods to control the magnitude and direction of spins, which can be used in applications such as spintronic devices. This work was supported by NRF of KOREA (Grant No. 2011-0018306) and KISTI supercomputing center (Project No. KSC-2015-C3-039).