



## Bulk-band Inversion and Three-dimensional Massive Dirac Fermions in ZrTe<sub>5</sub>

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### Introduction

Topological insulators (TIs) have attracted great attention due to their topologically nontrivial quantum states. People have been looking for ideal TIs to realize the applications of the topological quantum phenomena in spintronic devices. Experimental verifications of the theoretically predicted TIs are essential steps towards the applications. In the past, predicted TIs were mostly identified by the measurements of the topological surface states. However, as another hallmark of the topologically nontrivial states in TIs, an inversion between the bulk conduction- and valence-bands has seldom been investigated by experiments. Besides, three-dimensional (3D) massive Dirac fermions with nearly linear band dispersions were rarely observed in TIs.

### Experimental

Infrared spectroscopy is a powerful experimental technique for studying low-energy excitations of a material. To investigate the bulk-band inversion and the nature of the bulk fermions in a van der Waals crystal, ZrTe<sub>5</sub>, we measured the infrared transmission spectra of its multilayer flake with thickness  $d \sim 180$  nm at magnetic fields ( $B$ ) applied along the wave vector of the incident light.<sup>[1]</sup>

### Results and Discussion

A series of intra- and inter-Landau (LL) transitions are present in the relative transmission spectra  $T(B)/T(B_0 = 0 \text{ T})$  of the ZrTe<sub>5</sub> flake. The linear  $\sqrt{B}$  dependence of the LL transition energies at  $B \leq 4$  T and the nonzero intercept of the LL transitions at  $B = 0$  T, combined with the linear relationship between the zero-magnetic-field optical absorption and the photon energy, indicate 3D massive Dirac fermions with nearly linear band dispersions in the ZrTe<sub>5</sub> flake. More importantly, our analysis of the split LL transitions shows that the intra-LL transitions, which are associated to the two zeroth LLs and disappear at  $B \sim 2.5$  T, reemerge at  $B > 17$  T. The reemergence of the intra-LL transitions reveals the energy cross between the two zeroth LLs, which reflects the inversion between the bulk conduction and valence bands.

### Conclusions

The observation of 3D massive Dirac fermions with nearly linear dispersions and the revealed bulk-band inversion here not only provide spectroscopic evidence for the TI state in ZrTe<sub>5</sub> but also open up a new avenue for fundamental studies of Dirac fermions in van der Waals materials.

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### Reference

[1] Chen, Z.-G., *et al.*, **Proceedings of the National Academy of Sciences of USA** 114, 816-821 (2017).

