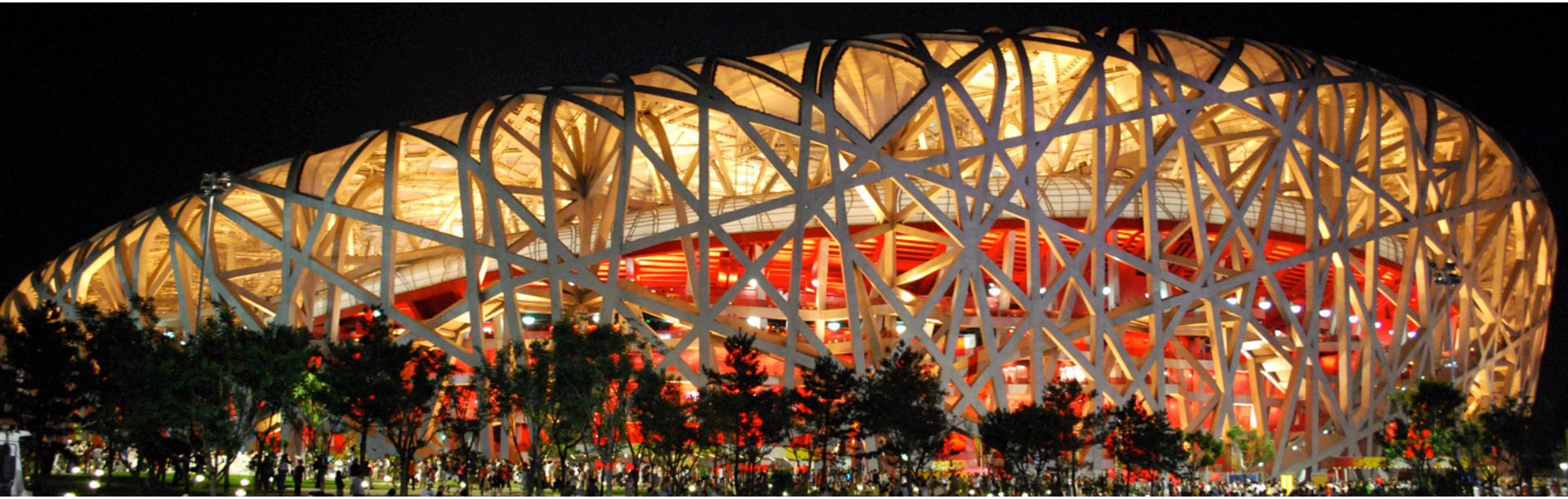
ARPES studies of iron-based superconductors



Hong Ding

Institute of Physics, Chinese Academy of Sciences

International Workshop on
"Recent developments in Fe-based high-temperature superconductors"
Long Island, US, *Sep. 3, 2013*

Outline
(focus on SC gap)

1. Brief review of our earlier ARPES measurements of SC gap in many Fe-SCs
2. A possible node observed in highly hole-doped $(Ba,K)Fe_2As_2$
3. A phenomenological understanding of Fe-SCs
4. In-gap states observed in $(Ba,K)Fe_2As_2$

Collaborators

ARPES:

IOP: T. Qian, P. Richard, J. Dong, Y.-B. Huang, X.-P. Wang, N. Xu, Y.-B. Shi, H. Miao, P. Zhang, J. Bowen

Boston College: Y.-M. Xu, M. Neupane, Z.-H. Pan

Tohoku Univ.: K. Nakayama, T. Kawahara, K. Sugawara, T. Arakane, Y. Sekiba, A. Takayama, S. Souma, T. Sato, T. Takahashi

Renmin Univ.: Z.-H. Liu, W.-C. Jin, S.-C. Wang

PSI: M. Shi, X.-Y. Cui, E. Razzoli, M. Radovic

BESSY: E. Rienks, S. Thirupathaiah

UVSOR: K. Terashima *ALS*: A. Fedorov

Theory:

IOP: X. Dai, Z. Fang *BC*: Z. Wang IOP/*Purdue*: J.-P. Hu

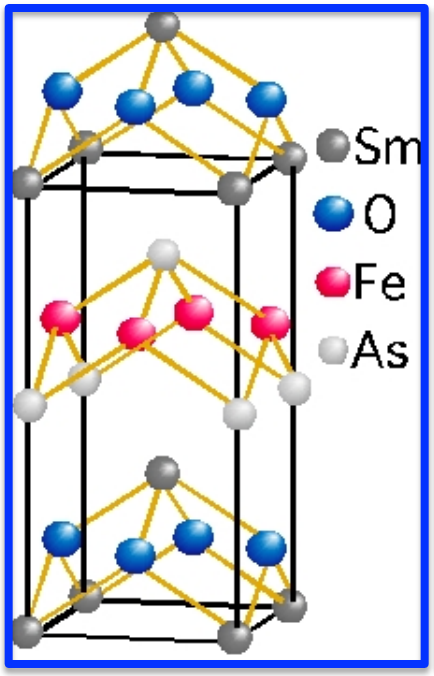
Samples:

IOP: G.-F. Chen , N.-L. Wang, X.-L. Chen

Nanjing Univ.: H.-H. Wen *Zhejiang Univ*.: G.-H. Cao, Z.-A. Xu, M.-H. Fang

UT: C.-L. Zhang, P.-C. Dai *BNL*: G.-D. Gu

Zoology of Fe-based superconductors



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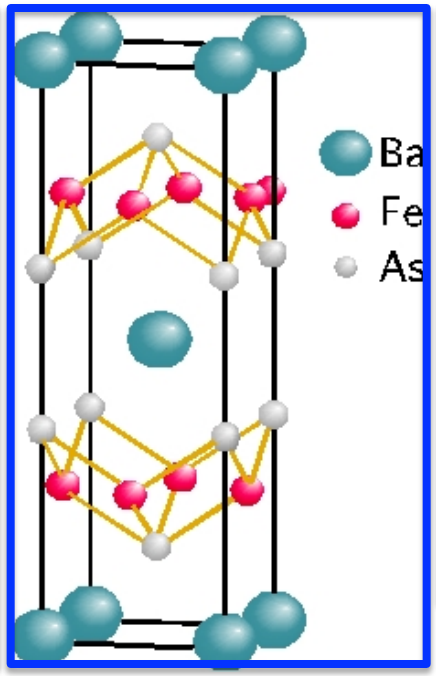
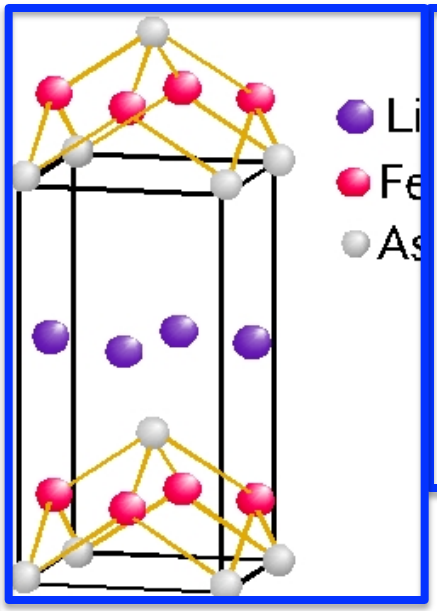


122



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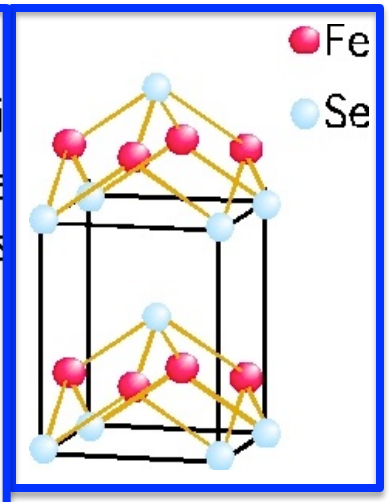

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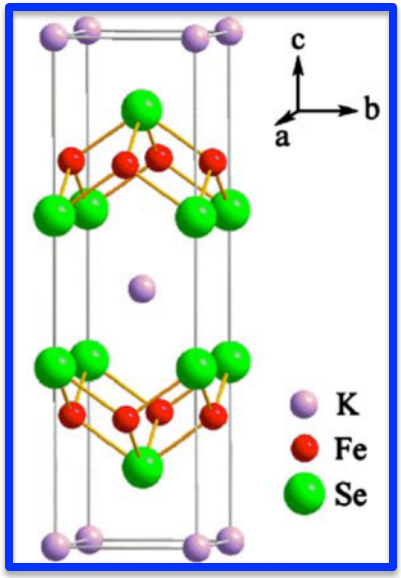
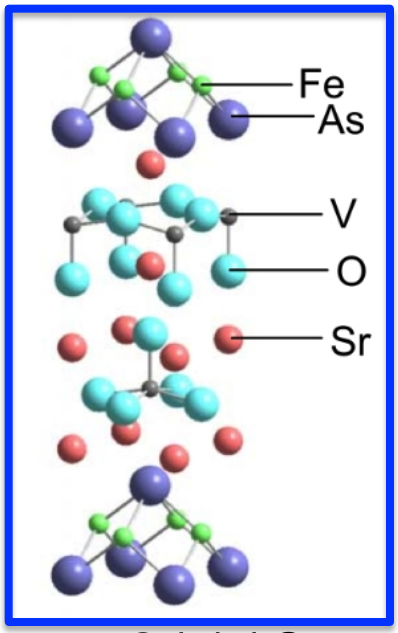
Universality in
Fermi surface topology
& superconducting gap?

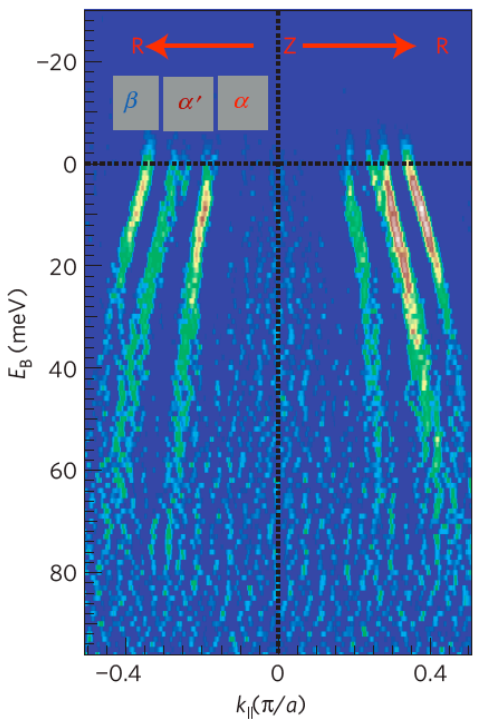


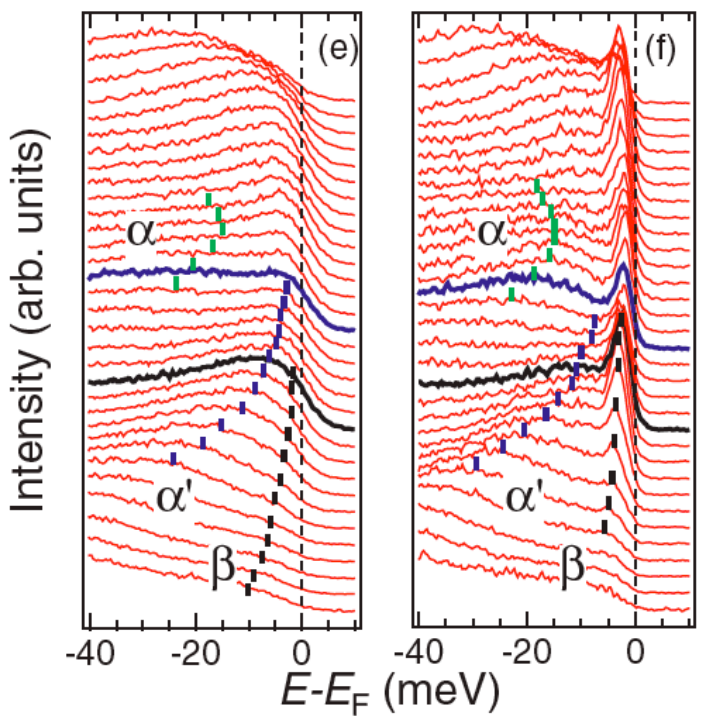
122'

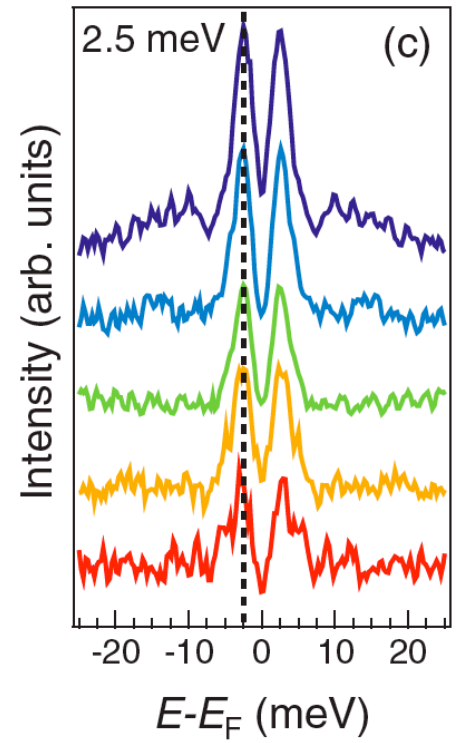


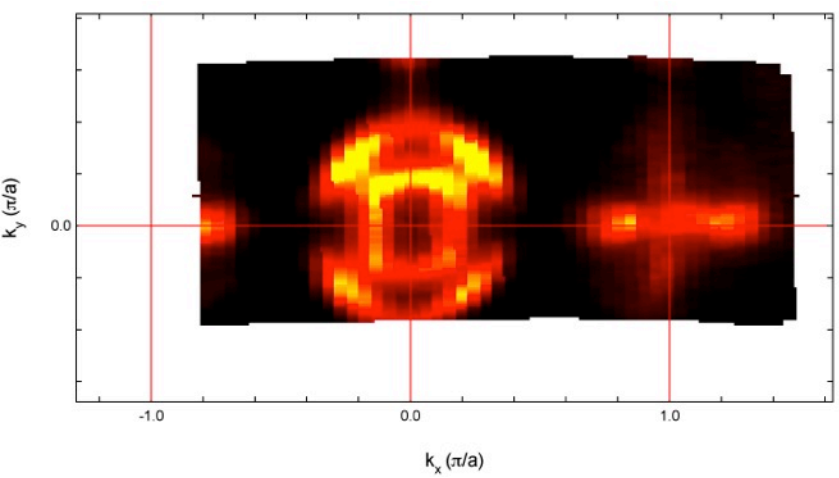
21113

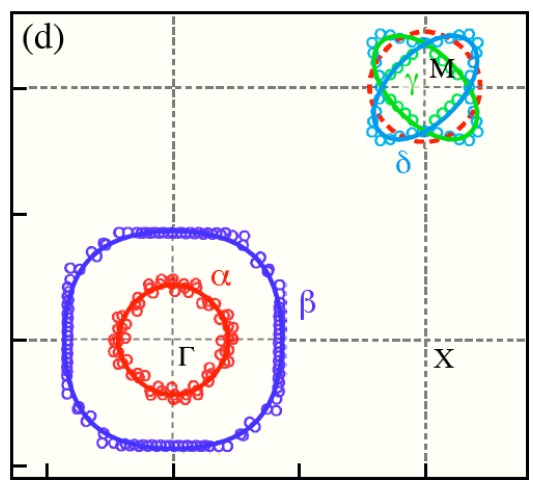
ARPES measures band structure, FS, & SC gap in Fe-SCs

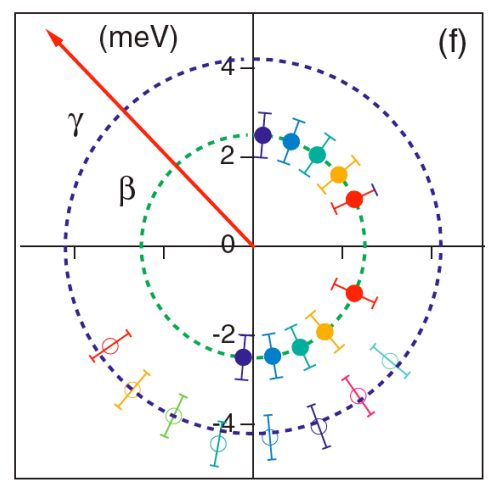




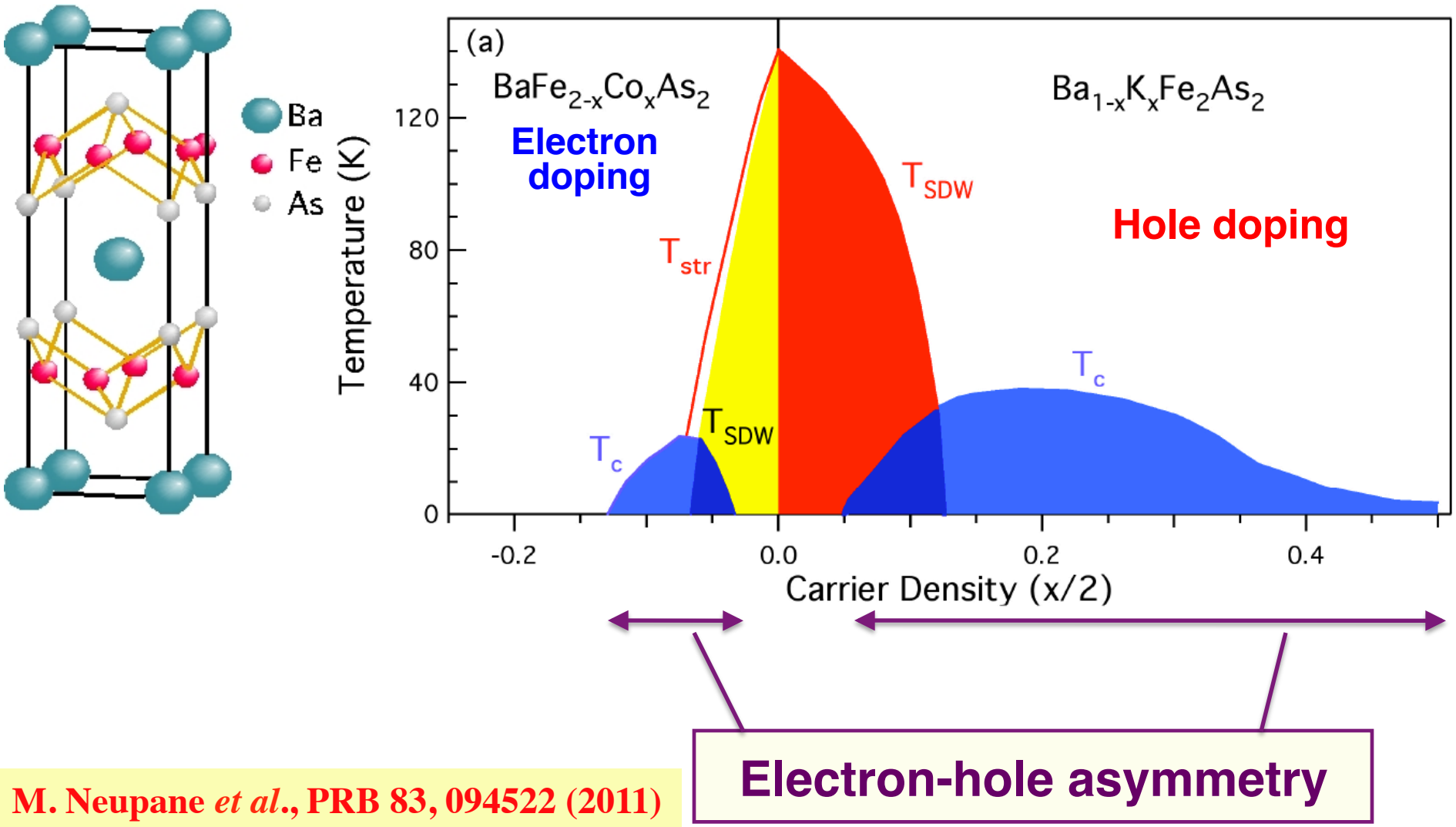








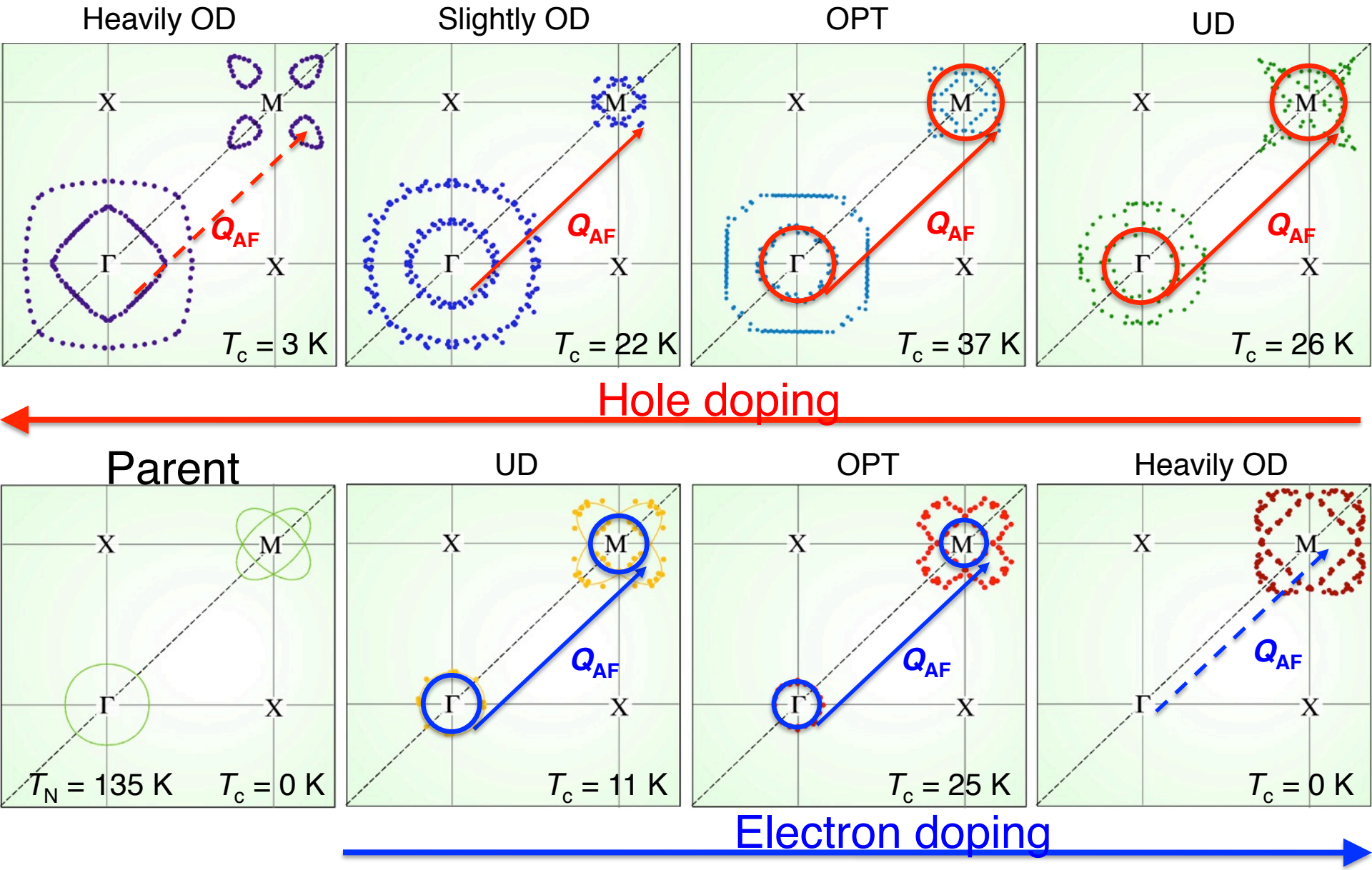
Phase diagram of Ba122 system



Electron-hole asymmetry

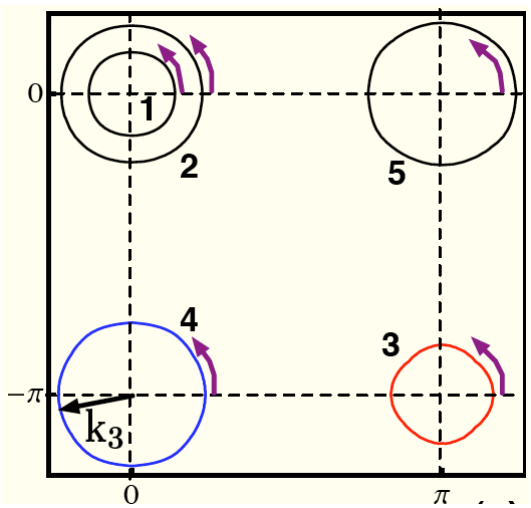
M. Neupane *et al*., PRB 83, 094522 (2011)

Fermi surface evolution in "122": quasi-nesting?

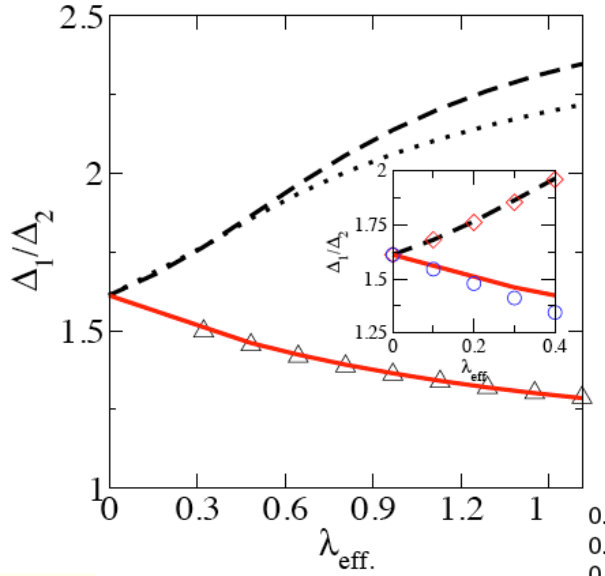


Most weak-coupling theories predict anisotropic s± gap

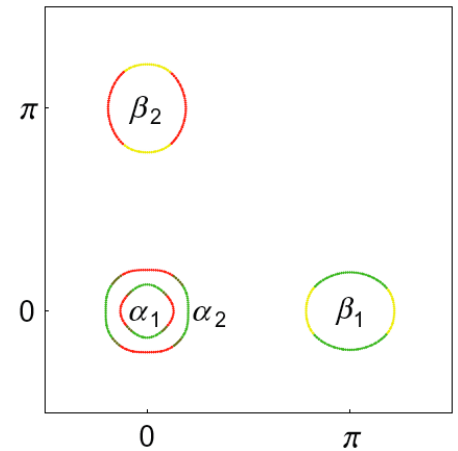
D.H. Lee
EPL 85, 37005 (2009)

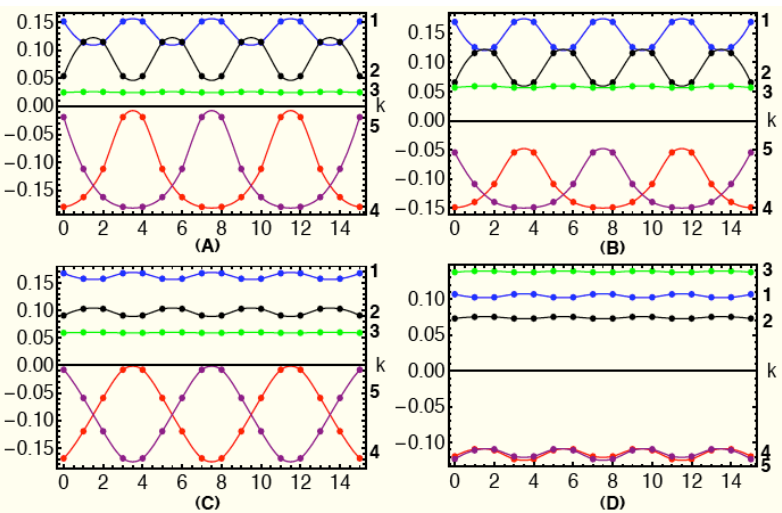


I. Mazin
PRB 79, 060502 (2009)



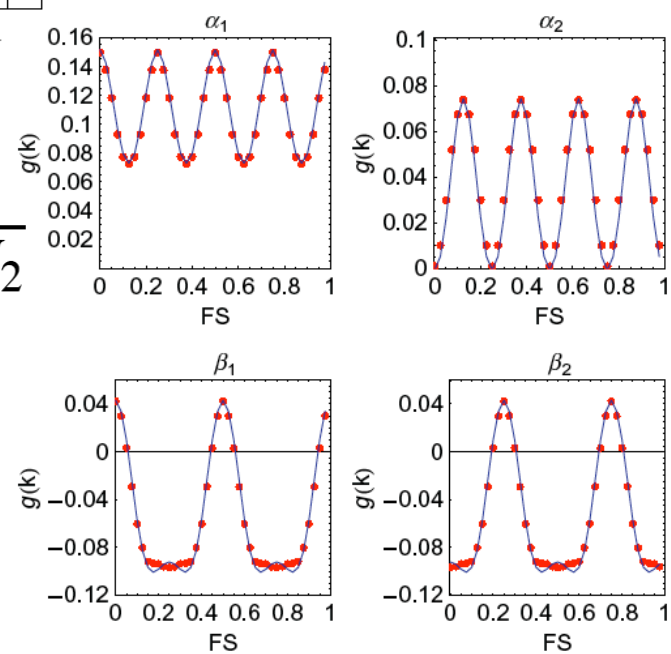
S. Graser
NJP 11, 025016 (2009)





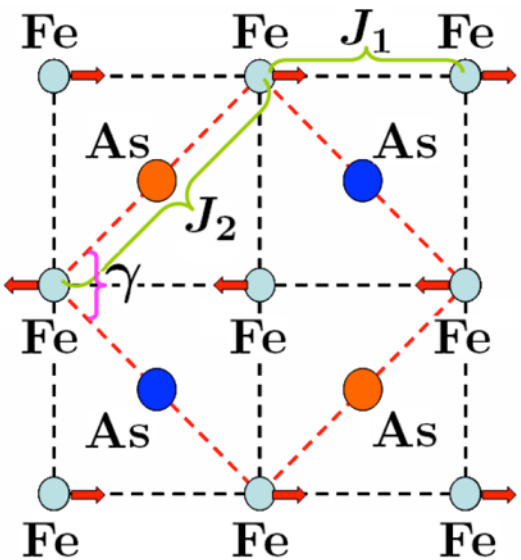
$$\Delta_2/\Delta_1 = \sqrt{N_1/N_2}$$

when $\lambda_{eff} \to 0$

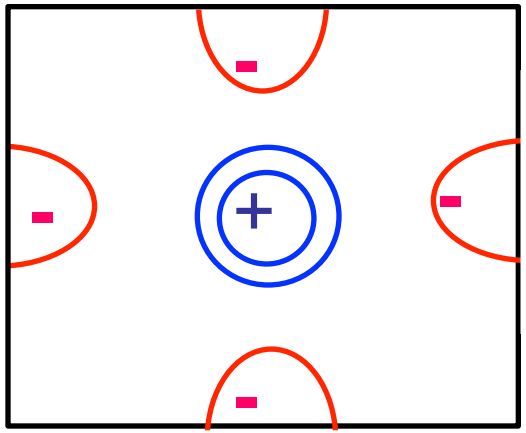


$J_1 - J_2$ model predicts almost isotropic s± gap

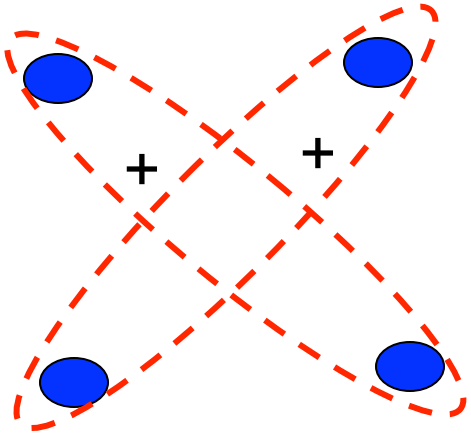
local interactions
J_1- J_2



Order parameters in momentum Space



Real space configuration of pairing symmetry

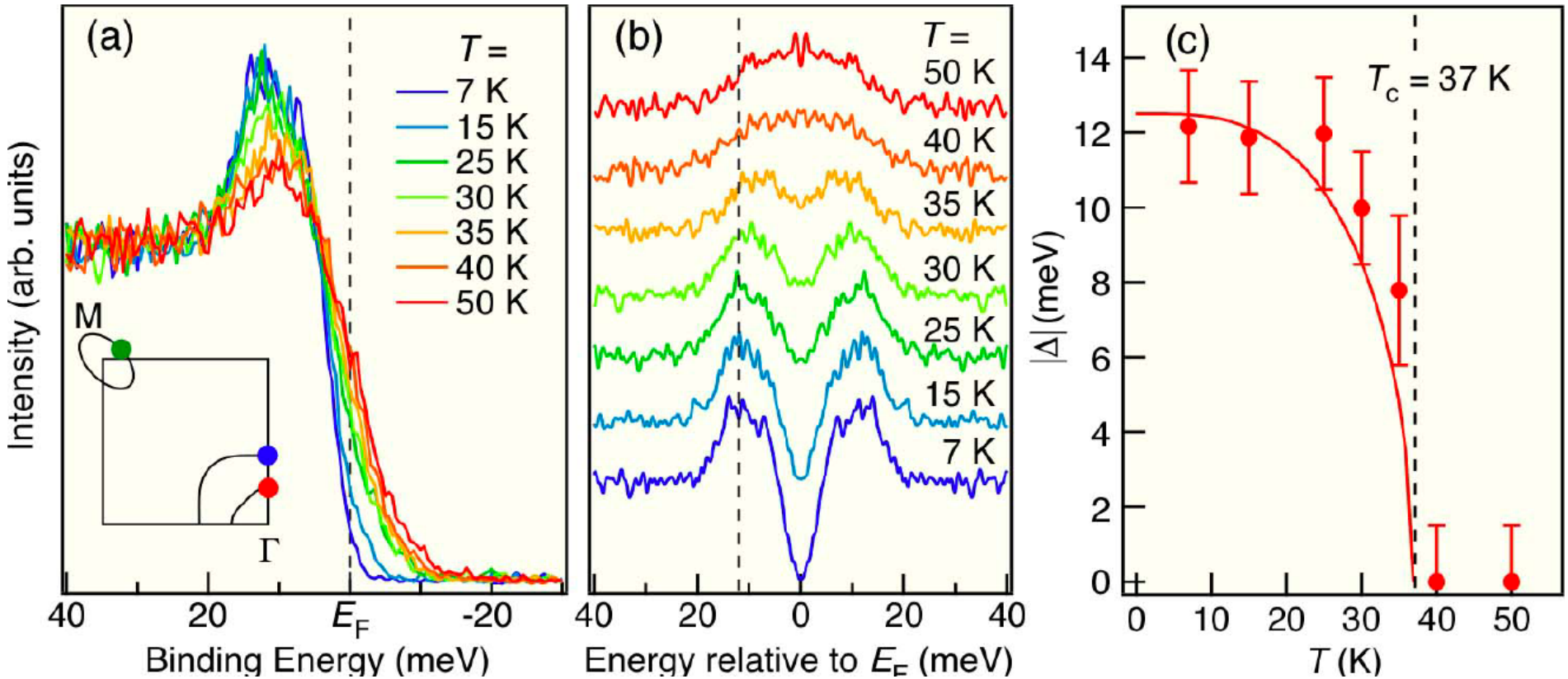


pnictides: large J_2 and FS topology favor $\Delta = \Delta_0 \cos k_x \cos k_y$, s±-wave

cuprates: large J_1 and FS topology favor $\Delta = \Delta_0 (\cos k_x - \cos k_y)/2$, d-wave

K. Seo, A. B. Bernevig, J. Hu PRL 101, 206404 (2008)

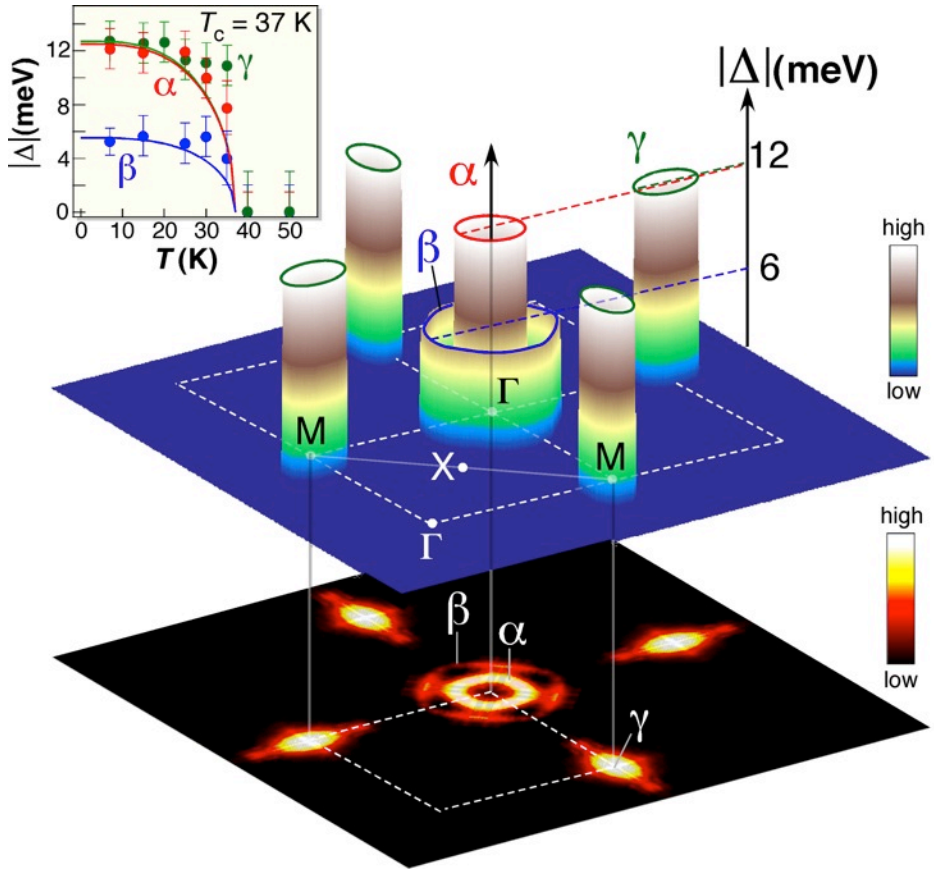
ARPES observation of superconducting gap

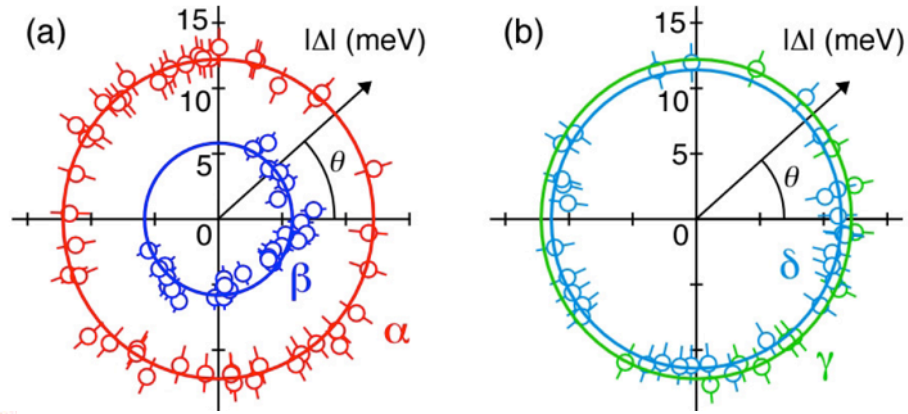


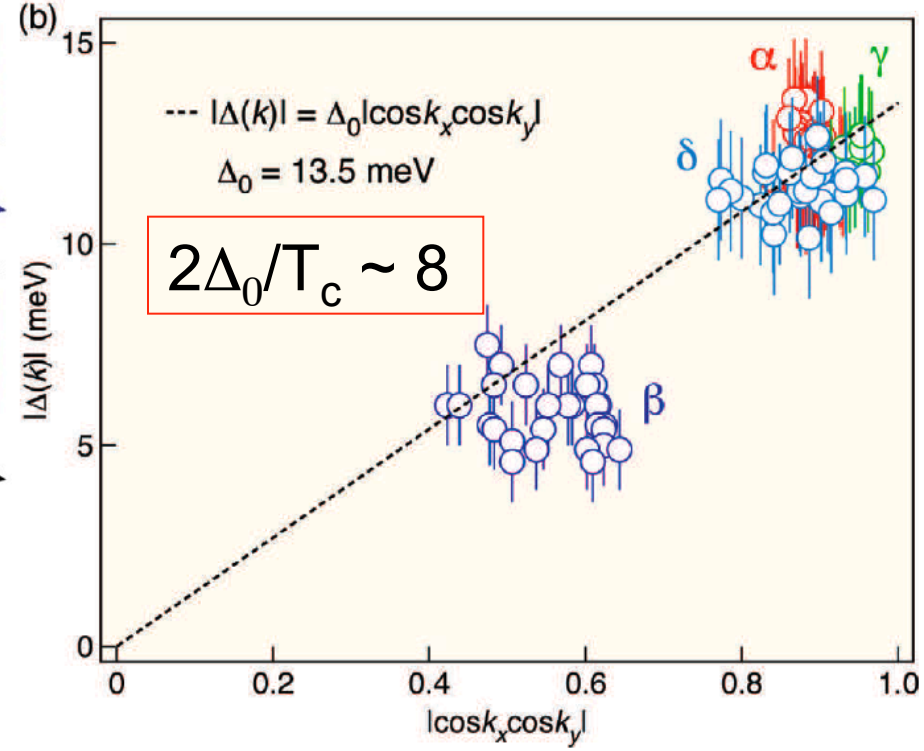
$2\Delta/T_c \sim 7$

H. Ding *et al.*, EPL 83, 47001 (2008)

Nodeless FS-dependent SC gap in $Ba_{0.6}K_{0.4}Fe_2As_2$ (T_c = 37K)



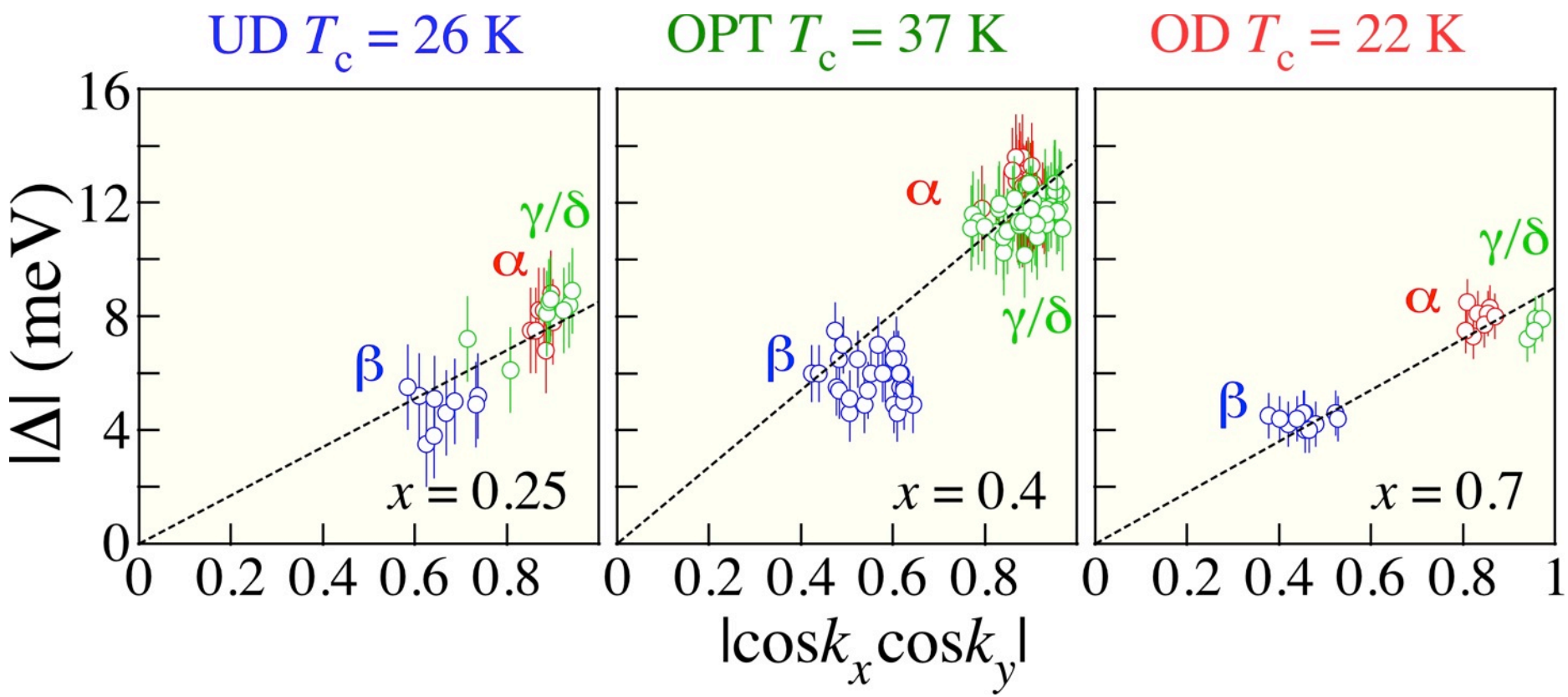




H. Ding *et al.*, EPL 83, 47001 (2008)

K. Nakayama *et al.*, EPL 85, 67002 (2009)

$\cos k_x \cos k_y$ plot of SC gap

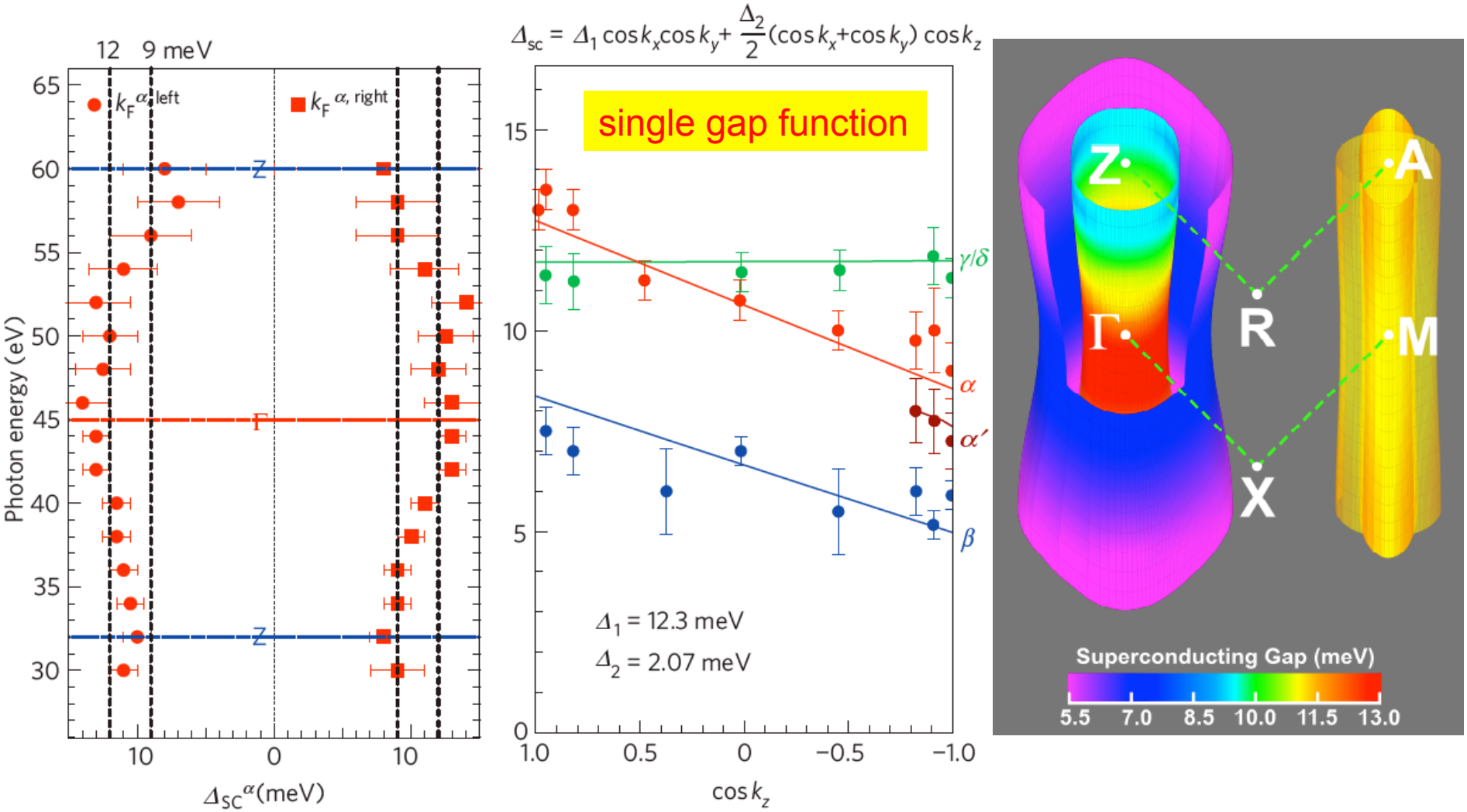


SC gap roughly follows $\Delta_0 \cos k_x \cos k_y$ irrespective of doping level

Y.-M. Xu *et al.*, Nature Comm. 2, 392 (2011)

K. Nakayama *et al.*, PRB 83, 020501(R) (2011)

kz dependence of SC gaps

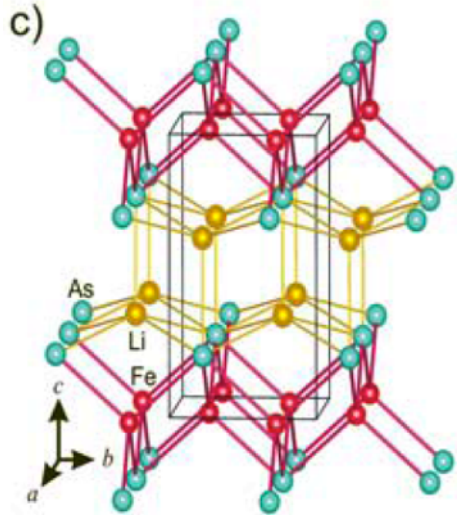


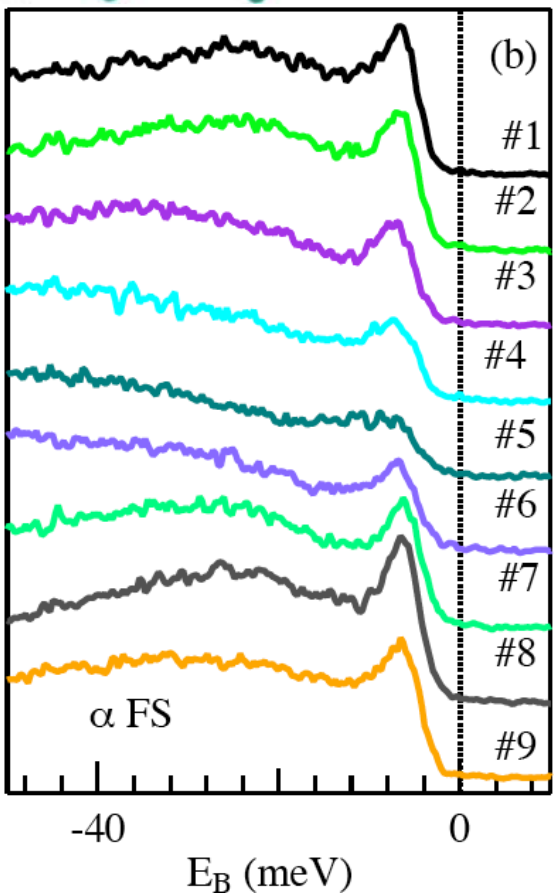
$J_{ab} = 30$
$J_c = 5$

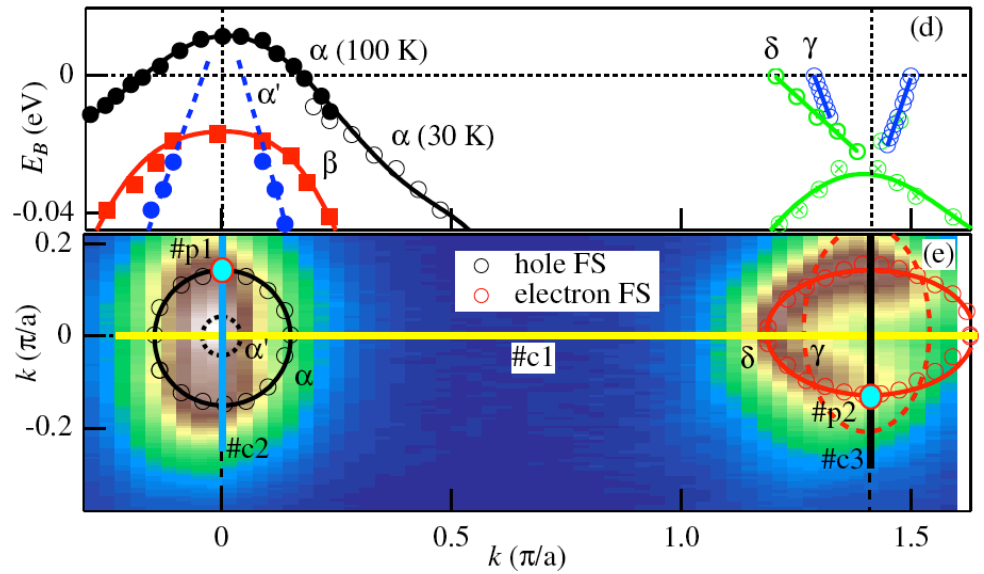
$\Delta_2/\Delta_1 \approx J_c/J_{ab} \approx 0.17$

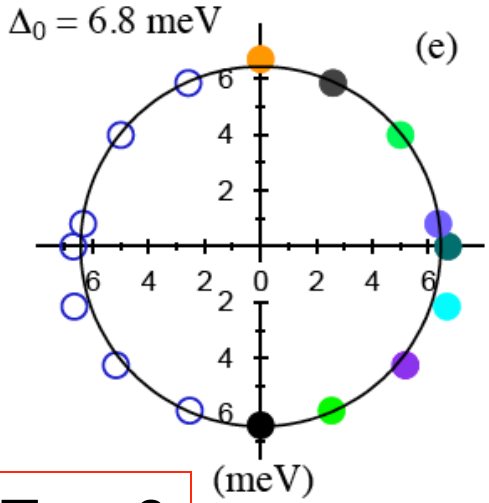
Y.-M. Xu *et al.*, Nature Physics 7, 198 (2011)

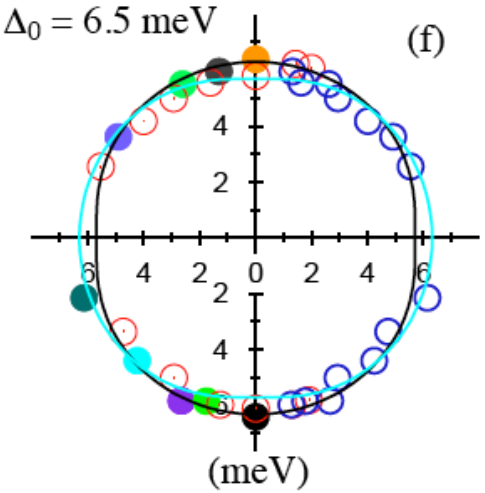
"111" - $NaFe_{0.95}Co_{0.05}As$ (T_c = 18K) non-polar surface











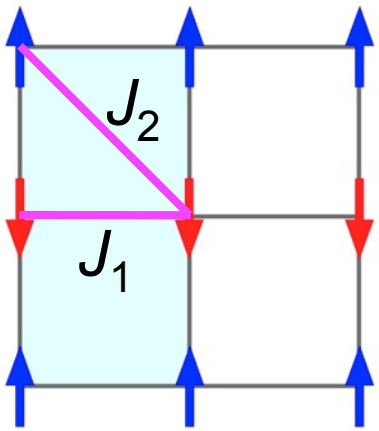
$2\Delta/T_c \sim 8$

Z.-H. Liu *et al.*, PRB 84, 064519 (2011)

Modification of SC gap function in $FeTe_{0.55}Se_{0.45}$

FeAs

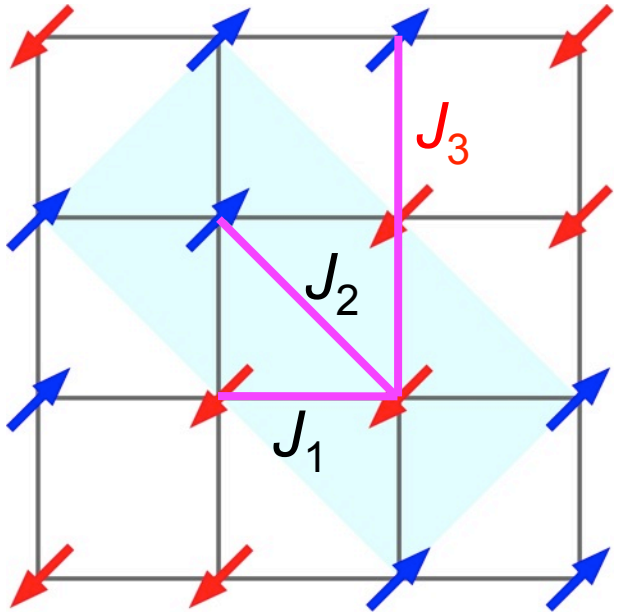
J_2 is large



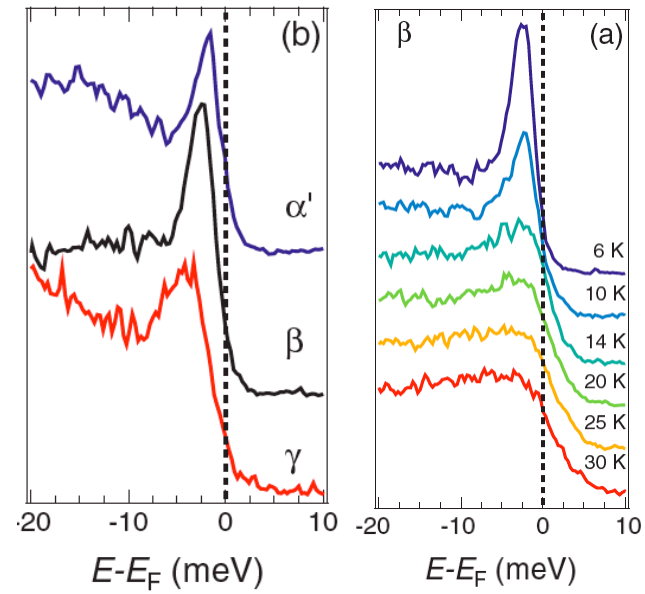
$s_{\pm}$-wave pairing
($\Delta_0 \cos k_x \cos k_y$)

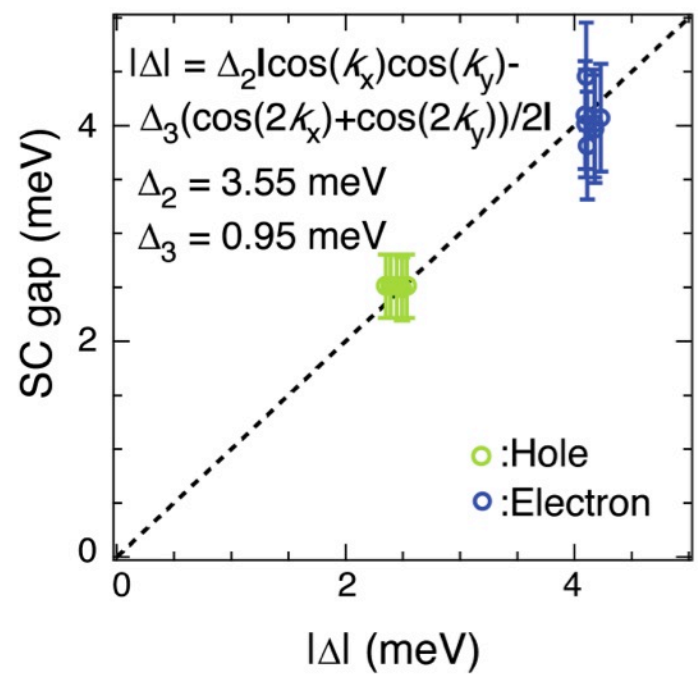
FeTe

J_3 is no longer negligible



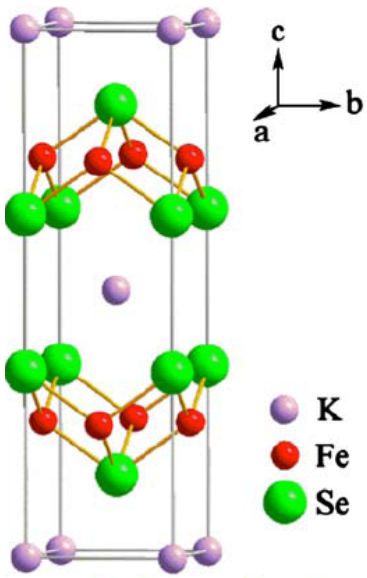
$s_{\pm}$-wave pairing
($\Delta_2 \cos k_x \cos k_y$
$- \Delta_3(\cos 2k_x + \cos 2k_y)/2$)

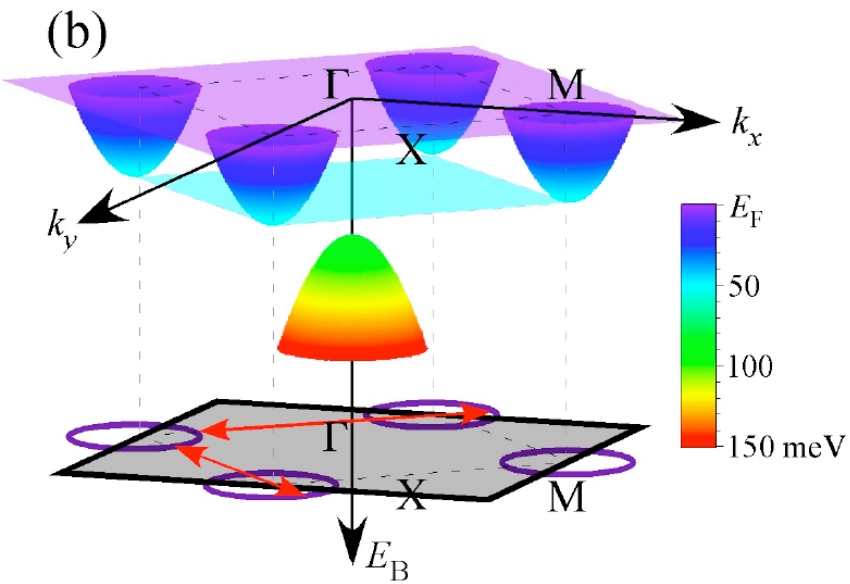


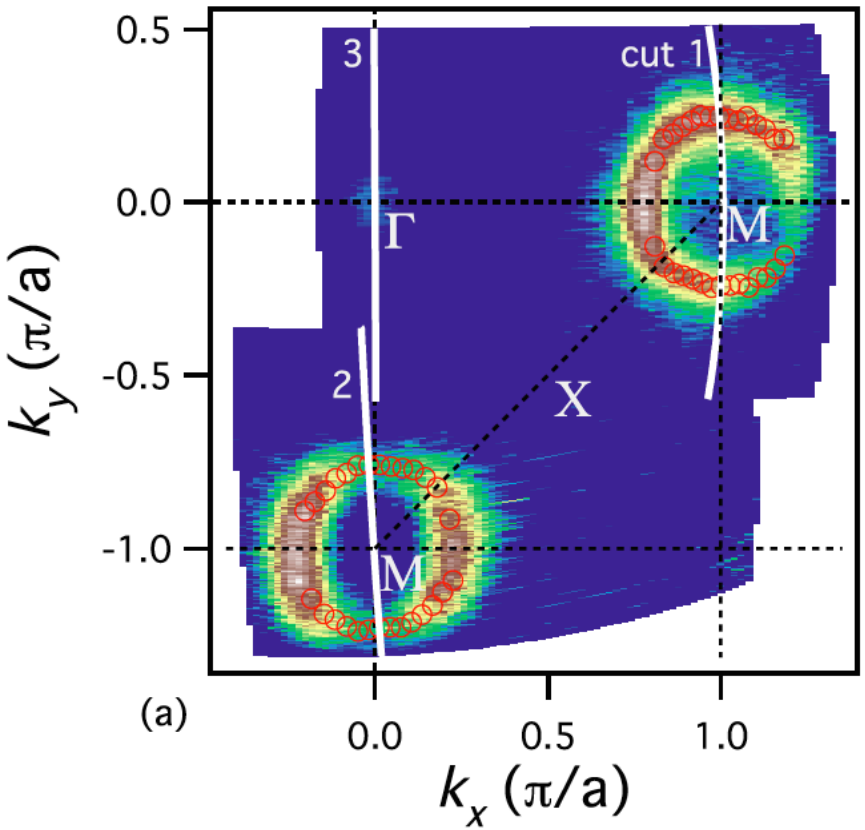


H. Miao *et al.*, PRB 85, 094506 (2012)

A new twist: $(Tl,K)_xFe_{2-y}Se_2$ ($T_c \sim 30K$)







T. Qian *et al.*, PRL 106, 187001 (2011)

$A_xFe_{2-y}Se_2$: electron doped SC

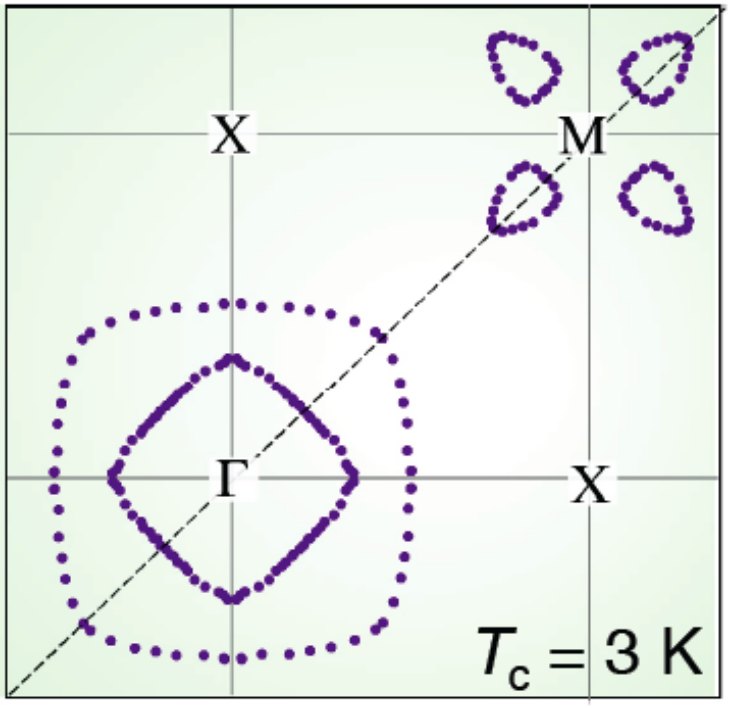
Se valence is 2-, while As valence is 3-

$A_xFe_{2-y}Se_2$: electron doping = x/2 – y,

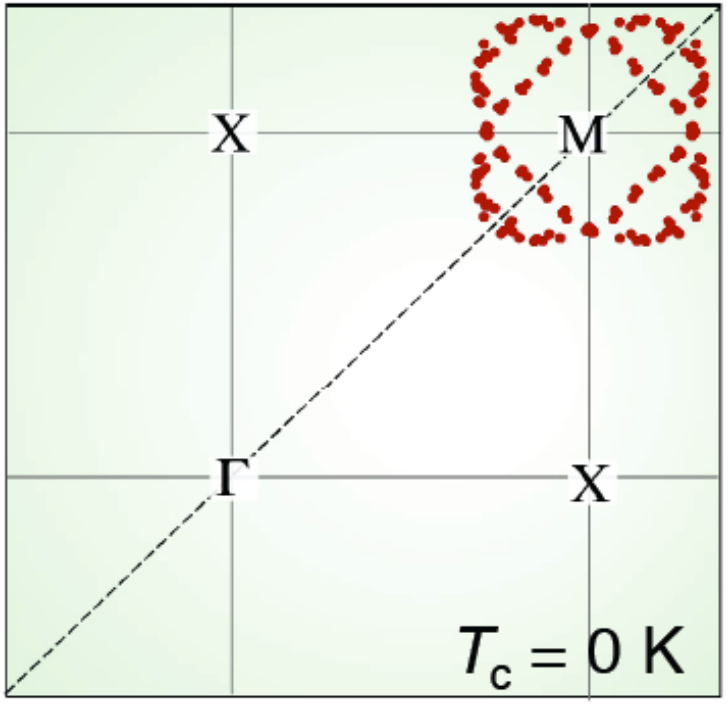
$K_{0.8}Fe_{1.8}Se_2$: electron doping = 0.2, T_c ~ 30K

$K_{0.8}Fe_{1.6}Se_2$ (245): electron doping = 0, insulator

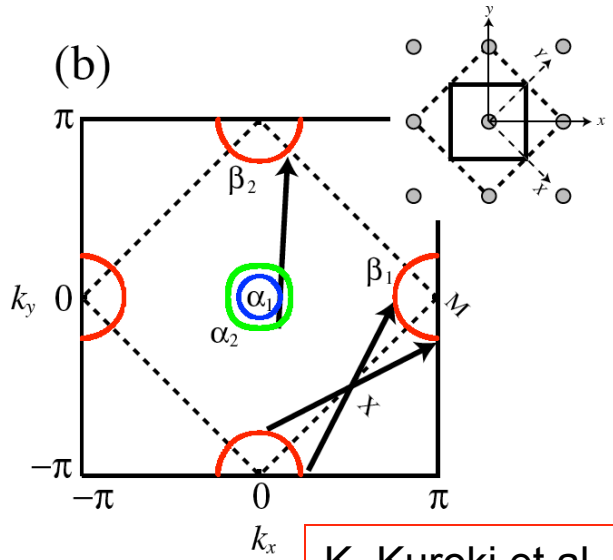
KFe_2As_2: heavily hole doped

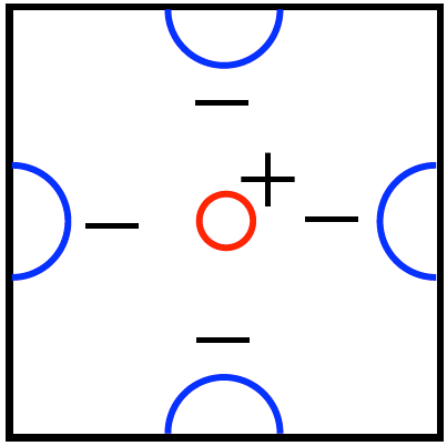


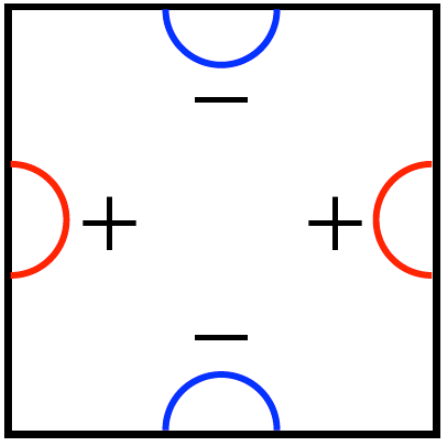
$K(Fe_{1.8}Co_{0.2})_2As_2$: 20% electron doped



Possible SC gap symmetries

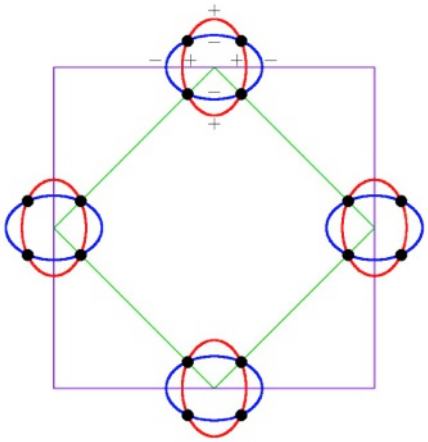




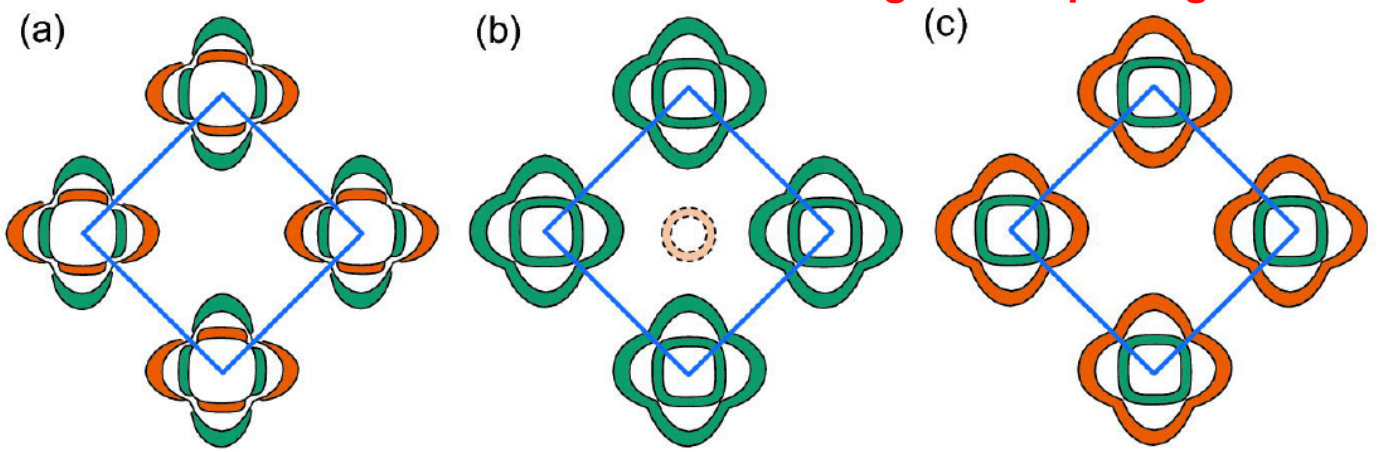


K. Kuroki et al., PRL **101**, 087004 (2008)

Note: Interband scattering between same type FSs is not good for pairing!



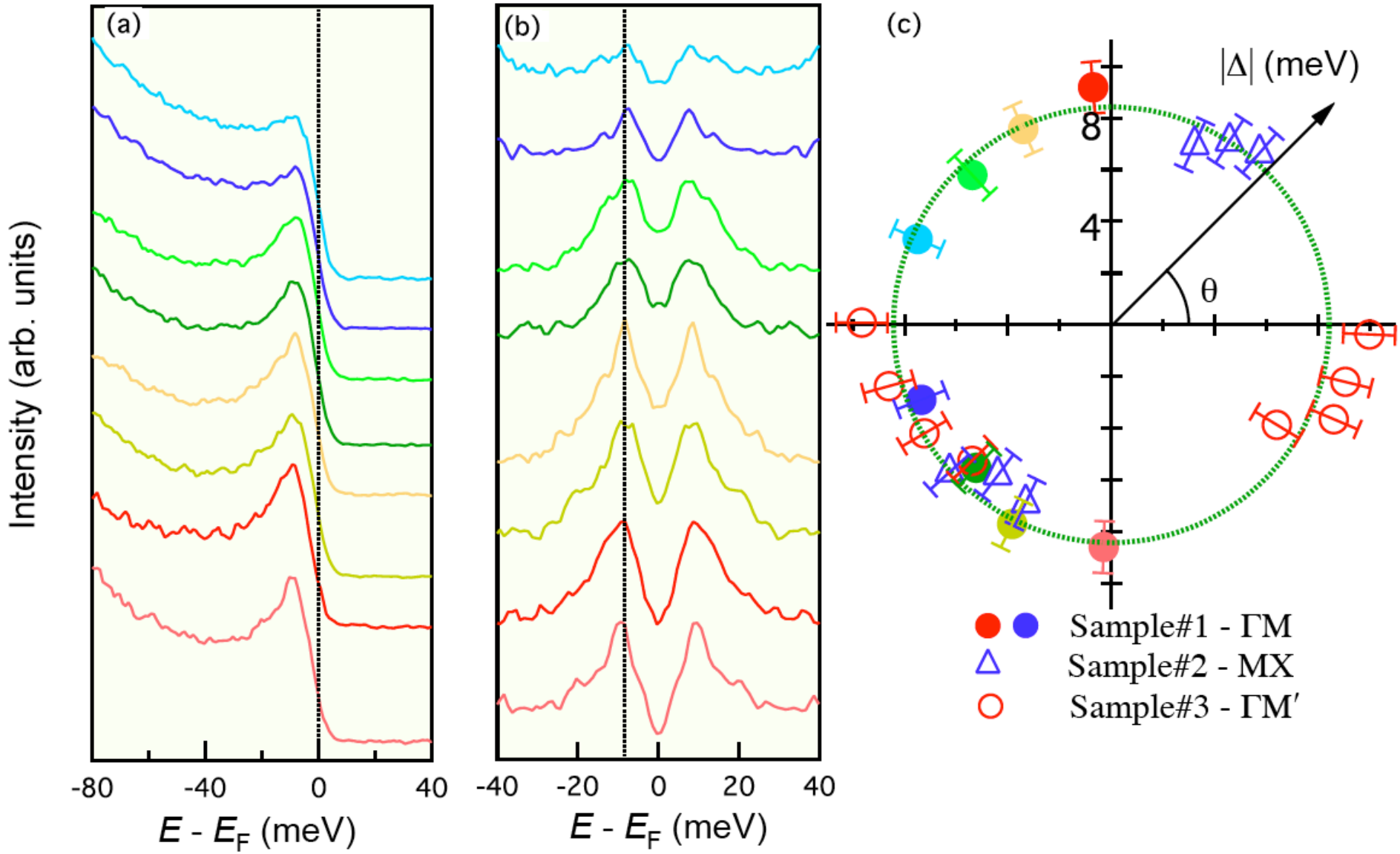
nodal d



"quasi − nodeless" d "incipient" $s_{\pm}$ "bonding − antibonding" $s_{\pm}$

P. J. Hirschfeld et al., Rep. Prog. Phys. **74**, 124508 (2011)

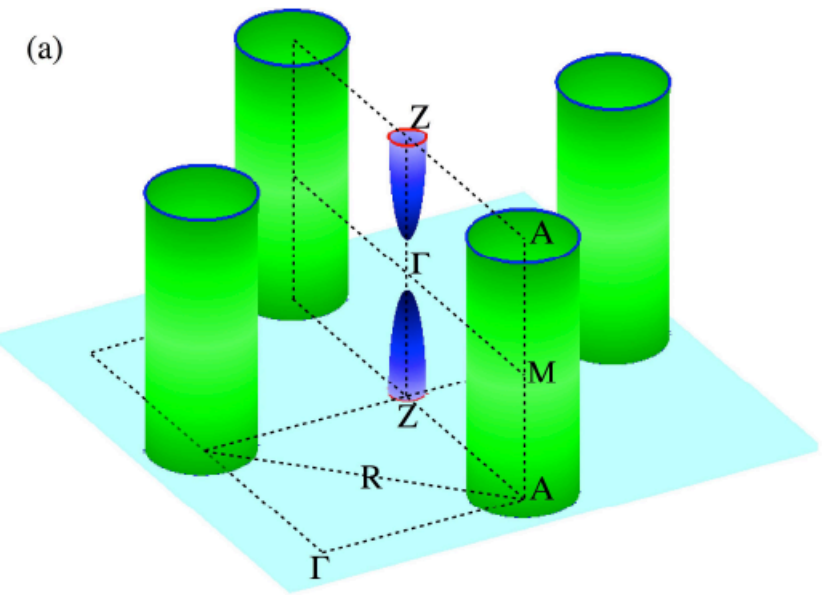
Isotropic SC gap on electron FS

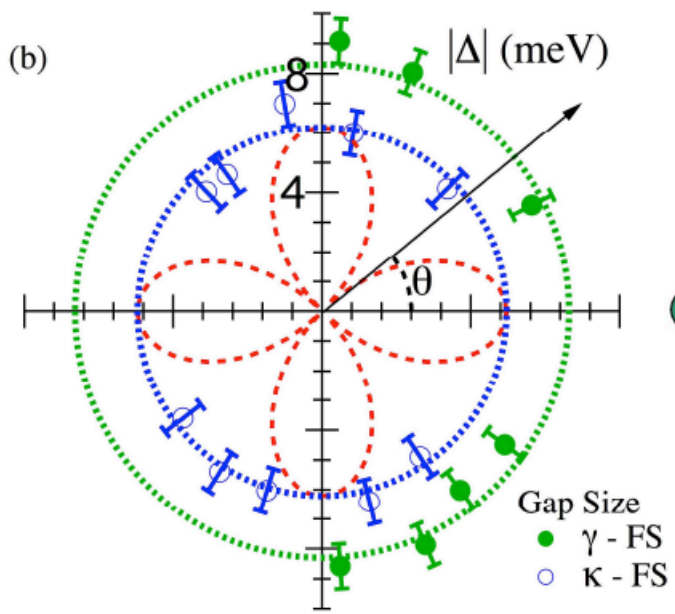


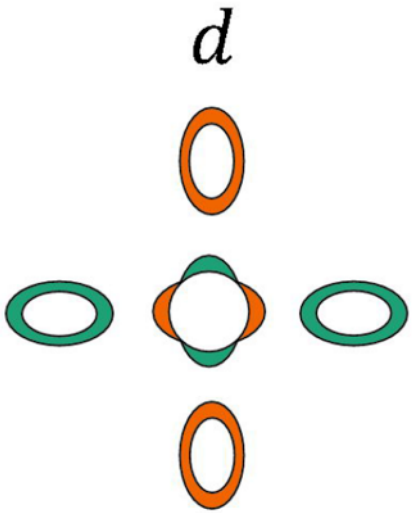
J1 < 0, FM, d-wave is not favored

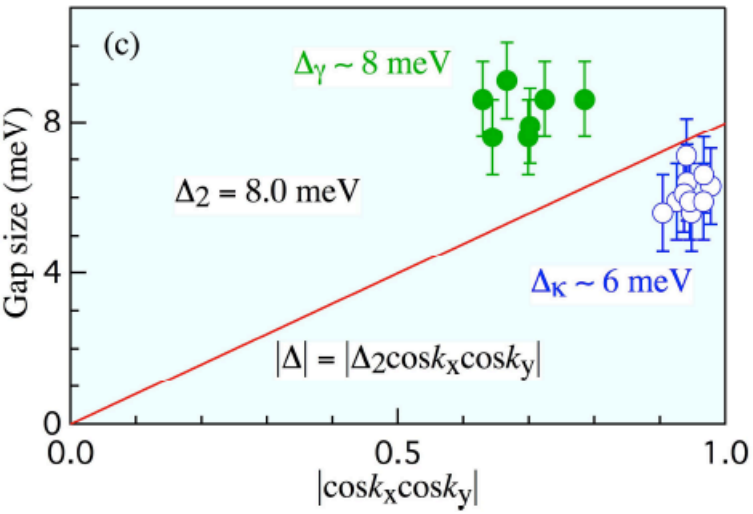
X.-P. Wang *et al.*, EPL 93, 57001 (2011)

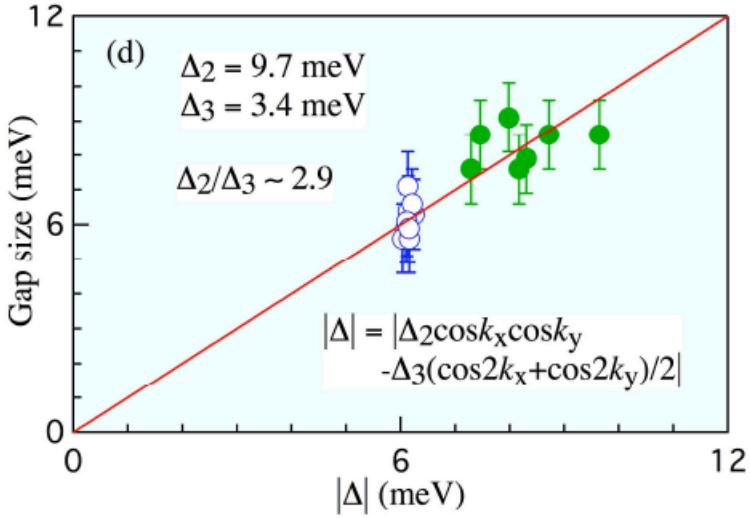
3D SC gap structure in $(Tl,K)Fe_{1.78}Se_2$







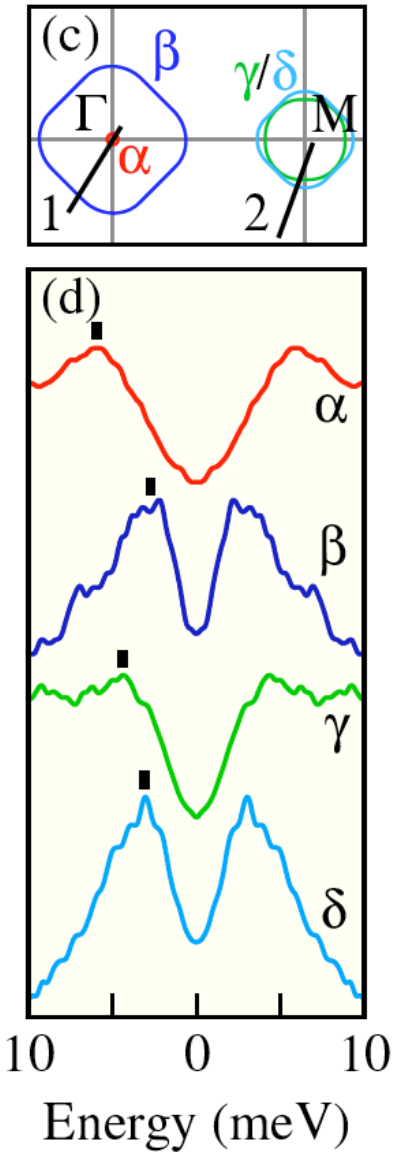


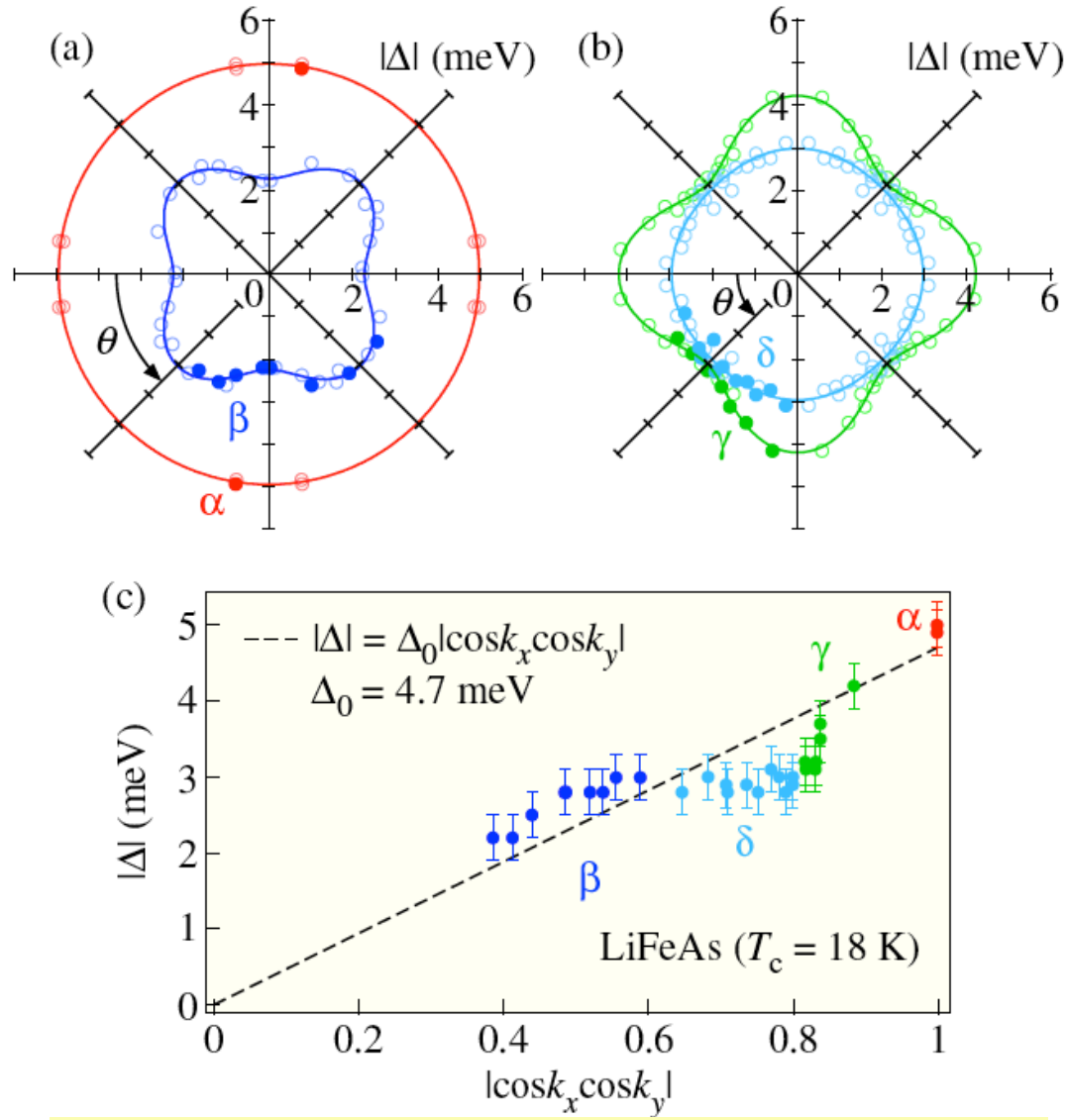


d-wave is ruled out!

X.-P. Wang *et al.*, EPL 99, 67001 (2012)

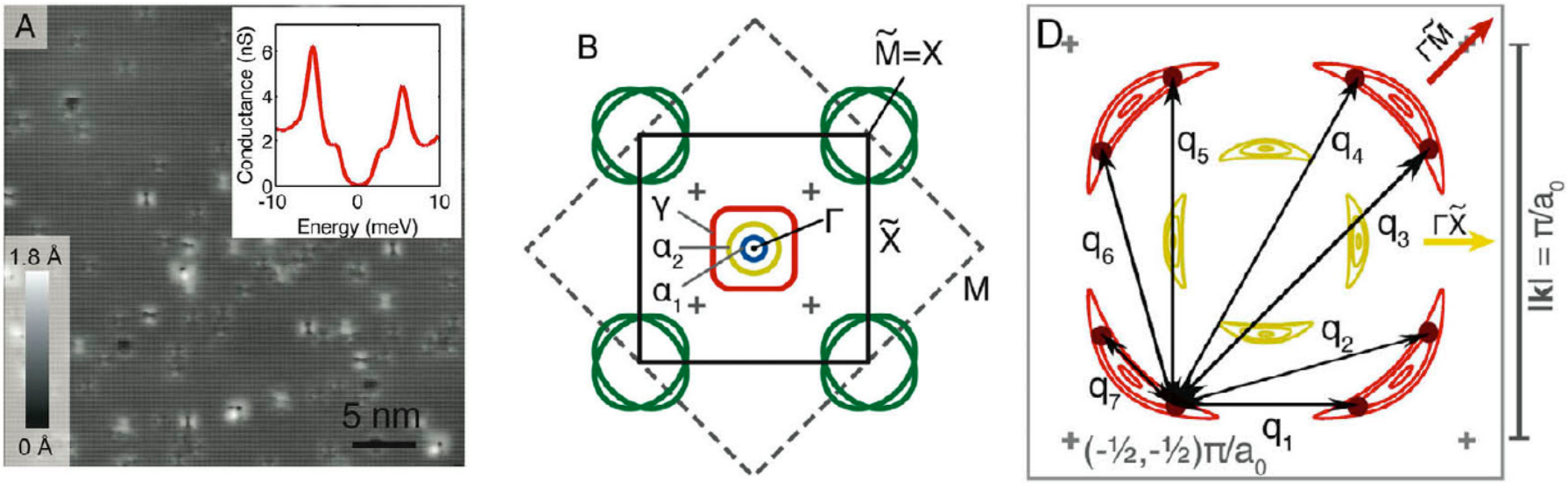
Moderate gap anisotropy in LiFeAs

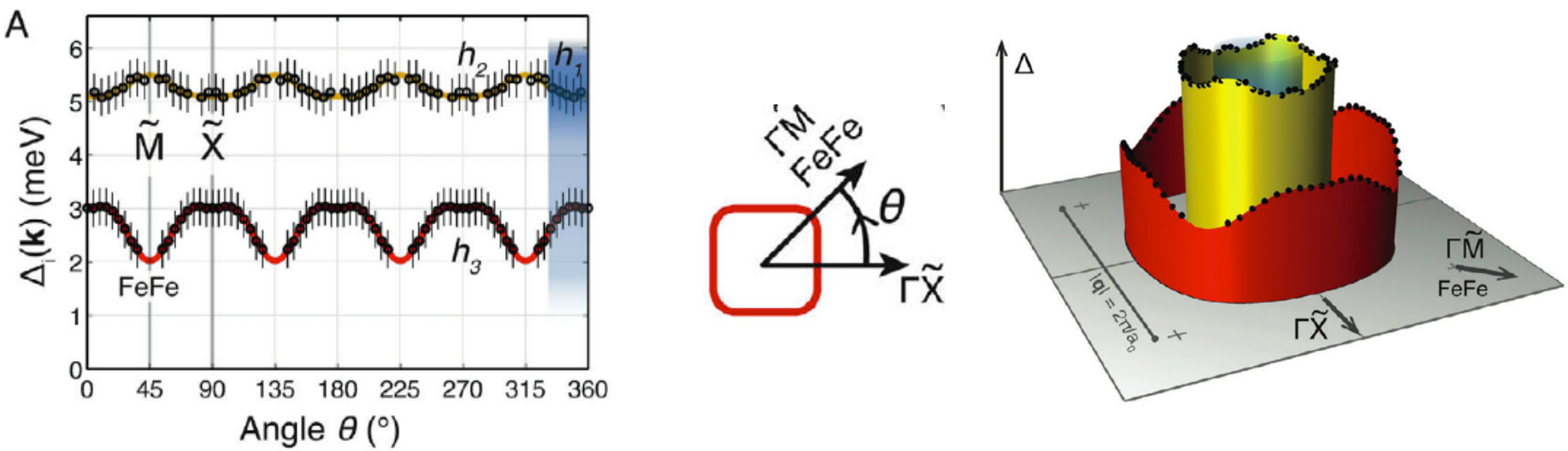




K. Umezawa et al, PRL 108, 037002 (2012)

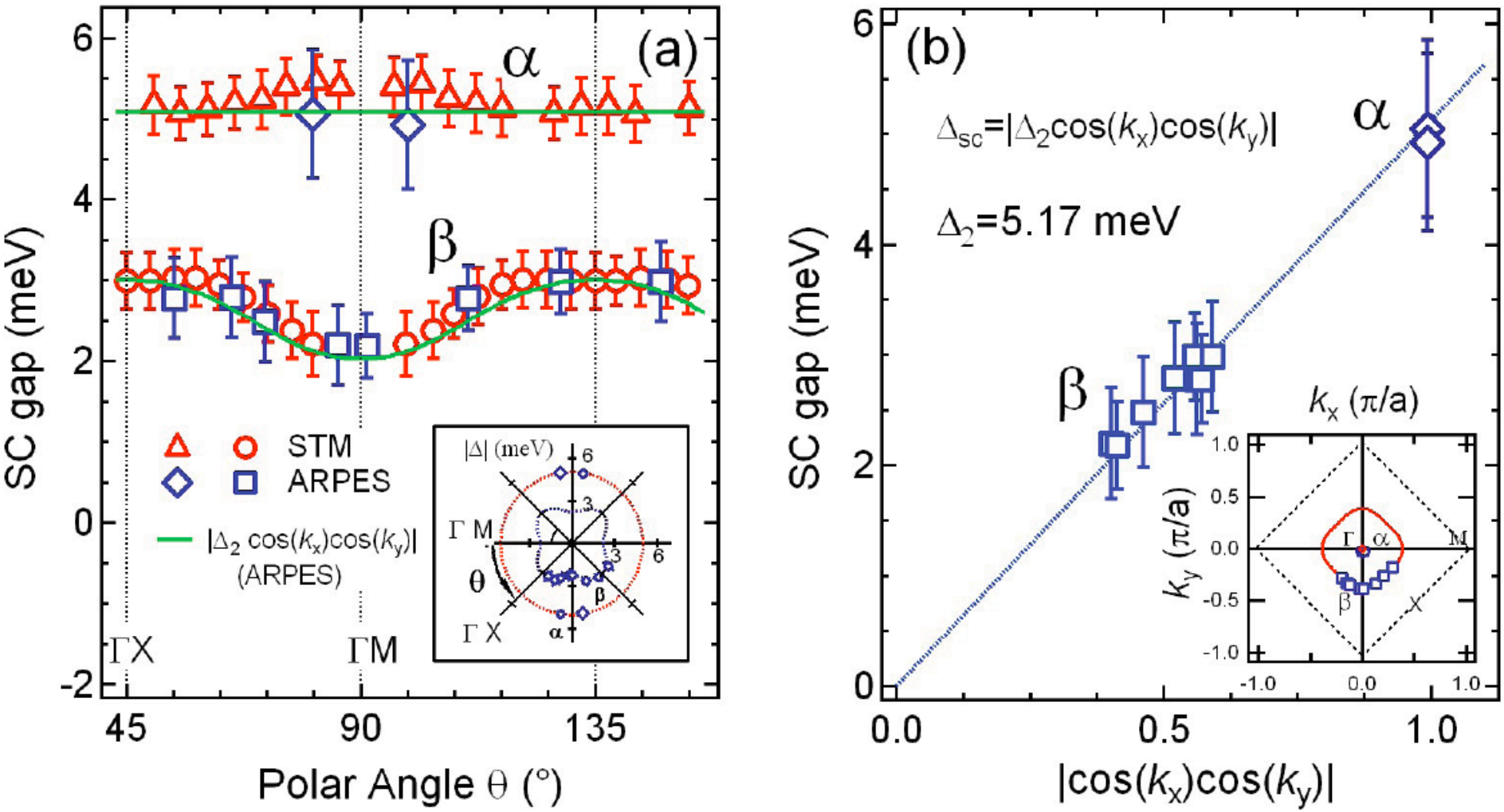
Moderate gap anisotropy in LiFeAs: STM results





M. P. Allan et al., Science 336 563 (2012)

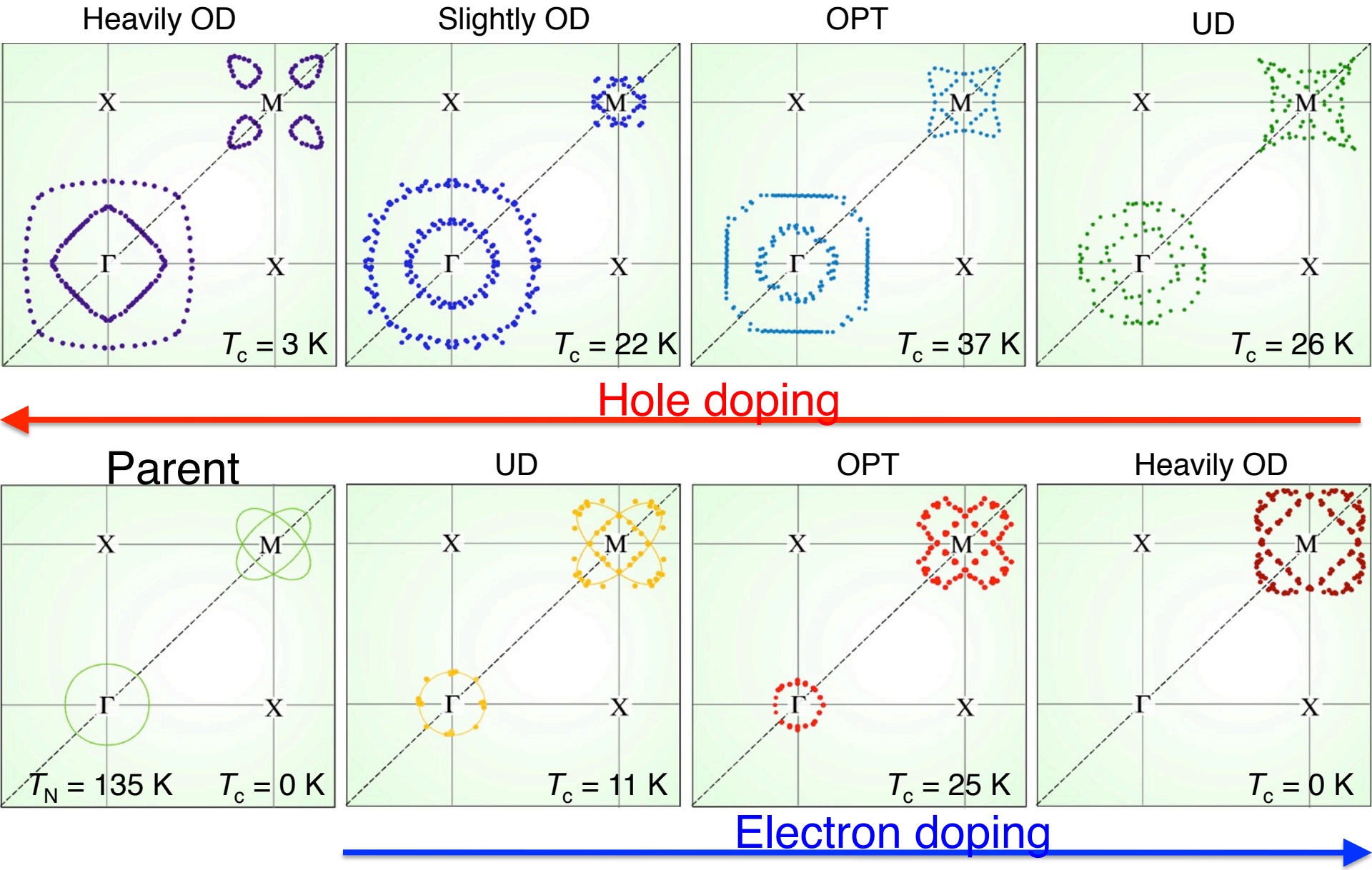
Comparison between ARPES and STM on LiFeAs consistent with $\cos k_x \cos k_y$



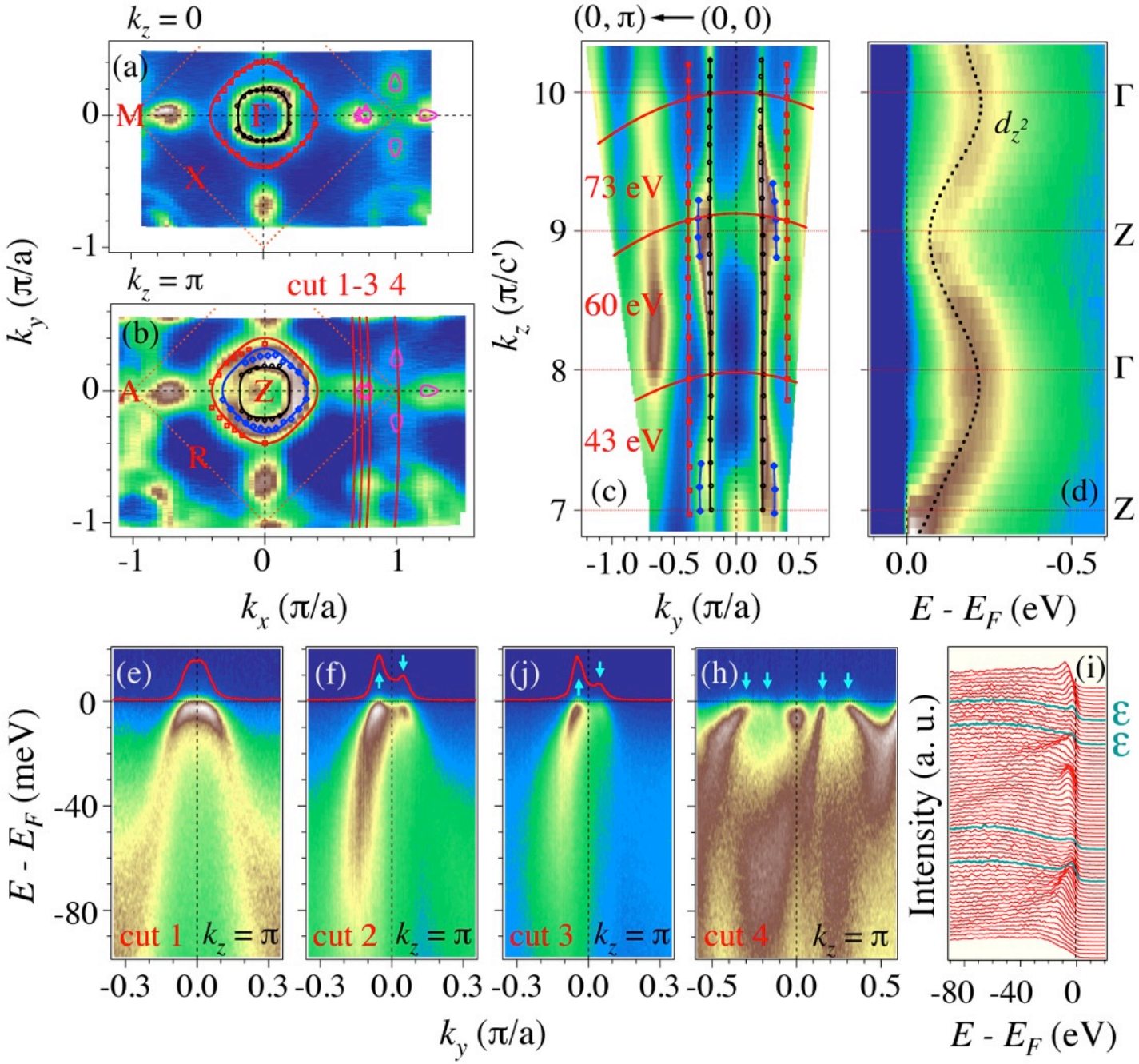
Y.-B. Huang *et al.*, AIP Advances 2, 041409 (2012)

A possible node in highly hole-doped $(BaK)Fe_2As_2$

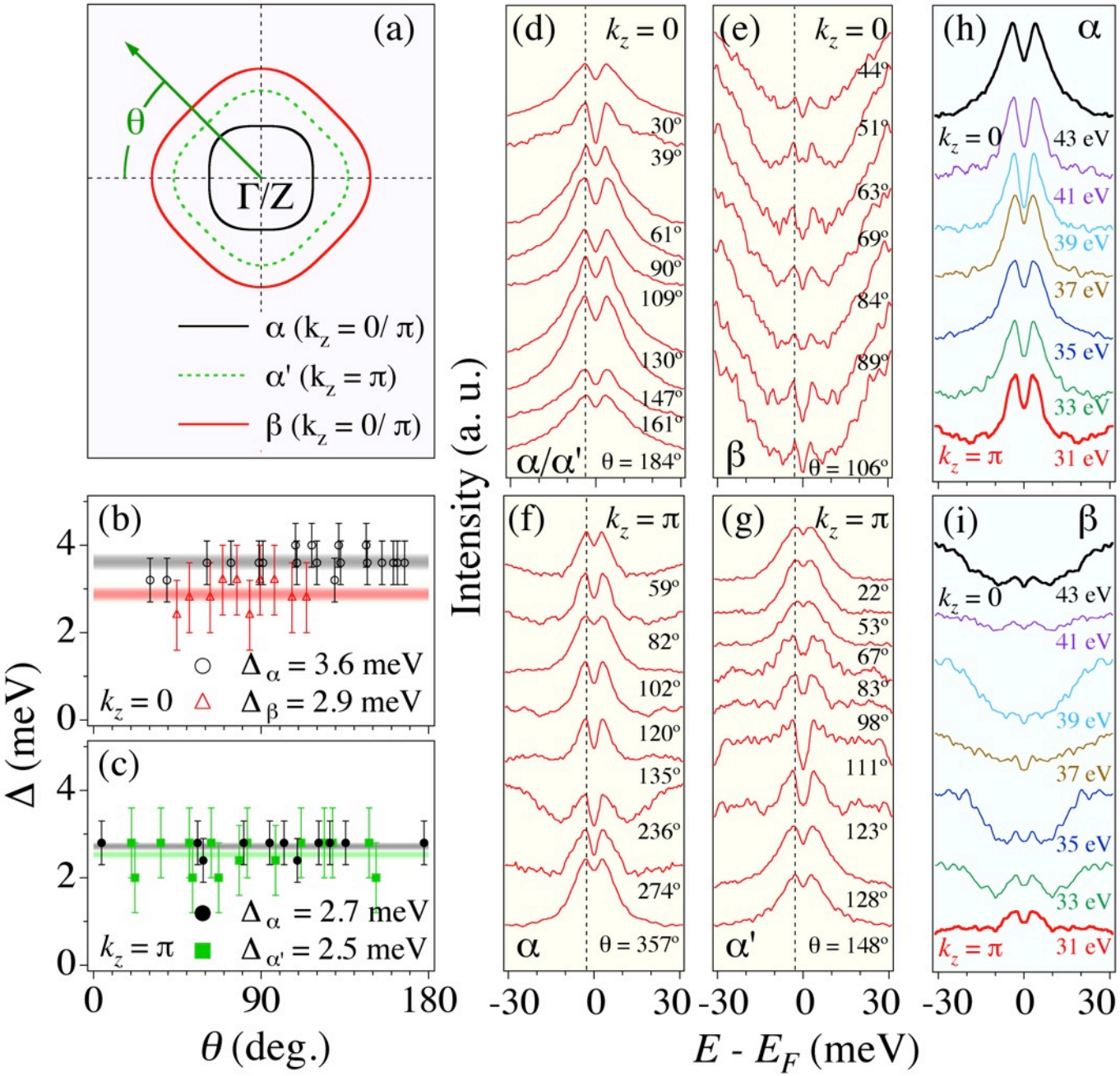
Fermi surface evolution in “122”



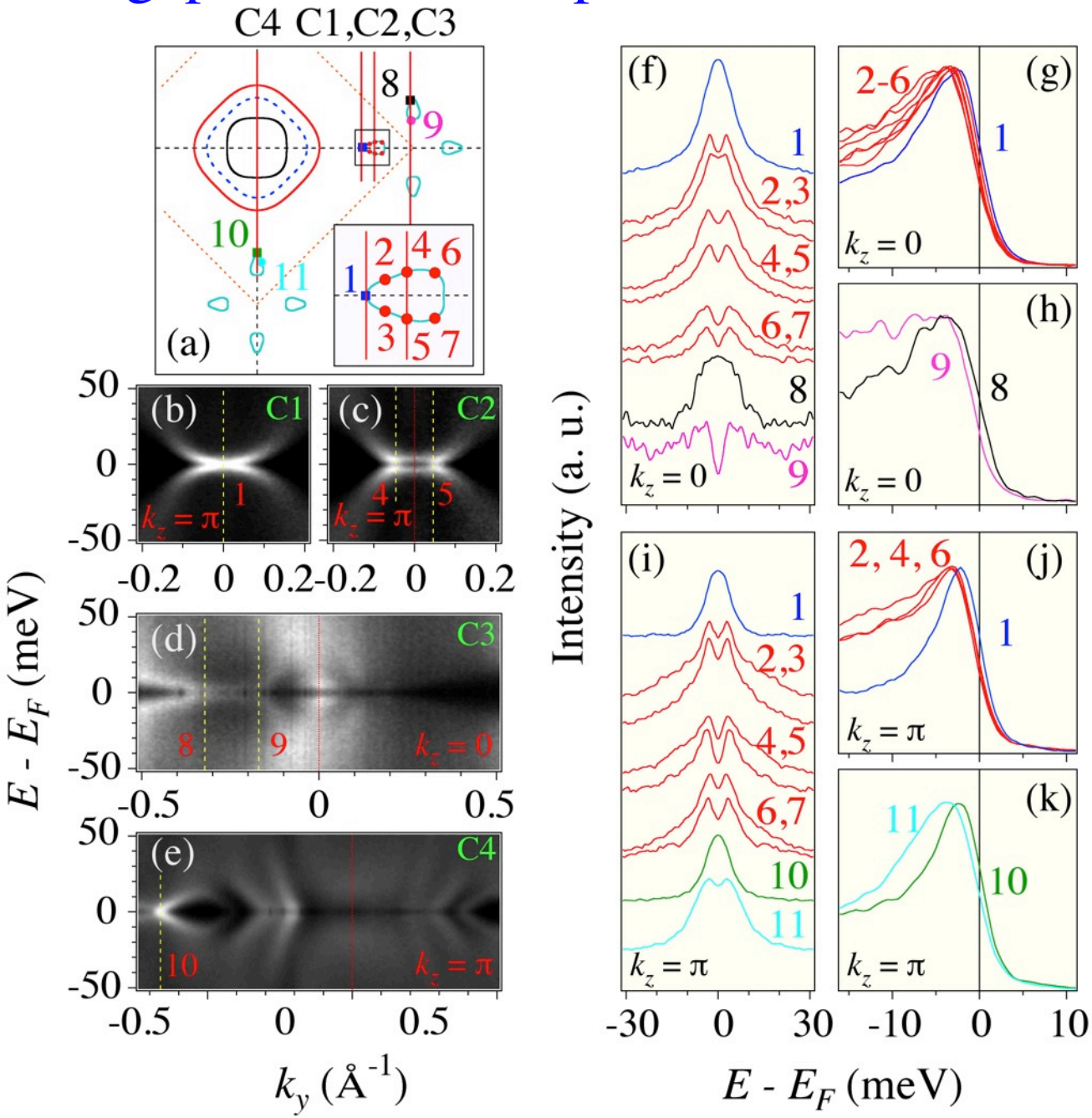
$Ba_{0.1}K_{0.9}Fe_2As_2$ (T_c = 9 K)

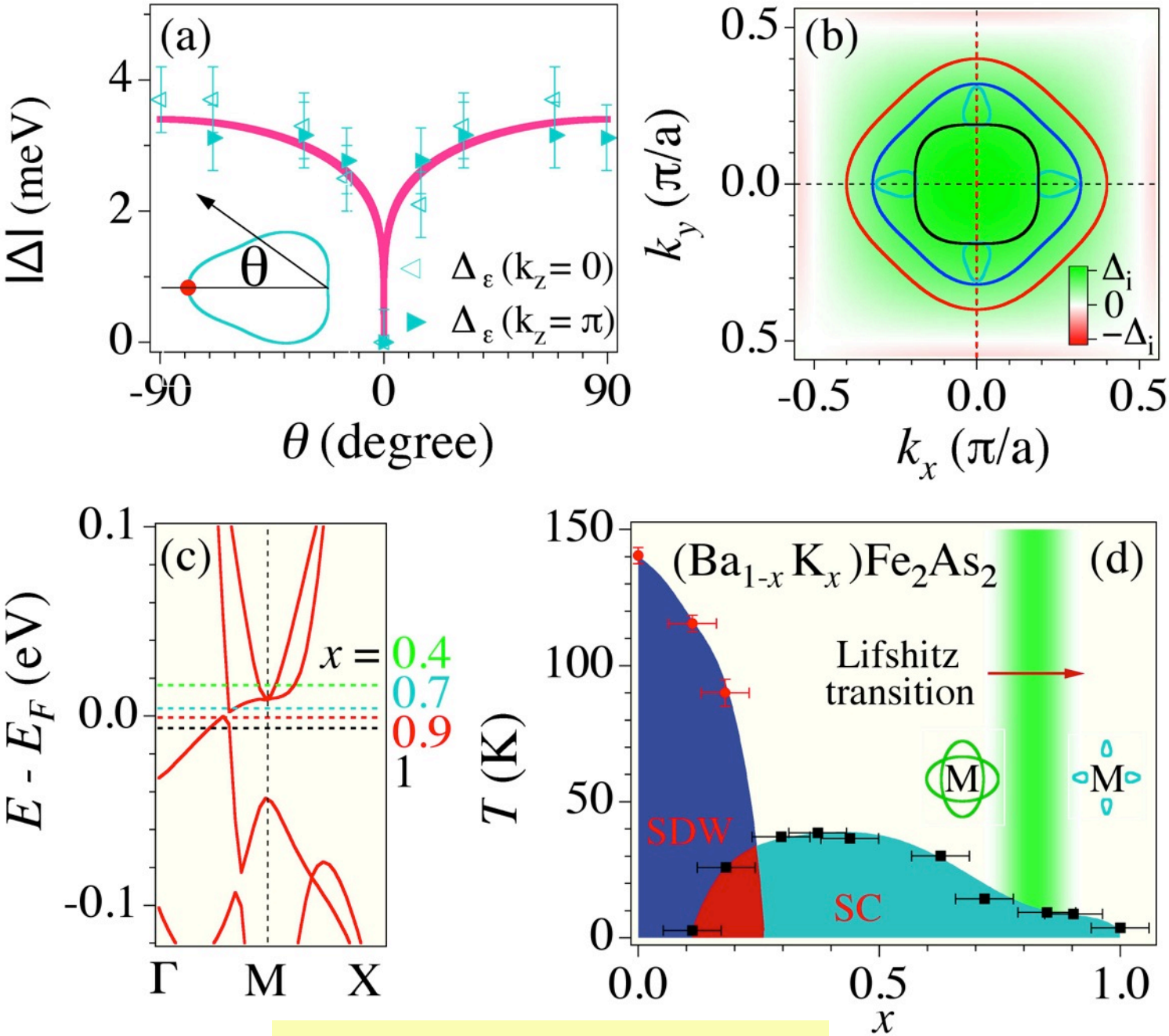


Nodeless SC gap on the large hole FSs around Γ



A possible gap node on the tip of small hole FS off M



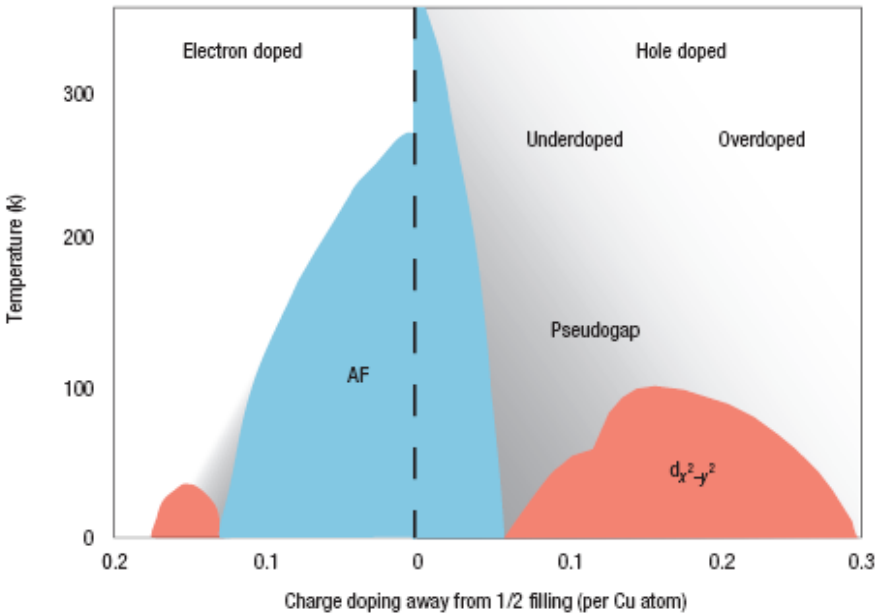


N. Xu *et al.*, arXiv:1308.3888

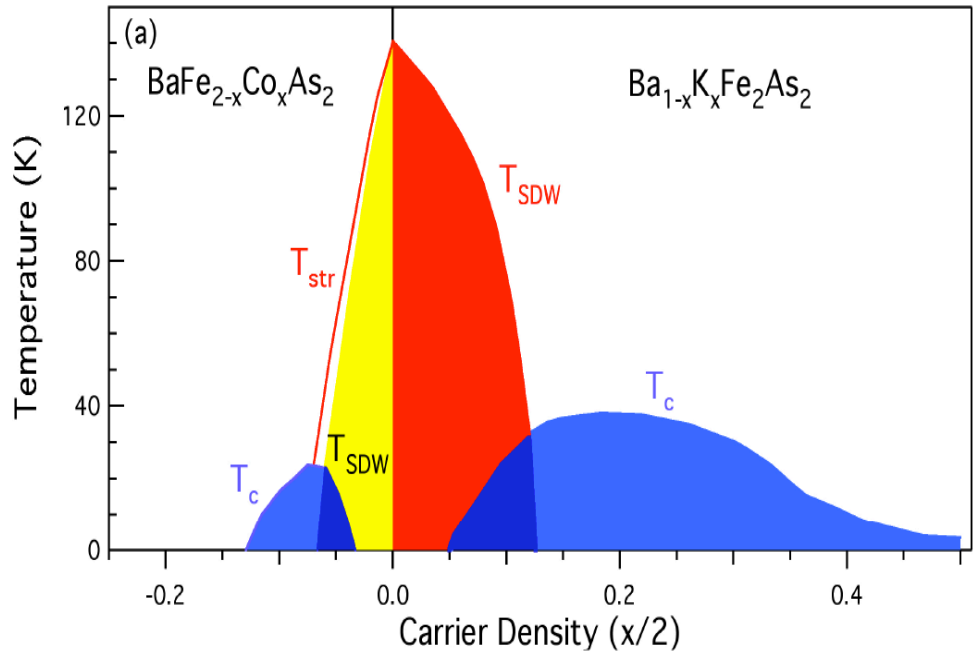
A phenomenological understanding of Fe-SCs

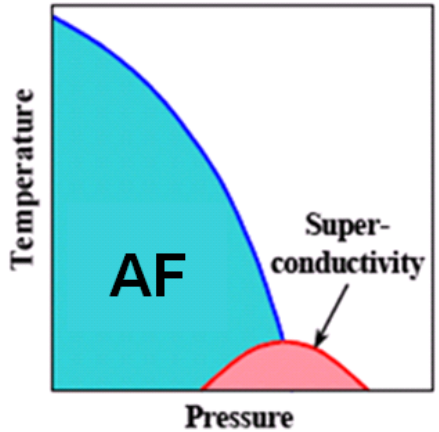
Phase diagrams of unconventional SCs

cuprate SC

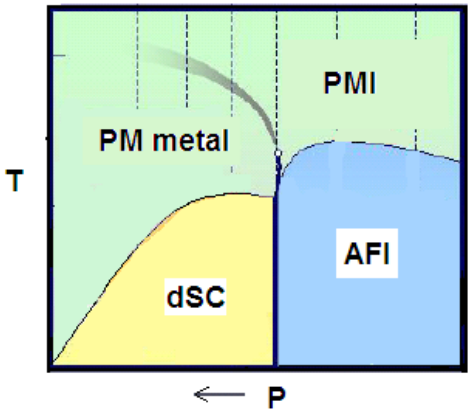


pnictide SC



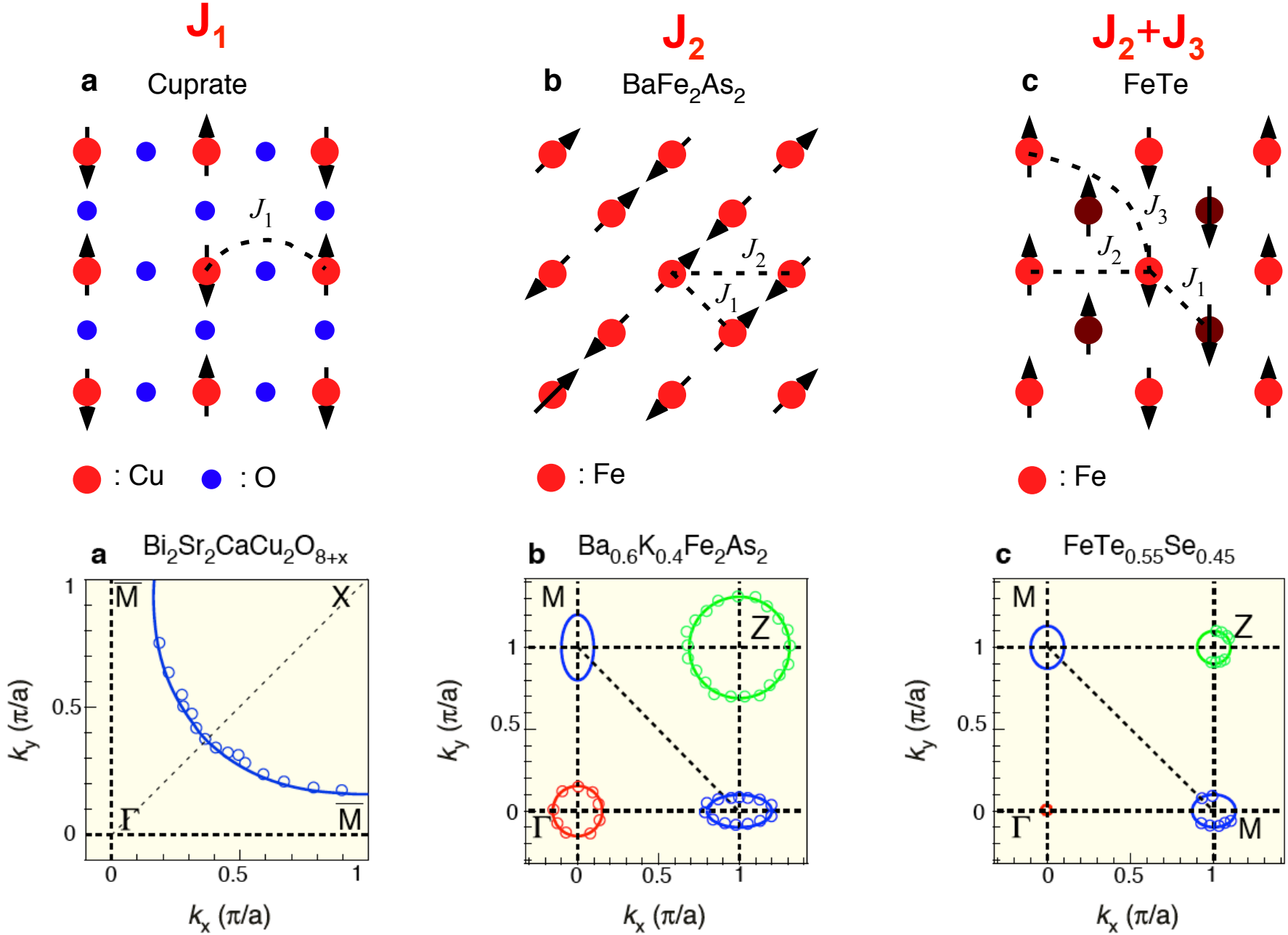


heavy fermion SC



organic SC

Three classes of high-T_c superconductors



Selection Rules of Pairing Symmetry

Self-consistent meanfield equation for t-J model

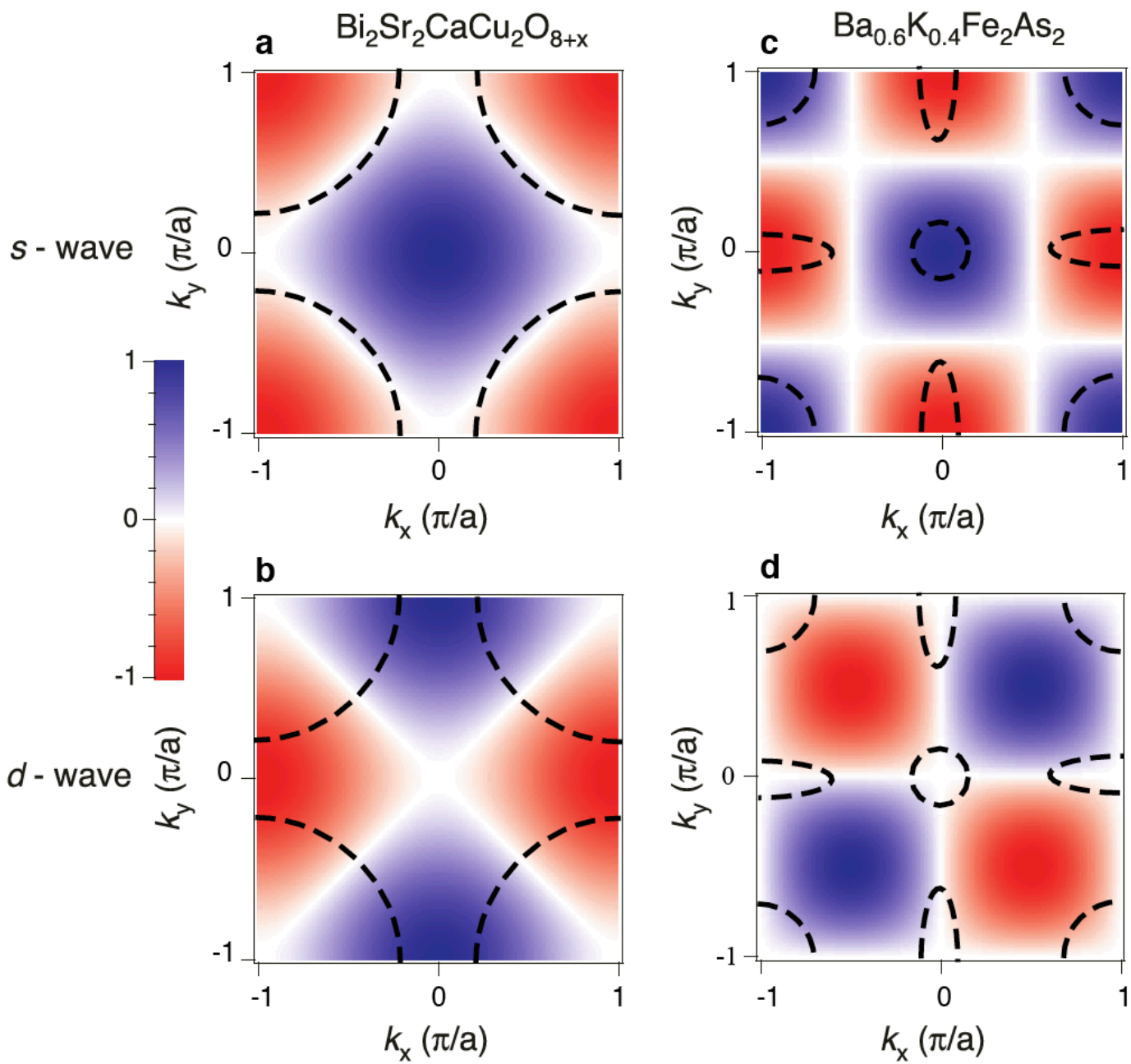
$$2T_c = J_\alpha \sum_k |f_\alpha(k)|^2 g(x(k, T_c)) \qquad g(x) = \frac{\tanh(x)}{x}, x(k, T_c) = \frac{(\varepsilon(k) - \mu)}{2T_c}$$

Overlap strength between pairing form factor and Fermi surface

$$\mathrm{OS} = \sum_k |f(k)|^2 \delta(\epsilon(k) - \mu)$$

AF couplings & gap form	$Bi_2Sr_2CaCu_2O_{8+x}$	$Pr_{1-x}Ce_xCuO_4$	$Ba_{0.6}K_{0.4}Fe_2As_2$	$FeTe_{0.55}Se_{0.45}$	$KFe_{1.7}Se_2$
J_1: s-wave $(cosk_x + cosk_y)/2$	0.03	0.01	0.43	(0.29)	(0.01)
J_1: d-wave $(cosk_x - cosk_y)/2$	0.61	0.40	0.36	(0.55)	(0.74)
J_2: s-wave $cosk_x cosk_y$	–	–	0.62	0.71	0.55
J_2: d-wave $sink_x sink_y$	–	–	0.03	0.01	0.05
J_3: s-wave $(cos2k_x + cos2k_y)/2$	–	–	–	0.52	0.31
J_3: d-wave $(cos2k_x - cos2k_y)/2$	–	–	–	0.07	0.11

Overlap strength between pairing form factor and Fermi surface

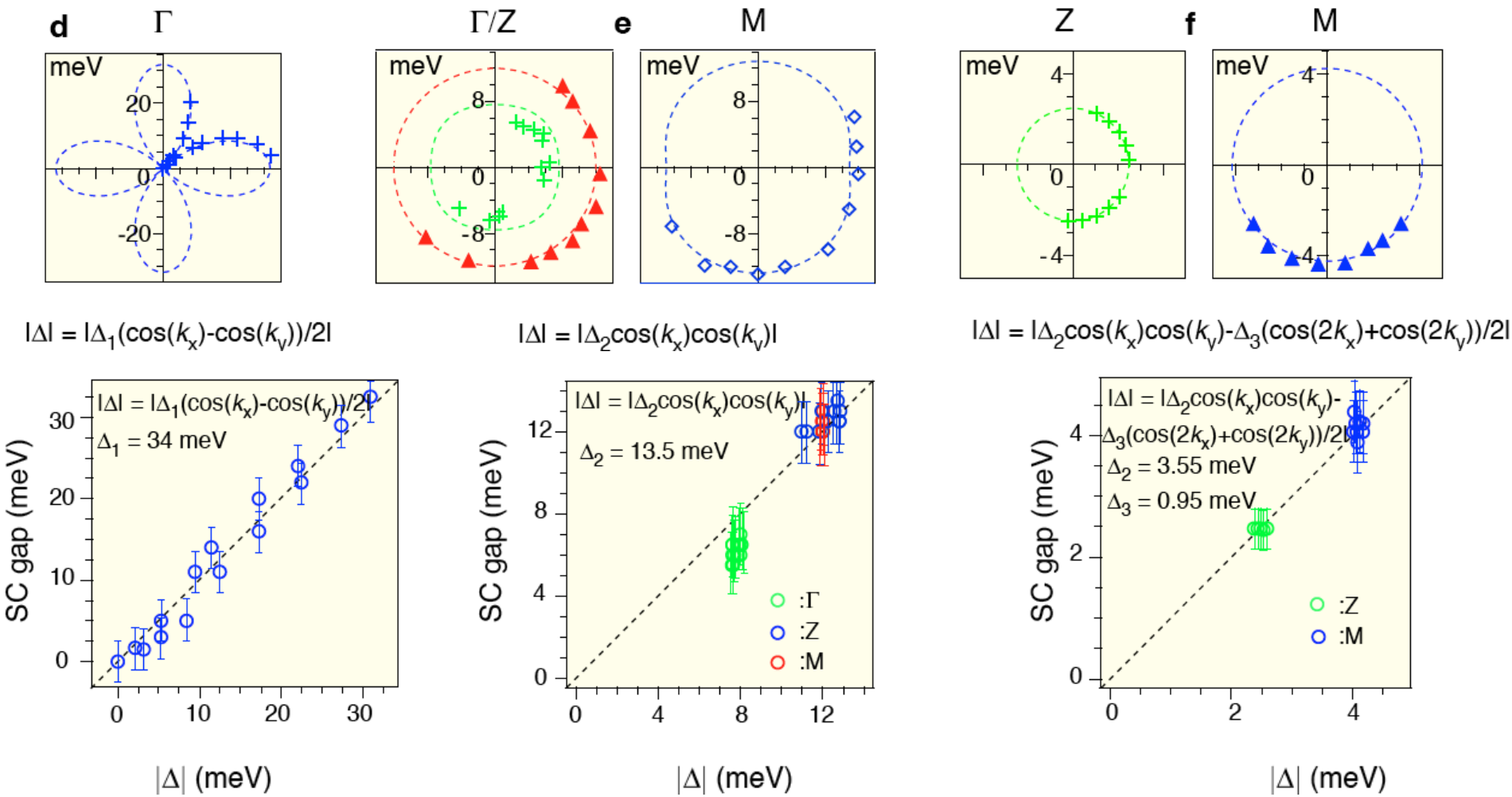


Three classes of high-T_c superconductors

J_1 — $Bi_2Sr_2CaCu_2O_{8+x}$

J_2 — $Ba_{0.6}K_{0.4}Fe_2As_2$

J_2+J_3 — $FeTe_{0.55}Se_{0.45}$



J.-P. Hu and H. Ding, Scientific Reports 2, 381 (2012)

Summary

1. The SC gap of all iron-based superconductors measured by ARPES is a simple sine/cosine function of (kx, ky, kz), strongly suggesting local pairing and strong coupling

2. On the first order, the gap function can by described by the J_1-J_2-J_3 model

3. A possible unified paradigm of high-T_c superconductivity:

local AFM magnetic exchange
+ collaborative FS topology

Thank you!