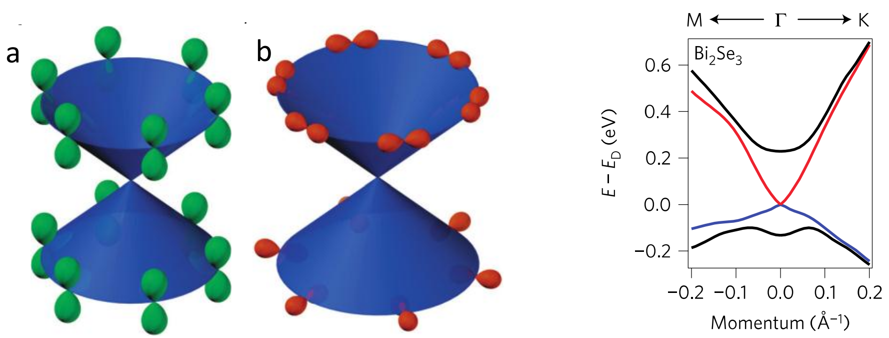
Discovery of Asymmetry in the Surface States of Topological Insulators

Scientific Achievement

The Center for Inverse Design (collaborating with Lawrence Berkeley National Laboratory, Brookhaven National Laboratory, and Rutgers University) has discovered novel asymmetry topological insulators, with the orbital texture of Dirac cone states asymmetric above and below the Dirac point. Inverse-design theory approaches were coupled with experimental characterization of synthesized Bi_2Se_3 and Bi_2Te_3 samples for validation.

Significance and Impact

The topological surface states of topological insulators (TI) protected by time-reversal symmetry pave new avenues to realize energy-efficient quantum computation based on spin degrees of freedom. The spin, locked to orbital wavefunction by spin-orbit coupling, is self-polarized in TI. The previous description of topological states assumes a symmetric orbital wavefunction that is widely used for quantum computation simulation. Our finding provides a new understanding of the orbital and the related spin wavefunction. This research is a key step toward understanding the topological insulators that may have the potential to be the building blocks of a super-fast quantum computer that could run on almost no electricity.



Experiment and theory unveil a new asymmetry character in topological insulators: the in-plane orbital wavefunction of surface states switches from tangential (a) to radial (b) when the energy surface varies from above to below the Dirac point.

Y. Cao, J.A. Waugh, X.-W. Zhang, J.-W. Luo, Q. Wang, T.J. Reber, S.K. Mo, Z. Xu, A. Yang, J. Schneeloch, G. Gu, M. Brahlek, N. Bansal, S. Oh, A. Zunger, and D.S. Dessau, *Nature Physics* **9**, 499–504 (2013).

Research Details

- Angle-resolved photoemission spectroscopy (ARPES) was used to measure the orbital character of the surface states of the Bi_2Se_3 TI, and the remarkable switch (asymmetry) of orbital wavefunctions was observed from tangential to radial near the Dirac point.
- Theoretical calculations and characterization of the orbital wavefunction of the surface states in Bi_2Se_3 and Bi_2Te_3 TIs were performed using first-principles methods. The orbital wavefunctions were found to switch exactly at the Dirac point for both TIs.