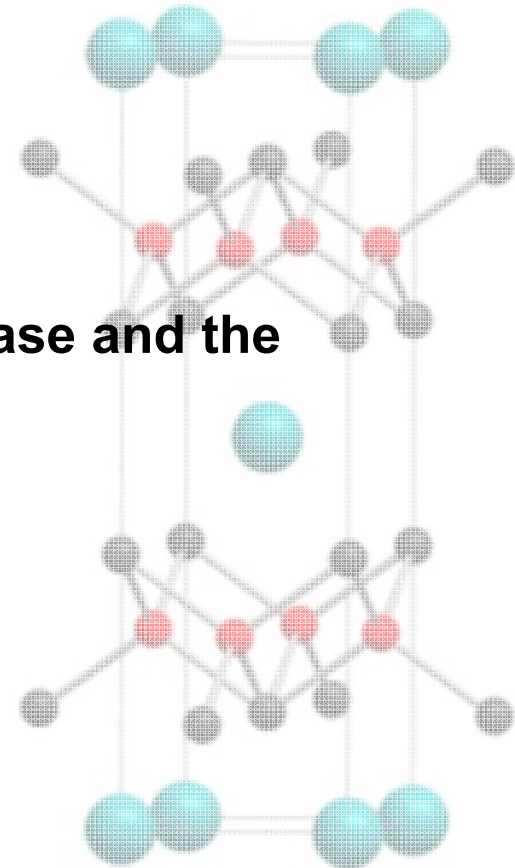


## ARPES studies of Fe pnictides: Nature of the antiferromagnetic-orthorhombic phase and the superconducting gap

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Atsushi Fujimori  
University of Tokyo

- Nature of the AFM-orthorhombic (AFO) phase and the “nematic phase”:
  - Band folding *versus*  $C_4$  symmetry breaking
- Superconducting gap anisotropy



# Collaborators

## *Photoemission expt*

K. Koshiishi, L. Liu, H. Suzuki, J. Xu, K. Okazaki, T. Shimojima (U of Tokyo),  
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## *Samples*

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S. Uchida (U of Tokyo)

Y. Matsuda, S. Kasahara, T. Terashima (Kyoto U), T. Shibauchi (U of Tokyo)

T. Kobayashi, S. Miyasaka, M. Nakajima, S. Tajima (Osaka U)

## *Theory*

R. Arita (RIKEN), H. Ikeda (Ritsumeikan U)

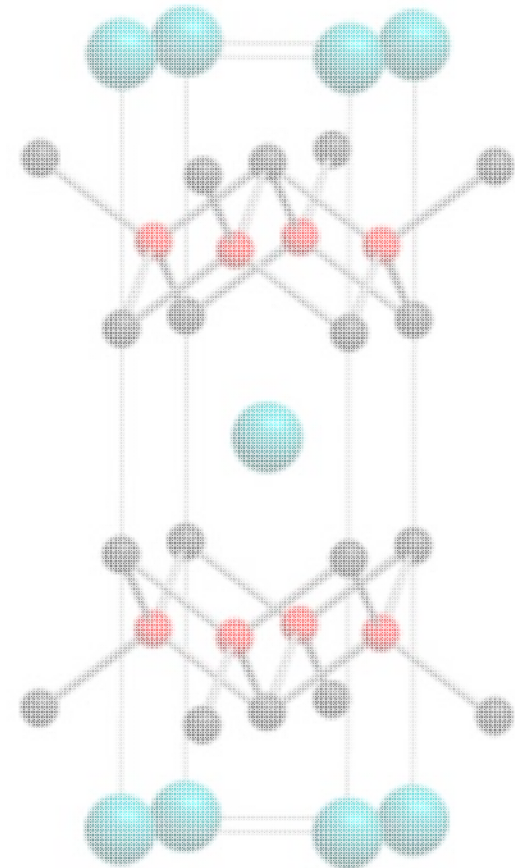
H. Kontani, T. Saito (Nagoya U.) S. Onari (Okayama U)



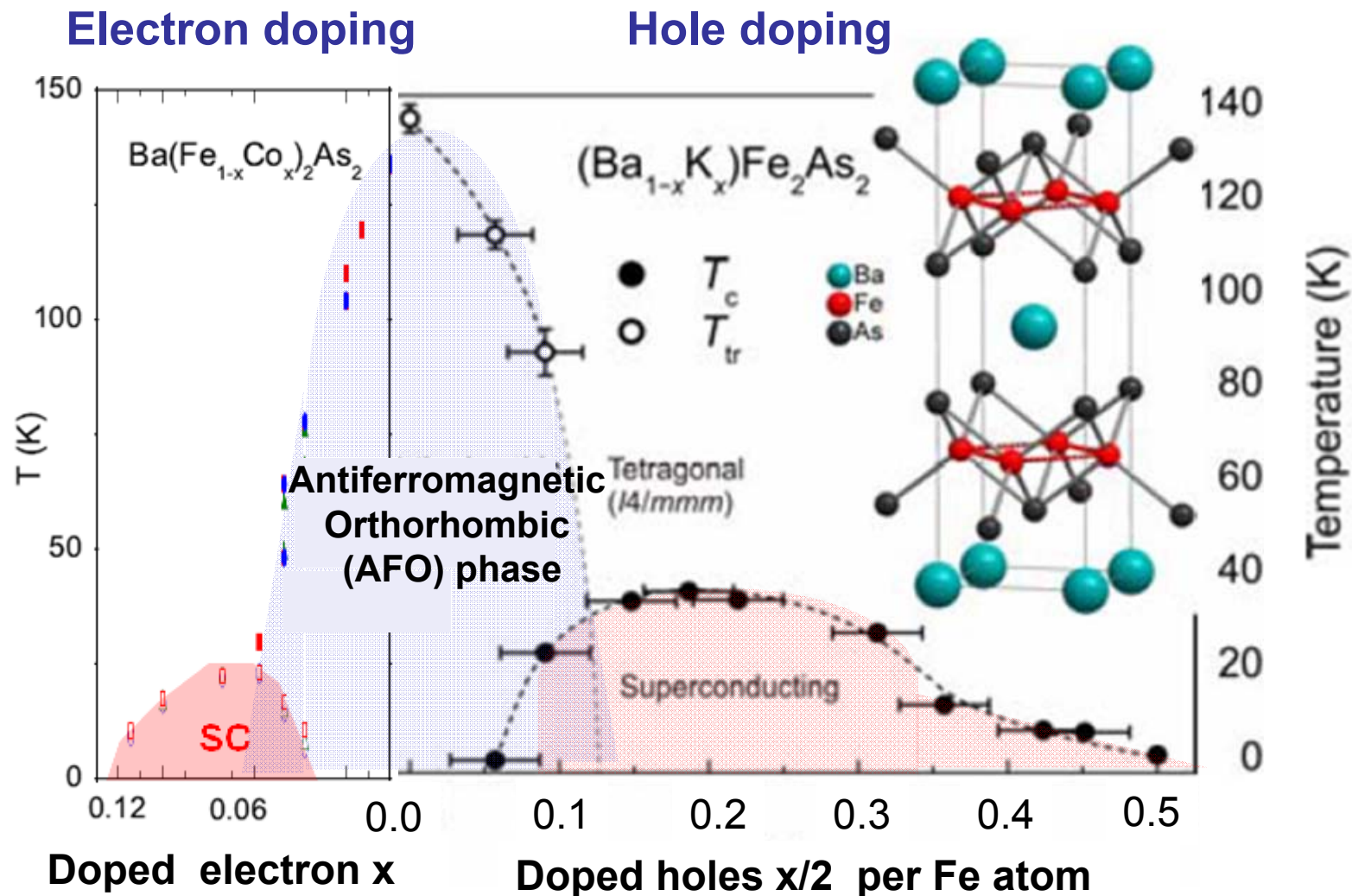
# Outline

---

- • **Nature of the AFM-orthorhombic (AFO) phase and the “nematic phase”:**
  - **Band folding *versus*  $C_4$  symmetry breaking**
- **Superconducting gap anisotropy**



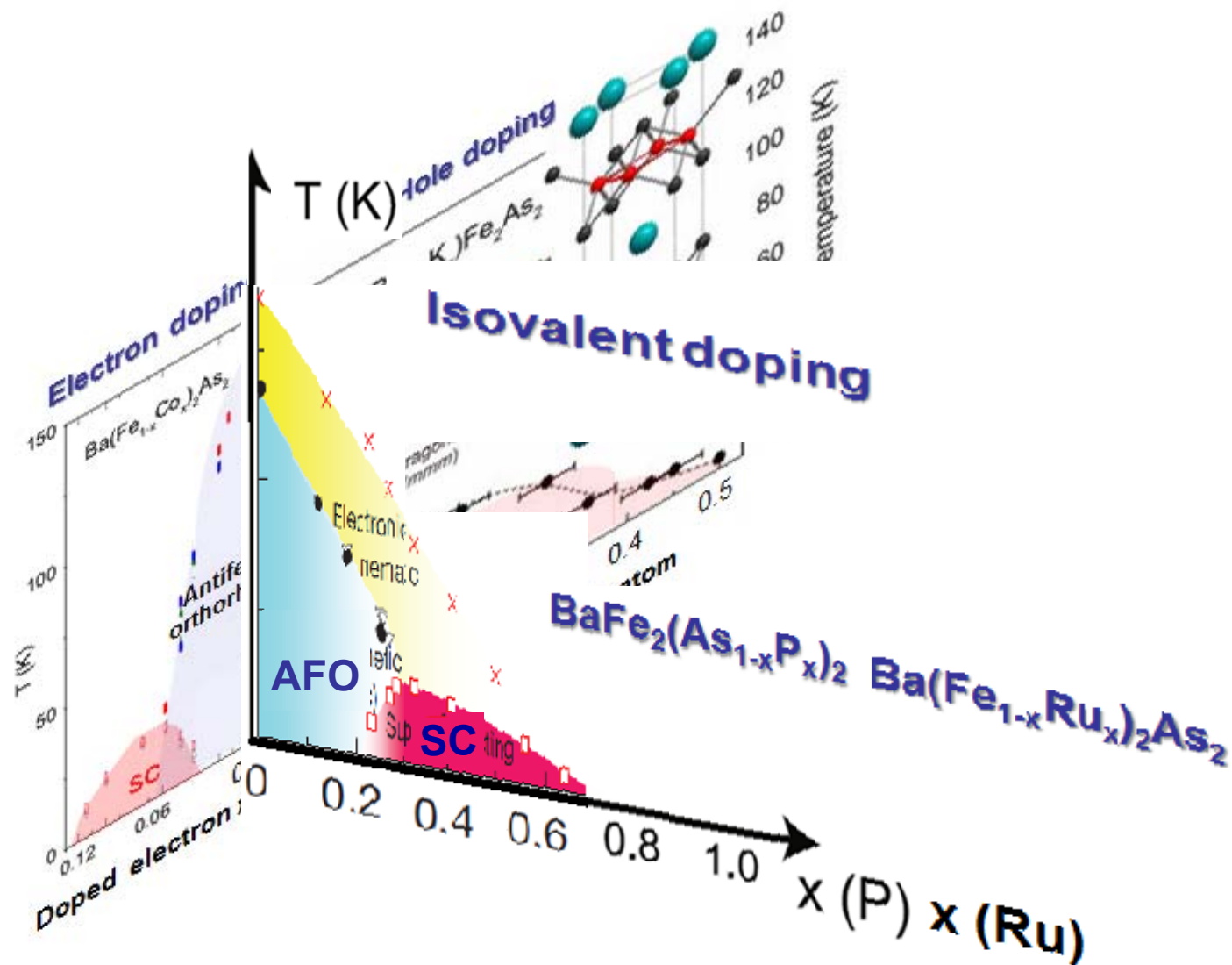
# Phase diagram of Fe-based superconductors



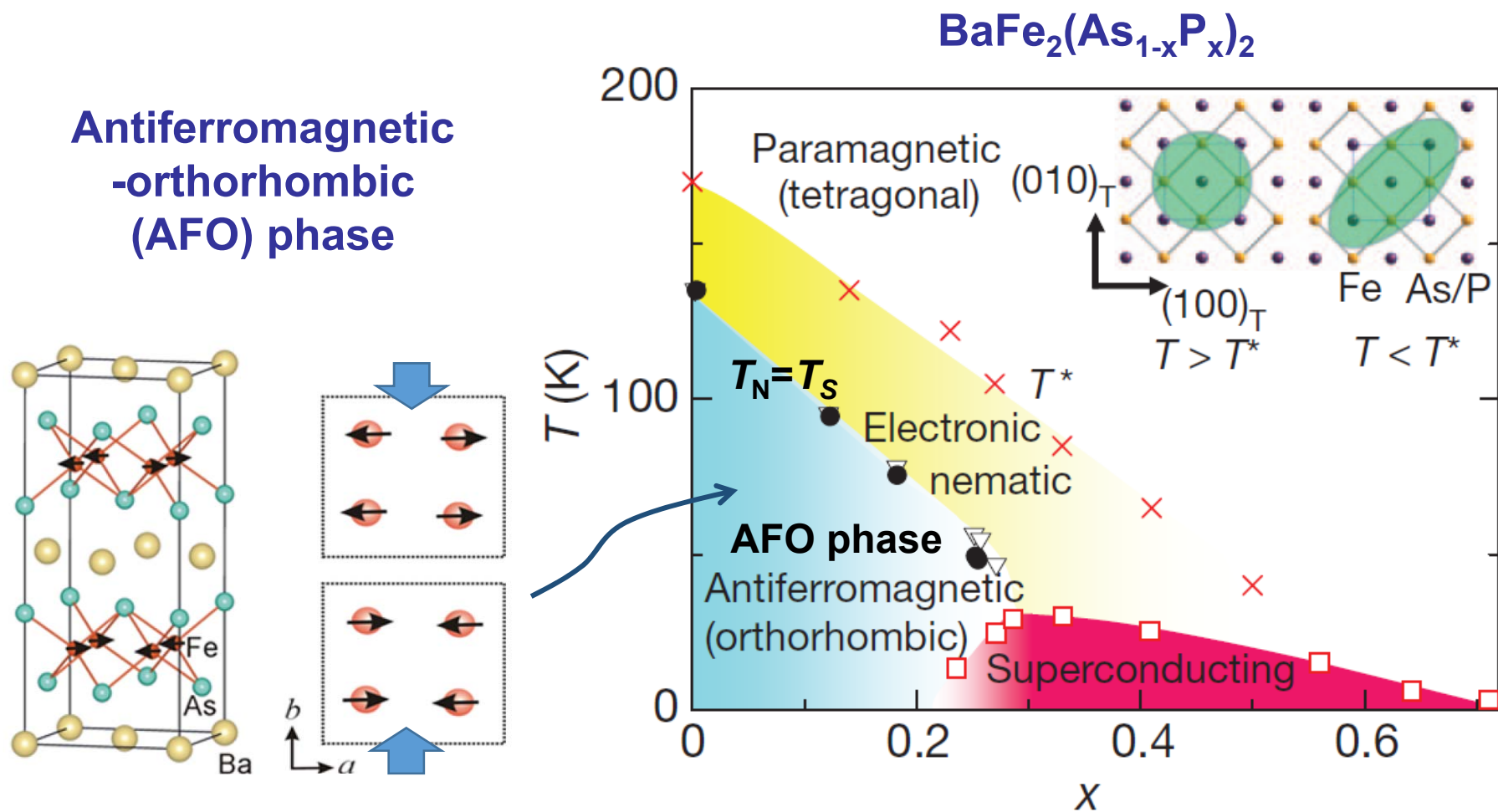
N. Ni *et al.*, PRL '08

M. Rotter *et al.*, Angew. Chem. Int. Ed. '08

# Phase diagram of Fe-based superconductors



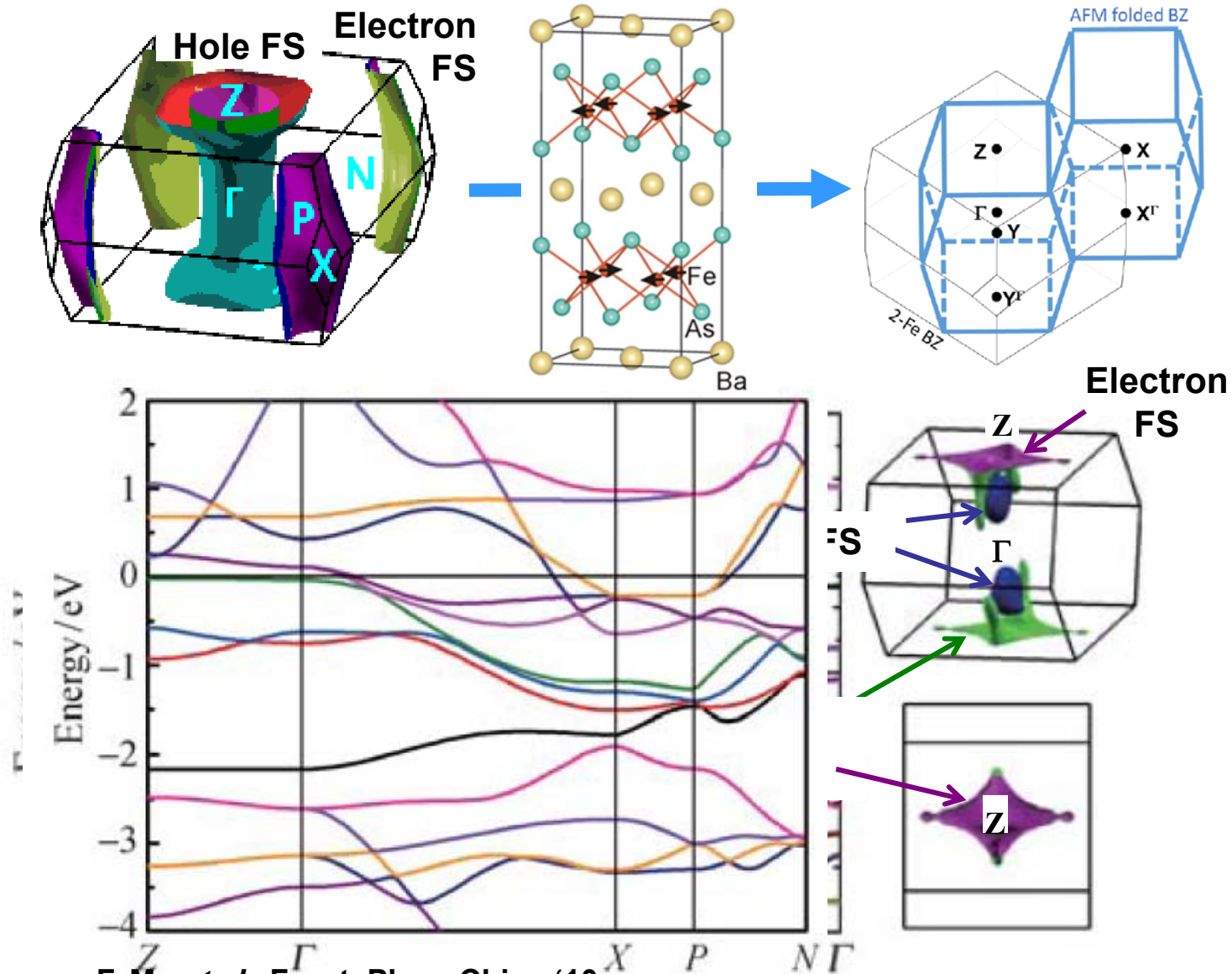
# Magneto-structural transition and possible electronic “nematic phase”



Q. Huang *et al.*, PRL '08

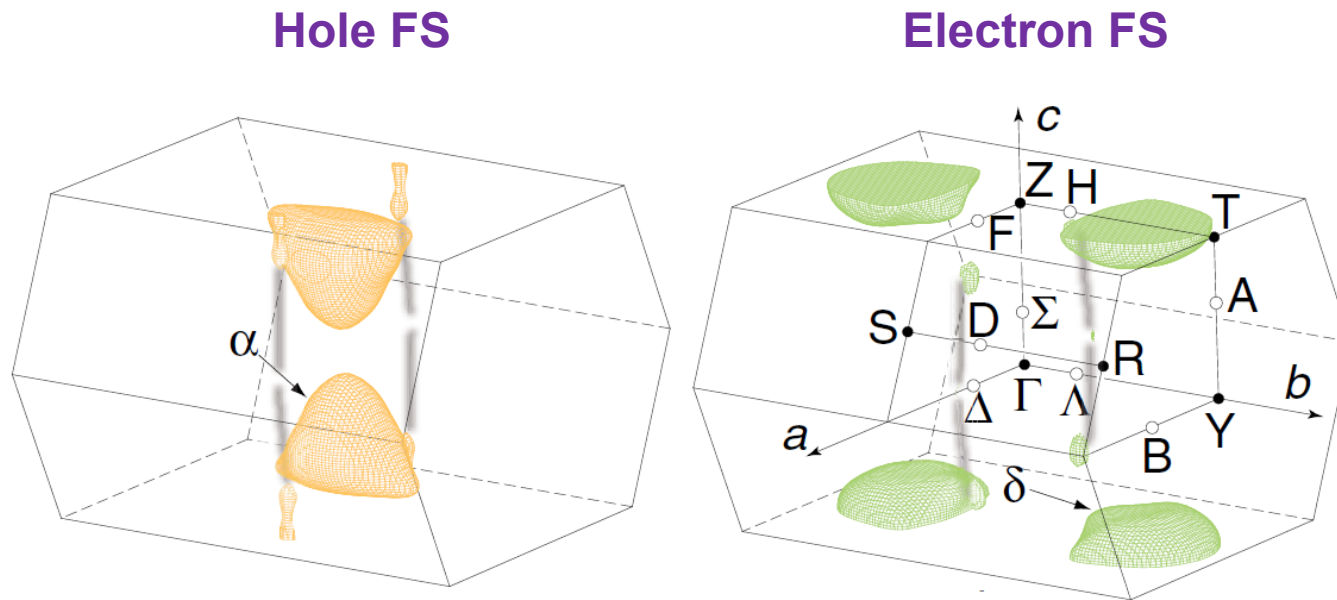
S. Kasahara *et al.*, Nature '13

# Folded Fermi surfaces of $\text{BaFe}_2\text{As}_2$ in the AFO phase



# Folded Fermi surfaces of $\text{BaFe}_2\text{As}_2$ in the AFO phase

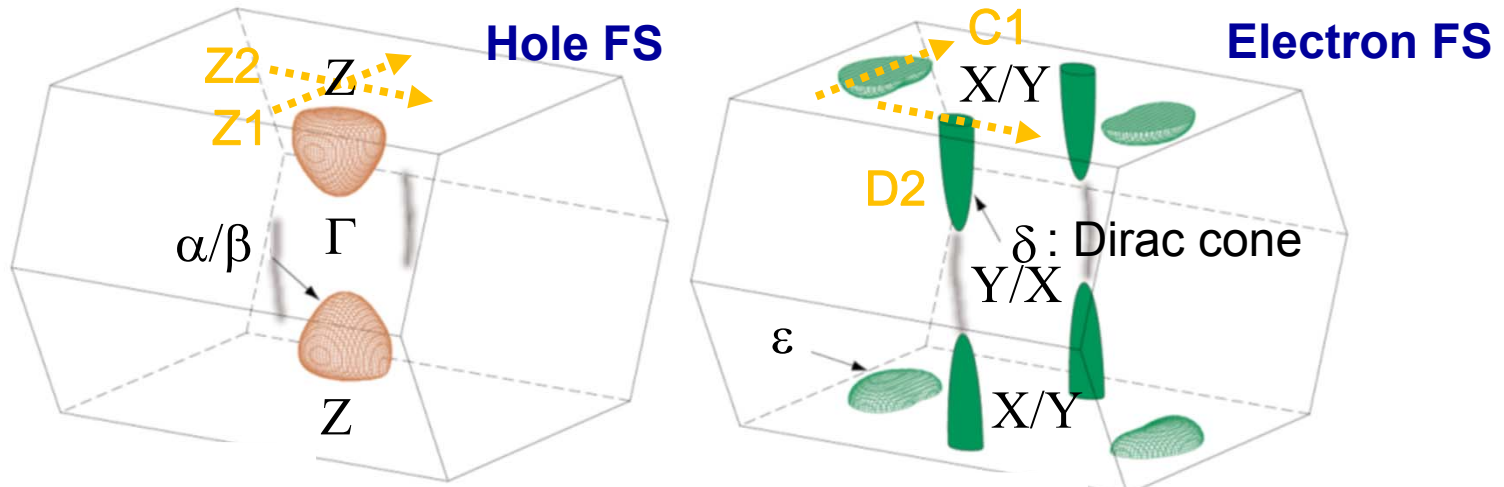
## LDA calculation





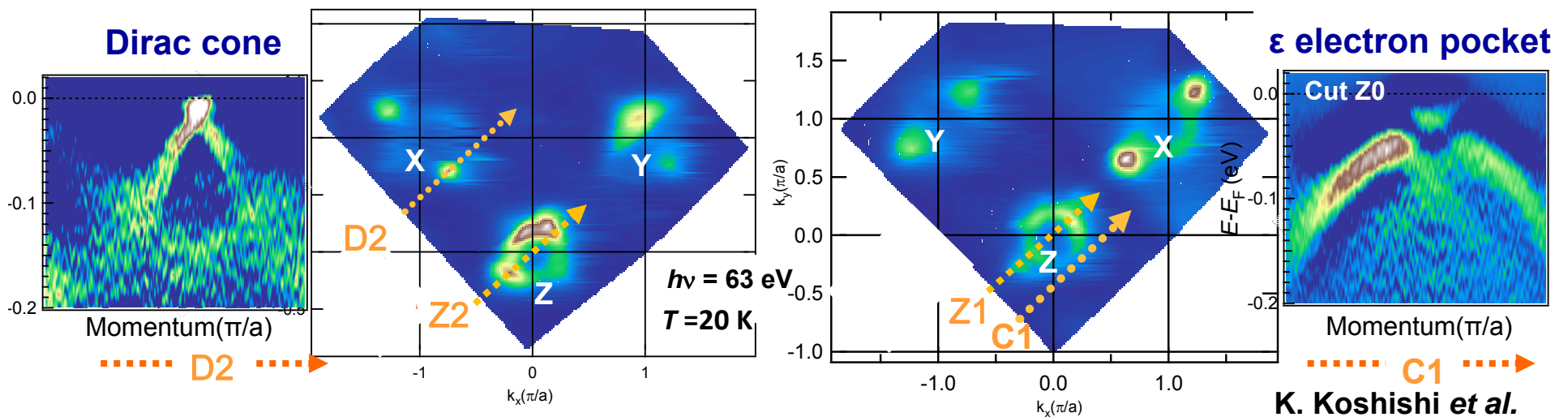
# Folded Fermi surfaces of BaFe<sub>2</sub>As<sub>2</sub> in the AFO phase by ARPES

LDA adjusted to de Haas-van Alphen experiment

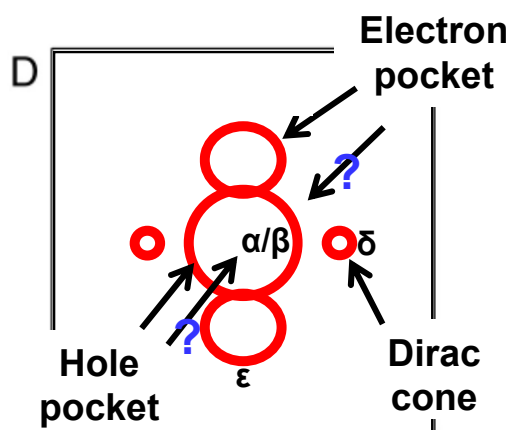
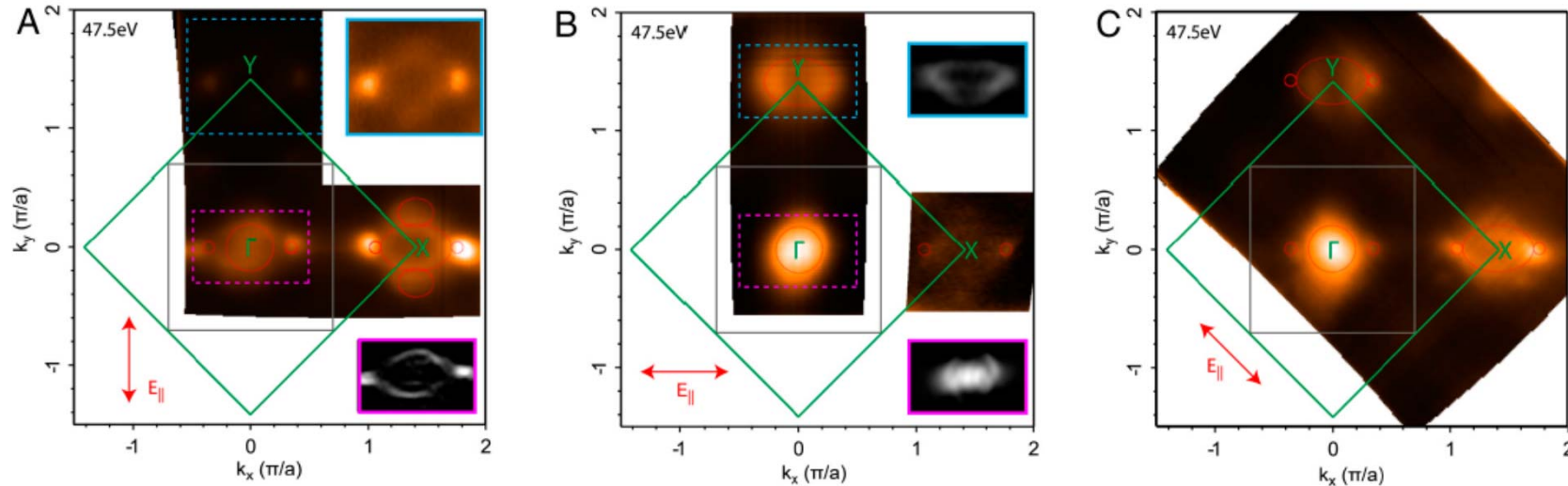


ARPES for  $k_z \sim Z$ , detwinned

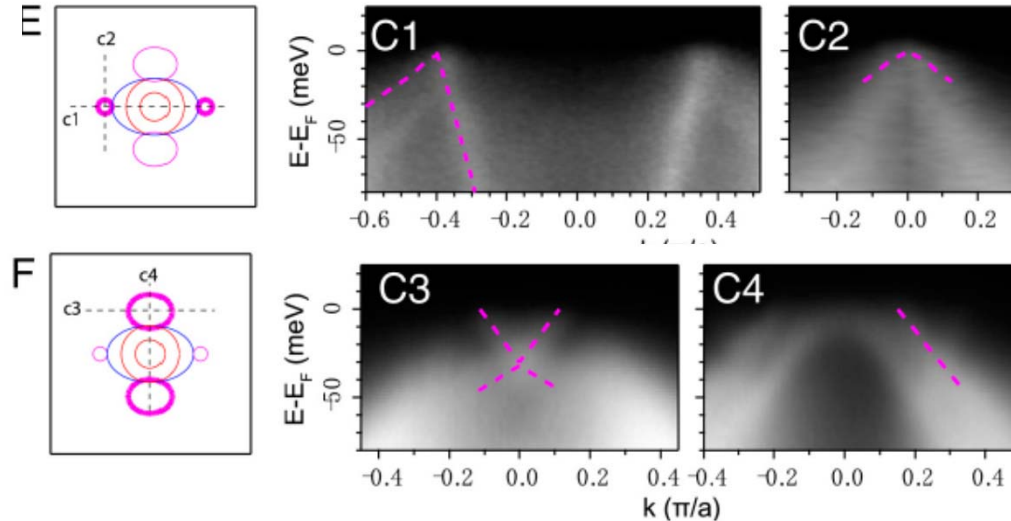
T. Terashima et al., PRL '11



# Folded Fermi surfaces of BaFe<sub>2</sub>As<sub>2</sub> in the AFO phase revealed by ARPES



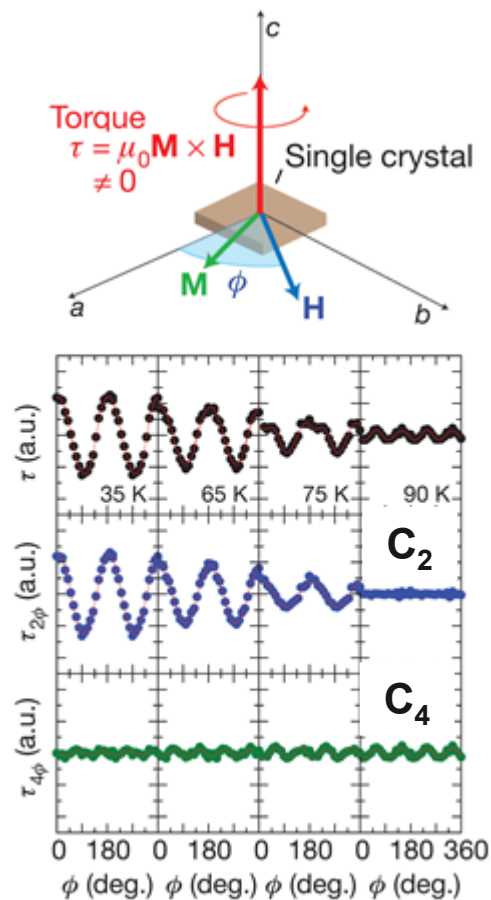
K. Koshiishi *et al.*



M. Yi *et al.*, PNAS '11

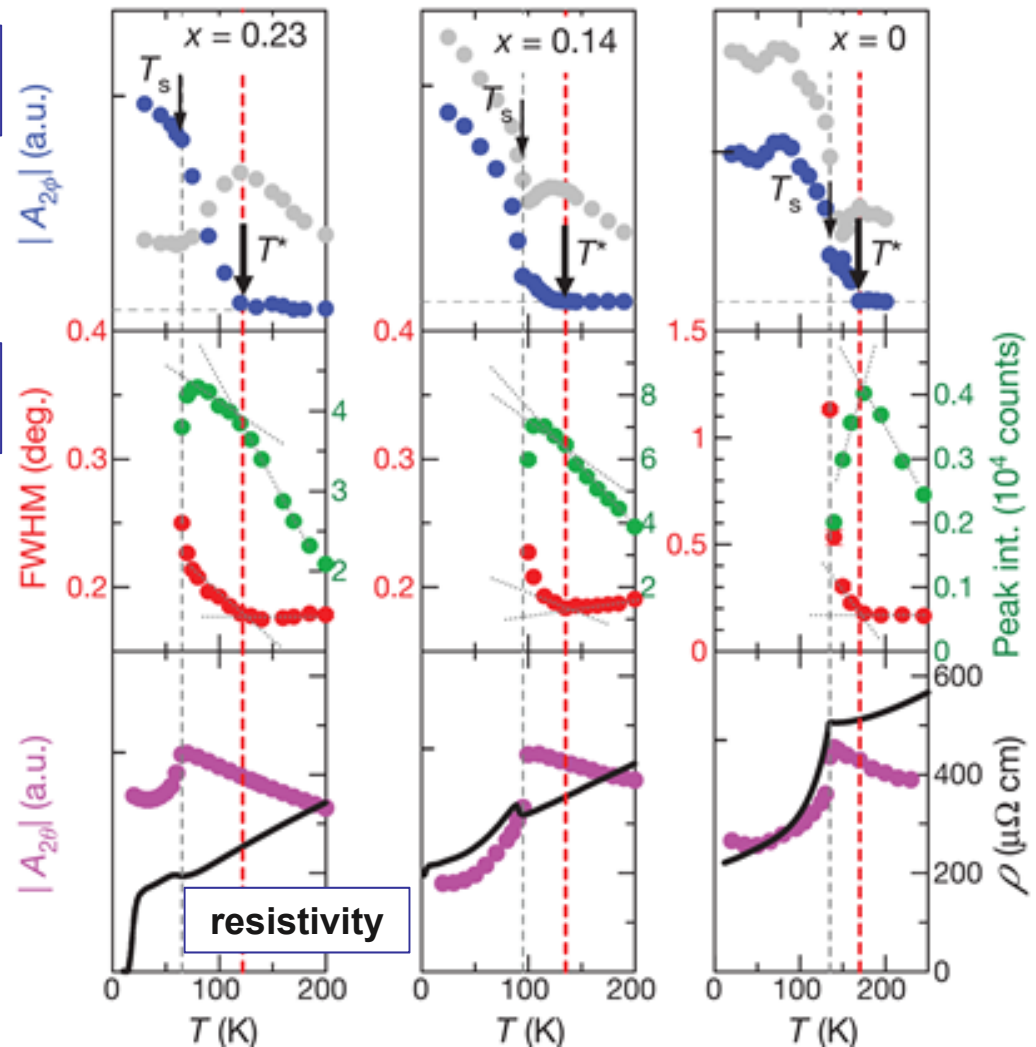
# $C_4$ symmetry breaking in the AFO and “nematic” phases of $BaFe_2(As_{1-x}P_x)_2$

## Magnetic torque measurements

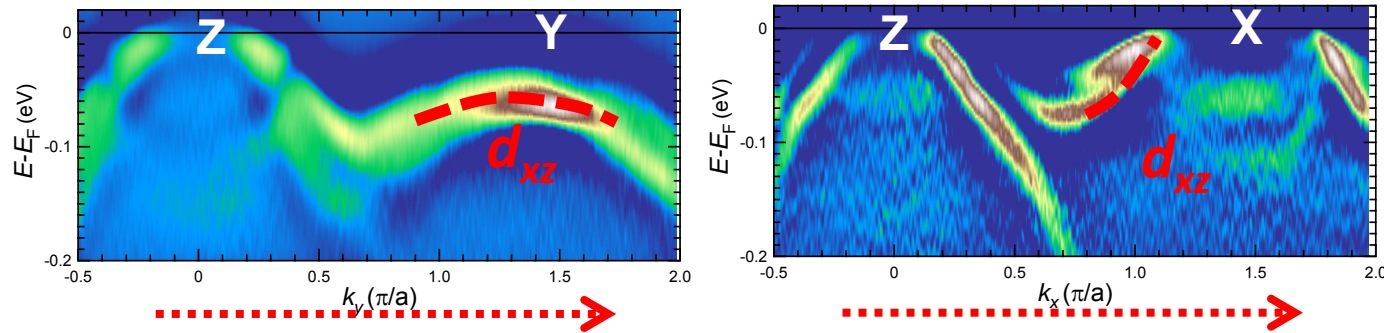


Magnetic torque

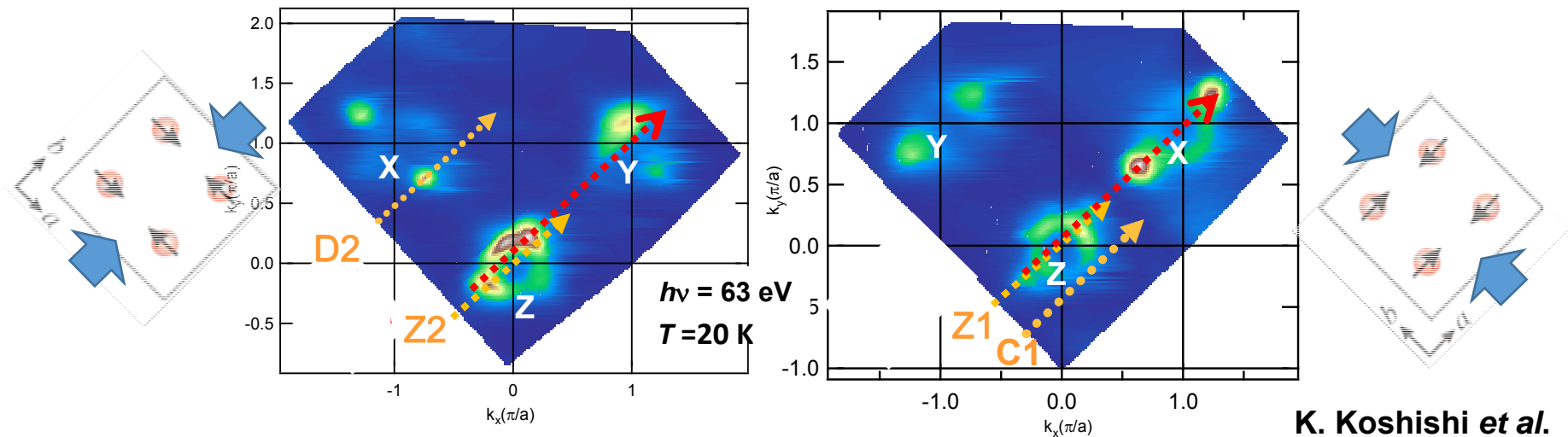
X-ray diffraction



# Anisotropic band dispersions in the AFO phase of $\text{BaFe}_2\text{As}_2$ – $C_4$ symmetry breaking

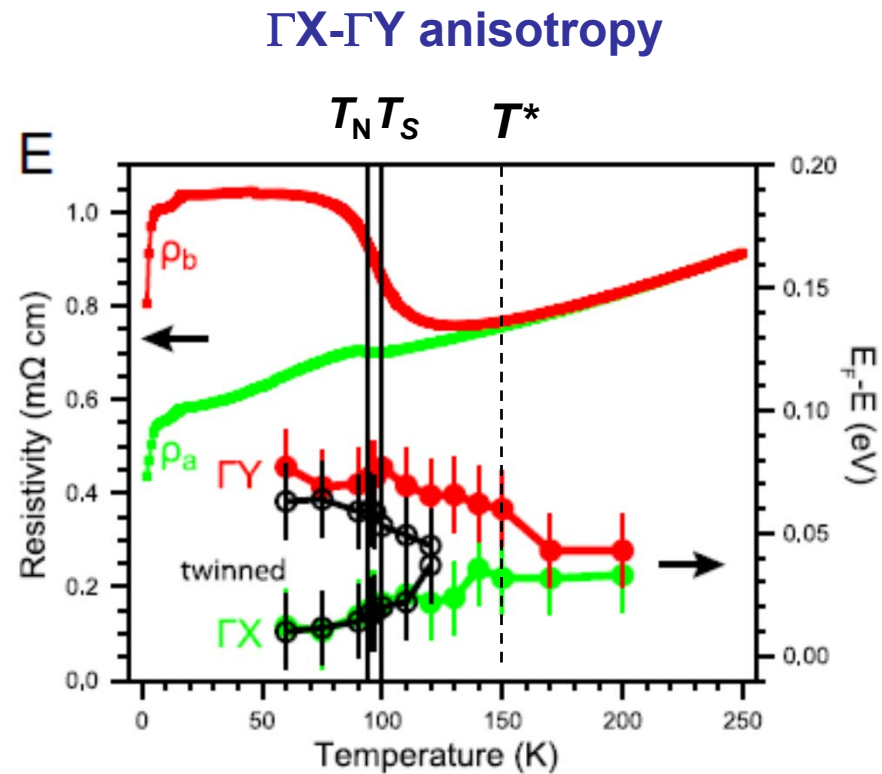
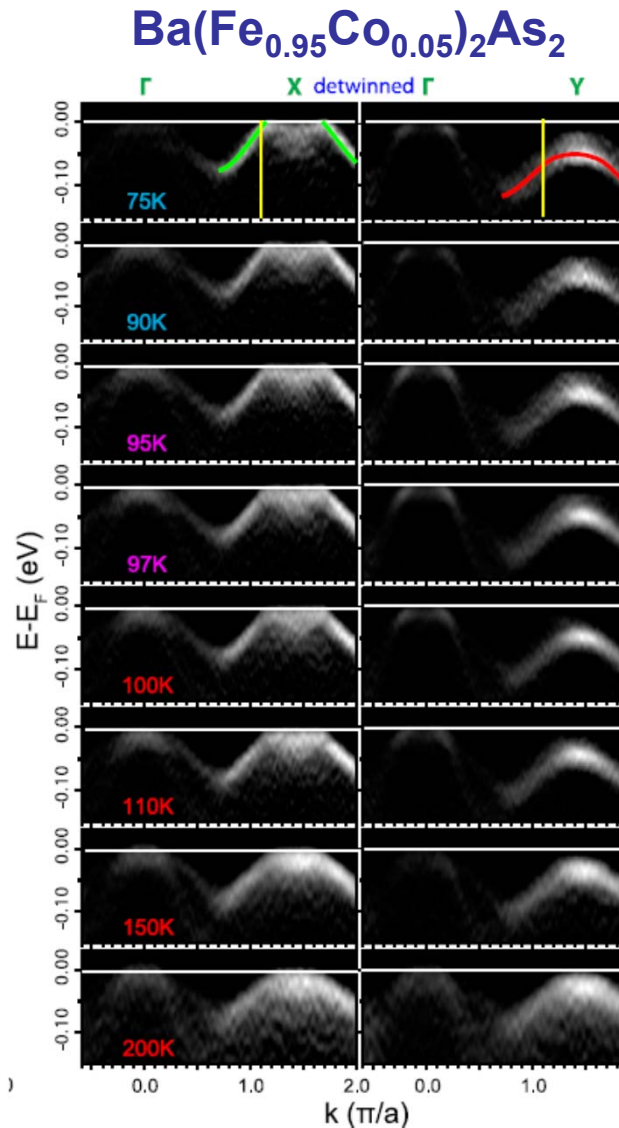


ARPES for  $k_z \sim Z$ , detwinned



K. Koshishi *et al.*

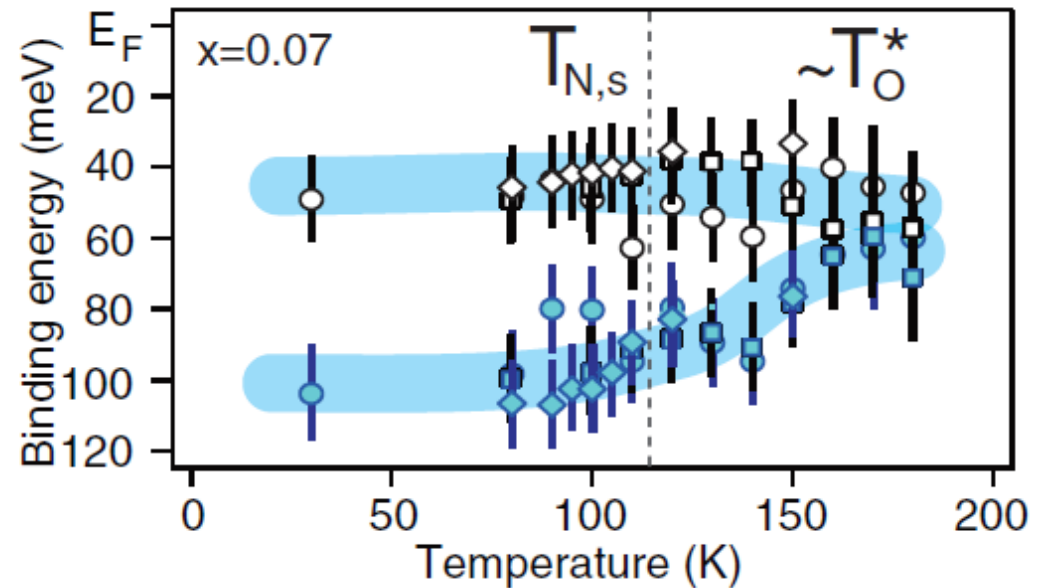
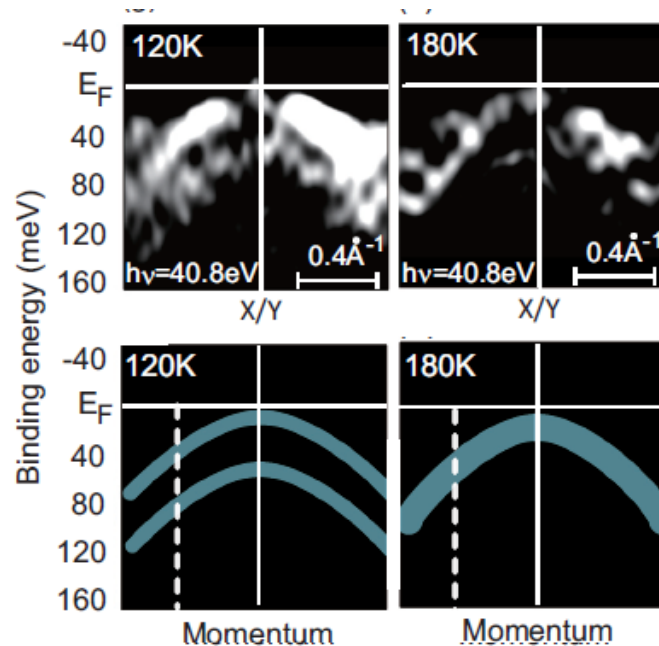
# Persistence of the anisotropic band dispersions above $T_{N,S}$



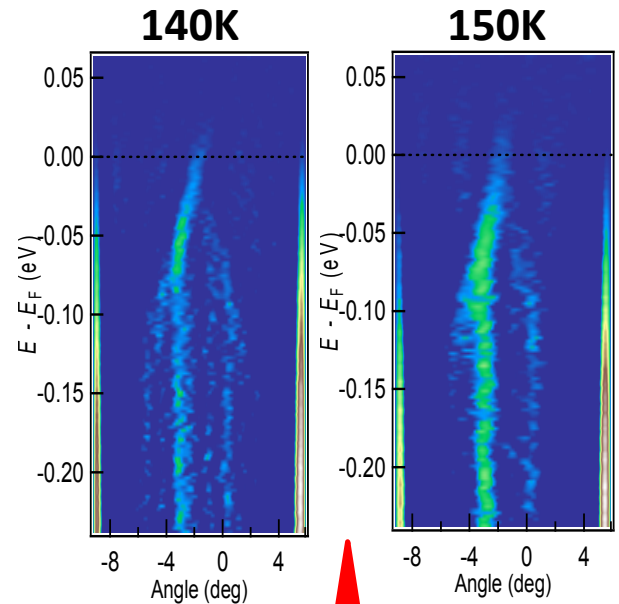
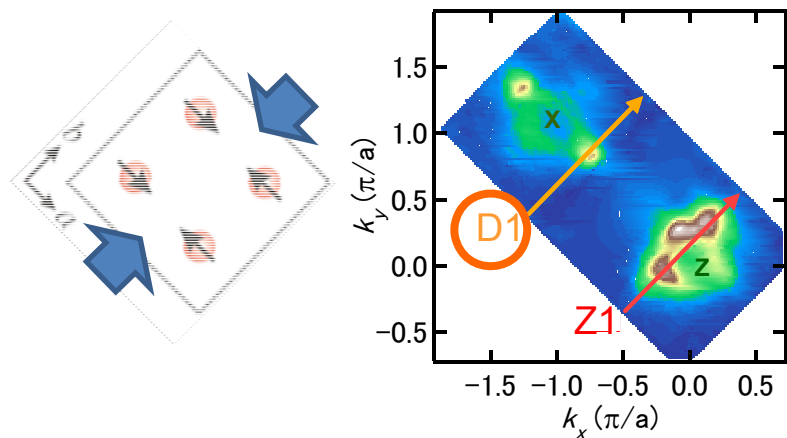
# Persistence of the anisotropic band dispersions above $T_{N,s}$



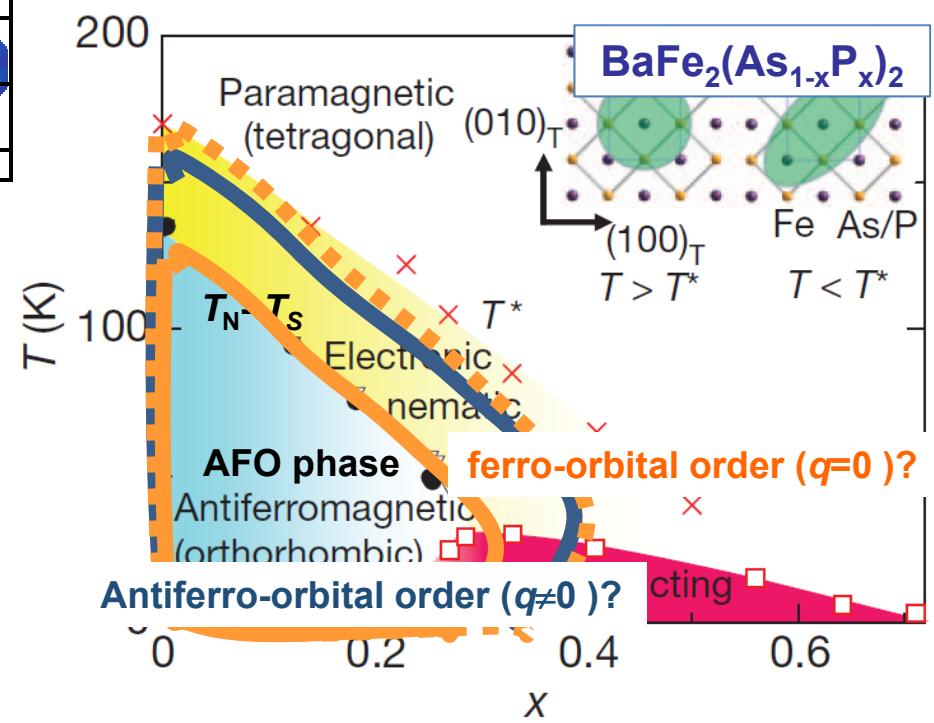
$\Gamma X-\Gamma Y$  anisotropy



# C<sub>4</sub> symmetry breaking and band folding in Fe-based superconductor: Possible antiferro-orbital order



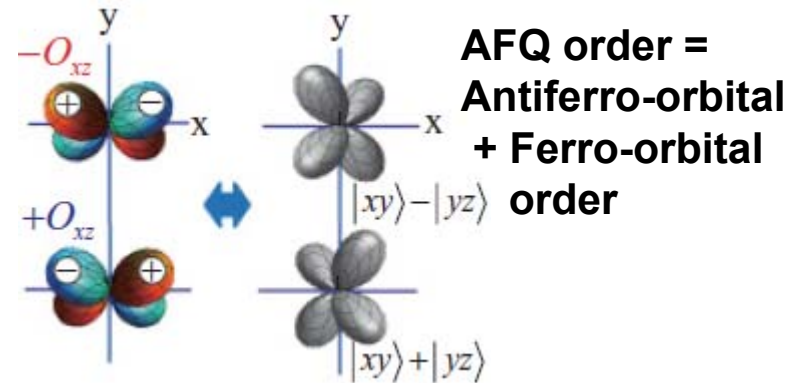
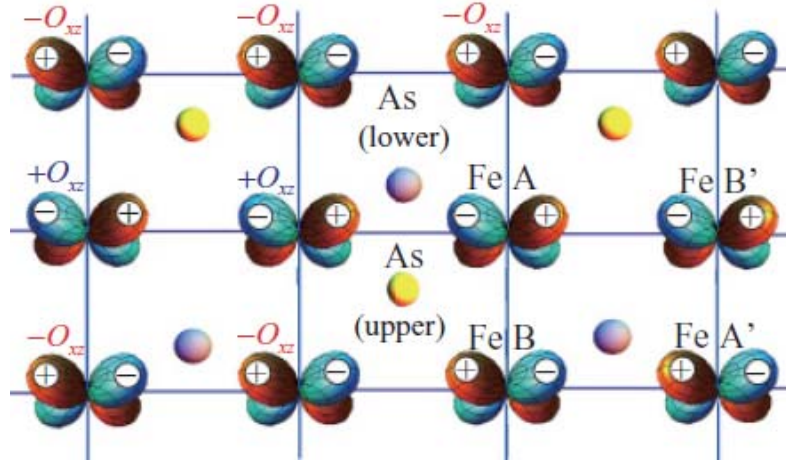
$T_{N,S} = 142 \text{ K}$



K. Koshishi *et al.*

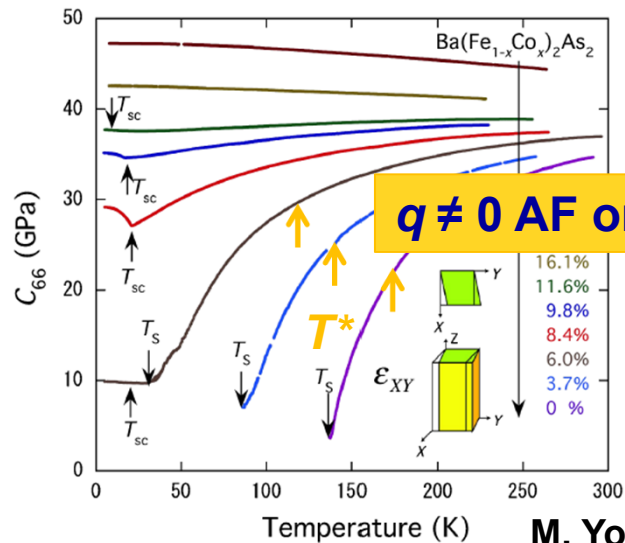
# Possible antiferro-orbital order below $T^*$

$O_{xz}$  antiferro-quadrupole (AFQ) order?

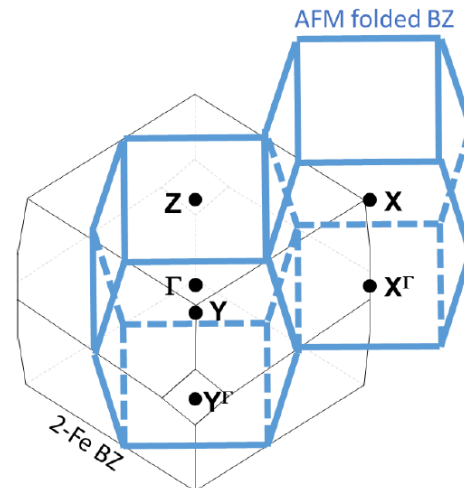


H. Kontani *et al.*, RB '11

Elastic constant  $C_{66}$



M. Yoshizawa *et al.*, JPSJ '12

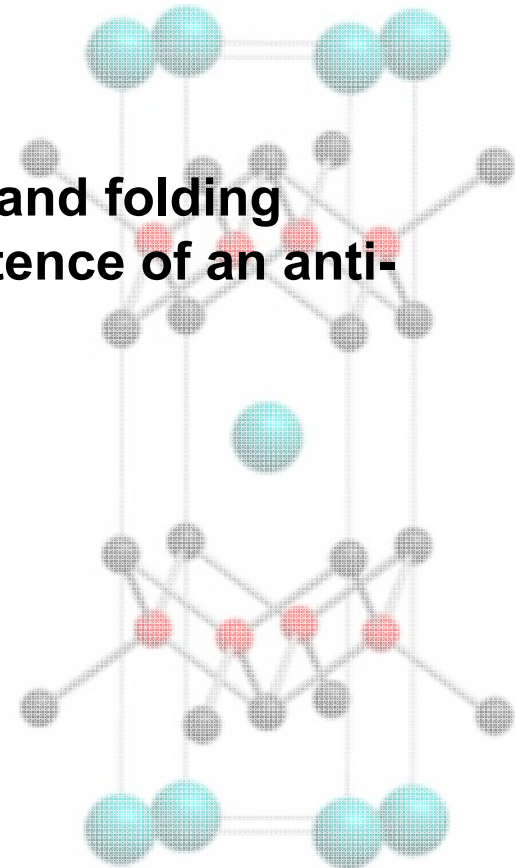




# Summary – AFO and “nematic” phases

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- **Folded electron and hole Fermi surfaces in the AFO phase revealed by ARPES are in almost perfect agreement with those deduced from the Subunikov-de Haas measurements.**
- **Not only  $C_4$  symmetry breaking but also band folding survive above  $T_{N,S}$ , suggesting the persistence of an anti-ferro-orbital order above  $T_{N,S}$  up to  $T^*$ .**

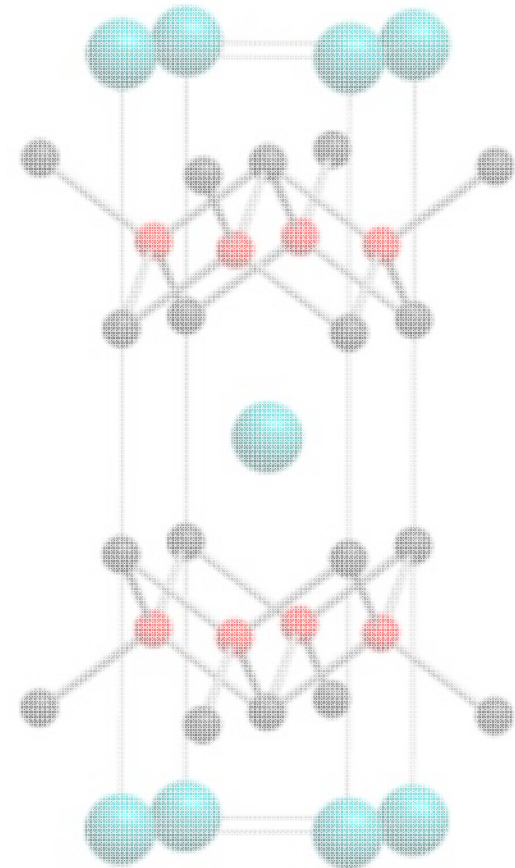


# Outline

- Nature of the AFM-orthorhombic (AFO) phase and the “nematic phase”:
  - Band folding *versus*  $C_4$  symmetry breaking

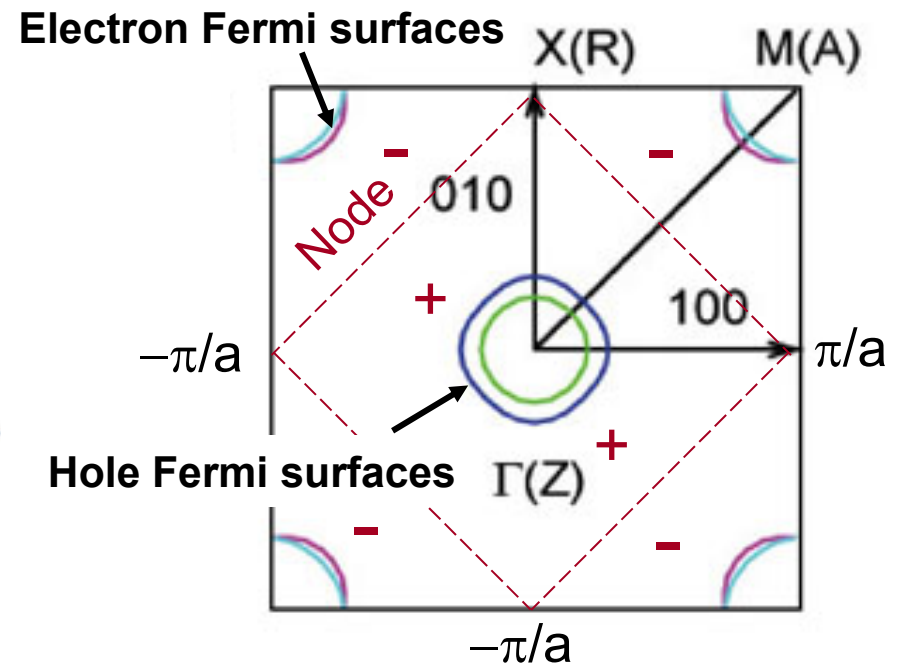
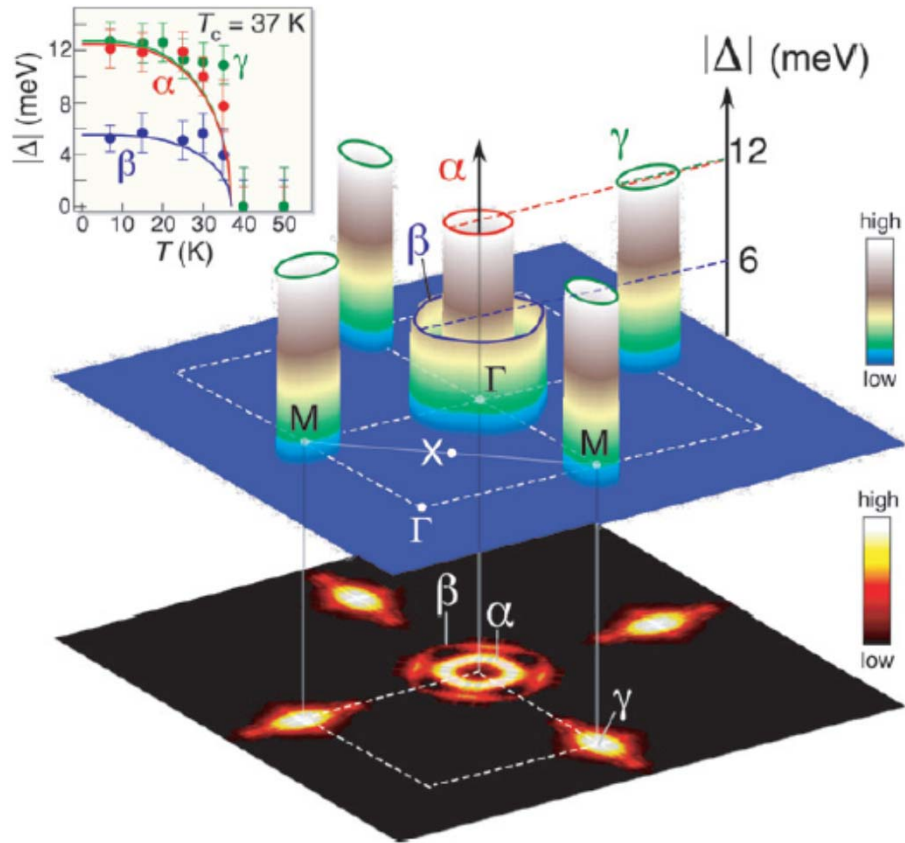


- Superconducting gap anisotropy



# Nodeless $s_{\pm}$ superconducting gap in Fe pnictides

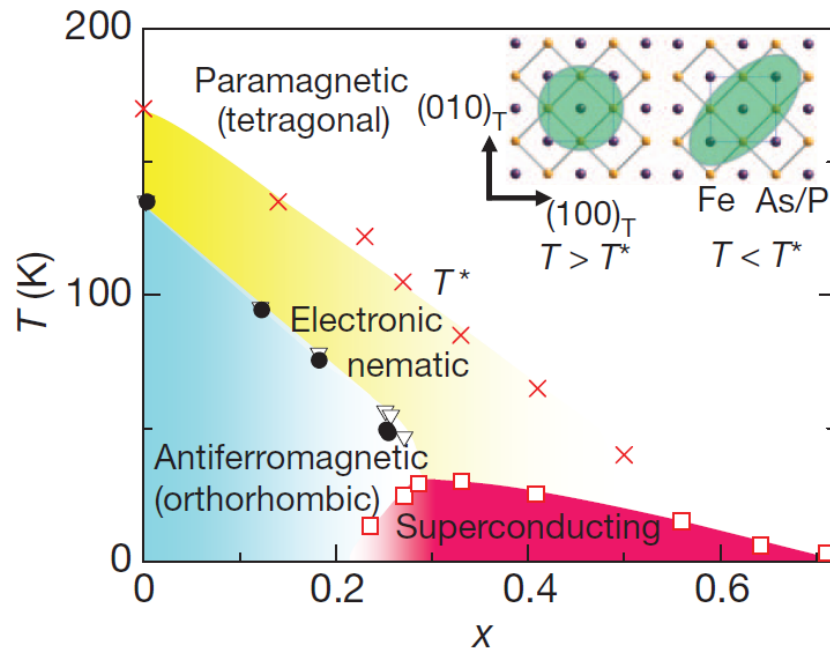
Superconducting gap of  $K_{0.4}Ba_{0.6}Fe_2As_2$   $s_{\pm}$ -wave superconductivity



**Order parameter**  
 $\Delta(k) = \Delta_0(\cos k_x a + \cos k_y a)/2$

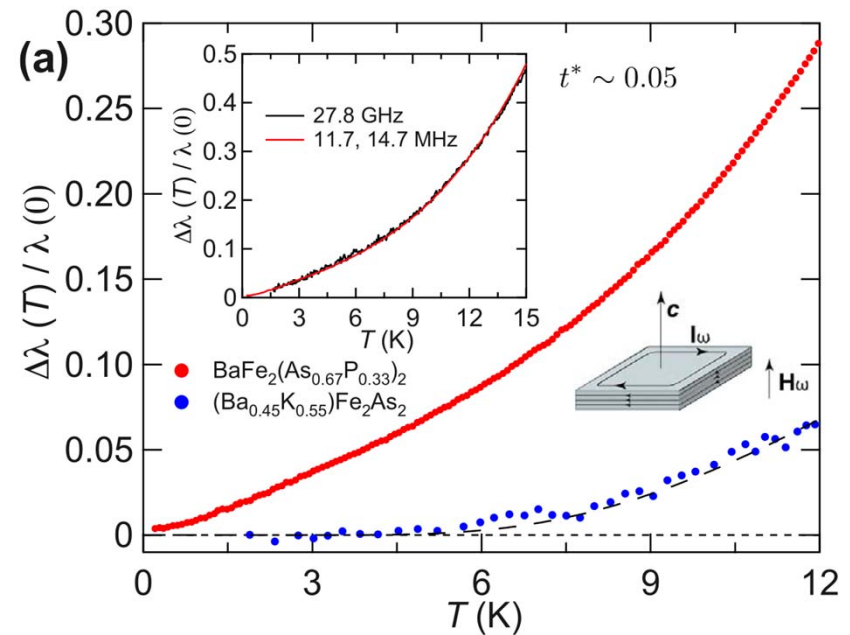
# Superconductivity with line nodes in $\text{BaFe}_2(\text{As}_{1-x}\text{P}_x)_2$

## Phase diagram



S. Kasahara *et al.*, Nature '13

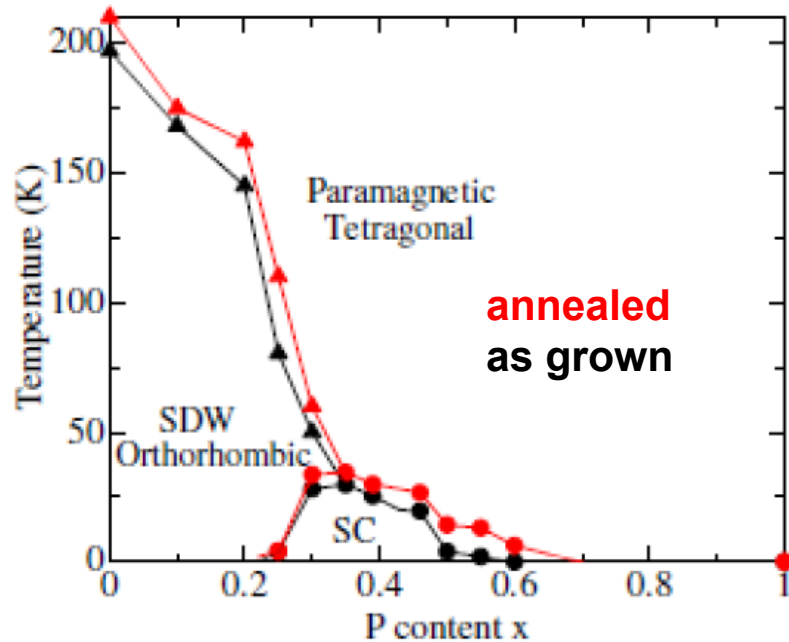
## Penetration depth



K. Hashimoto *et al.*, PRB '10

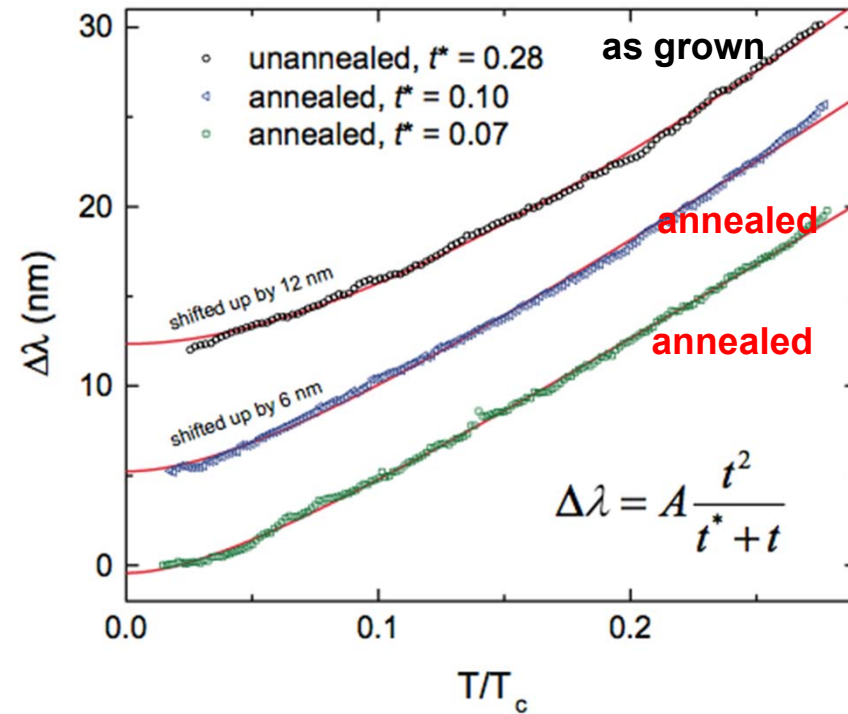
# Superconductivity with line nodes in $\text{SrFe}_2(\text{As}_{1-x}\text{P}_x)_2$

Phase diagram



T. Kobayashi *et al.*, PRB '13

Penetration depth

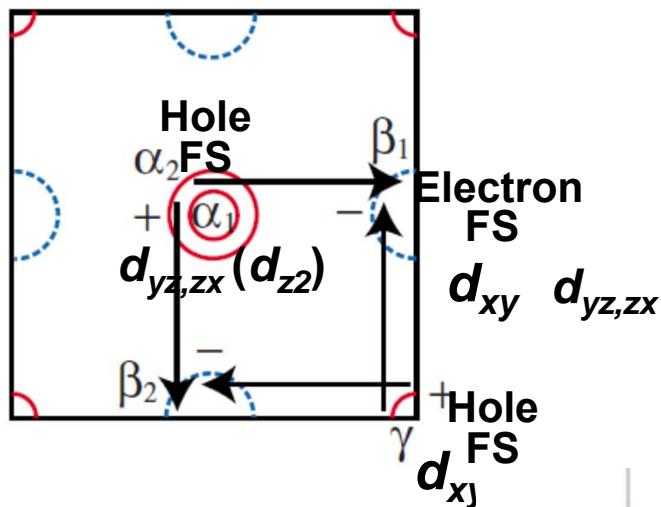


J. Murphy *et al.*, PRB '13

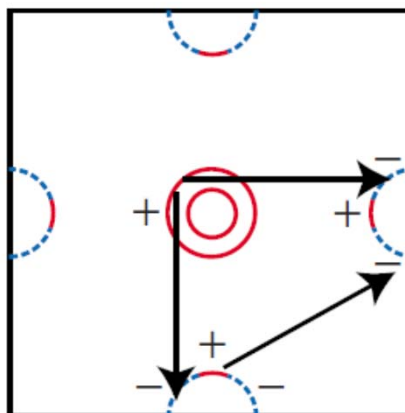
# Line nodes in order parameter according to spin-fluctuation mechanism

high ← Pnictogen height  $h_{pn}$  → low

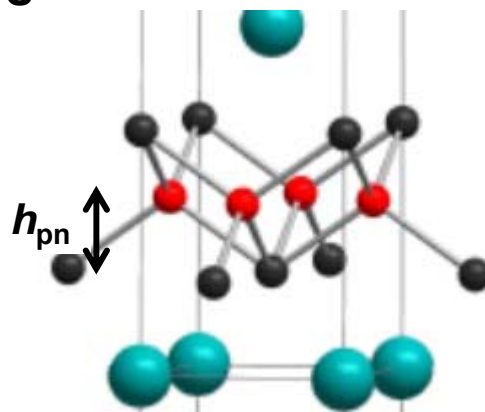
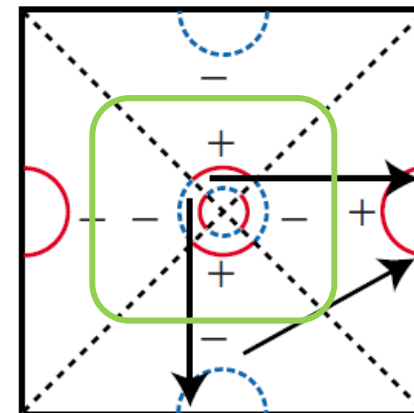
fully gapped  $s \pm$  wave



nodal  $s \pm$  wave

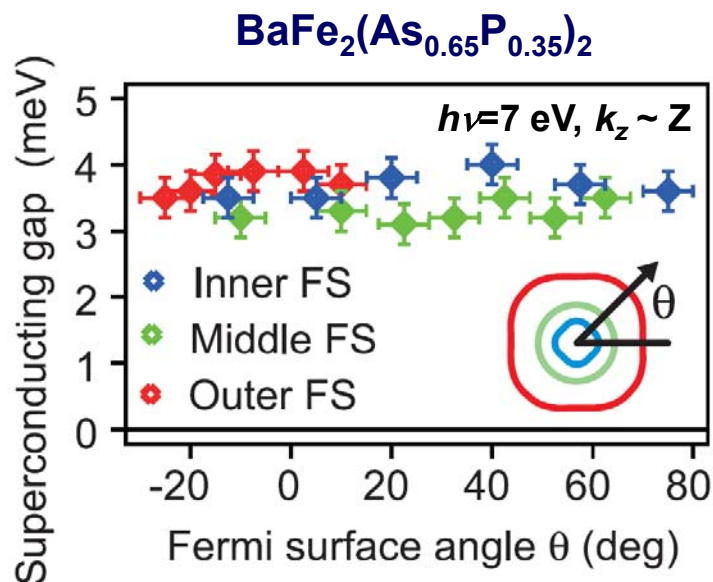


d-wave

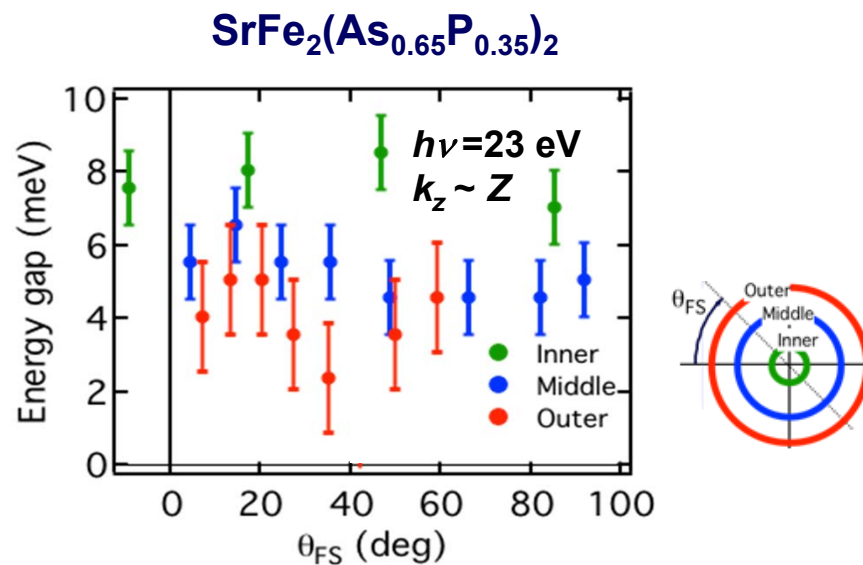


K. Kuroki *et al.*, PRB '09

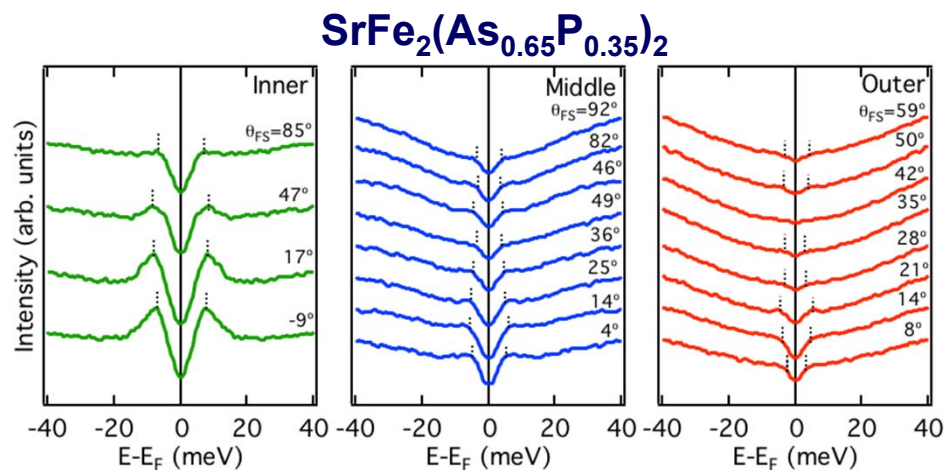
# Superconducting gap on hole Fermi surfaces of $\text{BaFe}_2(\text{As}_{0.65}\text{P}_{0.35})_2$ and $\text{SrFe}_2(\text{As}_{0.65}\text{P}_{0.35})_2$



**FS independent, nearly isotropic**



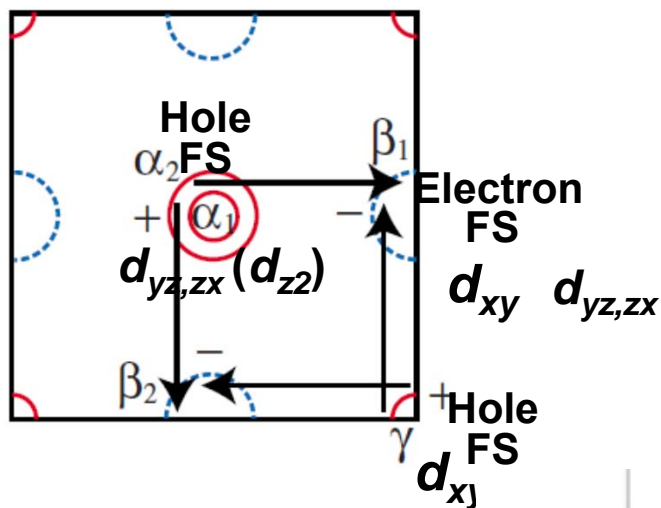
**FS dependent, nearly isotropic**



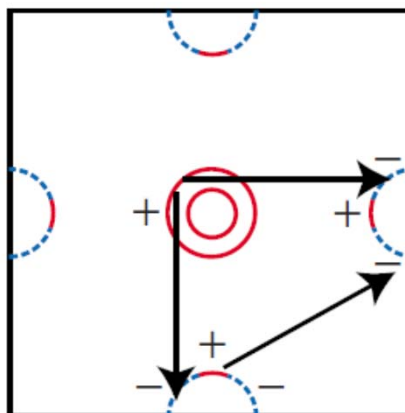
# Line nodes in order parameter according to spin-fluctuation mechanism

high ← Pnictogen height  $h_{pn}$  → low

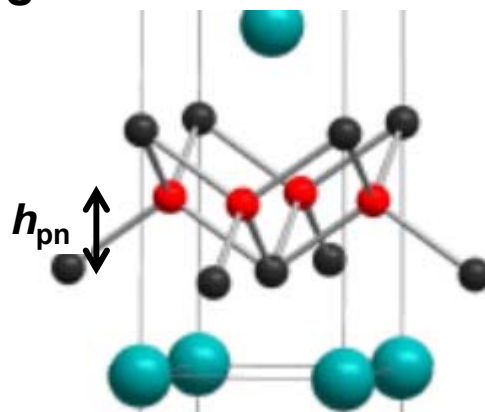
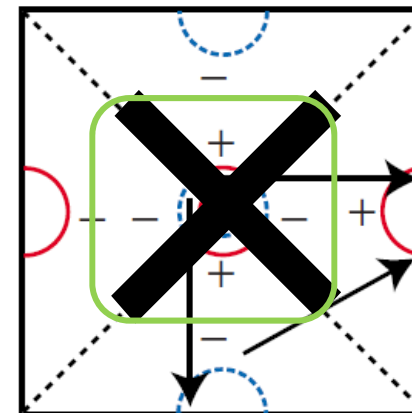
fully gapped  $s \pm$  wave



nodal  $s \pm$  wave



d-wave

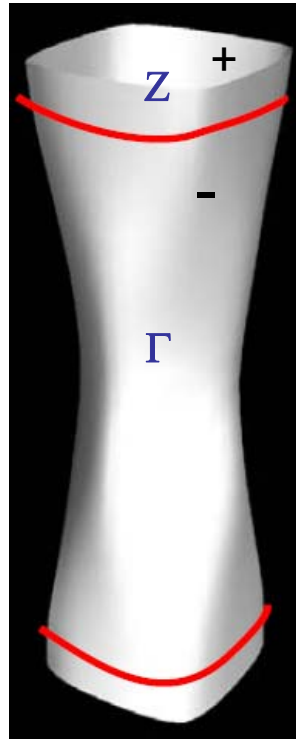


K. Kuroki *et al.*, PRB '09

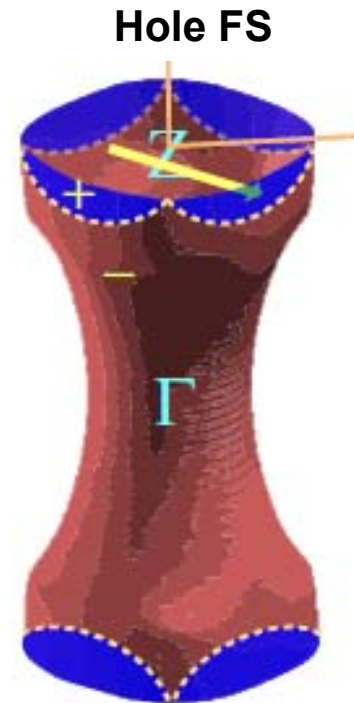


# Possibility of horizontal line nodes in spin-fluctuation mechanism

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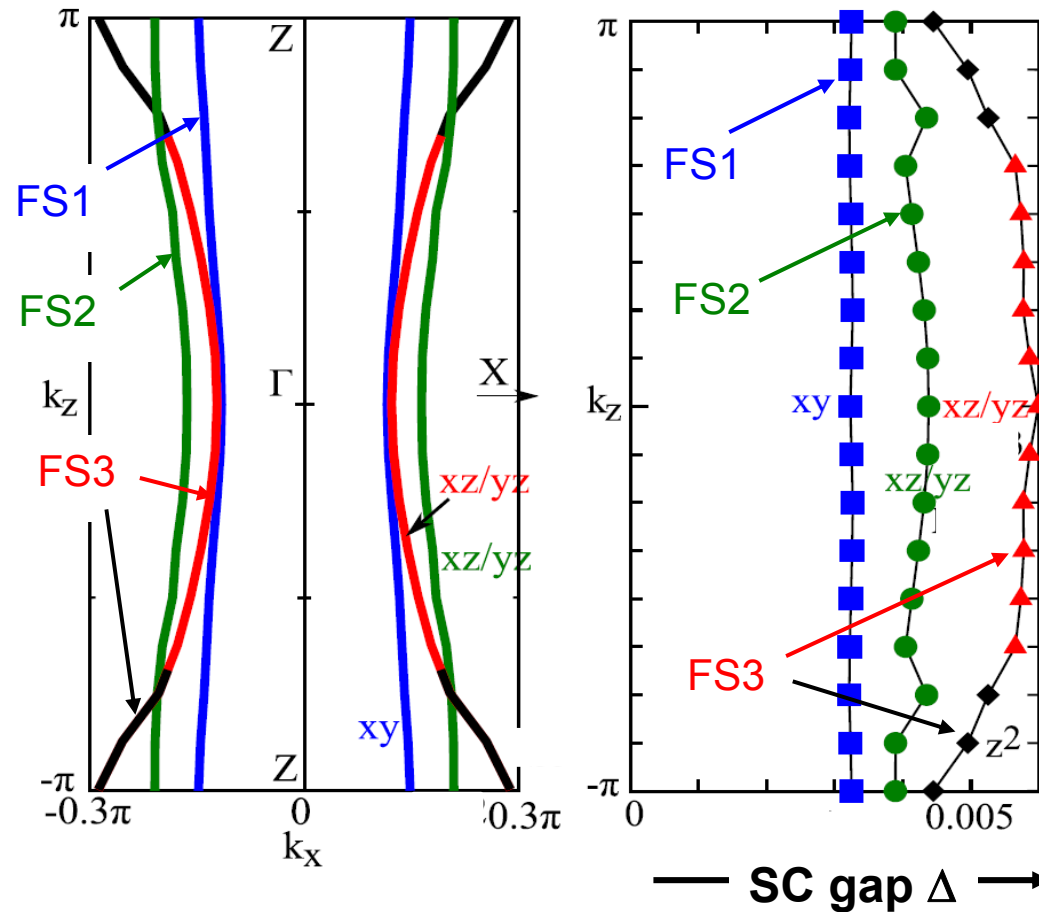


S. Graser *et al.*, PRB '10.



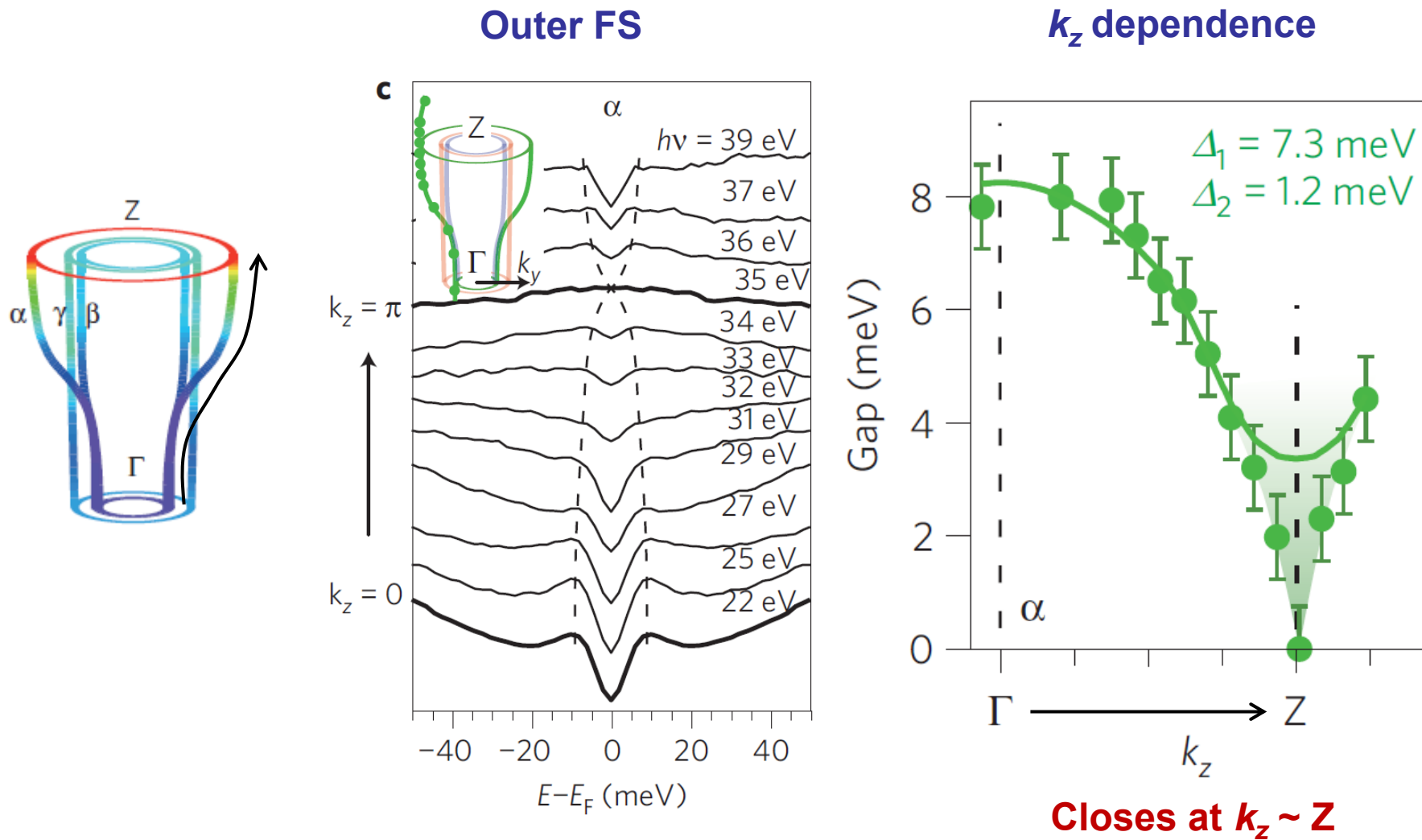
K. Suzuki *et al.*, JPSJ '11

# Superconducting gap on hole Fermi surfaces: Combined spin and orbital fluctuations

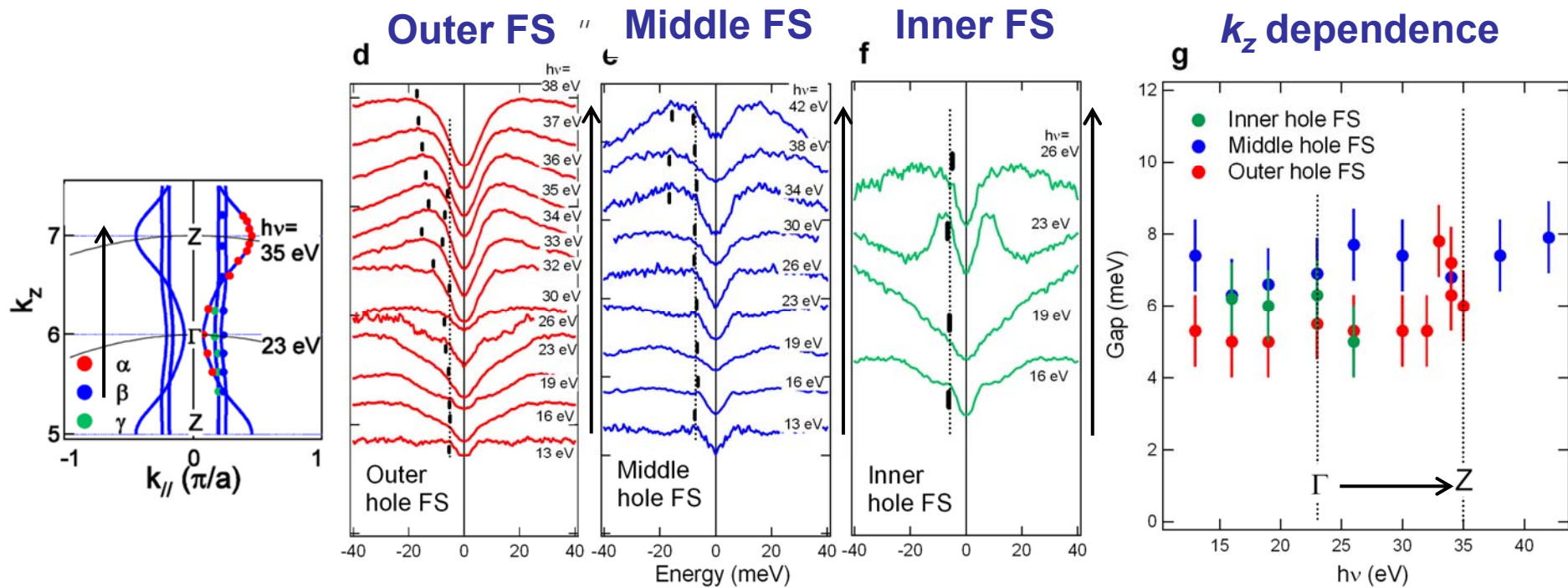


S. Onari and H. Kontani, PRL '12  
T. Saito, S. Onari, H. Kontani, PRB '13

# $k_z$ dependence of the superconducting gap on hole Fermi surfaces of $\text{BaFe}_2(\text{As}_{0.70}\text{P}_{0.30})_2$

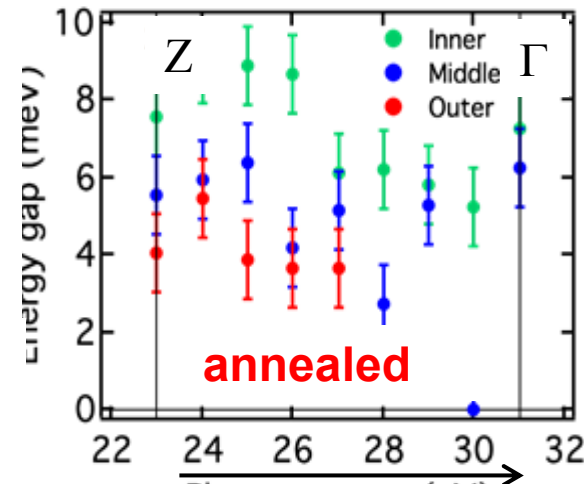
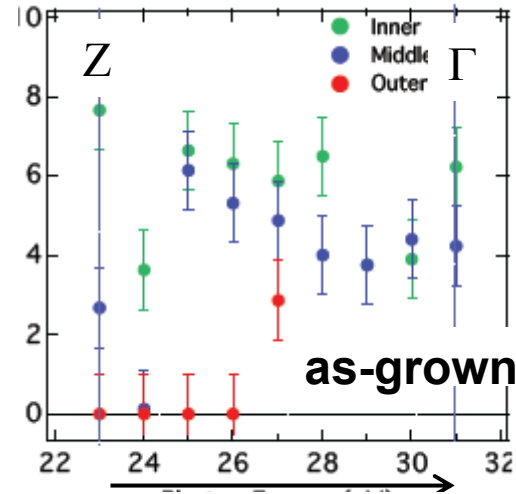
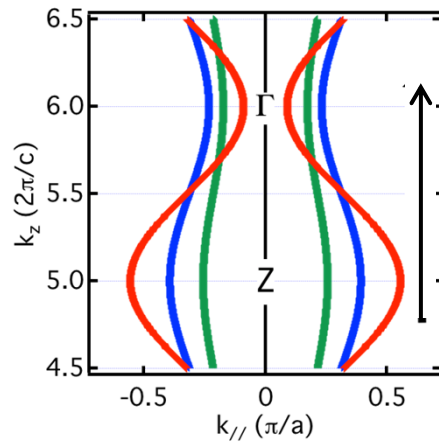


# $k_z$ dependence of the superconducting gap on hole Fermi surfaces of $\text{BaFe}_2(\text{As}_{0.70}\text{P}_{0.30})_2$

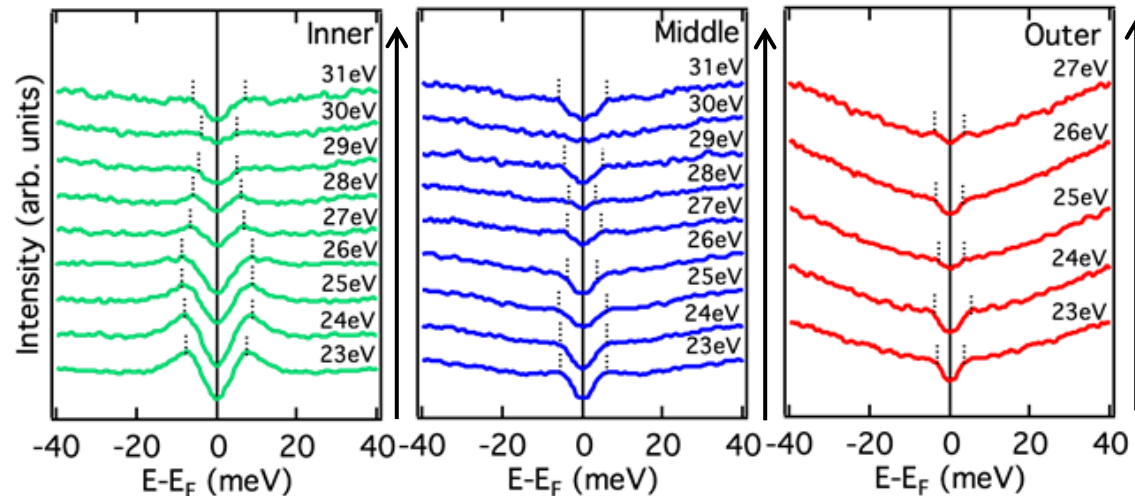


Nearly  $k_z$  independent

# $k_z$ dependence of the superconducting gap on hole Fermi surfaces of $\text{SrFe}_2(\text{As}_{0.65}\text{P}_{0.35})_2$



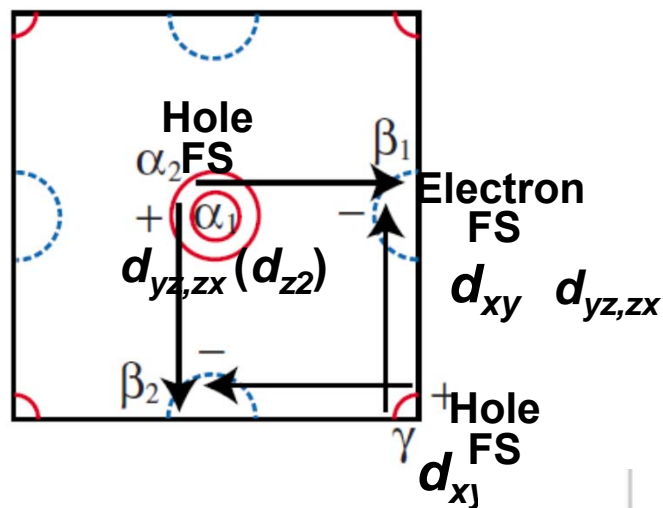
**Gap minimum around  $k_z \sim Z$     Gap opens around  $k_z \sim Z$**



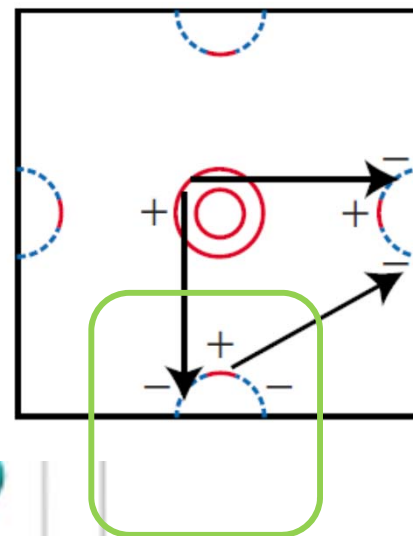
# Line nodes in order parameter according to spin-fluctuation mechanism

high ← Pnictogen height  $h_{pn}$  → low

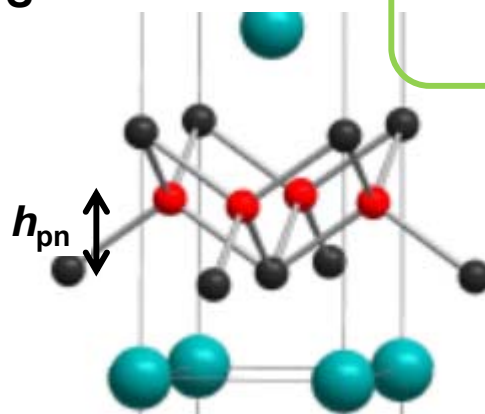
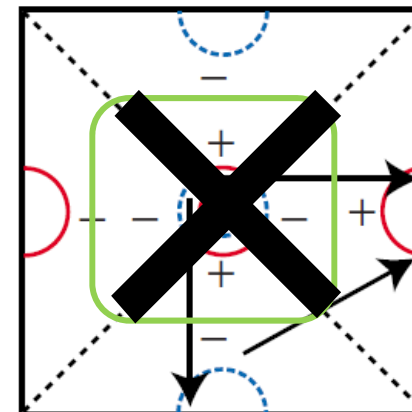
fully gapped  $s \pm$  wave



nodal  $s \pm$  wave



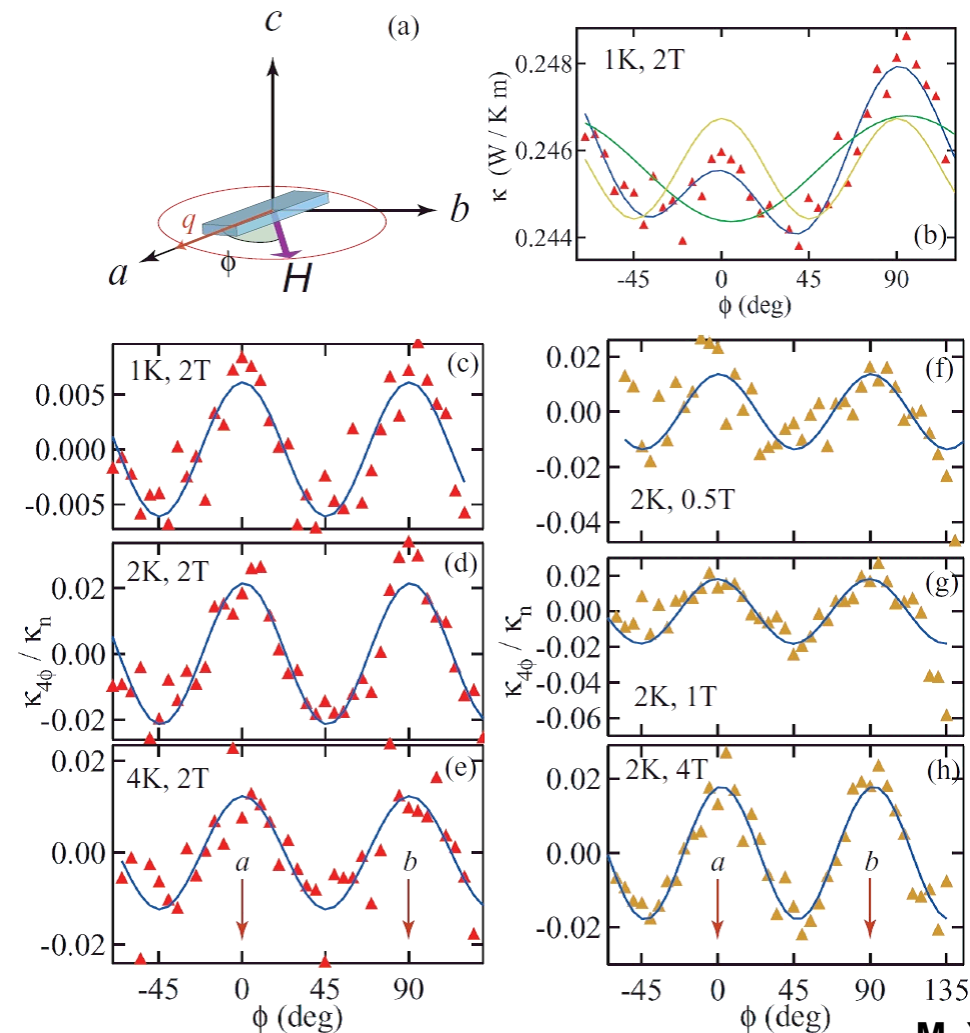
d-wave



K. Kuroki *et al.*, PRB '09

# Four-fold symmetry of thermal conductivity in magnetic fields in $\text{BaFe}_2(\text{As}_{1-x}\text{P}_x)_2$

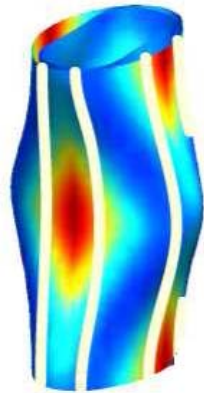
## Angular dependence



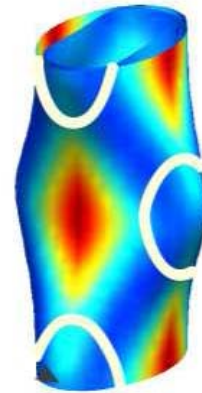
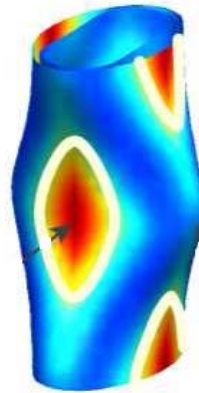
# Possible line nodes in superconducting gap on electron Fermi surfaces

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Vertical line nodes

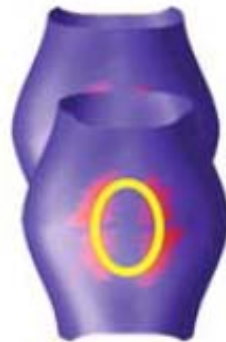


Loop-like line nodes



M. Yamashita *et al.*, PRB '11.

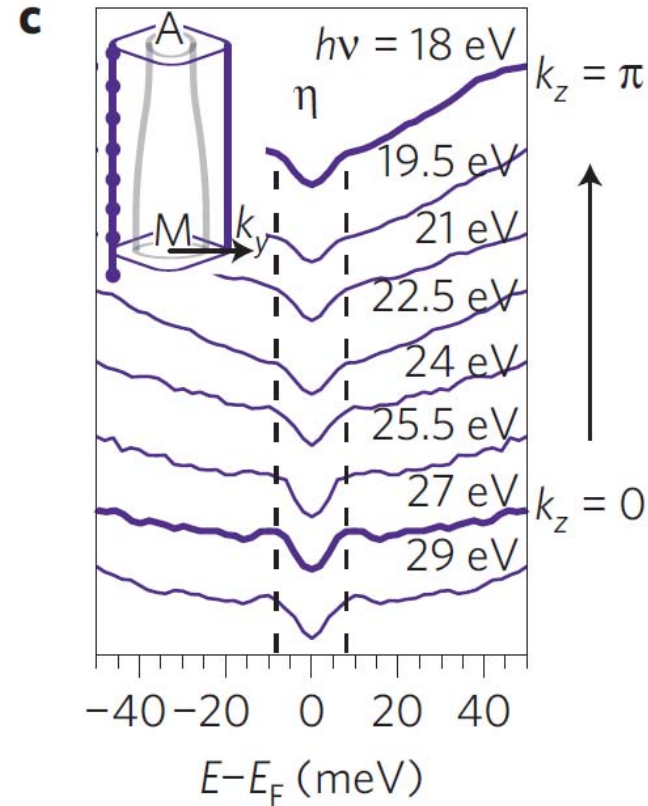
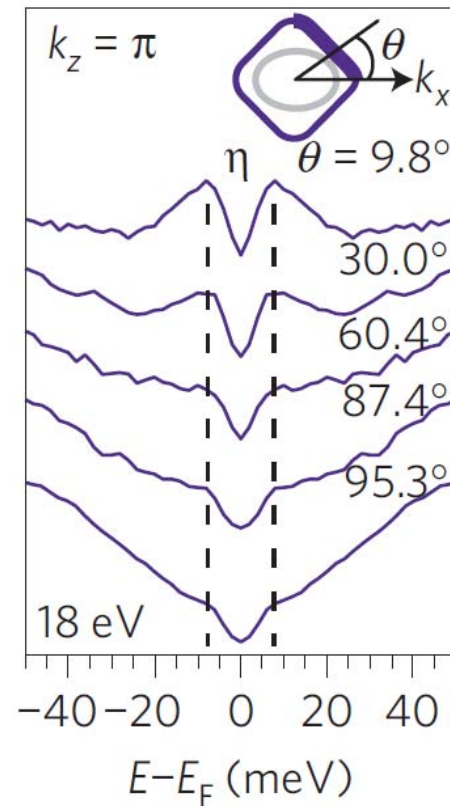
Loop-like line nodes



I. Mazin *et al.*, PRB '10



# Superconducting gap on electron Fermi surfaces of $\text{BaFe}_2(\text{As}_{0.70}\text{P}_{0.30})_2$



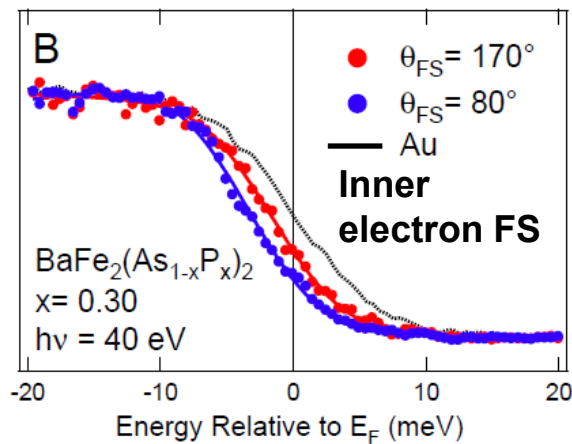
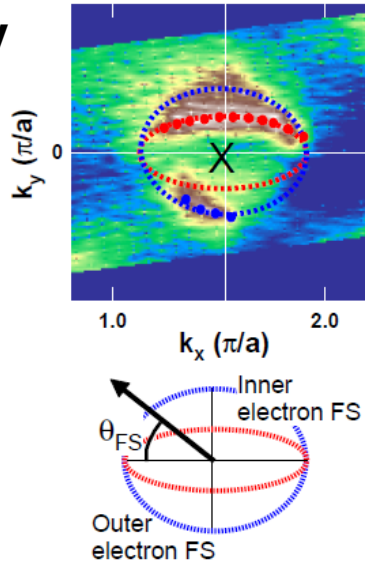
**Isotropic**

Y. Zhang *et al.*, Nat. Phys. '12

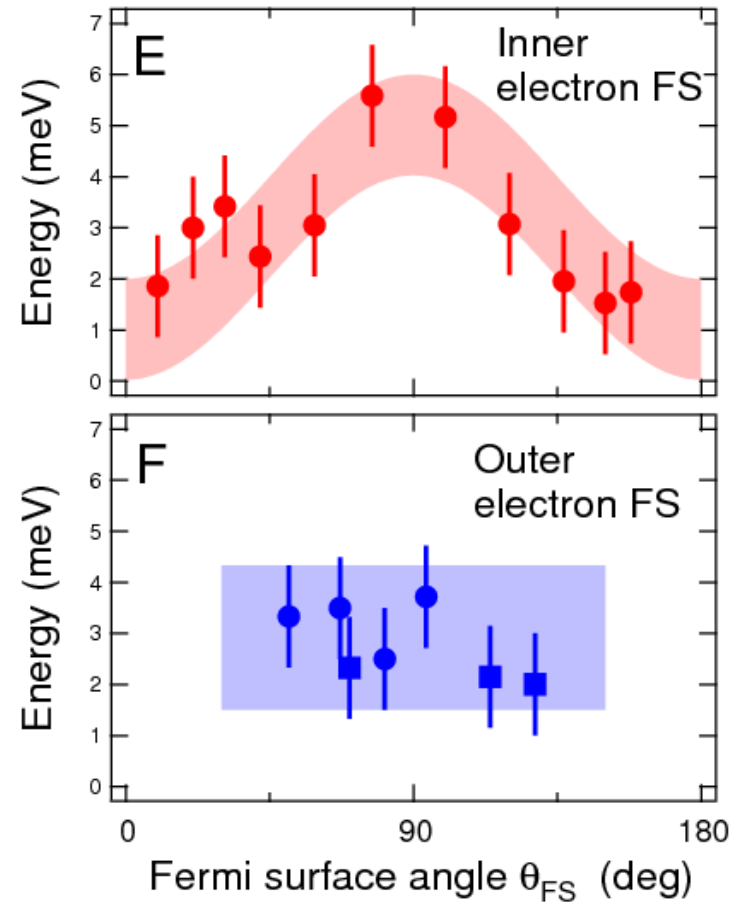
# Superconducting gap on electron Fermi surfaces of $\text{BaFe}_2(\text{As}_{0.70}\text{P}_{0.30})_2$

$h\nu=40$  eV

$T_c=30$  K

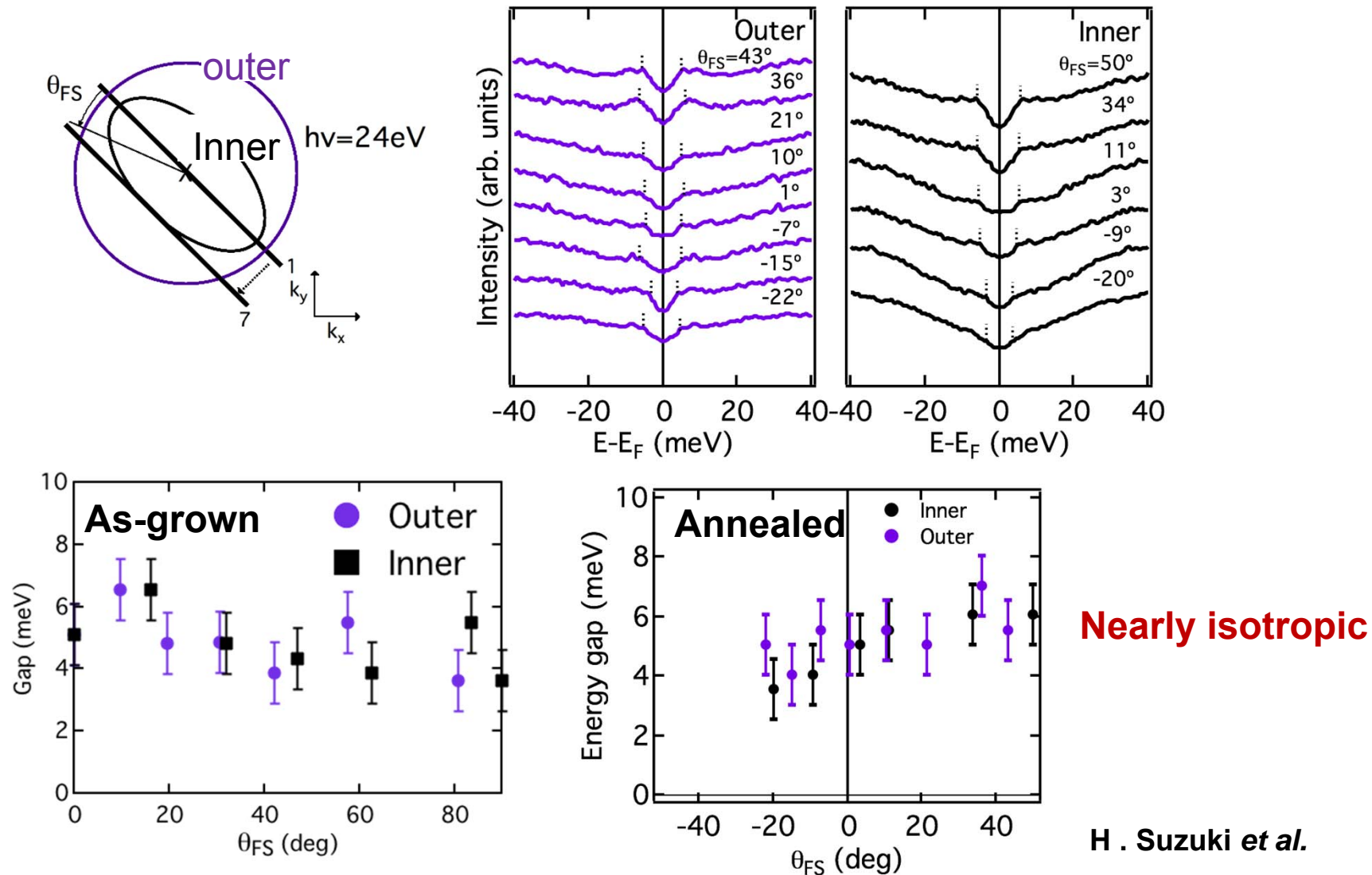


Gap magnitude



Anisotropy

# Superconducting gap on electron Fermi surfaces of $\text{SrFe}_2(\text{As}_{0.65}\text{P}_{0.35})_2$



# Summary of ARPES experiments on gap anisotropy in isovalent-substituted 122 systems

		Hole FS	Electron FS
BaFe <sub>2</sub> (As,P) <sub>2</sub> (x=0.30)	Y. Zhang <i>et al.</i>	$ \Delta  \sim 0$ at $k_z \sim Z$	isotropic
(x=0.30, 0.38) (x=0.35)	T. Yoshida <i>et al.</i> T. Shimojima <i>et al.</i>	$ \Delta  > 0$ for all $k_z$ $ \Delta  > 0$ at $k_z \sim Z$ FS-independent	anisotropic —
SrFe <sub>2</sub> (As,P) <sub>2</sub> (x=0.35) before annealing	H. Suzuki <i>et al.</i>	$ \Delta  \sim 0$ at $k_z \sim Z$	isotropic
after annealing		$ \Delta  > 0$ for all $k_z$	isotropic
Ba(Fe,Ru) <sub>2</sub> As <sub>2</sub> (x=0.35)	L. Liu <i>et al.</i>	$ \Delta  \sim 0$ at $k_z \sim Z$	isotropic

# Summary – Superconducting gap

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- Superconducting gap anisotropy is material, composition, and disorder dependent even in the limited number of isovalent P- and Ru-substituted systems:
  - Hole FS: Gap minimum or no minimum around  $k_z \sim Z$ .
  - Electron FS: Isotropic or anisotropic.

