Highlights

Innovative materials with strong interplay of spin orbital charge and topological degrees of freedom - 2019

Band splitting with vanishing spin polarizations in noncentrosymmetric crystals

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The Dresselhaus and Rashba effects are well-known phenomena in solid-state physics, in which spin–orbit coupling splits spin-up and spin-down energy bands of nonmagnetic noncentrosymmetric crystals. Here, we discuss a phenomenon we dub band splitting with vanishing spin polarizations (BSVSP), in which, as usual, spin-orbit coupling splits the energy bands in nonmagnetic non-centrosymmetric systems. Surprisingly, however, both split bands show no net spin polarization along certain high-symmetry lines in the Brillouin zone. In order to rationalize this phenomenon, we propose a classification of point groups into pseudo-polar and non-pseudo-polar groups. By means of first-principles simulations, we demonstrate that BSVSP can take place in both symmorphic (e.g., bulk GaAs) and non-symmorphic systems (e.g., two dimensional ferroelectric SnTe). Furthermore, we identify a linear magnetoelectric coupling in reciprocal space, which could be employed to tune the spin polarization with an external electric field. The BSVSP effect and its manipulation could therefore form the basis for future spintronic devices.

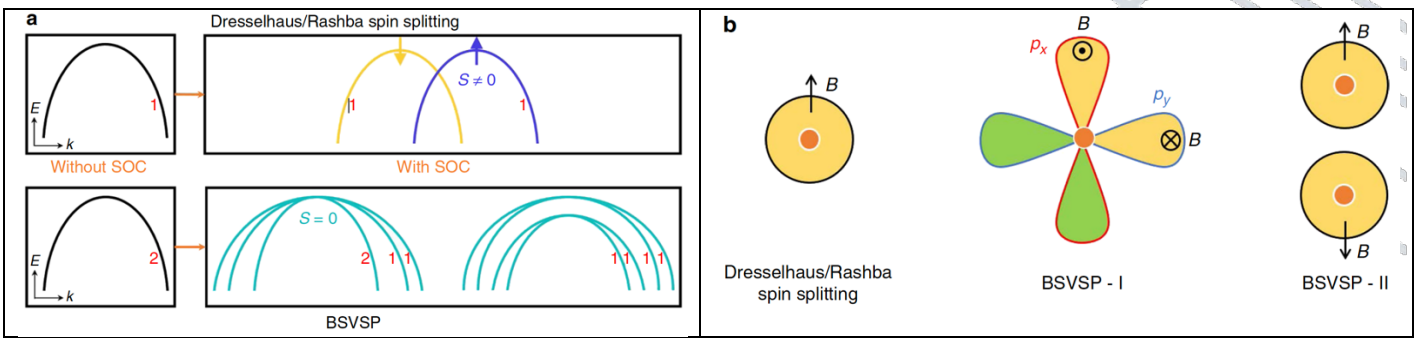

Fig. 1 The phenomena and mechanisms of Dresselhaus/Rashba spin splitting and BSVSP. a) Schematic depiction of Dresselhaus/Rashba spin splitting and BSVSP. "1" and "2" means single and double degenerate, respectively. In the Dresselhaus/Rashba spin splitting case, a non-degenerate band (without considering spin) splits into two bands with opposite nonzero spin polarizations. In the case of BSVSP, a double degenerate band (without considering spin) splits, resulting in some non-degenerate bands without net spin polarizations. b) Schematic illustration of the difference between Dresselhaus/Rashba spin splitting and BSVSP. In the case of Dresselhaus/Rashba spin splitting, a k-dependent magnetic field induces the band splitting. In BSVSP–I (II), the magnetic fields acting on two different p orbitals of the same atom (acting on different atoms of the same kind) are equal in strength but opposite, resulting in a band splitting with vanishing spin polarization