Origins of electronic bands in the antiferromagnetic topological insulator $MnBi_2Te_4$

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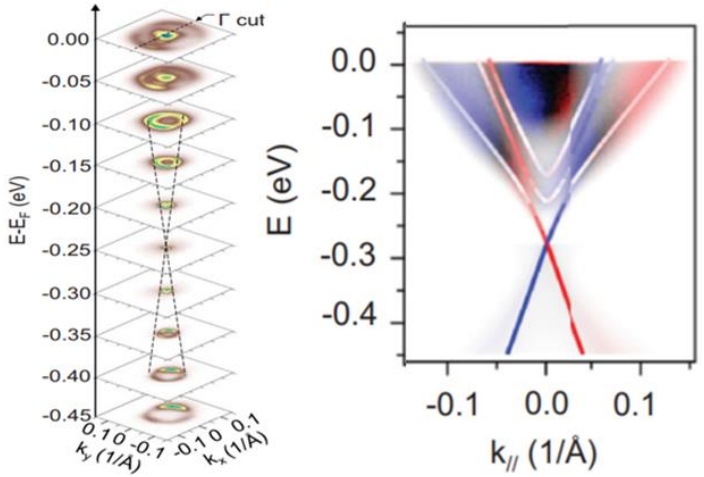
Project Summary: $MnBi_2Te_4$ has been established as the first intrinsic antiferromagnetic (AFM) topological insulator. Although the predicted exotic states such as quantum anomalous Hall insulator and axion insulator have been demonstrated in this material, the origin of the electronic bands is still unclear. Through an in-depth investigation by ARPES experiment and the numerical calculations, an upper bound of 3 meV for the gap size of the topological surface state (TSS) is estimated. Furthermore, we also reveal band chiralities for both the TSS and quasi-2D bands, which can be well reproduced in a band hybridization model based on the circular dichroism measurements. Importantly, we numerically simulate the energy-momentum dispersions based on a four-band model with an additional step potential near the surface. The step potential confines the spin-orbit-coupled quantum well states in addition to the TSS, providing a possible microscopic explanation for the quasi-2D bands. In this study, we offer a solid step forward in reconciling the existing controversies in the electronic structure of $MnBi_2Te_4$ and provides an important framework to understand the electronic structures of other relevant topological materials $MnBi_{2n}Te_{3n+1}$.

2DCC Role: This research resulted from a close collaboration between a 2DCC external user, Prof. Shuolong Yang at Univ. of Chicago, and the researchers of the 2DCC Bulk Growth and theory teams. The single crystals of $MnBi_2Te_4$ used for this study were grown using a flux method at the 2DCC Bulk Growth facility. The quantum well model used to interpret the ARPES data was developed by the 2DCC faculty.



(Left) ARPES constant energy maps at different binding energies. (Right) The chiral circular dichroism (CD) pattern of the resulting bands overlaid on the experimental CD map taken at 12 K. The simulated band structures are obtained by solving 2-band or 3-band Hamiltonians with hybridization terms.

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