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A mechanism for orbital angular momentum and giant spin-splitting in solids and nanostructures SEHOON OH, HYOUNG JOON CHOI, Department of Physics, IPAP, and Center for Computational Studies of Advanced Electronic Material Properties, Yonsei University, Seoul 03722, Korea — Giant spin-splitting (GSS) of electronic bands, which is several orders of magnitude greater than Rashba model, has been observed in various systems including noble-metal surfaces, thin film of transition-metal dichalcogenides, often accompanied by the orbital angular momentum (OAM). Here, we study structural and orbital conditions for emergence of a GSS 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 OAM at the atom. This OAM results in a GSS 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 GSS, 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).

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