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Hidden spin polarization in inversion-symmetric bulk crystals QIHANG LIU, XIUWEN ZHANG, Univ of Colorado - Boulder, JUN-WEI LUO, National Renewable Energy Laboratory, ARTHUR FREEMAN, Northwestern University, ALEX ZUNGER, Univ of Colorado - Boulder — Spin-orbit coupling (SOC) can induce spin polarization in nonmagnetic 3D crystals when the inversion symmetry is broken, as manifested by the bulk Rashba (R-1) and Dresselhaus (D-1) SOC effects. Here we note that these spin polarization effects originate fundamentally from atomic site asymmetries, producing site dipole field (DF) or being site inversion asymmetry (IA), rather than from the well-known bulk space-group crystal asymmetry. In non-centrosymmetric crystals where bulk inversion symmetry is absent, the local atomic polarizations due to site DF and site IA add up to create the bulk R-1 and D-1 net polarization effects, respectively. On the other hand, in centrosymetric crystals with sectors α and β that form together inversion partners, the ***total*** spin is zero in every twofold-degenerate energy bands (termed spin degenerate). Yet we find that ***local spin polarization*** can exist on each asymmetric sector, leading to "R-2" or "D-2" spin polarizations respectively. These local spin polarizations from asymmetric sectors $\alpha$and β compensated each other, forced by the bulk inversion symmetry. We demonstrate such remarkable R-2 and D-2 polarizations in some specific centrosymmetric crystals by first-principles calculations. This understanding leads to the recognition that a previously overlooked hidden form of spin polarization should exist in a much broader class of 3D bulk solids that own global inversion symmetry, and thus open the possibility to provide new routines for manipulating electron spins.

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