Designing a Higher-Order Topological Insulator Composed of Bismuth-Halide Chains

Low dimensional van der Waals (vdW) materials have been extensively studied as a platform to generate exotic quantum properties. Advancing this view, a great deal of attention is currently focused on topological materials with vdW structures, which are expected to bring a functionality in topological materials for future spintronics applications. In particular, a higher-order topological insulator (HOTI) in three-dimensions is highly sought after, since spin-polarized electrons are confined in one-dimensional (1D) hinges of a crystal, leading to a non-dissipative spin current that prohibits the mutual scattering of up- and down-spin. To date, only bulk bismuth has been experimentally shown to be in the higher-order topological phase. However, bulk bismuth is a semimetal, and thus it has been desired to find a bulk insulating HOTI in real materials, which allows one to extract the spin current without contamination by bulk conduction.

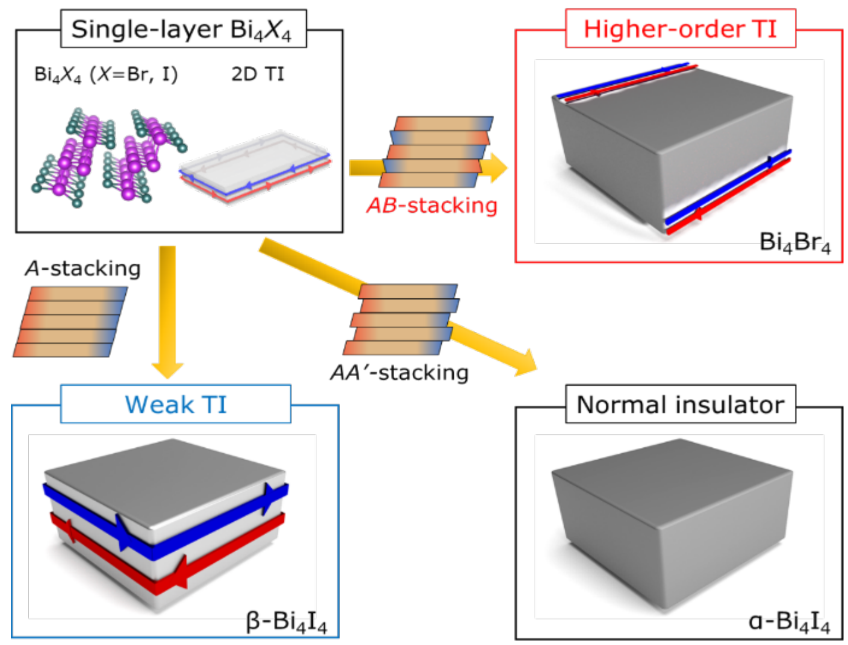

Figure 1. Construction of various topological phases based on quasi-1D bismuth halide chains. In a normal insulator, the whole crystal is insulating, whereas particular surfaces become metallic in a weak topological insulator (weak TI) with an insulating bulk. In a higher-order topological insulator (higher-order TI), only the hinges of a crystal become metallic, where dissipationless spin currents are expected to flow.

In the highlighted work, researchers provided evidence for a HOTI state in a vdW-stacked quasi-1D insulator Bi_4Br_4. Interestingly, various topological phases can be selected in quasi-1D bismuth halides Bi_4X_4 (X=Br, I) by changing the stacking sequences of Bi_4X_4 chains. In the form of a two-dimensional sheet consisting of the chains, bismuth halides are expected to be two-dimensional topological insulators (2D TIs) with metallic edge states (Fig. 1). By stacking these sheets to form a three-dimensional crystal as having a single-layer per unit cell (*A*-stacking: β-Bi_4I_4), a weak topological insulator (WTI) state will emerge, generating topological surface states on the side surfaces. In α-Bi_4I_4, the sheets are stacked with slight shifting (*AA′*-stacking) to form a double-layered structure, which inevitably makes the system a normal insulator, according to the Z_2 topological index. While Bi_4Br_4 also takes a double-layered structure, each layer is alternately rotated by 180° (*AB*-stacking). In this case, although the Z_2 is trivial, the criteria of Z_4 invariant expects a non-trivial topology, leading to a HOTI phase, in which metallic hinge states emerge in the bulk band gap. These hinge states, confined in one-dimension, could be the source of dissipationless spin currents.

The Bi_4Br_4 single crystals are ribbon-like (the top panel of Fig. 2a), reflecting the quasi-1D crystal structure. Importantly, the crystal exposes many terraces and steps in the chain directions on the surface after simple cleavage by a tape, as revealed in the laser-microscope image (the bottom panel of Fig. 2a). This indicates that a bunch of hinges are naturally created on the surface, offering a possibility to detect the strong enough photoemission intensities from the hinge state and uncover its electronic structure.

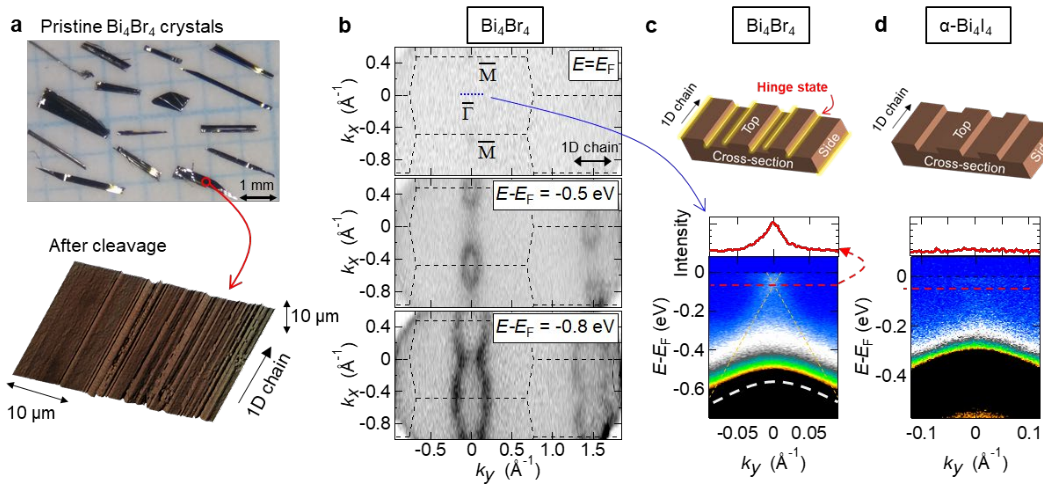

Figure 2. ARPES results of a higher-order topological insulator Bi_4Br_4. (a) Photograph of single crystals (top) and laser microscope images of cleaved crystals (bottom). Many hinges appear on the cleaved surface. (b) ARPES maps along k_y-k_x sheets at different binding energies. Highly anisotropic features are detected. (c) Magnified ARPES image of Bi_4Br_4. In gap states are detected in consistent with the HOTI phase. (d) No in-gap signals have been detected in a normal insulator α-Bi_4I_4.

The electronic structure of Bi_4Br_4 was investigated by angle-resolved photoemission spectroscopy (ARPES) at SSRL beam line 5-2 and at other facilities. Variable photon energies were employed to capture the band dispersions in the 3D momentum space. As shown in Fig. 2b, island-like patterns are observed at the Fermi level (E_F); these intensities most likely come from the spectral tail of the unoccupied conduction bands. At higher binding energies, highly anisotropic band structures with a strong dispersion are resolved along the chain direction. In contrast, the bands weakly disperse in the directions perpendicular to the 1D chain, reflecting the vdW-stacking between bismuth halide chains. In addition, a semiconducting gap of ~0.3 eV was observed, which is relatively large as a topological insulator. Additional high-resolution measurements were performed, and metallic in-gap states with quasi-1D Dirac-like linear dispersion was detected, consistent with the prediction for the topological hinge states in the HOTI state (Fig. 2c). The result is in sharp contrast to the case of a normal insulator α-Bi_4I_4, which shows no indication of the in-gap state (Fig. 2d). The difference in the ARPES results between Bi_4Br_4 and α-Bi_4I_4 clarifies the stacking dependence of the topological properties in quasi-1D bismuth halides.

The results presented in this study not only provide experimental evidence for the HOTI state in Bi_4Br_4, but also propose an excellent functionality of noble topological materials built from vdW-stacking, where the flow of spin currents can be switched by selecting different stacking sequences.

Primary Citation

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