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Surface State Bands in Superconducting $(Pt_xIr_{1-x})Te_2$ *

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Angle-resolved photoemission spectroscopy is performed to study the bulk and surface electronic structures of non-superconducting $IrTe_2$ and superconducting $Pt_{0.05}Ir_{0.95}Te_2$. In addition to the bulk electronic bands predicted by the local density approximation calculations, we observe two Dirac cone-like bands at the Brillouin zone center, which are non-dispersive along k_z, suggesting that the extra bands are surface state bands. As the experimental results are well consistent with the ab initio calculations of surface states, the parity analysis proves that these surface state bands are topologically trivial and thus exclude $(Pt_xIr_{1-x})Te_2$ as a possible topological superconductor candidate.

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Topological superconductivity is a new state of matter, which is expected to exhibit massless Marojana fermions and to provide a route for topological quantum computation.[1–5] While the realization of topological superconductors (TSCs) is highly demanded, the only serious TSC candidates are arguably the time-reversal breaking p-wave superconductor Sr_2RuO_4 and the chemically-substituted topological insulators.[6–16]

Very recently, the strong spin-orbit coupling (SOC) material $IrTe_2$ has attracted wide interest due to the emergence of superconductivity and the possible realization of a TSC in Pt-doped $(Pt_xIr_{1-x})Te_2$.[17–21] $IrTe_2$ is a layered compound with $1T$-structure at room temperature, where the Ir and Te atoms form regular triangle lattices in their respective (001) planes, as illustrated in Fig. 1(a). It exhibits a structural phase transition at $T_s = 265\,\mathrm{K}$, below which a new structural modulation with a wave vector $Q = (1/5, 0, -1/5)$ was revealed.[17] Substitution of Ir by Pt or Pd suppresses the structural phase transition and eventually induces bulk superconductivity.[17–21]

To justify whether the topological superconductivity can be realized in the $5d$ transition metal compound $(Pt_xIr_{1-x})Te_2$, we have performed angle-resolved photoemission spectroscopy (ARPES) studies on both the bulk and surface electronic structures of non-superconducting $IrTe_2$ and superconducting $Pt_{0.05}Ir_{0.95}Te_2$. While two Dirac cone-like bands at the Brillouin center are identified as surface state bands (SSBs), our local density approximation (LDA) calculations and parity analysis prove that these SSBs are topologically trivial and exclude $(Pt_xIr_{1-x})Te_2$ as a possible TSC candidate.

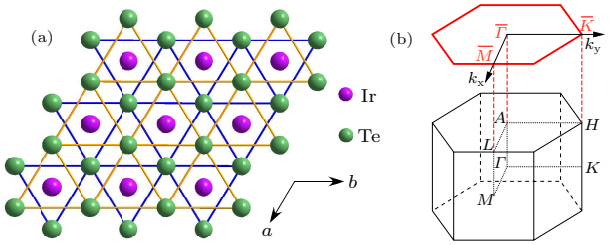

Fig. 1. (Color online) (a) Top view of an $IrTe_2$ layer. Blue and yellow lines represent Te–Te bonds within the Te layers above and below the Ir layer, respectively. (b) Hexagonal 3D Brillouin zone of $(Pt_xIr_{1-x})Te_2$ with the definitions of high-symmetry points.

Single crystals of $(Pt_xIr_{1-x})Te_2$ have been grown via the self-flux technique.[18] Mixtures of Ir(Pt) powder and Te pieces in an atomic ratio of 0.18:0.82 were placed in an Al_2O_3 crucible and were sealed in an evacuated quartz tube. The mixtures were initially heated up and kept at 950℃ for several hours, then at 1160℃ for one day, and finally cooled down slowly to 900℃ at a rate of 2℃/h. The Te flux was separated from single crystals by using a centrifuge. ARPES experiments were performed at beamlines PGM and Apple-PGM of the synchrotron radiation center (Wis-

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consin) equipped with a Scienta R4000 analyser and a Scienta SES 200 analyser, respectively. The energy and angular resolutions were set at 30 meV and 0.2°, respectively. The samples were cleaved *in situ* and measured in a vacuum better than 3×10^{-11} Torr.

We first focus on the electronic structure of the pristine material $IrTe_2$. In Fig. 2, we show the ARPES curvature intensity plots[22] of $IrTe_2$ along the K–Γ–M direction at different photon energies of $IrTe_2$. The LDA+SOC band structures along the high-symmetry path at k_z=π and 0 are also plotted in Figs. 2(b) and 2(c), respectively. We find qualitative agreement between the experimental data and the calculations without any band renormalization, indicating strong SOC effect but relatively weak electronic correlations in this material. In addition to the predicted bulk electronic bands, we observe two extra linearly dispersive bands marked with red dashed curves at several k_z planes, as shown in Figs. 2(b)–2(f). While the first one is fully occupied and locates at 1 eV below E_F, the second one is crossing E_F whereas it merges with the LDA predicted bulk band at $k_z = \pi$ at low binding energy. By comparing the extracted dispersions at different k_z, we find that, although the bulk band structure has strong three-dimensional character, the Dirac cone-like bands are non-dispersive along k_z, thus suggesting that the extra bands are likely surface state bands (SSBs).

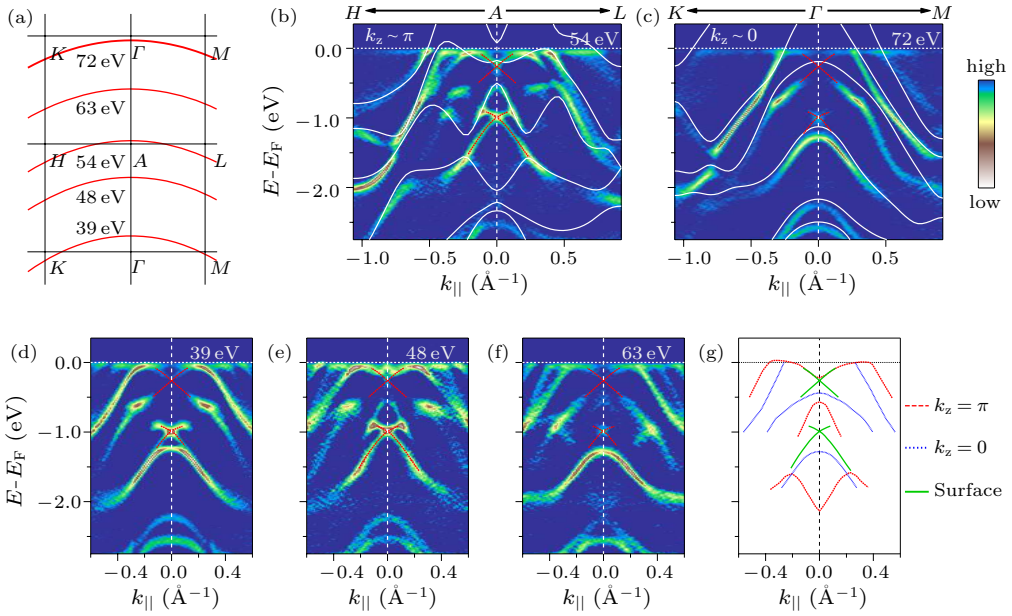

Fig. 2. (Color online) (a) Locations of photon energy dependent ARPES cuts in the momentum space. (b)–(f) ARPES curvature plots[22] of $IrTe_2$ at different phonon energies. Red dashed curves represent the extra SSBs. White solid curves in panels (b) and (c) represent the LDA+SOC band structures at $k_z = \pi$ and 0, respectively. (g) Extracted bulk bands at $k_z = \pi$ and 0 and SSBs.

To further justify this claim, we performed *ab initio* calculations of the surface states on the (001) surface of $IrTe_2$. We first construct the well-agreed maximally localized Wannier functions (MLWF)[23,24] from density function theory (DFT) calculations. We then use an iterative method[25,26] with these bulk MLWF hopping parameters to obtain the surface Greens function of the semi-infinite system. The imaginary part of the surface Greens function is the spectral function, from which we obtain the dispersion of the surface states, as shown in Fig. 3(b). In good agreement with the ARPES data, our calculations reveal two linearly dispersive SSBs.

In materials with strong SOC-like Bi_2Se_3, the linearly dispersive SSBs are topologically non-trivial and thus robust against non-magnetic impurities and weak crystal distortion. Since $IrTe_2$ also has a large SOC, it is important to check whether the experimentally observed SSBs are topologically non-trivial. Figure 3(a) shows the main orbital components and parities of the low energy bulk bands at time-reversal invariant points. To determine the topological properties, we use the green and orange curves to represent the fictitious Fermi level curves, where the SSBs are identified. Unfortunately, the calculated topological Z2 numbers below both the fictitious Fermi level curves are zero, proving that the observed surface states are topologically trivial.

To understand the origin of the SSBs, we analyze the dispersions and orbital components along the Γ–A line. As seen in Fig. 3(a), the slide-down $p_z\langle - \rangle$ band and the climb-up p_z $\langle + \rangle$ band have a band-change and open two hybridization gaps along Γ–A. This leads to two explicit Dirac cones at the projected point shown

in Fig. 3(b), corresponding to the fully occupied and the near-EF SSBs, respectively. As the parity analysis proves that the SSBs at the Γ point are topological trivial, one would expect Dirac cone-like SSBs at the M point. Such SSBs indeed exist at 1.6 and 2.2 eV below EF at the projected M point according to our calculations as shown in Fig. 3(b), which are located at the fictitious Fermi level curves represented by the green and orange curves in Fig. 3(a), respectively, confirming that the experimentally observed SSBs are topologically trivial.

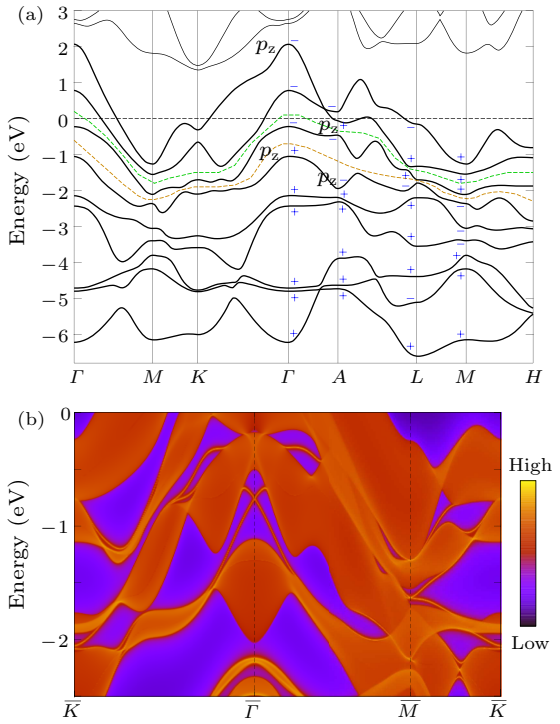

Fig. 3. (Color online). (a) Bulk band structure of IrTe2 with SOC, in which the main components and parities of the low energy bands at time-reversal invariant points are listed. The green and orange curves are the fictitious Fermi level curves used to determine the topological properties of the system. (b) Calculated spectral function illustrating the band dispersion on the (001) surface. Two linear topological sur- face states are obtained, in agreement with the experimental observations.

Finally, we study the evolution of the SSBs in the SC $(Pt_xIr_{1-x})Te_2$. The room temperature ARPES intensity plots, curvature plots and EDCs at $k_z \sim 0$ and π are shown in Figs. 4(a)–4(c) and Figs. 4(d)–4(f), respectively. As compared with pristine $IrTe_2$, both the bulk electronic bands and the SSBs of SC $Pt_{0.05}Ir_{0.95}Te_2$ barely change, proving that the parity analysis for $IrTe_2$ is still valid and thus that the Dirac cone SSBs observed in SC $Pt_{0.05}Ir_{0.95}Te_2$ are also topologically trivial. Moreover, by studying the electronic structure at low temperature, as shown in Figs. 4(g)–4(i), we find that the fully occupied SSB is shifted to higher binding energy and the near-E_F SSB is almost completely smeared out while the bulk states remain unchanged. The change of these SSBs at low temperature is consistent with the STM studies, where a complicated surface reconstruction at low temperature is observed in the SC $Pt_{0.05}Ir_{0.95}Te_2$.[27]

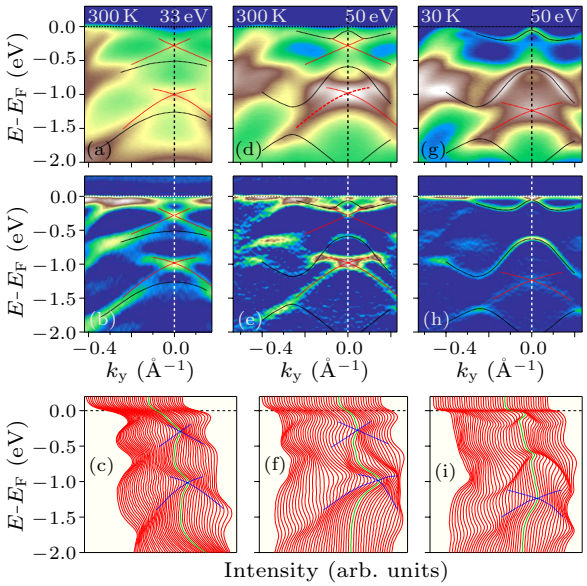

Fig. 4. (Color online) (a)–(c) Room temperature ARPES intensity plot, curvature plot and EDCs of $(Pt_xIr_{1-x})Te_2$ at $k_z \sim 0$. Red and black dashed curves represent the SSBs and bulk dispersions, respectively. Here (d)–(f) are the same as panels (a)–(c) while taken at $k_z \sim \Gamma$. (g)–(i) Low temperature ARPES intensity plot, curvature plot and EDCs at $k_z \sim \Gamma$.

In summary, we have resolved two Dirac cone-like SSBs in both non-SC $IrTe_2$ and SC $Pt_{0.05}Ir_{0.95}Te_2$. Combined with the LDA calculations and parity analysis, we find that the experimentally observed SSBs are topological trivial. Although our results exclude SC $(Pt_xIr_{1-x})Te_2$ itself as a possible TSC candidate, recent STM and transport studies prove that $(Pt_xIr_{1-x})Te_2$ is a fully gapped s-wave superconductor with large c-axis coherence.[21] By utilizing the proximity effect, the heterostructure of TIs/$(Pt_xIr_{1-x})Te_2$ could be an ideal system to study the novel topological superconductivity.

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