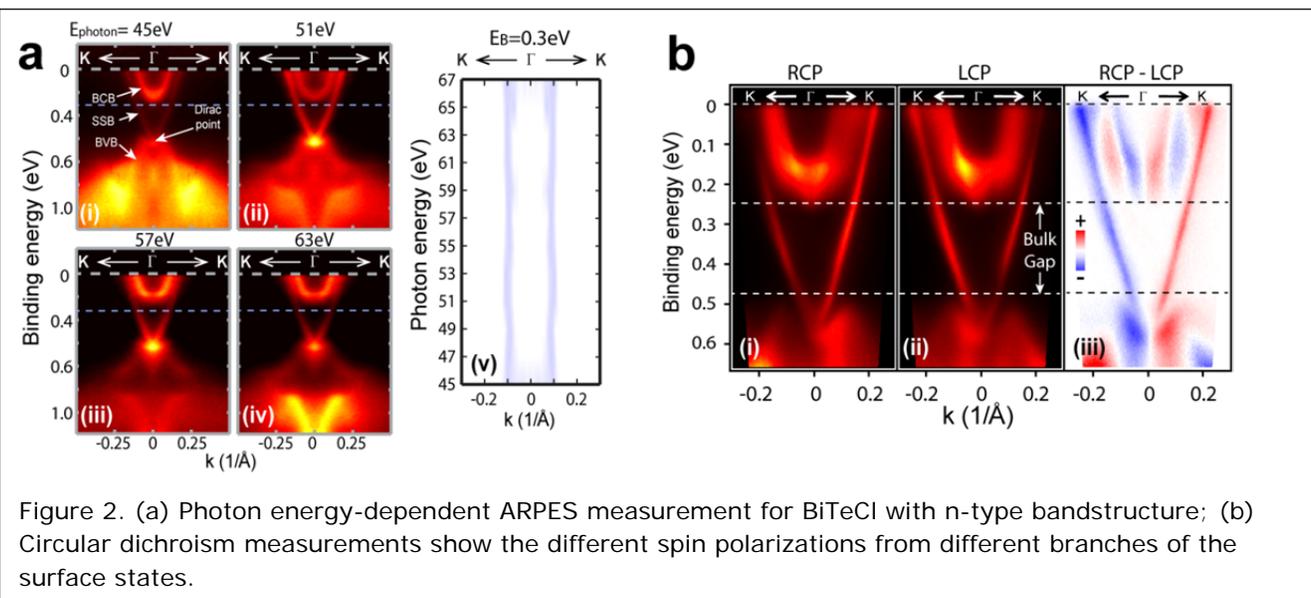
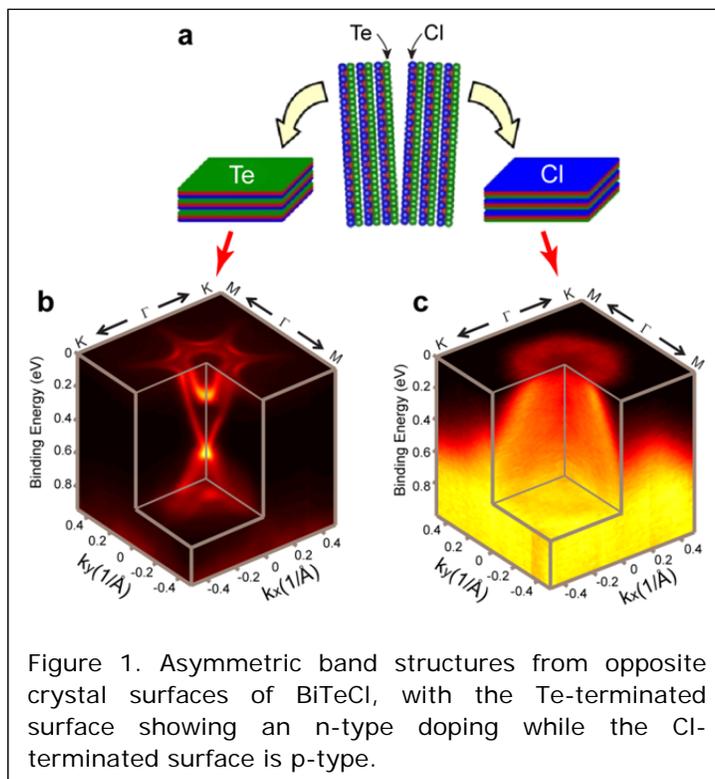


Discovery of a Single Topological Dirac Fermion in the Strong Inversion Asymmetric Compound BiTeCl

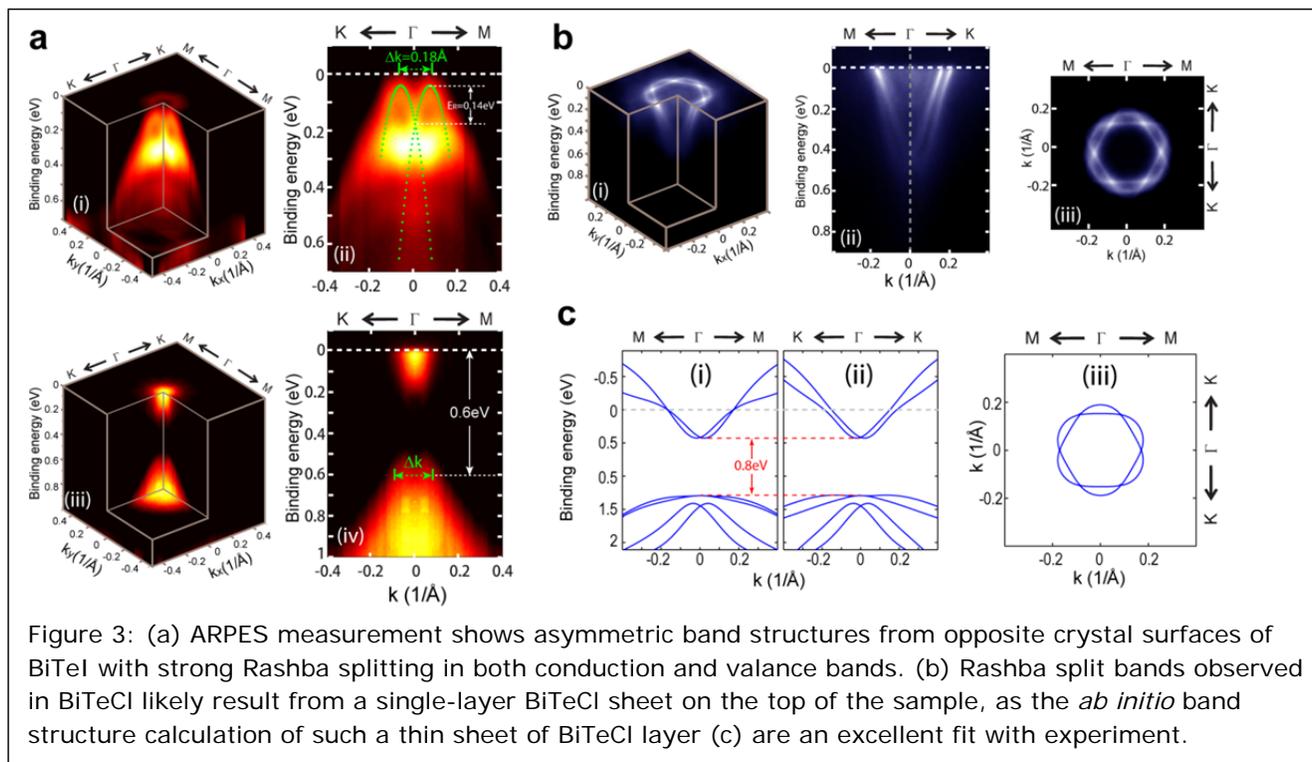
Topological insulators comprise a new state of quantum matter that has been predicted theoretically and realized experimentally in the past few years. Every topological insulator discovered so far in experiments has been inversion symmetric – except for strained HgTe, which has weak inversion asymmetry, but shows no bulk charge polarization. Strong inversion asymmetry in topological insulators would lead to many interesting phenomena, such as pyroelectricity and intrinsic topological p-n junctions, and would also serve as an ideal platform for realizing topological magneto-electric effects, which result from the modification of Maxwell's equations in topological insulators.

Researchers used SSRL's Beam Line 5-4 and Beam Line 10.0.1 at the ALS to study the electronic structure of BiTeCl with angle-resolved photoemission spectroscopy (ARPES). Their results, recently published in *Nature Physics*, revealed a single topological Dirac fermion and crystalline-surface-dependent electronic states resulting from the compound's strong inversion asymmetric crystal structure.

In their study, the researchers used ARPES to investigate the electronic structures of two V–VI–VII compounds: BiTeCl and BiTeI. In both materials, the researchers found that the electronic structures from opposite crystal surfaces (with halogen or chalcogen termination, respectively) were significantly different due to the strong inversion asymmetry in the lattice structure (Fig. 1).



The differences were so pronounced that the charge carriers on the two surfaces became opposite types, leading to strong bulk charge polarization (as confirmed by the *ab initio* calculation of the charge distribution). Surprisingly, the researchers observed a single Dirac cone inside the bulk energy gap in the BiTeCl n-type sample surface.



Next, the researchers confirmed the surface origin of the Dirac cone by performing photon-energy-dependent ARPES measurements (Fig. 2a). Circular dichroism measurements (Fig. 2b) then showed opposite spin polarization in different Dirac cone branches. Combined, both results prove the topological nature of the Dirac cone, thus making BiTeCl the first strong inversion asymmetric polar (and also pyroelectric) topological insulator candidate. Moreover, with an observed bulk energy gap of ~ 220 meV – a 10-fold increase over that of strained HgTe (~ 20 meV) – BiTeCl becomes a promising platform for realizing unusual topological phenomena and possible high-temperature applications.

In contrast, the researchers observed giant Rashba splitting in both the bulk conduction and valance bands of BiTeI (Fig. 3a) and sometimes in BiTeCl (likely to be from a single layer of BiTeCl sheet, Fig. 3b, c), making them promising materials for spintronic applications with both p- and n-type doping.

Primary Citation

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