Topological superconductivity in iron-based superconductors

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Introduction to Majorana modes and topological superconductors

In a topological superconductor, the opening of the superconducting gap is associated with the emergence of zero energy excitations that are their own antiparticles. These zero-energy states, generally called Majorana zero modes or Majorana bound states, have potential applications in quantum computing. Most of the proposed topological superconductors are realized with spin-helical states through proximity effect to *s*-wave superconductors. However, this approach generally requires complicated hetero-structures and a long superconducting coherence length which in principle prohibits the use of high temperature superconductors.

Topological superconductivity in high-T_c iron-based superconductors

In this work, we show that the Fe-based superconductor $FeTe_{0.55}Se_{0.45}$ single crystals host topological superconducting states at the surface, paving a distinct route for realizing topological superconductivity and Majorana bound states at higher temperatures.

Fe(Te,Se) has the simplest crystal structure among Fe-based superconductors (Fig. 1**A**). First-principles calculations show that, along ΓZ, the p_z band has a large dispersion; near E_F, SOC causes an avoided crossing with the d_{xz} band, and a SOC gap opens (Fig. 1**B**). This band inversion results in a non-trivial topological invariance. Thus, $FeTe_{0.5}Se_{0.5}$ should host strong topological surface states near E_F. To show the predicted topological surface states clearly, we project the band structure onto the (001) surface, as shown in Fig. 1**C**. The Dirac-cone type surface states are located near E_F, inside the SOC gap between the bulk valence band and bulk conduction band.

Three evidences are necessary to experimentally prove

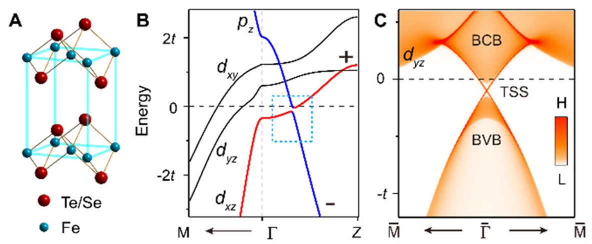

Fig. 1 (**A**) Crystal Structure of Fe(Te,Se). (**B**) Bulk band structure along ΓZ direction. (**C**) Calculated (001) surface spectrum.

that $FeTe_xSe_{1-x}$ (x ~ 0.5) is a topological superconductor, and they are all confirmed by our high-resolution ARPES experiments:

(i) *Dirac-cone–type surface states*. The overall band structure from the high resolution ARPES is summarized in Fig. 2**A**. We obtained clear Dirac-cone type band together with parabola-like band. Compare with the theory calculations, we conclude that the Dirac-cone–type band is the topological surface band, and the parabolic band is the bulk valence band.

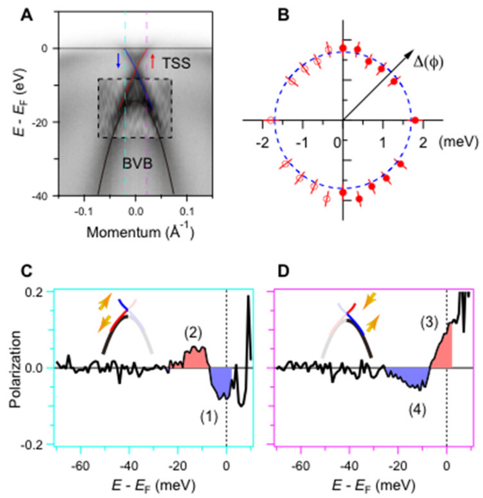

Fig. 2 (**A**) Intensity plot of the Fe(Te,Se) band structure from high-resolution ARPES measurements. (**B**) Polar representation of the superconducting gap size. (**C-D**) Spin polarization curve at the two cuts indicated in **A**.

(ii) *Helical spin polarization of the surface states.* Two curves at the cuts indicated in Fig. 2**A** were measured. The spin-resolved data show that the spin polarizations are reversed for the two cuts at the Dirac cone, whereas the background shows no spin polarization (Fig. 2**CD**). These data are consistent with the spin-helical texture, which is the direct consequence of "spin-momentum locking" of topological surface states.

(iii) *An s-wave superconducting gap of the surface states.* Since iron-based superconductors generally have isotropic *s*-wave superconducting gaps, it is natural that the surface states also open an *s*-wave gap, due to the proximity effect from bulk. Indeed, we observed a clear *s*-wave gap on the surface band, as shown in Fig. 2**B**.

Majorana modes in iron-based superconductors

When the spin-polarized topological surface states open an *s*-wave gap, the corresponding superconducting states are topologically non-trivial. Thus, when an external magnetic field is applied, a pair of Majorana bound states is expected to appear at the two ends of the vortices. Furthermore, if a magnetic domain is deposited on the surface, destroying superconductivity within that domain, there should be itinerant Majorana modes along the domain edge. It should be fairly easy to produce

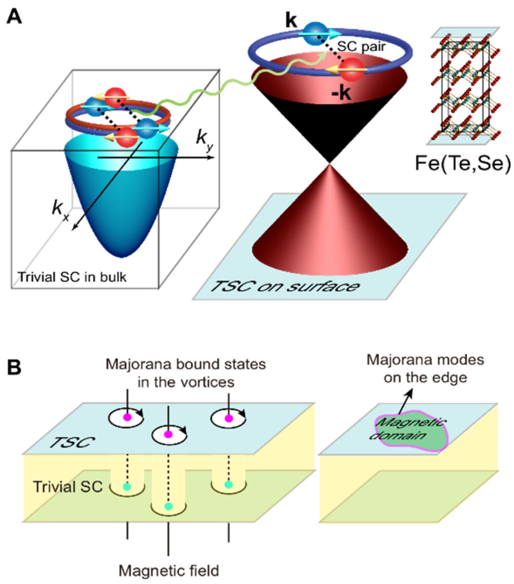

Fig. 3 (**A**) Topological superconductivity on the surface of $FeTe_{0.55}Se_{0.45}$. (**B**) Existence of Majorana bound states and itinerant modes with vortices and magnetic domains.

Majorana bound states and Majorana edge modes with Fe(Te,Se) single crystals. The relatively high T_c and facile growth of high-quality single crystals and thin films make Fe(Te,Se) a promising platform for studying Majorana bound states and may further advance research on quantum computing.

References:

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