International Workshop on Nanotechnology (Tnano20)
October 5 – 8, 2020, in Tbilisi, Republic of Georgia

UNUSUALLY STRONG "HIDDEN" RASHBA EFFECTS IN Si_2Bi_2

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In addition to spin-orbit coupling (SOC), it is an asymmetric crystal potential that induces Rashba (R-1) spin splitting observed at surfaces or interfaces. The R-1 states are characterized by a Mexican hat-like band dispersion with spin-momentum locking described by

$$H_R = -\alpha_R \boldsymbol{\sigma} \times \mathbf{k} \cdot \hat{z},$$

where $\alpha_R, \boldsymbol{\sigma},$ and $\mathbf{k}$ are Rashba strength coefficient, Pauli spin matrix, and crystal momentum; and $\hat{z}$ indicates the direction of local electric field created by the asymmetric crystal potential. Recently, it has, however, been found that even centrosymmetric materials can exhibit a similar but distinct spin splitting called "hidden" Rashba (R-2) effect, such as spatially-segregated spin splitting or spin-layer locking (SLL) as shown in Fig. 1. To understand the underlying physical origin of such R-2 phenomena, we used the first-principles density functional theory and model Hamiltonian calculation to investigate a new two-dimensional (2D) materials Si_2Bi_2, which we identified to possess an ideal condition for the strong R-2 SLL. Our study revealed that the hidden SLL can be determined by a competition between the SOC and sublayer-sublayer interaction. We evaluated the Rashba strength to be 2.16 eVÅ, which is the greatest value ever observed in 2D R-2 material to the best of our knowledge. [1, 2]

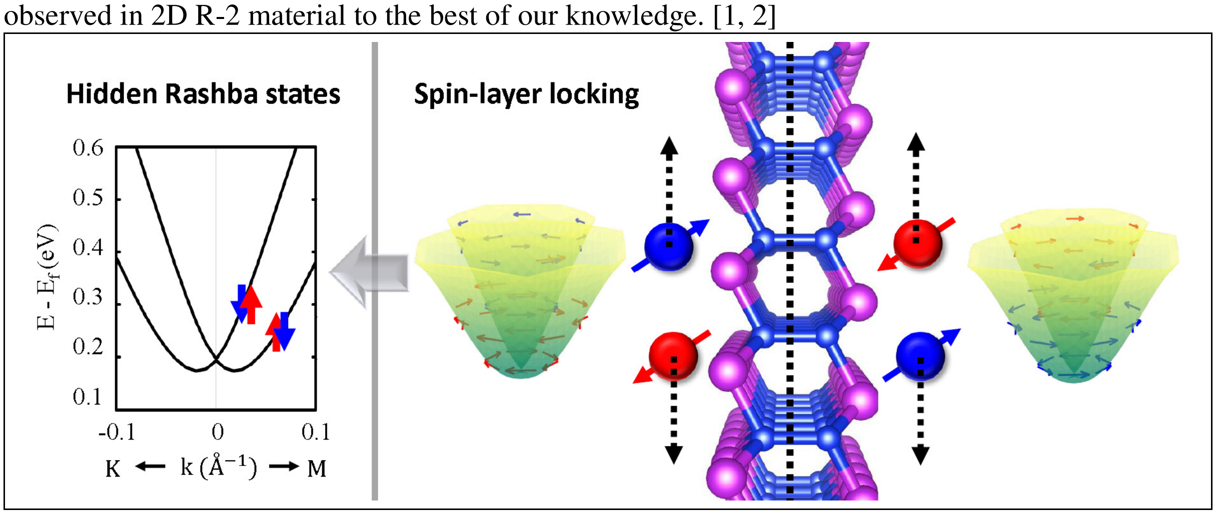

Figure 1. Hidden Rashba states corresponding to the spatially segregated Rashba spin splitting called spin-layer locking observed in an equilibrium phase of Si_2Bi_2 with the inversion symmetry.

References

[1] S. Lee and Y.-K. Kwon, arXiv:2007.06742 [cond-mat.mtrl-sci] (2020).
[2] S. Lee and Y.-K. Kwon, arXiv:2007.05137 [cond-mat.mtrl-sci] (2020).