Two-Dimensional Electronic Structure of La and P Co-Doped $CaFe_2As_2$ Studied by ARPES

The relation between the occurrence of high-temperature superconductivity and the underlying electronic structure in iron-based superconductors is a major unresolved problem. We revealed the electronic structure of La and P co-doped $CaFe_2As_2$ superconductor with the critical temperature (T_c) = 45 K by angle-resolved photoemission spectroscopy. Its Fermi surface topology consists of nearly two-dimensional hole- and electron-like Fermi surfaces. Compared to other high-T_c iron-based superconductors, we discuss the relationship between the dimensionality of Fermi surface topology and the value of T_c.

The discovery of high critical temperature (high-T_c) superconductivity in $LaFeAsO_{1-x}F_x$ [1] has triggered intensive research on iron-based superconductors [2-4]. Density functional theory calculations for iron-based superconductors predict that Fermi Surfaces (FSs) in these materials are composed of nearly cylindrical (two-dimensional) hole- and electron-like FSs at the Brillouin zone center and corner, respectively, as shown in Fig. 1(a) [5, 6]. For the emergence of iron-based superconductivity, the FSs nesting that can enhance spin and/or orbital fluctuations has been believed to be important for realizing exotic Cooper pairing [5-8].

Experimentally, FS topology and its nesting condition for several iron-based superconductors have been directly studied by angle-resolved photoemission spectroscopy (ARPES) [9-22]. The FS topology for AFe_2As_2 (so-called 122-type bulk superconductors, where *A* represents alkali or alkali-earth metals) has revealed that high-T_c 122-type bulk superconductors have both hole- and electron-like FSs with the electron-like FSs in common [19-22]. However, the dimensionality of the FSs, especially hole-like FSs, shows marked material dependence: while in hole-doped $Ba_{1-x}K_xFe_2As_2$ (T_c = 38 K), all hole-like FSs have a cylindrical shape [Fig. 1(b)] [19, 20], in electron-doped $Ba(Fe_{1-x}Co_x)_2As_2$ (T_c = 25 K), two- and three-dimensional hole-like FSs are present [Fig. 1(c)] [21, 22]. Since the presence of such a three-dimensional FS is not favorable for superconductivity

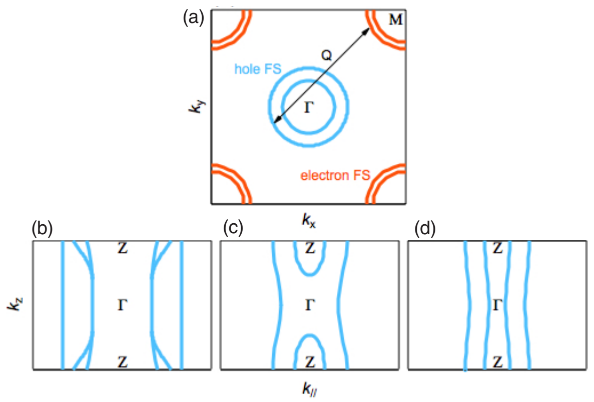

Figure 1: (a) Fermi surface (FS) and the nesting with nesting vector Q in the k_x-k_y plane for iron-based superconductors. The sky-blue and orange curved lines represent hole- and electron-like FSs, respectively. (b)-(d) Hole-like FSs in the k_z–k_x plane for $Ba_{1-x}K_xFe_2As_2$, $Ba(Fe_{1-x}Co_x)_2As_2$, and $Ca_{0.82}La_{0.18}Fe_2(As_{0.94}P_{0.06})_2$ obtained from refs. 19, 21 and 24, respectively.

resulting from the FS nesting, the relationship between the FS nesting and superconductivity is still unclear in iron-based superconductors. In this regard, the recent discovery of electron-doped $CaFe_2As_2$ with T_c = 45 K, namely La and P co-doped $Ca_{1-x}La_xFe_2(As_{1-x}P_x)_2$ [23], may be of importance. This value of T_c is the highest yet reported among iron-based bulk superconductors that have been studied by ARPES. In order to check the characteristic FS topology for the emergence of high-T_c in iron-based superconductors, we performed ARPES measurements for $Ca_{0.82}La_{0.18}Fe_2(As_{0.94}P_{0.06})_2$ superconductor [24].

High-quality single crystals of $Ca_{0.82}La_{0.18}Fe_2(As_{0.94}P_{0.06})_2$ were grown as described elsewhere [23]. ARPES measurements were carried out at BL-28A of the Photon Factory using circularly polarized light ($h\nu$ = 40–86 eV) and at BL-9A of the Hiroshima Synchrotron Radiation Center using circularly and linear polarized light ($h\nu$ = 19–31 eV). The total energy resolution was set to 10–30 meV. Clean surfaces were obtained by *in situ* cleaving of crystal in a working vacuum better than 3×10^{-8} Pa and measured at 60 K (above T_c).

In Figs. 2(a) and (b), we show ARPES intensity plots taken along the Γ-X direction with *s*- and *p*-polarized light, respectively ($h\nu$ = 31 eV). We observed one hole-like band whose top is located around 30 meV below E_F (α_1) and two hole-like bands with crossing E_F (α_2 and β). In the *s*-pol data along the Z-X [Fig. 2(c)], we found that the top of the α_1 band is located around 10 meV below E_F, indicating that the α_1 band cannot form FS between the Γ and Z points. On the other hand, the α_2 and β bands cross E_F at Z, as seen in the *p*-pol data [Fig. 2(d)]. Since the position of the Fermi wave vector (k_F) of the α_2 and β bands has almost no k_z dependence [Fig. 2(h)], we find these bands form nearly two-dimensional hole-like FSs. Around the M and A points, we observed two electron-like bands (ε and δ) as seen in Figs. 2(e) and (f). These form elliptical electron-like FSs [Fig. 2(g)], and their k_F position shows sizeable undulation along the k_z direction [Fig. 2(i)] reflecting the elliptical shape of these FSs and the shape of the boundary in the body-centered tetragonal Brillouin zone. Figs. 2(g-i) show the shape of the four FSs (α_2, β, ε, δ) observed by our ARPES measurements [24]. The total carrier number deduced from the volume of FSs of

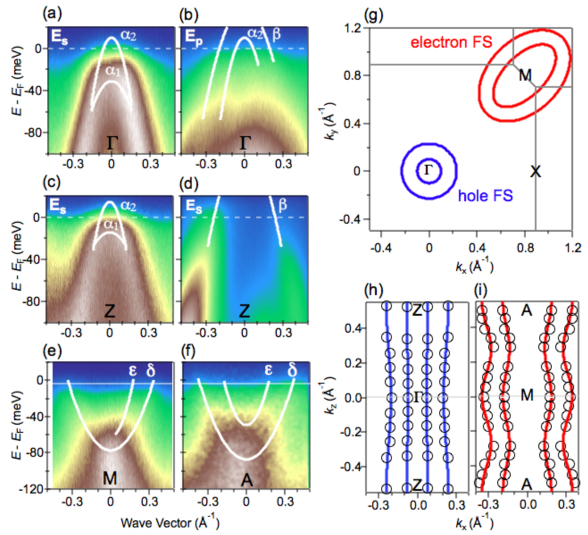

Figure 2: (a), (b) ARPES intensity plots taken along the Γ-X direction with *s*- and *p*-polarized light, respectively ($h\nu$ = 31 eV). (c), (d) are the same as (a), (b) but measured along the Z-X direction ($h\nu$ = 19 eV). (e), (f) ARPES intensity plots taken at M and A points, respectively ($h\nu$ = 69 eV and $h\nu$ = 86 eV). In (a)-(f), the white curves represent the band dispersion. (g) The FS topology in the k_x-k_y plane. The blue and red curved lines represent hole- and electron-like FSs, respectively. (h) and (i) The FS topology in the k_x-k_z plane. In (h) and (i), open circles show the positions of k_F deduced from the momentum distribution curve analysis of photon-energy dependent ARPES data [24].

0.12 ± 0.07 e/Fe agrees with the value expected from the chemical composition of 0.09 e/Fe.

Next we discuss the implications of the present ARPES results for iron-based superconductivity. As shown in Figs. 1(b) and (d), all hole-like FSs in hole-doped $Ba_{1-x}K_xFe_2As_2$ and electron-doped $Ca_{0.82}La_{0.18}Fe_2(As_{0.94}P_{0.06})_2$ have nearly a two-dimensional shape in common [19, 20]. From these results, we suggest that the two-dimensional FS topology, leading to the good FS nesting condition, is universal for high-T_c superconductivity regardless of the type of doped carrier. This supports the unconventional mechanisms for superconductivity in iron-based superconductors.

In summary, we investigated the three-dimensional electronic structure near E_F in electron-doped $Ca_{0.82}La_{0.18}Fe_2(As_{0.94}P_{0.06})_2$ (T_c = 45 K). We observed a nearly two-dimensional FS topology similar to that of $Ba_{1-x}K_xFe_2As_2$, demonstrating the common identity of the electronic structure to induce high-T_c in 122-type iron-based superconductors.

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