

Thesis Summary

Spin- and angle-resolved photoemission spectroscopy study of spin-momentum-layer locking in centrosymmetric BiOI

(スピン角度分解光電子分光による中心対称 BiOI におけるスピン・運動量・レイヤーで固定化された電子状態の研究)

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The electron spin in nonmagnetic crystal is degenerated under the protection of time-reversal and space inversion symmetries. The spin-orbit coupling (SOC), however, lifts the spin degeneracy if the space inversion symmetry is broken, termed as the Rashba or Dresselhaus spin splitting. Recently novel types of the Rashba spin splitting and/or Dresselhaus spin splitting have been predicted and confirmed in the centrosymmetric crystals, which is fundamentally derived from the asymmetry of the specific atomic site, rather than the asymmetry of the global crystal space group. Given the spin polarization or spin texture exists on a sector (quasi-2D sublattice) as well as its inversion partner sector in the unit cell, it is called the hidden spin polarization (HSP), as there is no net spin polarization for the whole crystal because spin polarization direction on a sector is anti-parallel to that on the inversion partner sector. The HSP on the sector, however, may be reduced via the interaction with its inversion partner, impeding potential applications of this effect.

Due to the compensation of the spin of the opposite sectors, it is not trivial at all to retain highly polarized spin texture of a given local sector. In order to obtain sizable net polarization in each sector, apart from a strong SOC, one should minimize the compensation between the sectors connected to the inversion symmetry point. A trivial strategy is to separate the opposite sectors as far as possible, for example, inserting a thick slab between the opposite sectors. However, even though the two opposite sectors are far away enough, there is still an unavoidable compensation of the opposite sectors, besides the difficulty in the realization of such type materials.

Here, we proof another non-trivial, symmetry-assisted strategy to minimize compensation and achieve a highly spin-polarized spin texture in each local sector protected by nonsymmorphic symmetries in centrosymmetric lattice. Based on the tight-binding model, if two opposing sectors are connected to each other through nonsymmorphic symmetry, the energy bands along the Brillouin zone (BZ) boundary have at least two-fold degeneracy derived from the energy bands on the two adjacent sectors with anti-parallel spin texture. These bands are fourfold degeneracy at the time-reversal invariant momentum (TRIM). The interaction

(compensation) between the adjacent sectors disappears along the BZ boundary and hence the HSP with high spin polarization can be realized on two sectors that are closely connected via the centrosymmetry point.

As a promising example, here we examined BiOI single crystal whose space group is $P4/nmm$ in which there exists a centrosymmetric point, glide planes and screw axes, such that the requirements on the symmetry properties are fulfilled and should have the HSP based on the theoretical considerations. In this study, we systematically investigated the electronic states of BiOI by means of spin and angle resolved photoemission spectroscopy (spin-ARPES). We find that the compensation of the spin polarization is substantially suppressed along the Brillouin zone boundary leading to a highly polarized spin state up to about 80% along the M-X direction, while the spin polarization is no more than 30% near the zone center (Gamma point) due to the strong compensation by its inversion partners. The observed band structure and spin texture show good agreements with our theoretical calculations, fully confirming the HSP protected by nonsymmorphic symmetry. Our study provides evidence how one can design and realize highly spin-polarized electronic states in nonmagnetic centrosymmetric solids using lattice symmetry, providing the guiding principle to design materials for the future spintronics devices.