# ARPES Results of '122' Iron-based Superconductors

Qinlong Luo
qluo@utk.edu
*Department of Physics and Astronomy, University of Tennessee, Knoxville, TN 37996, USA*
(Dated: April 23, 2010)

This paper shows several angle-resolved photoemission spectroscopy (ARPES) results of iron-based superconductors. It only contains the results for 122 system, which are very similar to 1111 system. The band structure and Fermi surfaces: two hole-like pockets around Γ point and one electron-like pocket around M point, are in a good agreement with band structure calculations

PACS numbers:

## I. INTRODUCTION

The discovery of superconductivity in iron pnictides has attracted considerable interest of the condensed matter physics community [1]. The superconductivity has been observed in both 1111 and 122 system. These superconductors display a fascinating interplay between magnetism and superconductivity. Two kinds of techniques are mainly performed to study these materials. One is the neutron scattering experiments which show a spin-density-wave (SDW) ground state [3–5] in the parent compounds. The other is the angle-resolved photoemission spectroscopy(ARPES) is a powerful technique to study this material, which can show the details of the electron structure of this material [7–13, 16–20].

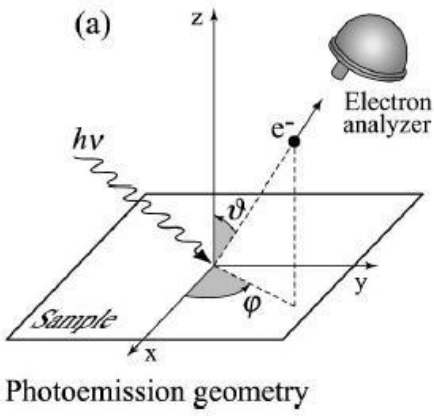


FIG. 1: geometry of an ARPES experiment in which the emission direction of the photoelectron is specified by the polar ($\vartheta$) and azimuthal ($\varphi$) angles.

To study the electronic structure of high-Tc superconductors, ARPES plays a major role because it is the most direct method to measure the energy and momentum of electrons simultaneously. The geometry of an ARPES experiment [2] is sketched in Fig. 1. With the incidence of monochromatic photons, the electrons in the sample are emitted by the photoelectric effect and escape into the vacuum in all directions. By measuring (calculating) the energy and momentum of these collective photoelectrons, one can plot the energy-momentum dispersions, which gives the band structure and FS of the sample.

The crystal structure of 122 parent compound is shown in Fig. 2 [6]. It contains the FeAs layer as the 1111 system

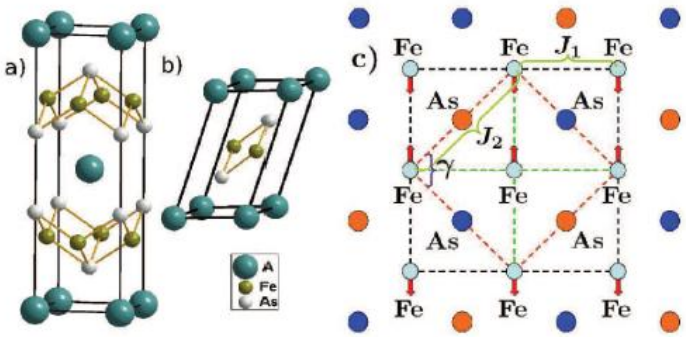


FIG. 2: Crystal structure of $AFe_2As_2$ (A=Ba, Sr, Ca).

does. The parent compounds undergo a tetragonal to orthorhombic structural transition accompanied by a magnetic transition which exhibits a SDW state below a transition temperature $T_{SDW}$.

## II. ARPES STUDY OF IRON-BASED SUPERCONDUCTORS

(1) $BaFe_2As_2$

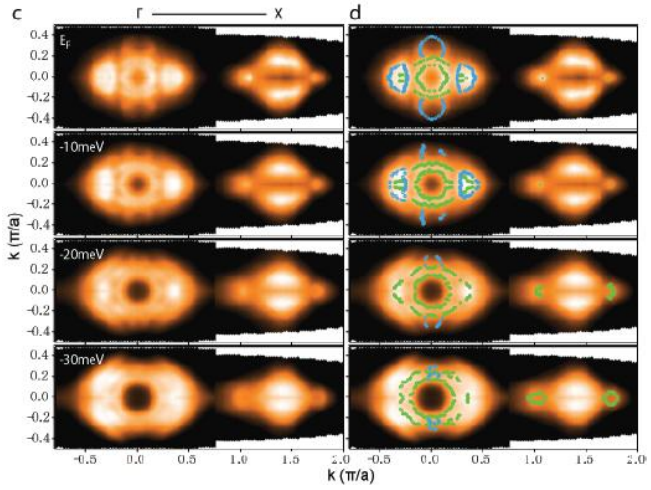


FIG. 3: Constant energy mapping of $BaFe_2As_2$ in the SDW state. (c) Constant energy maps across the Γ-X region at $E_B$=0, 10meV, 20meV, and 30meV. (d) Maps in (c) overlaid with dots marking the constant energy contours of the bands. Green marks donote hole-like features while blue marks denote electron-like features.

The Fermi surface (FS) of $BaFe_2As_2$ is shown in Fig. 3 [7]. Around the zone center (Γ point), there exist two enclosed pockets which are hole-like–increasing the binding energy results in a larger size of the pockets. Around these two pockets, four petal-like pockets are observed below the SDW transition temperature $T_{SDW}$, which disappear above $T_{SDW}$. These four petal-like pockets are electron-like because the size of the pockets become smaller with the binding energy increased. But these four pockets are absent in some experiments due to the low resolution of ARPES. Around the zone corner (M point), an electron-like pocket can be observed in both above and below $T_{SDW}$ cases. Four petal-like pockets are observed again around the M point, but they are hole-like which is opposite to the case around the Γ point.

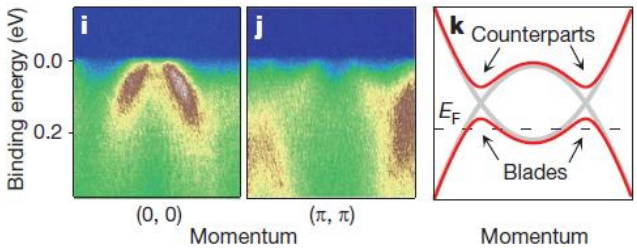


FIG. 4: Reconstruction of the electronic structure. (i) (j) Parallel cuts through the electronic structure of $BaFe_2As_2$, set apart by ($\pi$,$\pi$). (k) Simplest model showing the result of folding of single hole- and electron-like bands.

The band structure of $BaFe_2As_2$ is shown in Fig. 4 [8]. A simplest model illustrates that the hole-like petal pockets and the electron-like pocket around M point results from the folding of single hole- and electron-like bands, as shown in Fig. 4(k). In the LDA calculation [14–16], the interaction of the ($\pi$,$\pi$) replica of the Γ-centered hole-like band with the M-centered electron-like band implies that nesting plays an key role in the reconstruction of the Fermi surfaces of this material.

(2) $SrFe_2As_2$

A typical electronic structure of $SrFe_2As_2$ in Fig. 5 [17]. At high temperature, there are only two hole-like pockets around Γ point and one electron-like pocket around M point. At low temperature(SDW state), four petal like pockets appear around Γ point and four appear around M point. But the four pockets around Γ point are hole-like which is opposite to the $BaFe_2As_2$ case. Therefore, these two case are very similar except the only difference mentioned above.

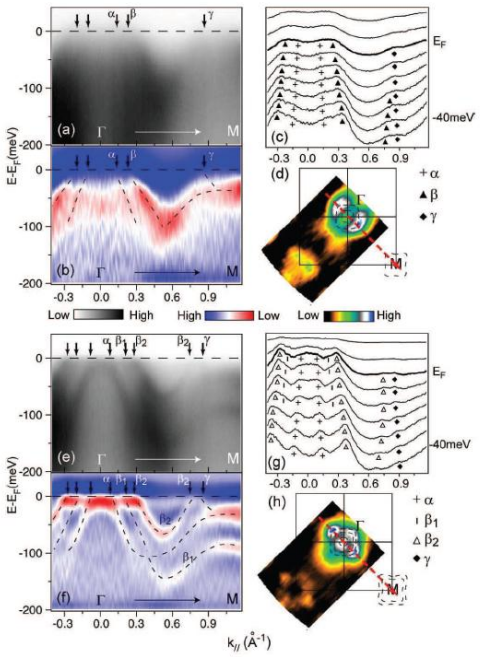


FIG. 5: Electronic structure of $SrFe_2As_2$. (a) Photonemission intensity along Γ - M cut as indicated in panel d. (b) The second derivative of the data in panel a. (c) The MDC's near Fermi energy for the data in panel a. (d) Photonemission intensity map at $E_F$ in the Brillouin zone, where the measured Fermi surface sheets are shown by dashed curves. Data were taken at 230K. (e,f,g,h) are the same as in panel a,b,c,d respectively, but taken at 10K.

(3) $CaFe_2As_2$

The ARPES data of $CaFe_2As_2$ at low temperature is presented in Fig. 6 [19]. At Γ point, the two hole-like pockets is given by the bands $\alpha$ and $\beta$. And the petal like pocket given by band $\gamma$ is hole-like, similar as the $SrFe_2As_2$ case. At M point, the shape of Fermi surface is identical to that of $BaFe_2As_2$.

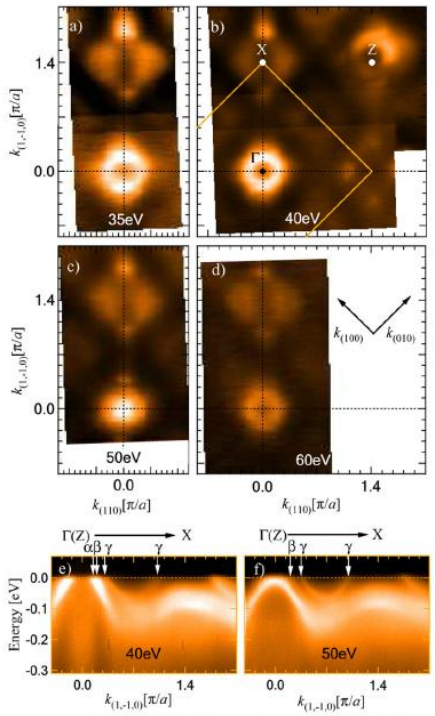


FIG. 6: ARPES data of $CaFe_2As_2$ low temperature orthorhombic phase (T=12K) for a few photon energies. (a)-(d) ARPES intensity integrated within 10 meV about $\mu$ for $h\gamma$ = 35, 40, 50, and 60 eV, respectively. (e)-(f) Band dispersion data along the Γ-X direction for $h\gamma$ = 40 and 50 eV. $\alpha, \beta, \gamma$ correspond to different bands that cross $\mu$.

(4) Three-dimensional property

This iron pnictides superconductors are more three-dimensional than cuprate superconductors. In ARPES experiments, the z component of the momentum is identified by the incident energy of the photon. In Fig. 6(a)(b)(c)(d), the bands that form the Γ pocket changes dramatically with the incident photon energies while the bands around the M stay invariable. The Fig. 7 gives a clearer illustration about this point with the $k_z$ dispersion [20].

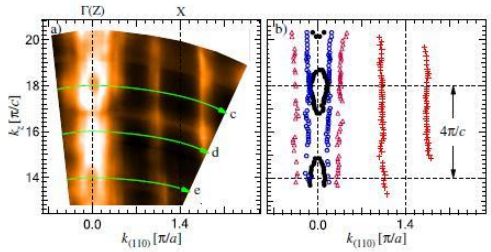


FIG. 7: $k_z$ dispersion data for $CaFe_2As_2$ low temperature orthorhombic phase (T = 40 K). (a) $k_z$ dispersion data obtained by plotting ARPES intensity integrated within 10 meV about $\mu$ as a function of $k_{(110)}$ and the energy of the incident photons. The photon energy range used was from 35 to 105 eV. (b) Fermi momentum $k_F$ was extracted from the data in panel (a) using the peak positions of the MDC's.

(5) Theoretical results

The Mean-field Approximation (MFA) is applied to the 5-orbital model [21]. The Hamiltonian reads:

$$H_0 = \sum_{\mathbf{k},\sigma} \sum_{\alpha,\beta} \left(\xi_{\alpha\beta}(\mathbf{k}) + \epsilon_\alpha \delta_{\alpha\beta}\right) d^\dagger_{\alpha\sigma}(\mathbf{k}) d_{\beta\sigma}(\mathbf{k}), \tag{1}$$

$$\begin{aligned} H_{\text{int}} &= U \sum_{\mathbf{i},\alpha} n_{\mathbf{i},\alpha,\uparrow} n_{\mathbf{i},\alpha,\downarrow} + (U' - \frac{J}{2}) \sum_{\mathbf{i},\alpha<\beta} n_{\mathbf{i},\alpha} n_{\mathbf{i},\beta} \\ &\quad -2J \sum_{\mathbf{i},\alpha<\beta} \mathbf{S}_{\mathbf{i},\alpha} \cdot \mathbf{S}_{\mathbf{i},\beta}. \end{aligned} \tag{2}$$

where $d^\dagger_{\alpha\sigma}(\mathbf{k})$ creates a particle with momentum $\mathbf{k}$ and spin $\sigma$ in the orbital $\alpha$, and $\epsilon_\alpha$ refers to the on-site energy of orbital $\alpha$. And $\mathbf{S}_{\mathbf{i},\alpha}$ ($n_{\mathbf{i},\alpha}$) is the spin (charge density) of orbital $\alpha$ at site $\mathbf{i}$, and $n_{\mathbf{i},\alpha} = n_{\mathbf{i},\alpha,\uparrow} + n_{\mathbf{i},\alpha,\downarrow}$. These terms refer to, accordingly, an on-site intra-orbital Hubbard repulsion, an inter-orbital repulsion, and a finite Hund coupling. Here we have $U' = U - 2J$.

Fig. 8 shows a typical result including the band structure from Γ point to M point and Fermi surface (FS). From the FS, there are two enclosed hole-like pockets around Γ point and one enclosed electron-like pocket around M point. Also four petal-like pockets are observed in this case, which is consistent with the ARPES results.

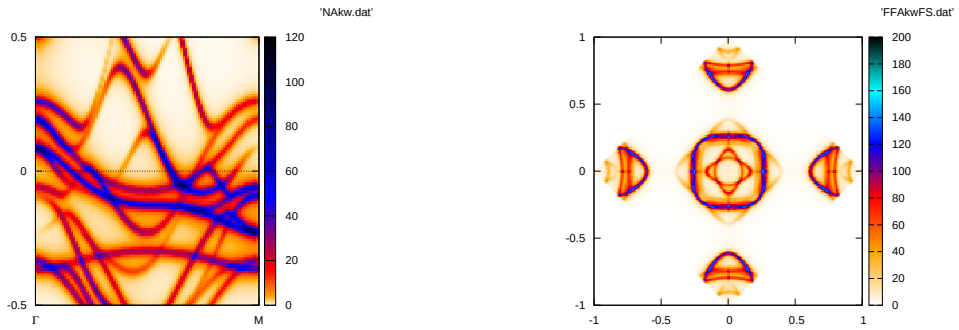


FIG. 8: band structure and Fermi surface. Here J/U=0.28 and U=1.45.

## III. CONCLUSIONS

In conclusion, the most recent ARPES results of 122 system of iron-based superconductors are summarized here. There are two hole-like pockets around the Γ point and four petal like pockets around these two pockets, which are electron-like in $BaFe_2As_2$ case but hole-like in other two cases. Referring to the M point, four petal like pockets, which are hole-like, are around an electron-like enclosed pocket. The electron structure of these materials shows an interesting point that they are more three-dimensional than the cuprates. Also the Mean-field calculation shows the consistency with the ARPES results.

[1] Y. Kamihara, T. Watanabe, M. Hirano, and H. Hosono, J. of the Am. Chem. Soc. **130**, 3296 (2008).
[2] A. Damascelli, Z. Hussain, Z.-X. Shen, Rev. Mod. Phys., **75**, 473 (2003).
[3] C. de la Cruz *et al.*, Nature (london) **453**, 899 (2008).
[4] Q. Huang, Y. Qiu, W. Bao, M. A. Green, J. W. Lynn, Y. C. Gasparovic, T. Wu, G. Wu, and X. H. Chen, Phys. Rev. Lett. **101**, 257003 (2008).
[5] J. Zhao, W. Ratcliff II, J. W. Lynn, G. F. Chen, J. L. Luo, N. L. Wang, J. Hu, and P. Dai, Phys. Rev. B **78**, 140504(R) (2008).
[6] Fengjie Ma, Zhong-Yi Lu, and Tao Xiang, arXiv:0806.3526.
[7] M. Yi, D. H. Lu, J. G. Analytis, J.-H. Chu, S.-K. Mo, R.-H. He, M. Hashimoto, R. G. Moore, I. I. Mazin, D. J. Singh, Z. Hussain, I. R. Fisher, and Z.-X. Shen, Phys. Rev. B **80**, 174510(R) (2009).
[8] V. B. Zabolotnyy, D. S. Inosov, D. V. Evtushinsky, A. Koitzsch, A. A. Kordyuk, G. L. Sun, J. T. Park, D. Haug, V. Hinkov, A. V. Boris, C. T. Lin, M. Knupfer, A. N. Yaresko, B. Buechner, A. Varykhalov, R. Follath, and S. V. Borisenko, Nature **457**, 569 (2009).
[9] Chang Liu, Takeshi Kondo, Rafael M. Fernandes, Ari D. Palczewski, Eun Deok Mun, Ni Ni, Alexander N. Thaler, Aaron Bostwick, Eli Rotenberg, Joerg Schmalian, Sergey L. Bud'ko, Paul C. Canfield, Adam Kaminski, arXiv:0910.1799.
[10] S. Thirupathaiah, S. de Jong, R. Ovsyannikov, H.A. Duerr, A. Varykhalov, R. Follath, Y. Huang, R. Huisman, M.S. Golden, Yu-Zhong Zhang, H.O. Jeschke, R. Valenti, A. Erb, A. Gloskovskii, J. Fink, arXiv:0910.0147.
[11] Chang Liu, G. D. Samolyuk, Y. Lee, Ni Ni, Takeshi Kondo, A. F. Santander-Syro, S. L. Budko, J. L. McChesney, E. Rotenberg, T. Valla, A. V. Fedorov, P. C. Canfield, B. N. Harmon, and A. Kaminski, Phys. Rev. Lett. **101**, 177005 (2008).
[12] P. Richard, K. Nakayama, T. Sato, M. Neupane, Y.-M. Xu, J. H. Bowen, G. F. Chen, J. L. Luo, N. L. Wang, H. Ding, T. Takahashi, arXiv:0909.0574.
[13] Y Sekiba, T Sato, K Nakayama, K Terashima, P Richard, J H Bowen, H Ding, Y-M Xu, L J Li, G H Cao, Z-A Xu, and T Takahashi, New J. Phys. **11**, 025020 (2009)
[14] D. Singh and M.-H. Du, Phys. Rev. Lett. **100**, 237003 (2008).
[15] I.I. Mazin, D.J. Singh, M.D. Johannes and M.H. Du, Phys. Rev. Lett. **101**, 057003 (2008).
[16] J. Fink, S. Thirupathaiah, R. Ovsyannikov, H. A. Duerr, R. Follath, Y. Huang, S. de Jong, M.S. Golden, Yu-Zhong Zhang, H.O. Jeschke, R. Valenti, C. Felser, S. Dastjani Farahani, M. Rotter, and D. Johrendt, arXiv:0903.0967.
[17] Y. Zhang, J. Wei, H. W. Ou, J. F. Zhao, B. Zhou, F. Chen, M. Xu, C. He, G. Wu, H. Chen, M. Arita, K. Shimada, H. Namatame, M. Taniguchi, X. H. Chen, D. L. Feng, arXiv:0808.2738.
[18] D. Hsieh, Y. Xia, L. Wray, D. Qian, K. Gomes, A. Yazdani, G.F. Chen, J.L. Luo, N.L. Wang, and M.Z. Hasan, arXiv:0812.2289.
[19] Chang Liu, Takeshi Kondo, Ni Ni, A. D. Palczewski, A. Bostwick, G. D. Samolyuk, R. Khasanov, M. Shi, E. Rotenberg, S. L. Budko, P. C. Canfield, and A. Kaminski, Phys. Rev. Lett. **102**, 167004 (2008).
[20] Takeshi Kondo, R. M. Fernandes, R. Khasanov, Chang Liu, A. D. Palczewski, Ni Ni, M. Shi, A. Bostwick, E. Rotenberg, J. Schmalian, S. L. Bud'ko, P. C. Canfield, A. Kaminski, arXiv:0905.0271.
[21] S. Graser, T. A. Maier, P. J. Hirschfeld, and D. J. Scalapino, New J. Phys. **11**, 025016 (2009)