

Topological nature of the FeSe_{0.5}Te_{0.5} superconductorZhijun Wang,^{1,2} P. Zhang,¹ Gang Xu,^{1,3} L. K. Zeng,¹ H. Miao,¹ Xiaoyan Xu,¹ T. Qian,¹ Hongming Weng,^{1,4} P. Richard,¹ A. V. Fedorov,⁵ H. Ding,^{1,4,*} Xi Dai,^{1,4,†} and Zhong Fang^{1,4,‡}¹*Beijing National Laboratory for Condensed Matter Physics, and Institute of Physics, Chinese Academy of Sciences, Beijing 100190, China*²*Department of Physics, Princeton University, Princeton, New Jersey 08544, USA*³*Department of Physics, McCullough Building, Stanford University, Stanford, California 94305-4045, USA*⁴*Collaborative Innovation Center of Quantum Matter, Beijing, China*⁵*Advanced Light Source, Lawrence Berkeley National Laboratory, Berkeley, California 94720, USA*

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We demonstrate, using first-principles calculations, that the electronic structure of FeSe_{1-x}Te_x ($x = 0.5$) is topologically nontrivial and characterized by an odd \mathbb{Z}_2 invariant and Dirac cone type surface states, in sharp contrast to the end member FeSe ($x = 0$). This topological state is induced by the enhanced three-dimensionality and spin-orbit coupling due to Te substitution (compared to FeSe), and characterized by a band inversion at the Z point of the Brillouin zone, which is confirmed by our ARPES measurements. The results suggest that the surface of FeSe_{0.5}Te_{0.5} may support a nontrivial superconducting channel in proximity to the bulk.

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I. INTRODUCTION

Among the Fe-based superconductors, the FeSe_{1-x}Te_x family of compounds [1–4] is of particular interest. First, it has the simplest PbO structure (space group $P4/nmm$) with Se (or Te) atoms forming distorted tetrahedra around Fe [see Fig. 1(b)] similar to the structure of FeAs planes in the families of FeAs-based high- T_c superconductors [5]. Second, the internal parameters can be systematically tuned by the substitution of Se by Te [6–8], which provides us a platform for in-depth study of possible superconducting mechanisms and topological characters. Third, superconductivity has been observed for a wide range of composition x [2–4], and the transition temperature T_c can be further enhanced by pressure [9–11]. More recently, superconductivity with T_c higher than 77 K was suggested for single unit cell FeSe films [12] epitaxially grown on SrTiO₃ substrates.

Despite these interesting properties though, the particularities of the system have still not been fully explored. Earlier studies, both theoretical and experimental, suggest the similarity of the electronic structures of the Fe chalcogenides (FeSe, FeTe) [13–15] and the FeAs-based [16–18] superconductors. Indeed, the low-energy physics around the Fermi level is dominated by the Fe-3d states, and the morphology of the Fermi surfaces is similar. On the other hand, a surprisingly stable (no splitting under external magnetic field) zero-energy bound state (ZBS) at randomly distributed interstitial excess Fe sites was observed in very recent scanning tunneling microscopy (STM) measurements on the surface of superconducting Fe(Te,Se) [19], suggesting a possible topological feature of its electronic structure. Obviously, the 5p orbitals of Te are more extended and have stronger spin-orbit coupling (SOC) than the 4p orbitals of Se. The consequences of Te substitution, particularly for the bulk topological character of FeSe_{1-x}Te_x, have been largely ignored in the literature and will be the

main purpose of the present paper. Based on first-principles calculations combined with angle-resolved photoemission spectroscopy (ARPES) measurements, here we report that the electronic structure of FeSe_{0.5}Te_{0.5} is topologically nontrivial, in sharp contrast to its end member FeSe. The topological properties of FeSe_{0.5}Te_{0.5} can be characterized by an odd \mathbb{Z}_2 number, and the existence of Dirac cone type surface states, in proximity to bulk superconductivity, should favor topologically superconducting surface states, as suggested by Fu and Kane [20]. After introducing our methodology in Sec. II, we present the DFT band structures and main results in Sec. III, and provide a section on the ARPES experimental data in Sec. IV, which is followed by our conclusion in Sec. V.

II. METHODOLOGY

The electronic structures of FeSe and FeSe_{0.5}Te_{0.5} are calculated with SOC included. The calculations are performed based on the density functional theory (DFT) [21,22] and the generalized gradient approximation (GGA) for the exchange-correlation potential [23], as implemented in the plane-wave pseudopotential based BSTATE (Beijing Simulation Tool of Atomic TEchnology) package [24]. The experimental lattice parameters [6,25] are used in the calculations. Maximally localized Wannier functions (MLWF) [26] are constructed from bulk calculations, and then used to study the surface states in the semi-infinite system. To treat the substitution properly, we have calculated FeSe_{0.5}Te_{0.5} by using both the virtual crystal approximation and the two-formula cell with ordered Se and Te sites. Both calculations give converging results.

III. RESULTS AND DISCUSSION**A. Electronic structures without SOC and band inversion**

We first neglect the SOC and concentrate on the comparison between the electronic structures of FeSe and FeSe_{0.5}Te_{0.5} [as shown in Figs. 2(a) and 2(b)]. The band structure of FeSe is very similar to that of LaOFeAs as reported before [17]. At the Γ point, the valence band top is not occupied, leading to

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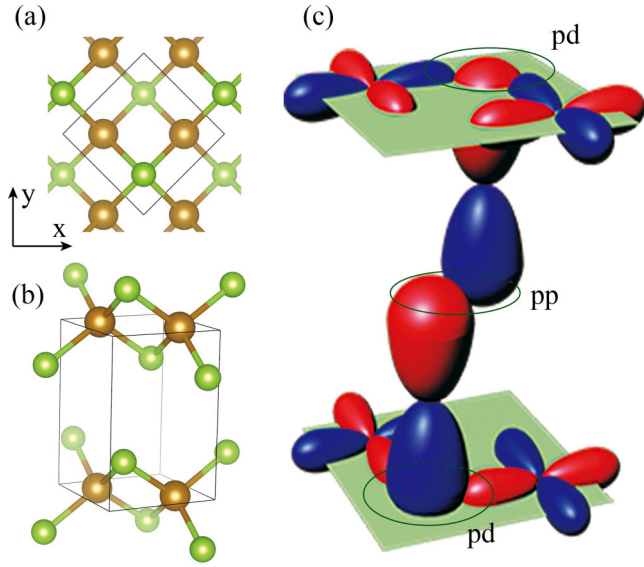


FIG. 1. (Color online) Unit cell of FeX ($X = \text{Se}_{0.5}\text{Te}_{0.5}$), with the x axis pointing along Fe nearest neighbors. (a) Top view. (b) Crystal structure. Gray and green balls represent Fe and X atoms, respectively. (c) Schematic plot of the hybridization along the z axis between the combined orbitals D_{xy}^- and P_z^- (see details in Appendix B), consisting of intralayer pd bonding and interlayer pp bonding.

the well known hole pockets of Fermi surfaces around Γ . The three topmost states at Γ can be labeled as twofold degenerate Γ_5^+ states (d_{yz}/d_{xz} orbitals) and nondegenerate Γ_4^+ state (d_{xy}

orbital), respectively. There is a clear band gap larger than 0.6 eV above the valence band top at the Γ point. All the $d-d$ antibonding states (with negative parity) are located above the gap except the d_{z^2} orbital that has a weaker antibonding state. Among them, the most interesting state is the second highest one with remarkable red circles, which belongs to the Γ_2^- representation and comes from the antibonding d_{xy} orbitals of Fe and p_z orbital of chalcogen. The weight of the p_z component is illustrated by the size of red circles, which suggest that the Γ_2^- state can be affected by hybridizing with the d_{xy} and p_z orbitals. Looking along the Γ -Z direction, the band dispersion of the Γ_2^- state is the strongest among all d states. Nevertheless, since it is energetically high, the band structure around the Z point of the Brillouin zone (BZ) is only slightly affected and remains similar to that around Γ . The result suggests that FeSe is quite two-dimensional.

Immediate differences can be seen in comparing these results with the band structure of $\text{FeSe}_{0.5}\text{Te}_{0.5}$ shown in Fig. 2(b): (1) the Γ_2^- state in $\text{FeSe}_{0.5}\text{Te}_{0.5}$ is significantly pushed down and almost touches the valence band top, and the band gap at Γ (above the valence and top) is nearly closed; (2) the band dispersion of this Γ_2^- state along the Γ -Z direction is strongly enhanced. As a result, a band inversion occurs at the Z point, which implies a change of topological property.

Compared to FeSe, the c axis and the experimental intralayer distance d_z of $\text{FeSe}_{0.5}\text{Te}_{0.5}$ are enlarged by 7.8% and 9.7%, respectively (see Appendix A), while the a axis and the interlayer distance change only very little. As a result, the intralayer hybridizations, especially the pd bonding as shown in Fig. 1(c), are seriously weakened, and the Γ_2^- band

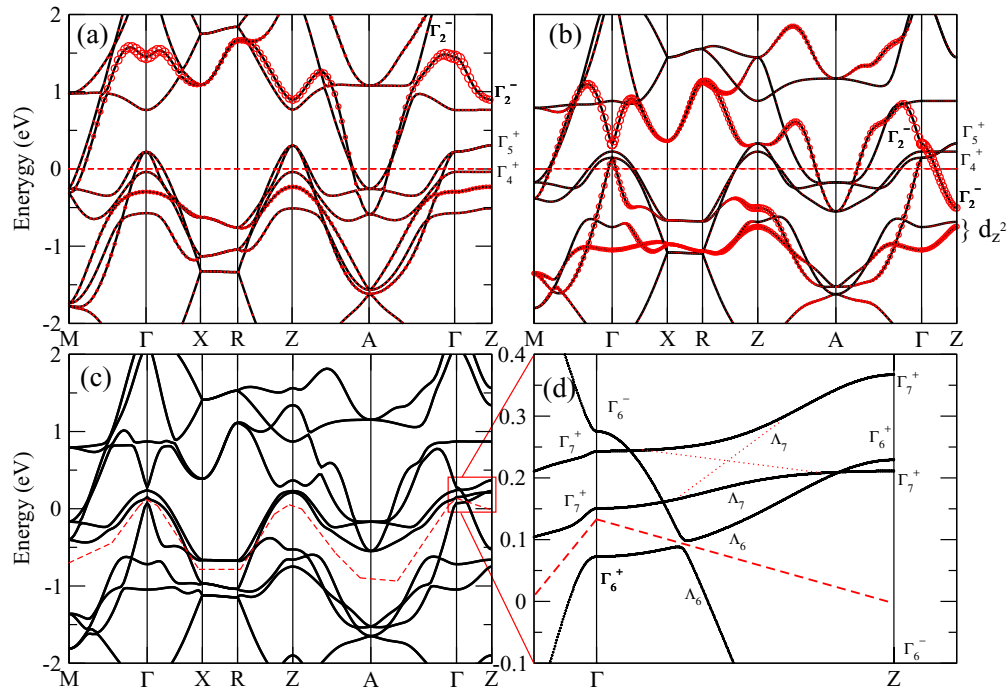


FIG. 2. (Color online) DFT electronic band structures. (a) Band structure of FeSe with internal parameter $z_X = 0.2345$ without SOC. (b) Band structure of $\text{FeSe}_{0.5}\text{Te}_{0.5}$ ($z_X = 0.2719$) without SOC. (c) Band structure of $\text{FeSe}_{0.5}\text{Te}_{0.5}$ with SOC. (d) Zoom-in view of the solid red box area in (c). The size of the red circles in (a) and (b) indicates the weight of the p_z component of the chalcogen atoms. The two d_{z^2} bands are indicated below E_F in (b). The original Λ_5 bands split into Λ_6 and Λ_7 . Along the Γ -Z line, two Λ_6 bands cross and hybridize to open a SOC gap of about 10 meV. The red dashed line corresponds to a Fermi curve across the gap.

center is lowered very much and becomes close to E_F , as shown in Fig. 2(b). On the other hand, because the Te 5*p* orbitals are much more extended than the Se 4*p* orbitals, the interlayer hybridization through the *pp* bonding becomes stronger. Therefore, the Te substitution enhances the hopping between layers and gives rise to a larger dispersion for Γ_2^- in $\text{FeSe}_{0.5}\text{Te}_{0.5}$. These two observations are in good agreement with the band structure of $\text{FeSe}_{0.5}\text{Te}_{0.5}$ shown in Fig. 2(b). Therefore, the band inversion in $\text{FeSe}_{0.5}\text{Te}_{0.5}$ is a consequence of the weakened intralayer hopping and enhanced interlayer hopping originating from the Te substitution.

B. Electronic structures with SOC and nontrivial \mathbb{Z}_2 invariant

Once SOC is included, the band structure of $\text{FeSe}_{0.5}\text{Te}_{0.5}$ opens a direct SOC gap and a nontrivial \mathbb{Z}_2 invariant can be defined by assuming a “curved chemical potential”—the red dashed line in Fig. 2(c)—lying between the 10th and 11th bands (neglecting the spin-doublet degeneracy of the bands). Generally, the doubly degenerate Γ_5^+ states split into Γ_6^+ and Γ_7^+ , and the odd Γ_2^- state turns into Γ_6^- (see details in Appendix B). Along the Γ -Z high-symmetry line, two Λ_6 bands under C_{4v} symmetry hybridize and open a gap of about 10 meV, which is clearly shown in Fig. 2(d). When defining a Fermi curve through the SOC gap, the \mathbb{Z}_2 invariant is easily calculated from the parity criterion, which comes out to 1. [The parities at all time-reversal-invariant momenta (TRIM) are presented in Appendix B.] This nonzero \mathbb{Z}_2 invariant indicates that $\text{FeSe}_{0.5}\text{Te}_{0.5}$ is in a topological phase that can support the nontrivial surface states (SS). Due to the substantial SOC of Te, increasing the content *x* enlarges the SOC gap, which is beneficial for the detection of the SS in the gap. Moreover, we also performed dynamical mean-field theory (DMFT) calculations to confirm the band inversion and identify the strong band renormalization due to electronic correlations (see Appendix C for details). The correlation effects do not change the detail of the electronic bands, but simply reduce the bandwidth.

C. Spin-resolved Fermi surface

Next, we analyze the spin-resolved Fermi surfaces around the Dirac point of the semi-infinite system formed by the SS to identify the nontrivial topology. With the surface Green’s function calculated from the modified effective Hamiltonian considering DMFT on-site modification, the spin-filter surface states and the corresponding Fermi surfaces can be obtained directly. From the dispersion of the SS shown in Fig. 3(a), the protected SS emerges in the SOC gap around E_F due to the nontrivial topological nature of the bulk system. The Fermi surface of the SS ($E_F = 50$ meV) is illustrated as a bright yellow circle in Fig. 3(b), and the spin orientation for the SS around the Fermi surface is marked by green arrows, which form a π Berry phase enclosed. The magnitude of the *z* spin component is very small compared to the in-plane component. The π Berry phase signifies the topological nontrivial properties of the bulk. By inducing an *s*-wave superconducting gap, the chiral SS can play an important role in producing the Majorana zero energy mode.

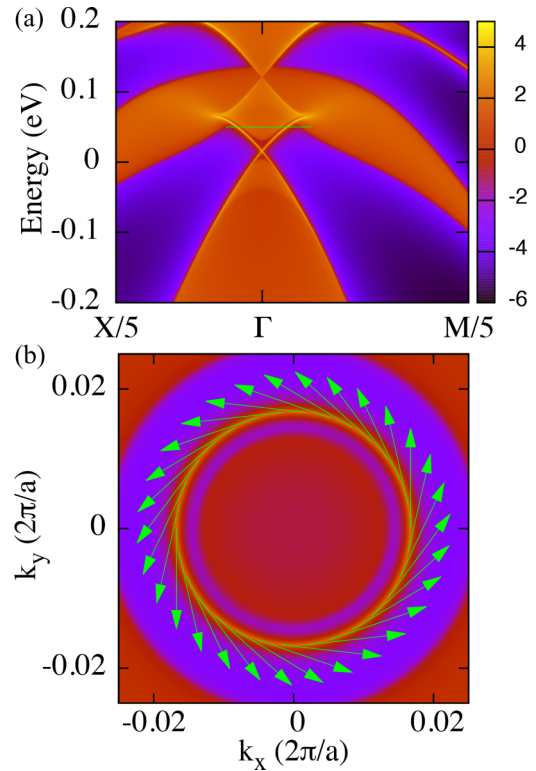


FIG. 3. (Color online) Topological nontrivial 001 surface states and spin-resolved Fermi surface of these states. (a) Surface LDOS on the (001) surface for $\text{FeSe}_{0.5}\text{Te}_{0.5}$ considering DMFT on-site modification. (b) Fermi surface of the topological state (bright yellow circle beside the projected bulk states). The in-plane spin orientation is indicated by green arrows.

IV. ARPES MEASUREMENTS

We performed ARPES measurements in order to demonstrate experimentally the existence of the Γ_2^- band with strong p_z orbital character crossing E_F along the Γ -Z direction. Large single crystals of $\text{FeSe}_{0.45}\text{Te}_{0.55}$ were grown using the self-flux method, and LiFeAs with FeAs flux method. ARPES measurements were performed at the Advanced Light Source and at Synchrotron Radiation Center, using a VG-Scientia electron analyzer. The K source used for evaporation is made of a SAES K dispenser. In the experiments, the largest coverage is less than one monolayer. All data were recorded with linear horizontal polarized photons with a vertical analyzer slit (σ geometry). Under this configuration, odd orbitals with respect to the emission plane are visible, such as the d_{xy} and d_{yz} orbitals, while the d_{xz} band should not be detected. In addition, our experimental setup leads to a *z* component of the light polarization, and thus orbitals with mainly *z* components such as d_{z^2} and p_z orbitals are also observable [27].

The comparison of the DFT band calculations on FeSe and $\text{FeSe}_{0.5}\text{Te}_{0.5}$, shown in Figs. 2(a) and 2(b), suggests that while it is pushed far above E_F at Γ in FeSe, the Γ_2^- band in $\text{FeSe}_{0.5}\text{Te}_{0.5}$ forms an electron band just above E_F . To prove its existence, we raised the chemical potential by performing *in situ* K doping, and we measured ARPES spectra along Γ -M at $h\nu = 30$ eV, which coincides with $k_z = 0$ [28]. The results before and after evaporation (6 minutes) are shown in Figs. 4(a)

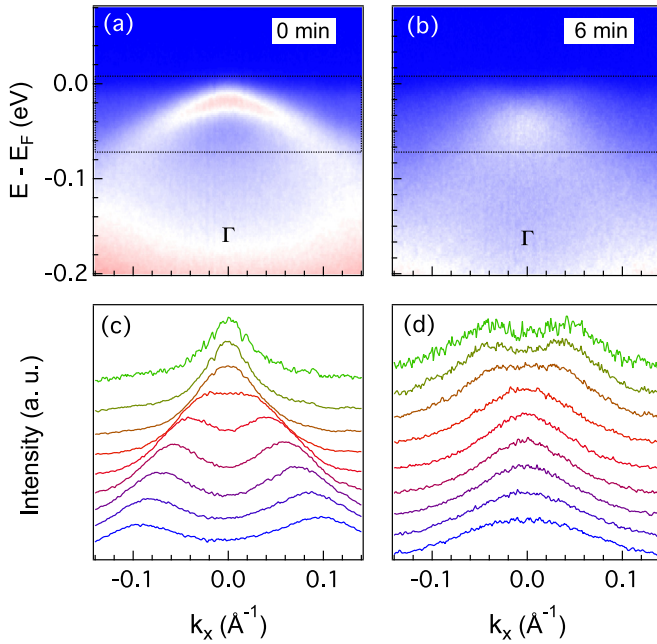


FIG. 4. (Color online) ARPES spectra along the Γ - M direction in the σ -polarization geometry. (a) $\text{FeSe}_{0.5}\text{Te}_{0.5}$ before surface evaporation. (b) $\text{FeSe}_{0.5}\text{Te}_{0.5}$ after 6 minutes of K surface doping. (c), (d) MDCs corresponding to data from the dashed boxes in panels (a) and (b), respectively.

and 4(b), respectively. As expected, the hole band is sinking further below E_F after evaporation. Interestingly, an additional electron band is observed, as clearly shown by contrasting the momentum distribution curves (MDCs) obtained before [Fig. 4(c)] and after [Fig. 4(d)] evaporation. This band, locating about 30 meV above the top of the valence band in $\text{FeSe}_{0.5}\text{Te}_{0.5}$, is very similar to the small 3D electron pocket reported in $(\text{Ti,Rb})_y\text{Fe}_{2-x}\text{Se}_2$ [27], which mainly has a p_z component.

In the presence of SOC, the DFT calculations indicate that the Γ_6^+ , Γ_7^+ , and Γ_7^+ states at the Γ point mostly come from the d_{xz} , d_{yz} , and d_{xy} orbitals, respectively, while the Γ_6^- state (labeled as Γ_2^- without SOC) have an important p_z component besides the d_{xy} orbital. As shown in Fig. 5(a), while the p_z band locates above E_F at Γ , it is shifted below E_F upon moving along Γ - Z and it reaches its minimum at the Z point. On its way down, the p_z band crosses the d_{xy} , d_{yz} , and d_{xz} bands, opening a SOC gap with the d_{xz} band. This situation is illustrated schematically in Fig. 5(a). We now ask how the hybridization of the p_z band with the d_{xz} band should affect the ARPES measurements. Around the Γ point, the p_z band forms an electron-like band located above E_F along the Γ - M direction. Therefore, it should not be observed in our experimental geometry. Due to selection rules, the d_{xz} band should not be observed either and only the d_{xy} and d_{yz} band can possibly be seen, as shown schematically in Fig. 5(b). However, because it hybridizes with the p_z band, one should expect to be able to detect the d_{xz} band near the crossing point below E_F , as illustrated schematically in Fig. 5(c). Finally, our calculations indicate that the p_z band has a hole-like dispersion near the Z point, and we should be able to observe it. On the other hand, the d_{xz} band no longer hybridizes strongly with

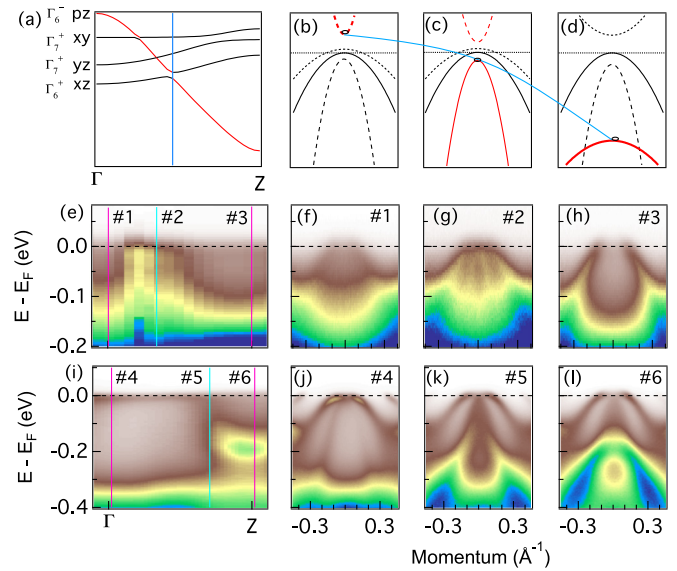


FIG. 5. (Color online) Normal-emission ARPES spectra. First row: Schematic band dispersions. The main feature is the p_z band crossing the d_{xy} , d_{yz} , and d_{xz} bands, opening a SOC gap with the d_{xz} band. Second row: ARPES data on $\text{FeSe}_{0.5}\text{Te}_{0.5}$. Third row: ARPES data on LiFeAs . First column: Dispersion at $k_x = 0$ along the Γ - Z direction. Second, third, and fourth columns: Electronic dispersions along cuts indicated in the first column.

the p_z band and its intensity should be significantly suppressed again in the σ polarization, as described in Fig. 5(d).

In order to confirm this dispersion, we compare in Fig. 5(e) ARPES spectra recorded on $\text{FeSe}_{0.45}\text{Te}_{0.55}$ with different photon energies. We see some intensity between the Γ and Z points that we assign to the p_z band sinking down from Γ to Z . At the Z point, this band has merged with the strong d_{z^2} band and it is thus undistinguishable. We display in Figs. 5(f)–5(h) three ARPES intensity cuts along Γ - M recorded on $\text{FeTe}_{0.55}\text{Se}_{0.45}$ and corresponding respectively to k_z values around Γ [cut 1, Fig. 5(f)], the hybridization between the p_z and d_{xz} bands [cut 2, Fig. 5(g)], and around Z [cut 3, Fig. 5(h)]. As the d_{xy} band heavily renormalizes compared to the d_{xz}/d_{yz} bands, it is shallower and hardly resolved with weaker intensity [29]. In cut 1 [Fig. 5(f)], as expected, none of the p_z and d_{xz} bands are detected near $k_z = 0$. In contrast, not only the d_{yz} band is observed in cut 2 [Fig. 5(g)], but the d_{xz} band as well due to its hybridization with the p_z band. At the Z point, away from hybridization, the d_{xz} band disappears from the ARPES spectrum [Fig. 5(h)]. Unfortunately, the p_z band is too close to the strong d_{z^2} band to be distinguished unambiguously.

As shown in Figs. 5(i) to 5(l), the strong k_z dispersion of the p_z band is also observed in LiFeAs , which exhibits very clear spectral features. Because its bottom is located away from the d_{z^2} band, the dispersion of the p_z band along Γ - Z can be identified very clearly, as illustrated in Fig. 5(i). As with $\text{FeSe}_{0.45}\text{Te}_{0.55}$, the intensity of the d_{xz} band is the strongest along cut 5 [Fig. 5(k)], where it hybridizes with the p_z band. Figures 5(k) and 5(l) also show clearly that the p_z band has a hole-like dispersion below E_F , as expected theoretically.

TABLE I. Structural parameters of PbO-structure FeX. The lattice parameters are from experimental data [6,25], and both optimized (Opt.) and experimental (Exp.) internal chalcogen positions z_X are shown. d_z is the Cartesian distance in the z direction from the X plane to the Fe plane.

	a (Å)	c (Å)	$z_X(\text{Opt.})/d_z$ (Å)	$z_X(\text{Exp.})/d_z$ (Å)
FeSe [25]	3.7724	5.5217	0.2345/1.2948	0.2673/1.4759
$\text{Fe}_{1.068}\text{Te}$ [6]	3.8123	6.2517	0.2496/1.5604	0.2829/1.7686
$\text{FeSe}_{0.493}\text{Te}_{0.507}$ [6]	3.7933	5.9552	0.2476/1.4745	0.2719/1.6192

V. CONCLUSION

In conclusion, we have presented both theoretical and experimental evidence for a topologically nontrivial phase in $\text{FeSe}_{0.5}\text{Te}_{0.5}$. From the DFT calculations, we show that the band topology is sensitive to the intralayer and interlayer hopping terms, which can be tuned by the Te substitution. The Te substitution content x strongly affects the structural, electronic, and topological properties of these materials. We have identified the topologically nontrivial electronic band structure of $\text{FeSe}_{0.5}\text{Te}_{0.5}$ with a band inversion, characterized by an odd \mathbb{Z}_2 invariant and spin-moment-locked SS. Our ARPES data strongly support that the Γ_2^- band forms a band inversion at the Z point. Similar results can also be applied to iron pnictides such as LiFeAs. Due to the topologically nontrivial surface states, the $\text{FeSe}_{1-x}\text{Te}_x$ materials would be an ideal system for realizing possible topological superconductors and Majorana fermions on the surface.

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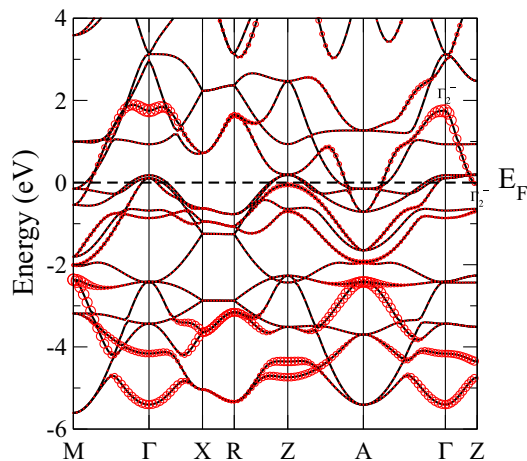


FIG. 6. (Color online) Electronic band structure of LiFeAs. The p_z component is highlighted by the size of the red circles.

APPENDIX A: STRUCTURAL PARAMETERS OF FeX AND BAND STRUCTURE OF LiFeAs

The experimental parameters of Iron chalcogenides (FeX) are used in Table I. For LiFeAs, we used the experimental lattice parameters [30] and relaxed the free internal coordinates. The experimental structure (space group $P4/nmm$, No. 129) has the Li sites in 2c positions, which lie above and below the centers of the Fe squares opposite the As. The calculated DFT band structure is given in Fig. 6. The Γ_2^- band shows a large dispersion and a band reversion along the z direction.

APPENDIX B: SYMMETRY AND PARITY ANALYSIS

Since the system has inversion symmetry, it is convenient to combine these orbitals into bonding and antibonding states with definite parity as

$$|D_\alpha^\pm\rangle = \frac{1}{\sqrt{2}}(|\text{Fe}_\alpha\rangle \pm |\text{Fe}'_\alpha\rangle),$$

$$|P_\beta^\pm\rangle = \frac{1}{\sqrt{2}}(|X_\beta\rangle \mp |X'_\beta\rangle).$$

Using the orbitals with definite parity defined in the main text, we can label all the non-spin-orbital (NSO) bands with the irreducible representations (IRs), which are given in Table II. The Γ_2^- band is composed of the antibonding states with both d_{xy} and p_z characters. At both the Γ and Z points, the IRs of the D_{4h} group are labeled as Γ_n^\pm , whereas along the Γ - Z high-symmetry line, we label these IRs as Λ_n because of its C_{4v} symmetry. In our conventions, the (x, y) axes are rotated by 45° as compared to the crystallographic axes, so that the d_{xy} orbital in our definition is the one pointing from Fe to chalcogen atoms, as shown in Fig. 1(a).

The IR labels along the Γ - Z line are shown in Fig. 7(a). Around E_F , the $D_{xz/yz}^+$ bands can mix with the $P_{x/y}^+$ orbitals with the same Γ_5^+ representations, although the P - D hybridization is not strong due to the little orbital overlap in the real space. For the Γ_2^- representation, the D_{xy}^- character can mix

TABLE II. Combined orbitals and related irreducible representations

D/P	(+/-)	z^2	yz/xz	xy	$x^2 - y^2$	x/y	z
D_{4h}	+	Γ_1^+	Γ_5^+	Γ_4^+	Γ_3^+	Γ_5^+	Γ_1^+
	-	Γ_3^-	Γ_5^-	Γ_2^-	Γ_1^-	Γ_5^-	Γ_2^-
C_{4v}	+	Λ_1	Λ_5	Λ_4	Λ_3	Λ_5	Λ_1
	-	Λ_4	Λ_5	Λ_1	Λ_2	Λ_5	Λ_1

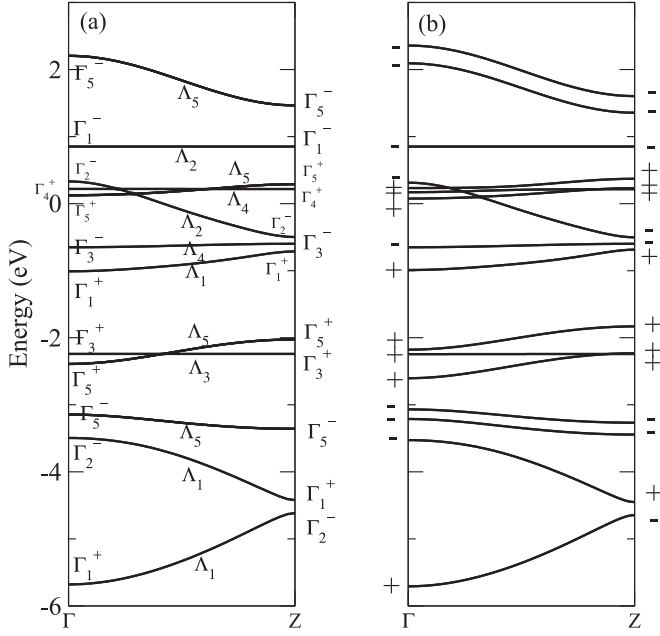


FIG. 7. Electronic band structure along Γ -Z. (a) The IRs are labeled in the NSO bands. (b) The parities are labeled in the SOC bands.

with the P_z^- band, and the d_{xy} and p_z orbitals have a strong hybridization along the z direction. However, as shown in Table I, the distance d_z becomes larger with the Te substitution content x increasing, thus leading to weaker hybridization. As a result, the Γ_2^- band, consisting of d_{xy} and p_z orbitals, sinks down to E_F and has a large dispersion in $\text{FeSe}_{0.5}\text{Te}_{0.5}$. Moreover, due to selection rules, the bonding state of D_{xy}^+ cannot mix with the p_z band, including along the Γ -Z line. As a consequence, the Γ_4^+ band characterized by the D_{xy}^+ representation exhibits a weak dispersion in the z direction, which is not sensitive to the height d_z . Beside, all the IRs in NSO bands and parities in SOC bands are presented in Table III. “(+, -)” denotes that the quadruple bands consist of two Kramers pairs with opposite parity. The nontrivial \mathbb{Z}_2 index is presented beside the vertical line, which denotes the hypothetical Fermi level in the main text.

TABLE III. The D_{4h} IRs and parities for each band.

IRs (NSO)	P							D								
Γ	Γ_1^+	Γ_2^-	Γ_3^-	Γ_4^+	Γ_5^+	Γ_6^+	Γ_7^+	Γ_1^+	Γ_3^-	Γ_5^+	Γ_4^+	Γ_2^-	Γ_1^-	Γ_5^-		
Z	Γ_2^-	Γ_1^+	Γ_5^-	Γ_3^+	Γ_5^+	Γ_6^+	Γ_7^+	Γ_1^+	Γ_3^-	Γ_5^+	Γ_4^+	Γ_2^-	Γ_1^-	Γ_5^-		
Parities (SO)	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16
Γ	+	-	-	-	+	+	+	+	-	+	+	-	-	-	-	-
Z	-	+	-	-	+	+	+	+	-	-	+	+	+	-	-	-
X	(+ -)	(+ -)	(+ -)	(+ -)	(+ -)	(+ -)	(+ -)	(+ -)	(+ -)	(+ -)	(+ -)	(+ -)	(+ -)	(+ -)	(+ -)	(+ -)
M	(+ -)	(+ -)	(+ -)	(+ -)	(+ -)	(+ -)	(+ -)	(+ -)	(+ -)	(+ -)	(+ -)	(+ -)	(+ -)	(+ -)	(+ -)	(+ -)
R	(+ -)	(+ -)	(+ -)	(+ -)	(+ -)	(+ -)	(+ -)	(+ -)	(+ -)	(+ -)	(+ -)	(+ -)	(+ -)	(+ -)	(+ -)	(+ -)
A	(+ -)	(+ -)	(+ -)	(+ -)	(+ -)	(+ -)	(+ -)	(+ -)	(+ -)	(+ -)	(+ -)	(+ -)	(+ -)	(+ -)	(+ -)	(+ -)
\mathbb{Z}_2											1					

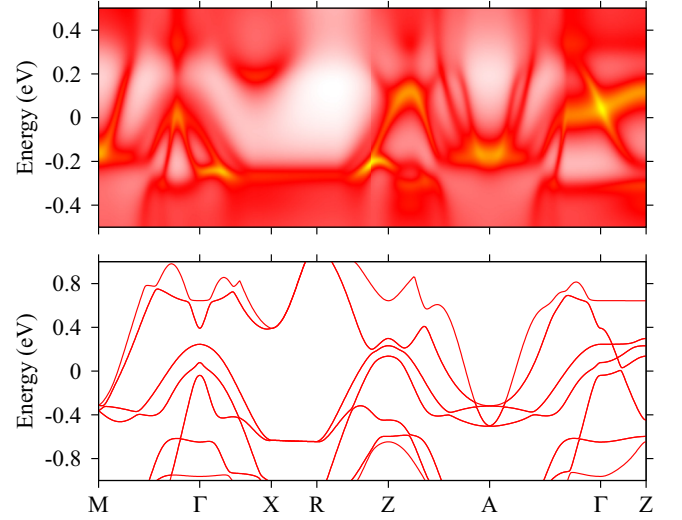


FIG. 8. (Color online) Upper panel: LDA+DMFT calculations. Lower panel: SOC band structure only taking the LDA+DMFT on-site modification into consideration.

APPENDIX C: LDA+DMFT CONFIRMATION

The LDA+DMFT method has proven to be a powerful technique to study the electronic structure of correlated systems. In this section, we apply this method to $\text{FeSe}_{0.5}\text{Te}_{0.5}$ with a local Coulomb integral $U = F_0 = 4.0$ eV and a Hund’s coupling $J = 0.7$ eV, and confirm that it has a topological character of band inversion by computing the topological invariants within the DMFT framework.

The one-electron spectral function is defined as

$$A_{\mathbf{k}}(\omega) = -\frac{1}{\pi} \frac{\text{Im} \Sigma(\omega)}{[\omega + \mu - \epsilon_{\mathbf{k}} - \text{Re} \Sigma(\omega)]^2 + \text{Im} \Sigma(\omega)^2}$$

in terms of the LDA band dispersion $\epsilon_{\mathbf{k}}$ and the self-energy $\Sigma(\omega)$. This momentum-resolved spectra $A_{\mathbf{k}}(\omega)$ is shown in the upper panel of Fig. 8, where the overall renormalization of the bands and the bandwidth reduction are apparent. However, the relative positions of different bands almost do not change. The Γ_2^- and Γ_5^+ band crossing near E_F remains in the correlated system.

In a previous work [31], only the Green’s function at zero frequency $G_{\mathbf{k}}^{-1}(0) = \mu - \epsilon_{\mathbf{k}} - \Sigma_{\mathbf{k}}(0)$ is needed to determine

the topology of the quasiparticle states, since renormalization does not change the nontrivial topological nature of the bulk system. Following Refs. [32], we compute the topological invariant of an interacting system with the Hamiltonian defined by $H_t(\mathbf{k}, \omega) = H(\mathbf{k}, \omega) + \Sigma_{\mathbf{k}}(0) - \mu$. A modified effective dispersion of $H_t(\mathbf{k})$ for which we neglected the imaginary part

of $\Sigma_{\mathbf{k}}(0)$ is given in the lower panel of Fig. 8. By introducing correlations, the bandwidth is reduced by approximately half, but the band inversion character still exists. According to the parity criteria, we conclude that $\text{FeSe}_{0.5}\text{Te}_{0.5}$ remains a topological correlated system. The topological surface state is derived from this modified effective TB Hamiltonian.

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