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The appearance of a switch in orbital texture and the resulting absence of complete spin polarization in a Rashba semiconductor[1] QIHANG LIU, XIUWEN ZHANG, ALEX ZUNGER, University of Colorado, Boulder — We consider spin-orbit coupling (SOC) induced spin splitting and spin polarization in nonmagnetic bulk materials lacking inversion symmetry, in which a pair of side-by-side bands that cross at some wavevector K is formed. We find that (i) even though in the semi-classical single-electron model the two bands manifest complete spin polarization, we find via density functional theory and $k \bullet p$ modeling that SOC-induced spin splitting in real materials does not necessarily manifest complete spin polarization. (ii) Away from band crossing point K and looking at the same wavevector, the spin polarization in different branches does not compensate each other. When considering the full pair of spin-split bands this leads to a net spin texture. We explain this unexpected phenomenon and find that the key factor here is the complex interplay between spin and orbital textures entangled by SOC. (iii) In surprising analogy to the surface states of topological insulators (such as Bi_2Se_3), a bulk Rashba compound (such as BiTeI) also exhibits a switch of in-plane orbital character between radial and tangential orbital at the critical band crossing point K. These observations provide a different thinking on the fundamental concept of SOC-induced spin polarization, and opens a new route for manipulating spin degree of freedom by the atomic-orbital feature.

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Qihang Liu
University of Colorado, Boulder

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