Iron-based superconductors

With a focus on ARPES studies thereof

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Physics 250 (Special topics: spectroscopies of quantum materials)

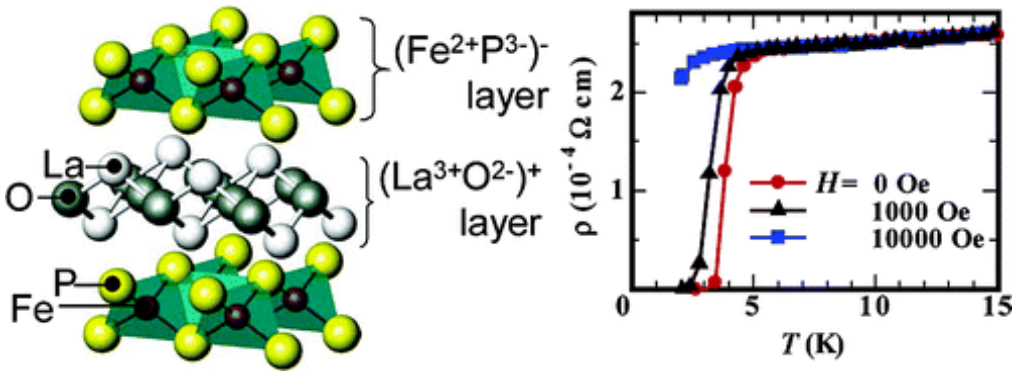
UC Davis, Fall 2016

Outline

- Introduction
  - Discovery
  - Materials and phase diagrams
  - Correlations
  - Potential mechanisms
- ARPES studies of FeSCs
  - Fermiology
  - Magnetism/SDW
  - Superconducting gap
  - Monolayer FeSe on STO

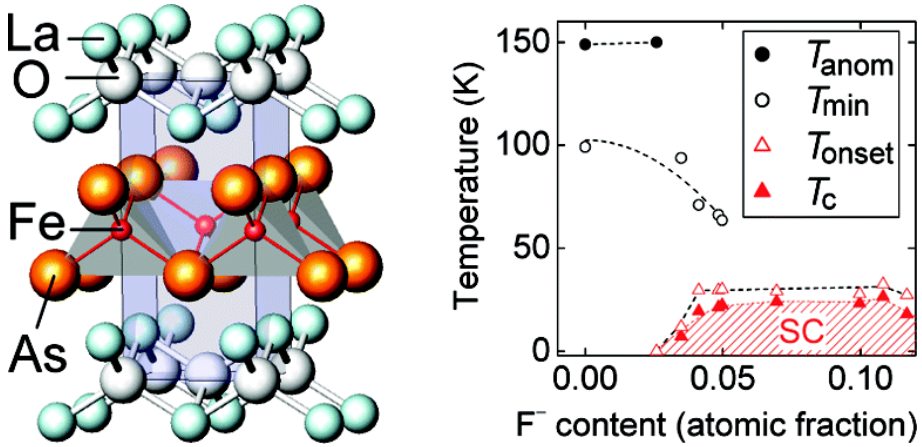
Discovery of Fe-based SCs

2006: LaFePO, Tc=**5K**



Kamihara et al, *J. Am. Chem. Soc.*, ***128***, pp 10012–10013 (2006)

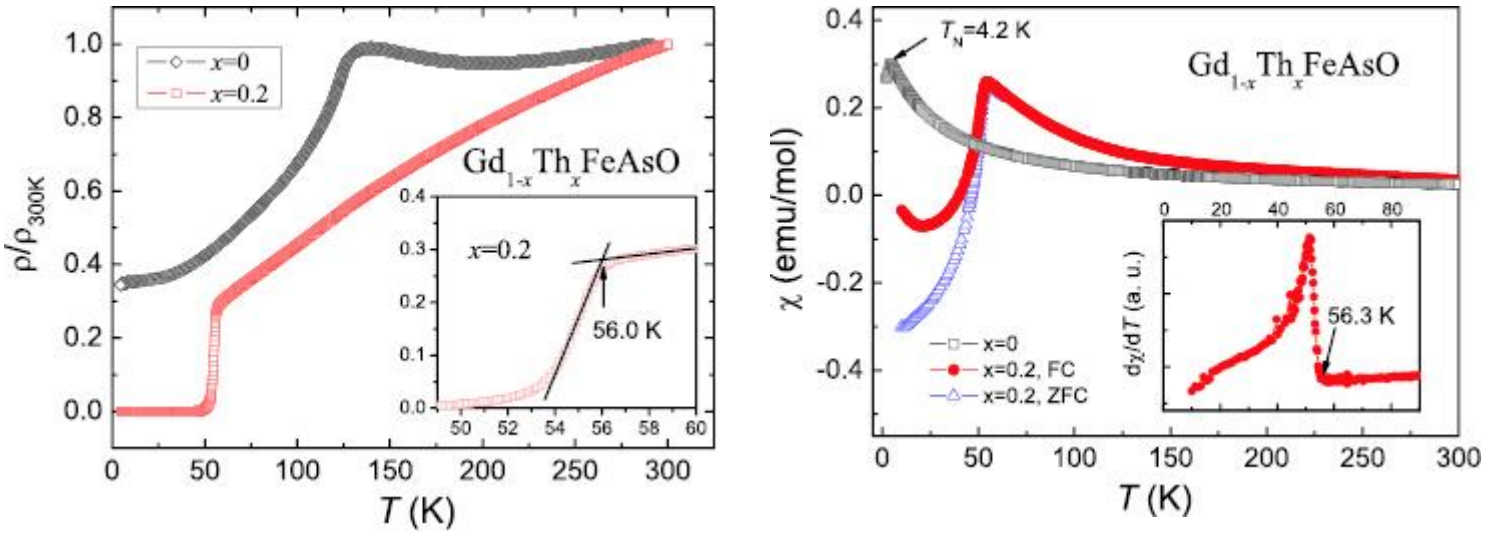
2008: LaFeP[$O_{1-x}F_x$], Tc=**26K**



Kamihara *et al. . Am. Chem. Soc.*, ***130***, pp 3296–3297 (2008)

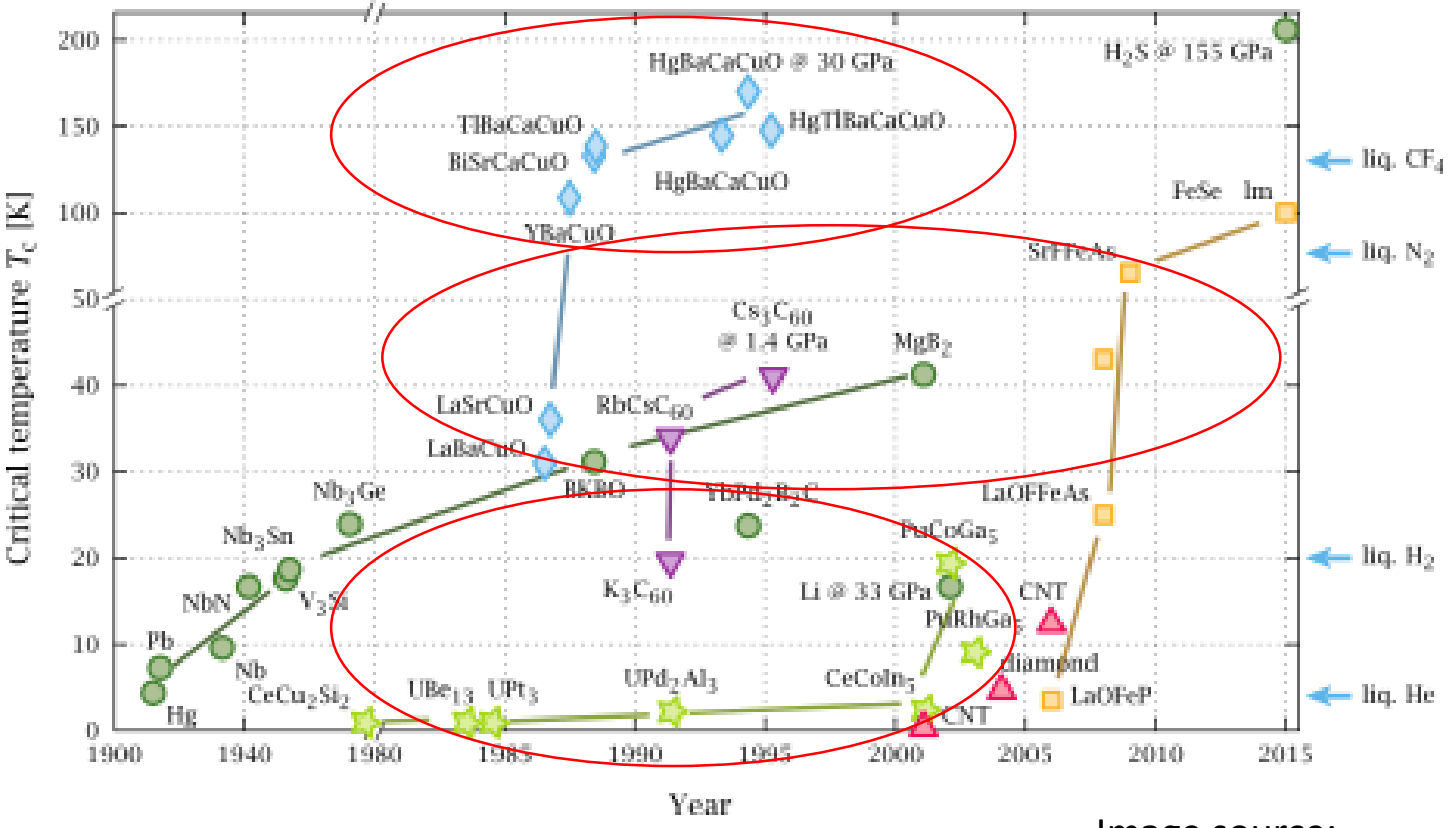
Discovery of Fe-based SCs

2008: $Gd_{1-x}Th_xFeAsO$, Tc=**56K**



Wang *et al.* Europhys. Lett. **83** 67006 (2008)

What is high T_c?

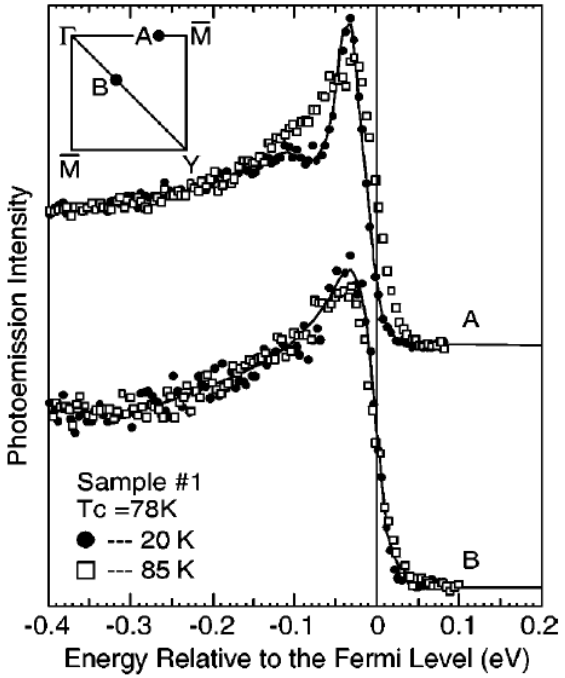


- T_c>77K (boiling point of liquid nitrogen)
- T_c>30K (former BCS "limit")
- T_c large relative to Fermi energy
- Mechanism unknown (not BCS)

Image source: https://en.wikipedia.org/wiki/High-temperature_superconductivity

A second family of high-T_c materials!!

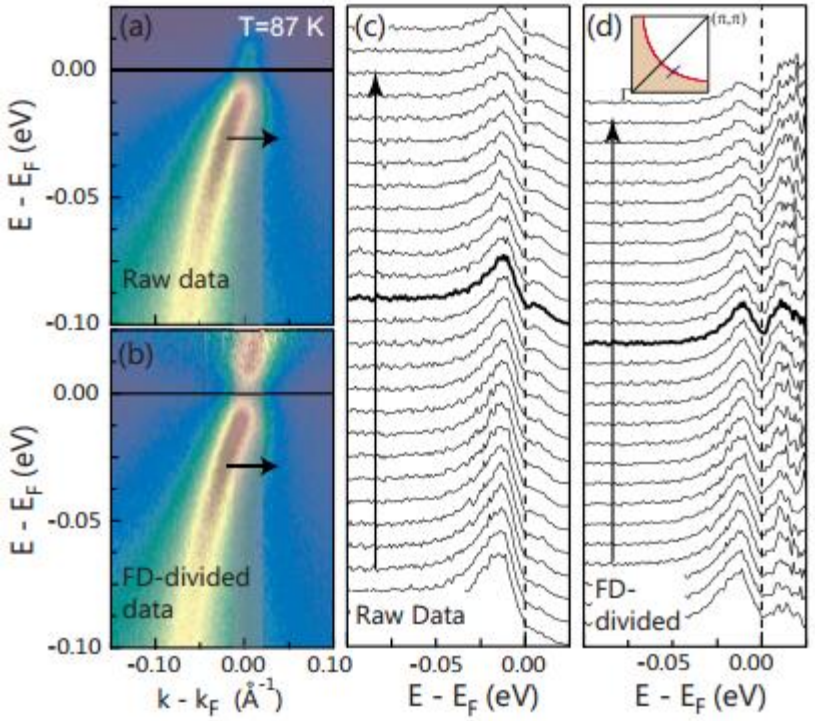
- High-T_c is not unique to one material class
- Benefit of hindsight
- Better tools



Shen *et al.* PRL **70** (1993)

1993:

- 6hrs per trace
- One momentum at a time



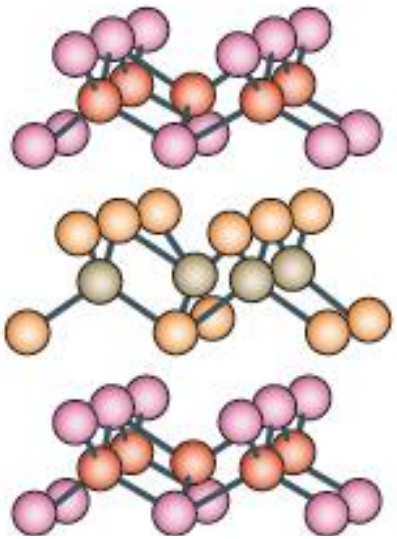
Balatsky, Lee, Shen, PRB **79** (2009)

~2008

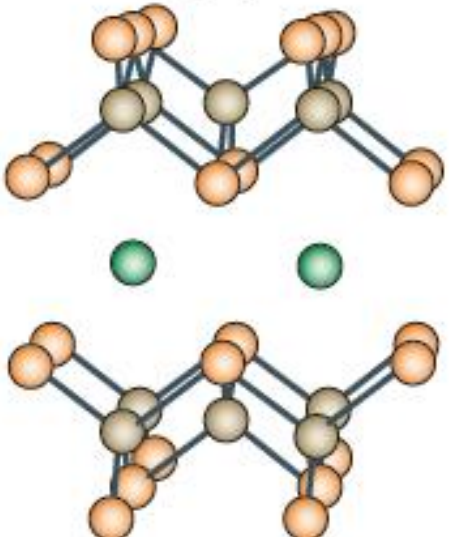
- ~10 mins per cut
- Many momenta at a time, along 1D trajectory in k-space

Fe-SC materials

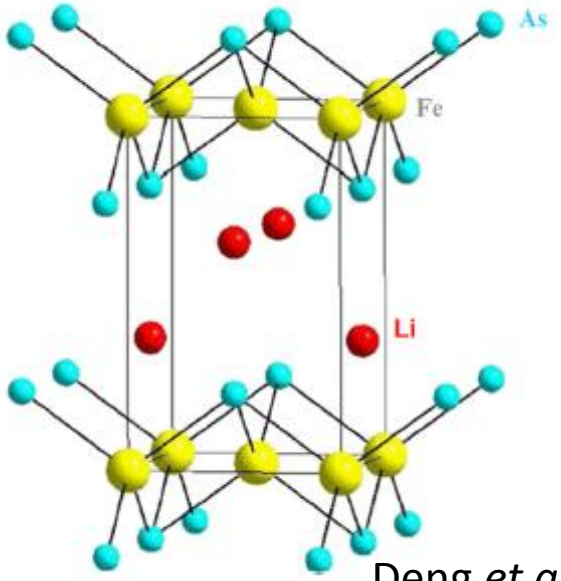
LaFeAsO (1111)



$BaFe_2As_2$ (122)



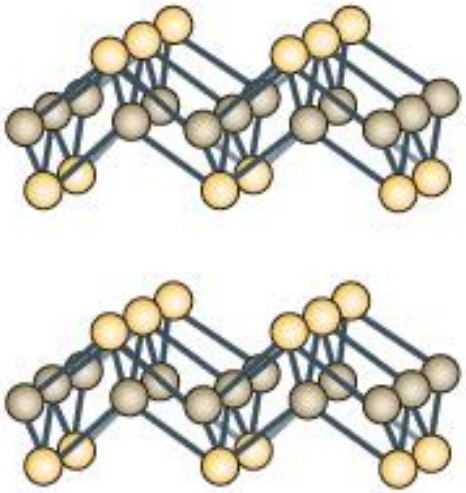
LiFeAs (111)



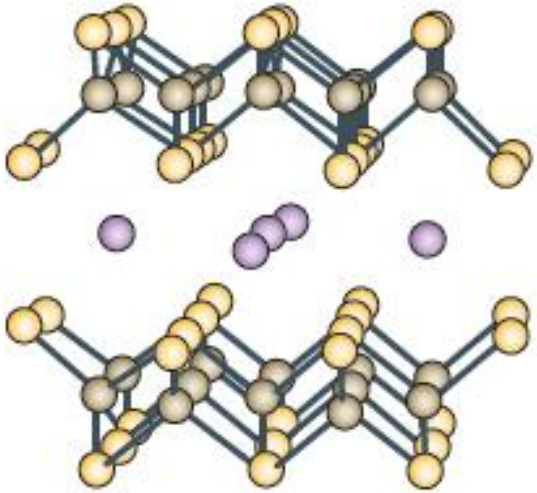
Fe-Arsenides
Fe-Pnictides

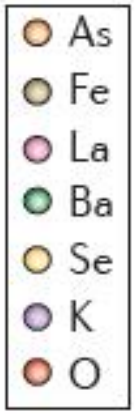
Deng *et al,* EPL (2009)

FeSe (11)



$K_xFe_{2-y}Se_2$



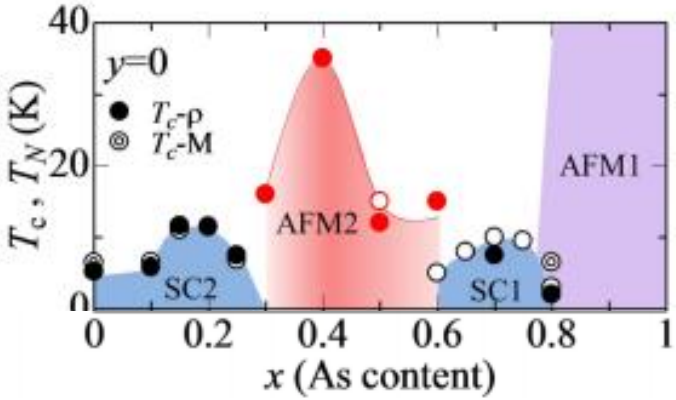


Fe-Selenides
Fe-Chalcogenides

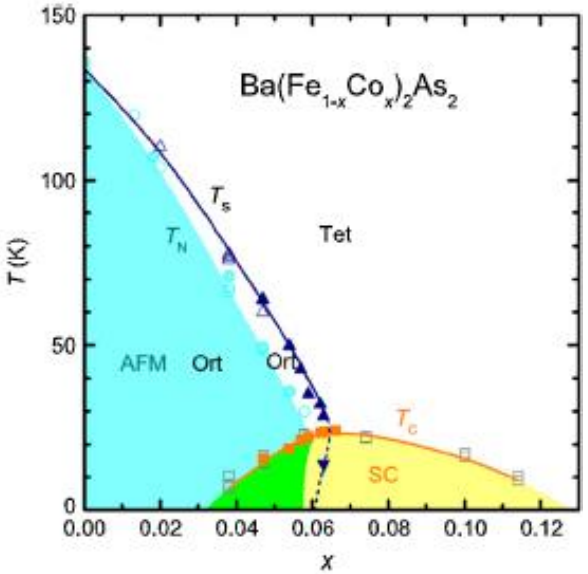
Si *et al.* Nat. Rev. Mater. (2016)

(A small selection of) Fe-SC phase diagrams

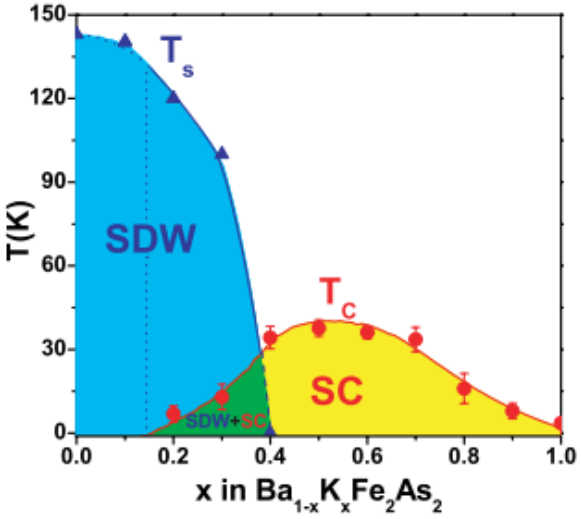
LaFe(P,As)O



Lai *et al,* PRB **90**, 064504 (2014)

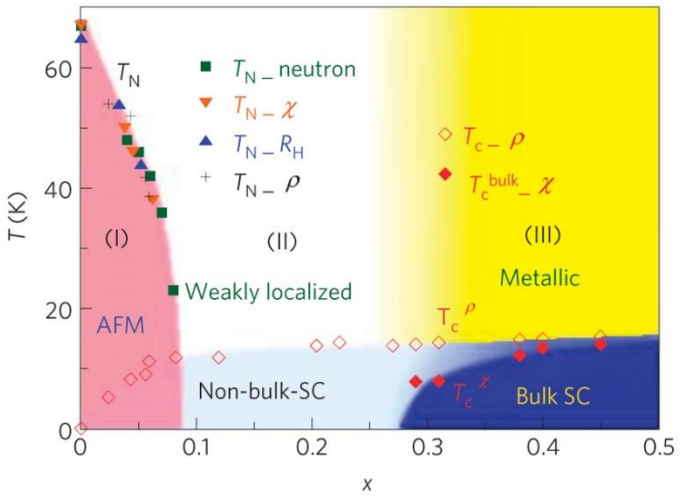


Nandi *et al,* PRL **104**, 057006 (2010)

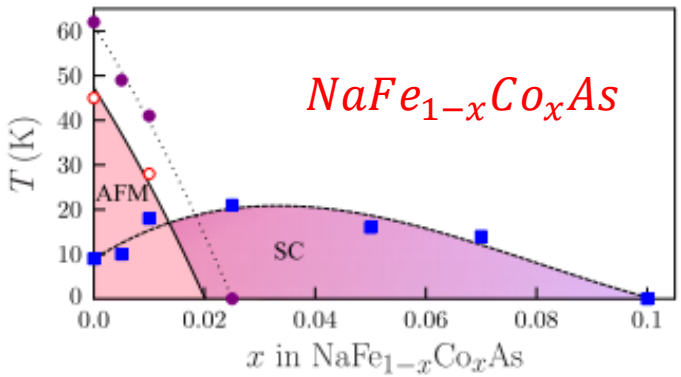


Chen *et al.,* EPL **85** 17006 (2009)

$Fe_{1.02}Te_{1-x}Se_x$



Liu *et al., Nat. Mater.* **9**, 718–720 (2010)



Parker *et al.* PRL **104**, 057007 (2010)

Comments on phase diagrams

- Electron, hole, and isovalent doping produces superconductivity
- Most materials can be tuned through entire phase diagram
- Proximity of antiferromagnetism and superconductivity
- AFM often is preceded by structural phase transition

Are Fe-SCs correlated electron systems?

How does one assess if a material is a strongly correlated electron system?

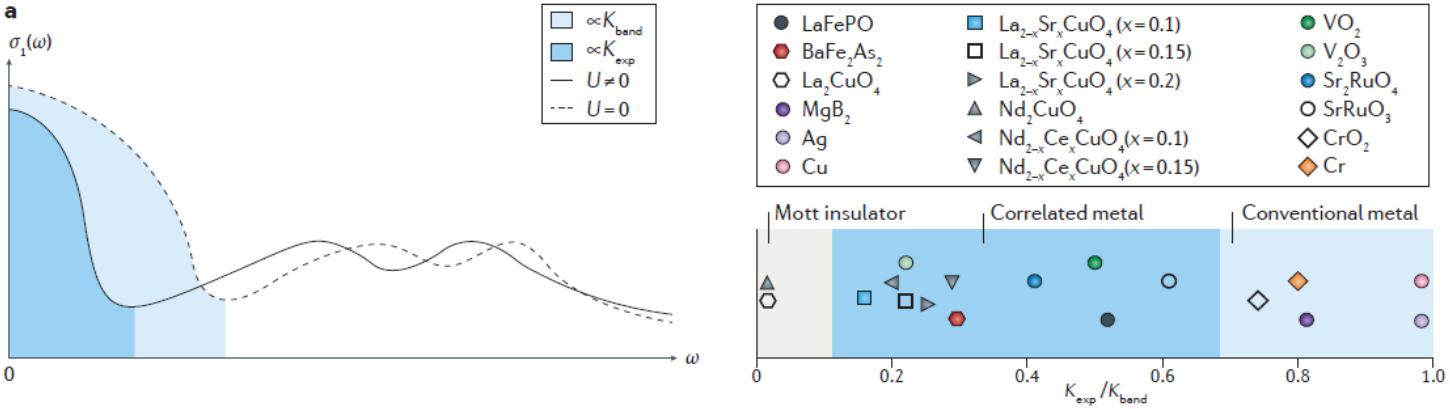
- Specific heat (large m*)
- ARPES (strong renormalization of band relative to LDA)
- U/W
- High-temperature transport (larger resistivity→more types of scattering)
- Optics (Drude weight depletion)

No

- Small renormalization relative to LDA in some materials
- On-site coulomb repulsion (U) smaller than bandwidth (W) (Yang *et al,* **80**, 014508 (2009))

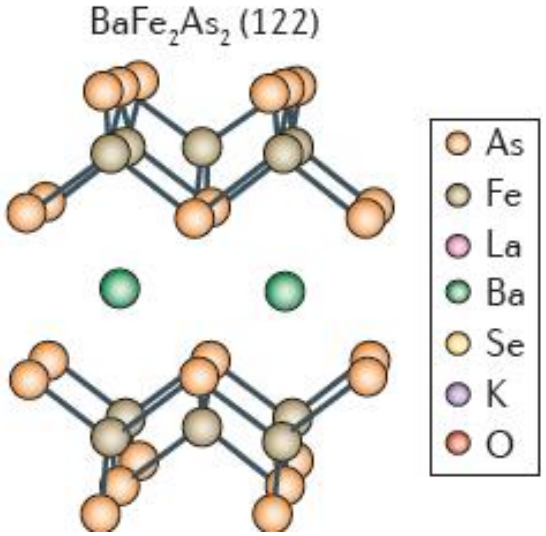
Yes

- Some materials have large band renormalization
- Optical drude weight depletion consistent with cuprates and other correlated systems
- Bad metal conductivity at high temperature
- Some systems show orbital-selective Mott transitions

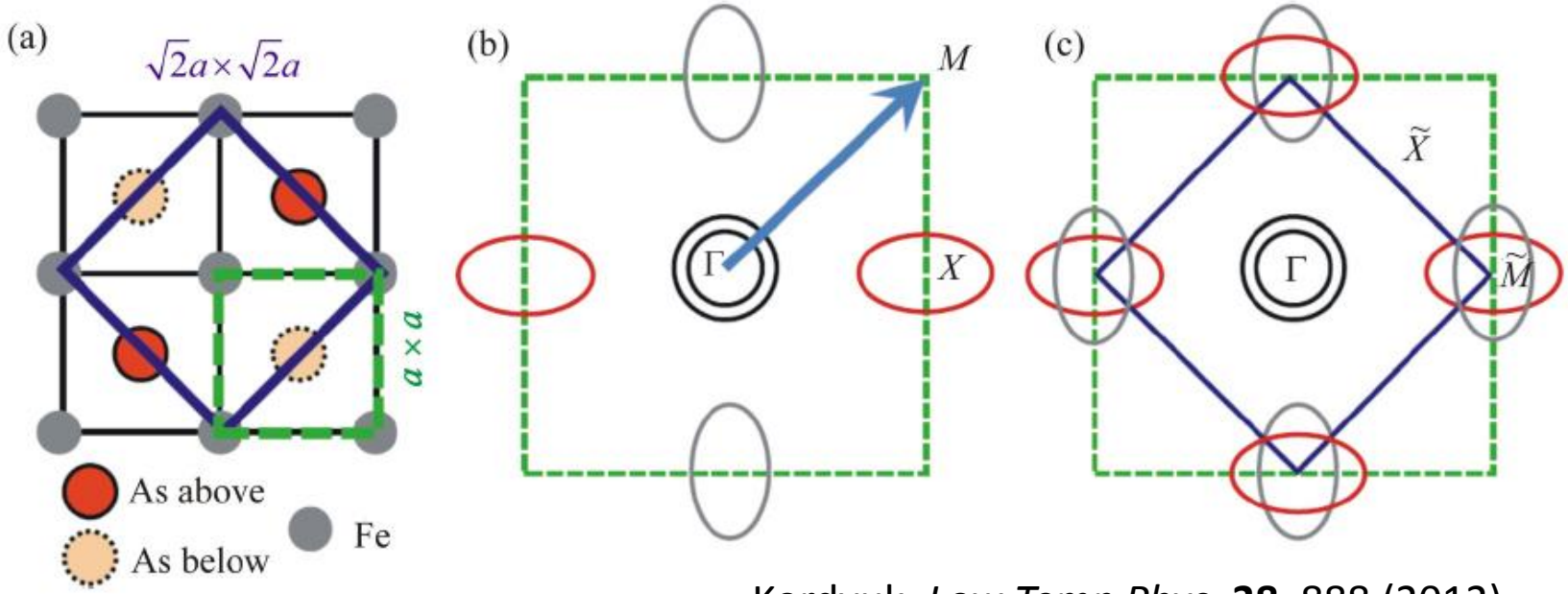


Si *et al,* Nat. Rev. Mater. **1** 1 (2016)

Fe-SC Brillouin zone



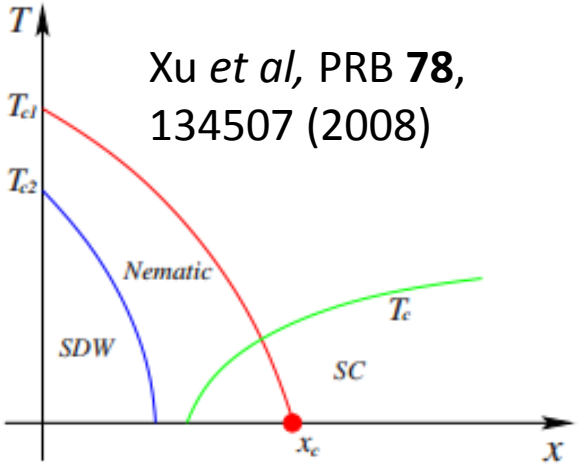
- 1-Fe unit cell (ignore As/Se)
- 2-Fe unit cell (consider larger unit cell due to Fe/Se)
- Multiple Fermi surfaces: momentum-resolved tool is very useful!



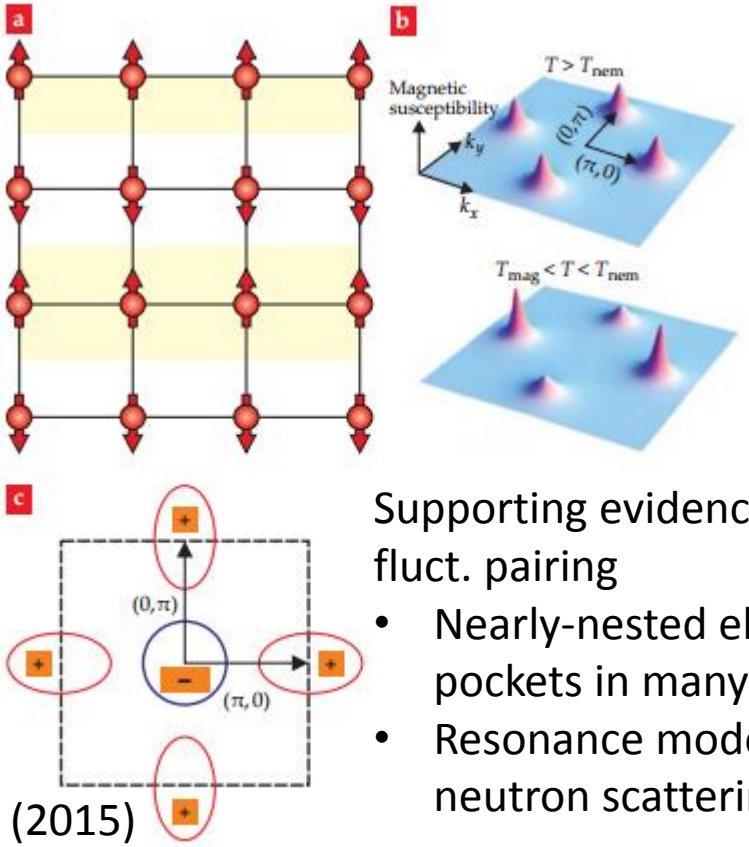
Kordyuk, *Low Temp Phys,* **38**, 888 (2012)

Potential mechanisms of superconductivity in iron-based superconductors

- Spin-fluctuation-mediated *interband* pairing with $s_{\pm}$ superconducting order parameter
- Fluctuations around nematic quantum critical point
- Orbital fluctuations
- Others



Xu *et al,* PRB **78**, 134507 (2008)

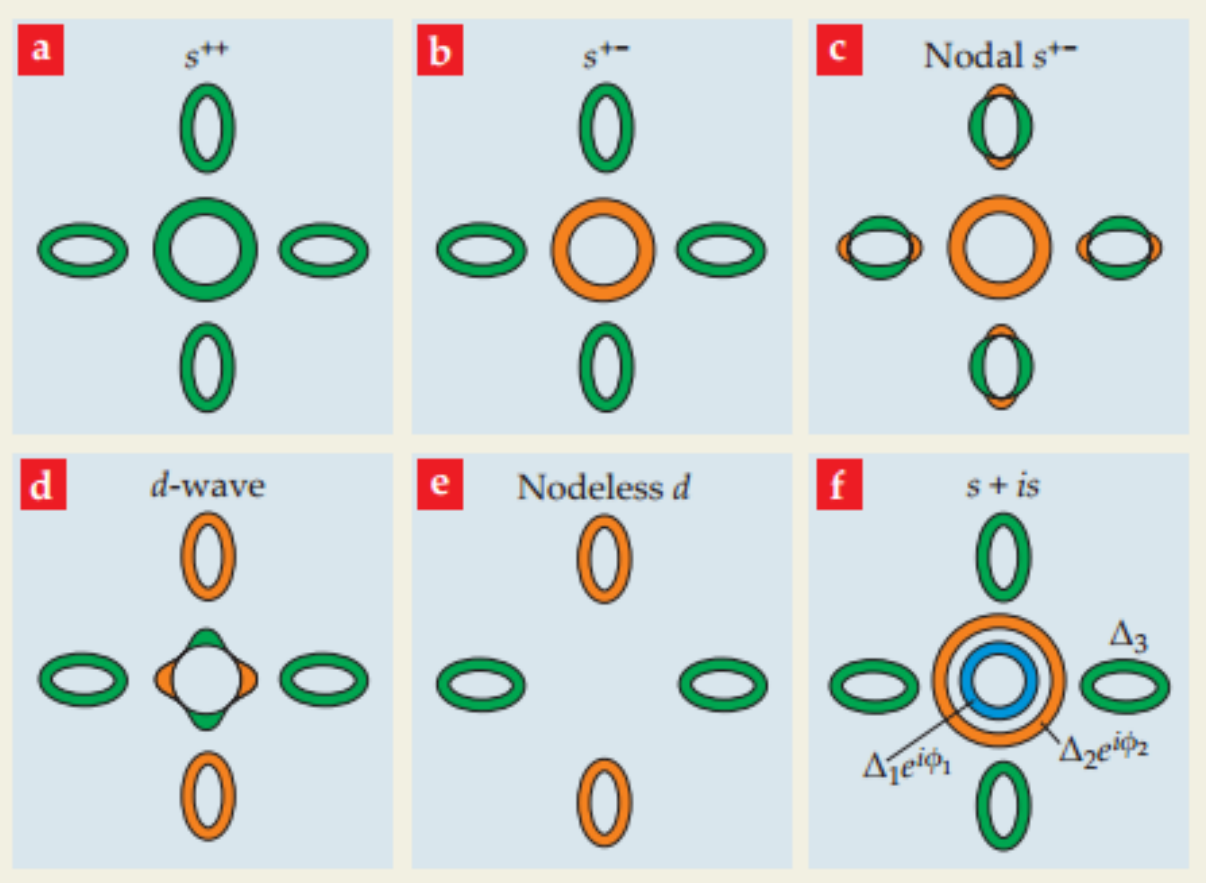


Supporting evidence for spin fluct. pairing

- Nearly-nested electron/hole pockets in many materials
- Resonance mode in inelastic neutron scattering

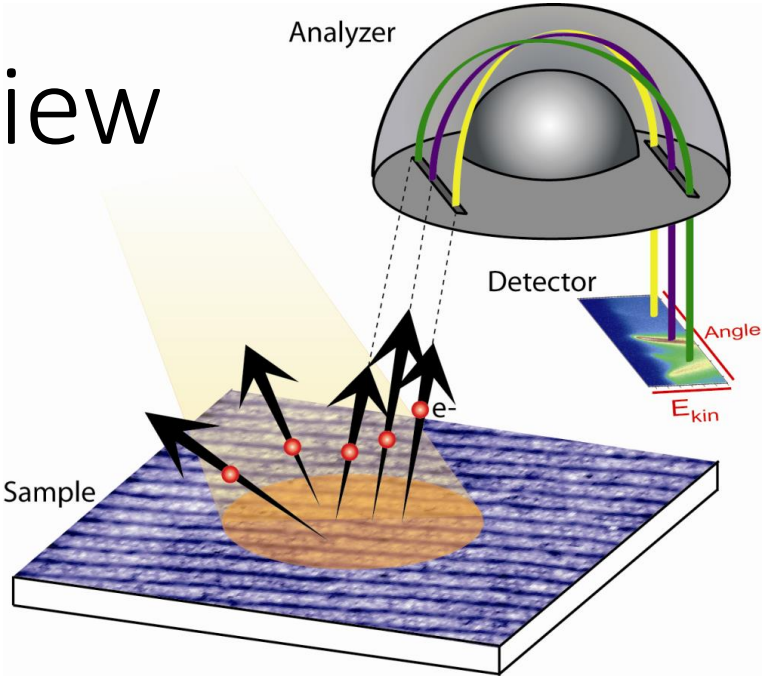
Chubukov and Hirschfeld, Phys. Today **68**, 46 (2015)

Potential gap symmetries



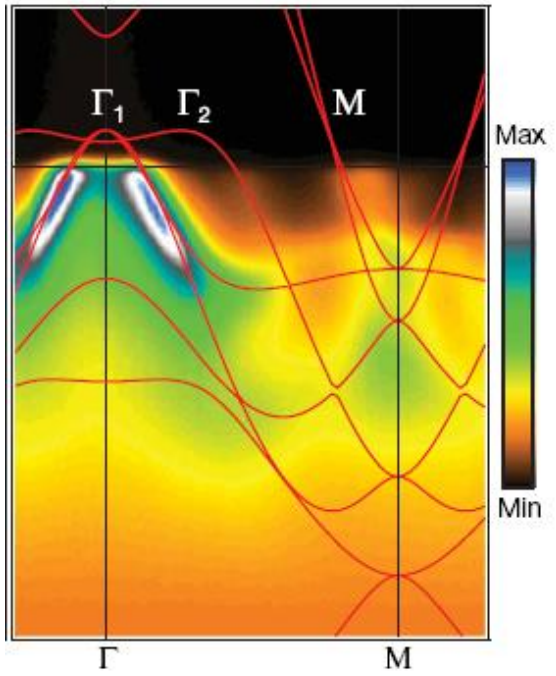
Chubukov and Hirschfeld, Phys. Today **68**, 46 (2015)

ARPES review



$$E_{kin} = h\nu - \phi - |E_B|$$

$$\mathbf{p}_{\parallel} = \hbar\mathbf{k}_{\parallel} = \sqrt{2mE_{kin}} \cdot \sin\vartheta$$



$$I(\mathbf{k},\omega) = I_0(\mathbf{k},\nu,\mathbf{A})\, f(\omega) A(\mathbf{k},\omega) \otimes R(\Delta k, \Delta\omega)$$

Fermi-dirac cutoff

Instrument resolution

$$|M_{f,i}^{\boldsymbol{k}}|^2 \equiv |<\phi_f^{\boldsymbol{k}}| - \frac{e}{mc}\boldsymbol{A}\cdot\boldsymbol{p}|\phi_i^{\boldsymbol{k}}>|^2$$

"matrix elements"→prefactor from experimental conditions

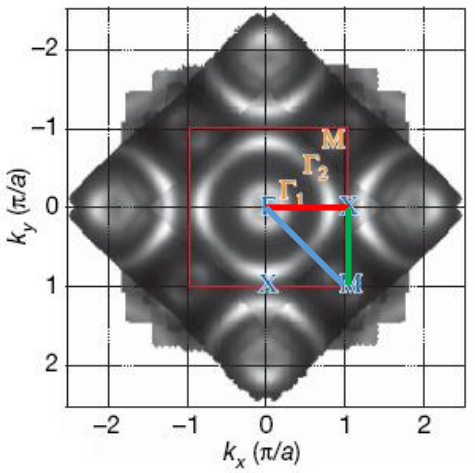
Single-particle spectral function: band structure + interactions

$$A(\mathbf{k},\omega) = -\frac{1}{\pi}\frac{\Sigma''(\mathbf{k},\omega)}{[\omega - \varepsilon_{\mathbf{k}} - \Sigma'(\mathbf{k},\omega)]^2 + [\Sigma''(\mathbf{k},\omega)]^2}$$

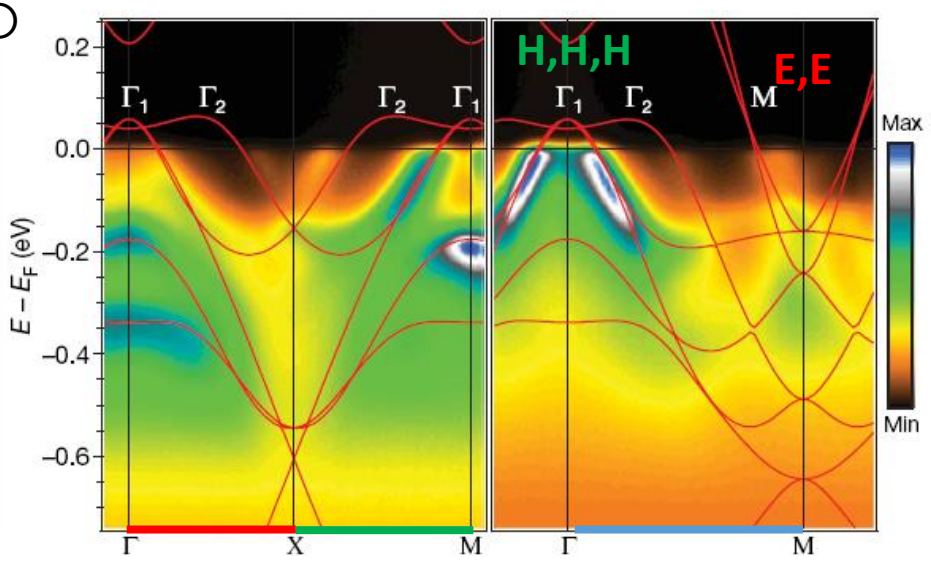
D. H. Lu, *et al.* Nature **455** 81 (2008)

1111-Fermi surface

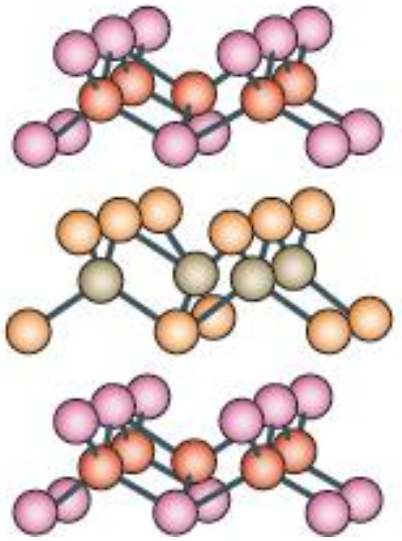
LaOFeP
Now called: LaFePO



T=20K



LaFeAsO (1111)



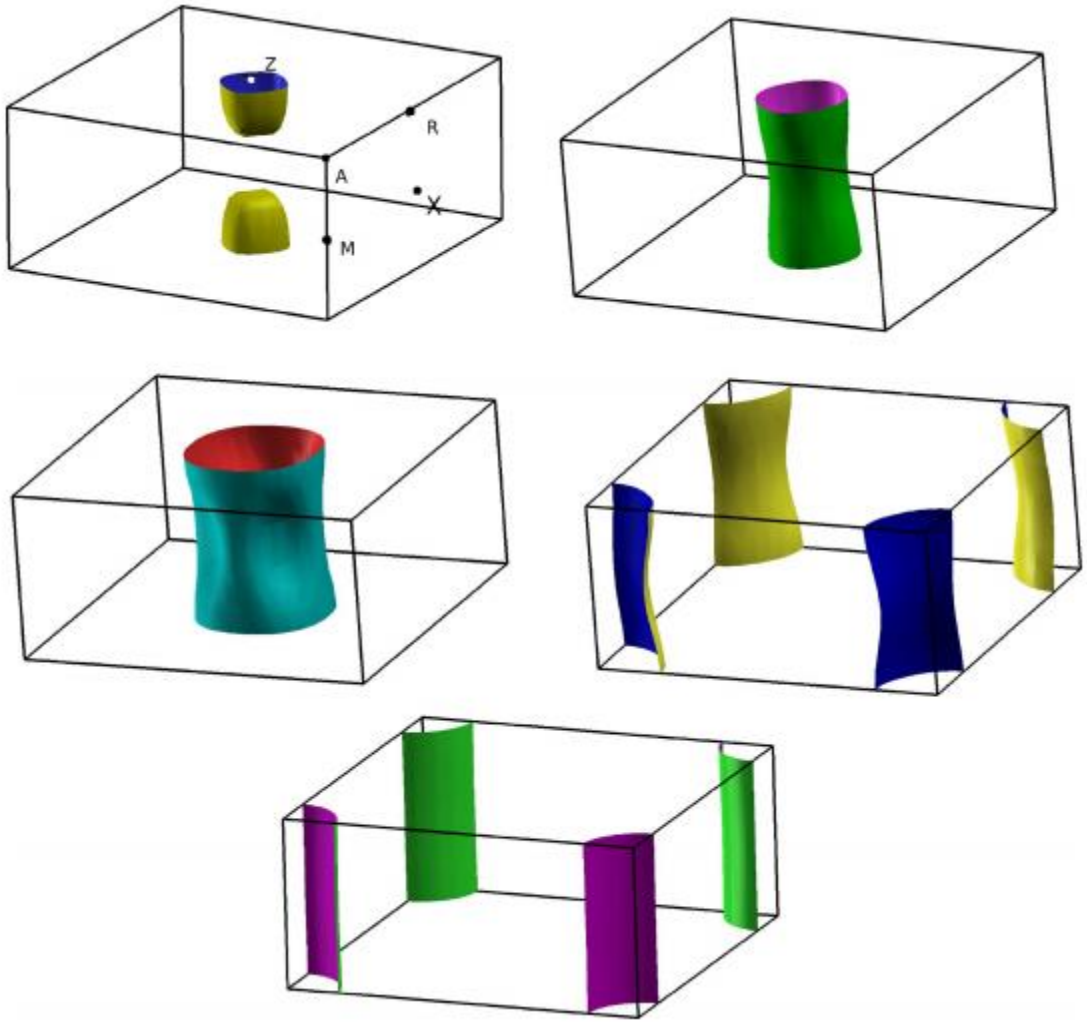
D. H. Lu, *et al.* Nature **455** 81 (2008)

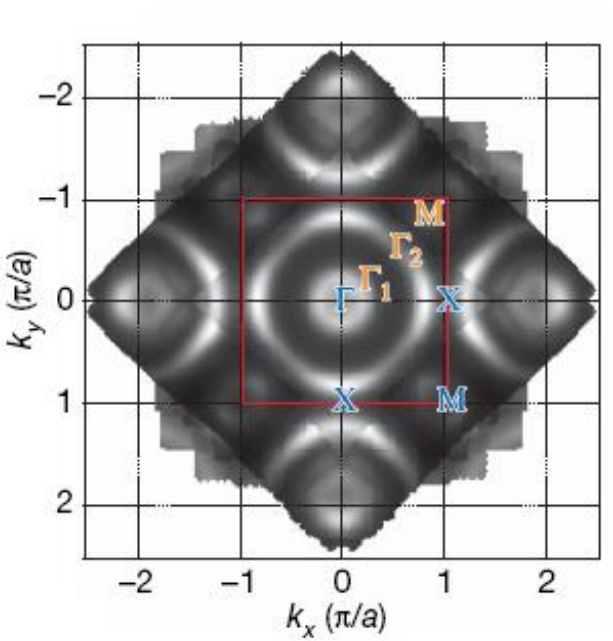
"A quantitative agreement can be found between the angle-resolved photoemission spectra and the calculated band dispersions after shifting the calculated bands up by 0.11 eV and then renormalizing by a factor of 2.2."

How does one distinguish electron pockets from hole pockets?

How many pockets are there?

Comparison to Fermi surface calculations





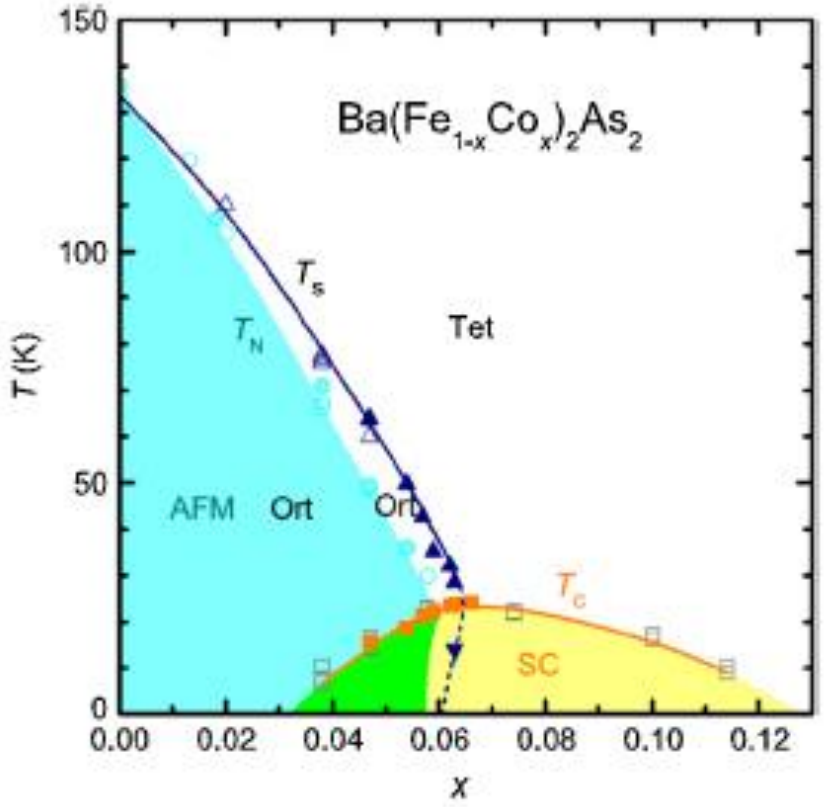
S. Lebègue, PRB **75**, 035110 (2007)

What information does ARPES give about Fermi surfaces and electronic band structure?

(+answers specific to LaFePO)

- Fermi surface size and number (related to charge count)
  - 5 total Fermi surfaces, giving electron count of ~5 per unit cell
  - 6 are expected
  - Discrepancy may arise from polar surface
- Electron vs hole pockets + their locations
  3 hole pockets at Γ, 2 electron pockets at M
- Band mass renormalization
  2.2 relative to LDA (one way of parametrizing correlations)

Effect of magnetism and orthorhombicity on fermiology



112 Fe-pnictides are easier to prepare as single crystals and can be doped in many ways

122 materials

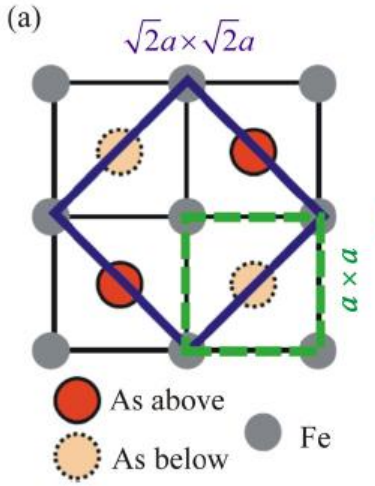
TABLE II. T_c versus composition in $M_{1-x}A_xFe_{2-y}TM_yAs_{2-z}P_z$. T_cs given are the maxima versus composition. Only one site is doped at a time.

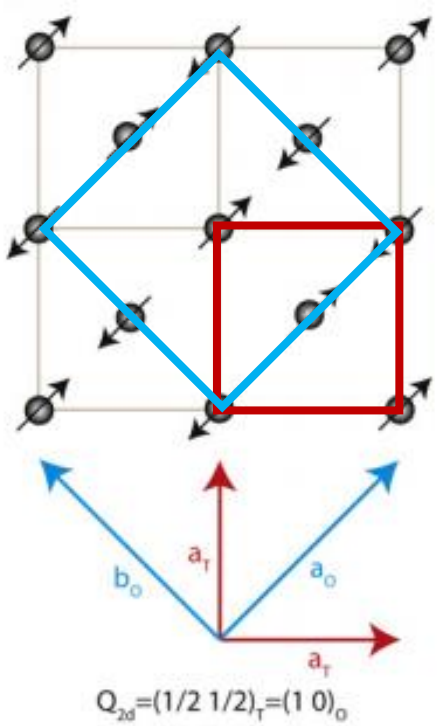
Material	M-site dopant	T_c (K) vs x, $y = z = 0$	Ref.	Fe-site dopant	T_c (K) vs y, $x = z = 0$	Ref.	As-site dopant	T_c (K) vs z, $x = y = 0$	Ref.
$BaFe_2As_2$	K	38/0.4	Rotter, Tegel, and Johrendt (2008)	Co	22/0.2	Sefat *et al.* (2008b)	P	30/0.7	Kasahara *et al.* (2010); Jiang *et al.* (2009)
	Rb	23/0.1	Bukowski *et al.* (2009)	Ni	20.5/0.1	L. J. Li *et al.* (2009)			
				Pd	19/0.11	Ni *et al.* (2009)			
				Rh	24/0.11	Ni *et al.* (2009)			
				Ru	21/0.9	Sharma *et al.* (2010)			
				Pt	25/0.1	Zhu *et al.* (2010); Saha *et al.* (2010b)			
$SrFe_2As_2$	K	36.5/0.5	Sasmal *et al.* (2008)	Co	20/0.2	Leithe-Jasper *et al.* (2008)	P	27/0.7	Shi *et al.* (2009)
	Na	35/0.5	Goko *et al.* (2009)	Ni	10/0.15	Saha *et al.* (2010a); Leithe-Jasper *et al.* (2008)			
	Cs	37/0.5	Sasmal *et al.* (2008)	Pd	9/0.15	F. Han *et al.* (2009)			
	La	22/0.4	Muraba *et al.* (2010)	Rh	22/0.25	F. Han *et al.* (2009)			
				Ru	13.5/0.7	Qi *et al.* (2009a)			
				Ir	22/0.5	F. Han *et al.* (2009)			
				Pt	16/0.16	Kirshenbaum *et al.* (2010)			
$CaFe_2As_2$	Na	33/0.66	K. Zhao *et al.* (2010) (see also Wu *et al.*, 2008a)	Co	17/0.06	Kumar *et al.* (2009b)	P	13/0.3	Shi *et al.* (2009)
				Ni	15/0.06	Kumar *et al.* (2009a)			
				Rh	18/0.1	Qi *et al.* (2011)			
$EuFe_2As_2$	K	32/0.5	Jeevan *et al.* (2008b), Anupam *et al.* (2009)				P	26/0.6	Ren *et al.* (2009); Jeevan *et al.* (2011)
	Na	35/0.3	Y. Qi *et al.* (2008)						

[a]Note: Cu substituted for Fe in $BaFe_2As_2$ suppresses T_S and T_{SDW} but does not induce superconductivity (Canfield *et al.*, 2009b) while Mn substituted for Fe in $SrFe_2As_2$ up to $x = 0.3$ is relatively ineffective in suppressing T_S and T_{SDW} (Kasinathan *et al.*, 2009).

G. R. Stewart, Rev. Mod. Phys. **83** p1589 (2011)

Magnetism and structural phase transition in 122 materials





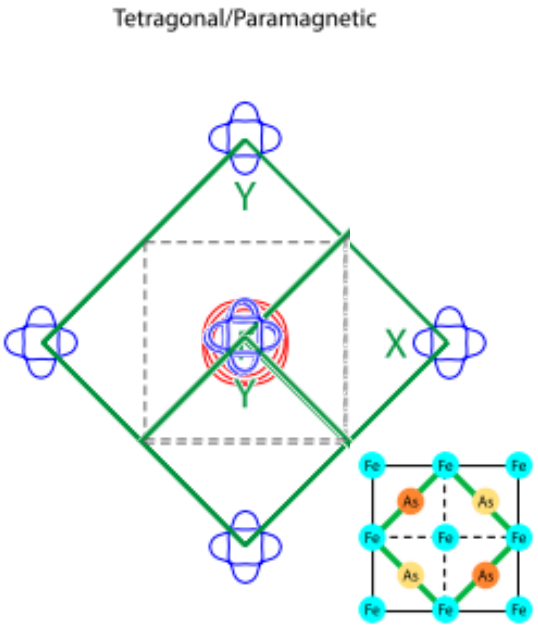
2 Fe tetragonal unit cell

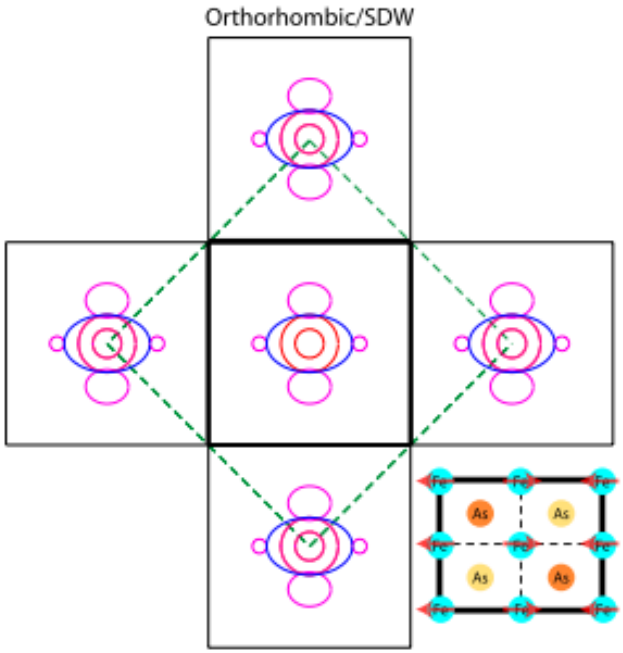
Magnetic order with orthorhombic unit cell

*Structural and magnetic ordering have same unit cell, but orthorhombic phase transition usually happens first

Lumsden *et al*, J. Phys.: Condens. Matter **22** 203203 (2010)

Expected FS reconstruction





Note broken 4-fold rotation symmetry!

Yi *et al.* PNAS **108** 6878 (2011)

Problem: twinning

$BaFe_2As_2$

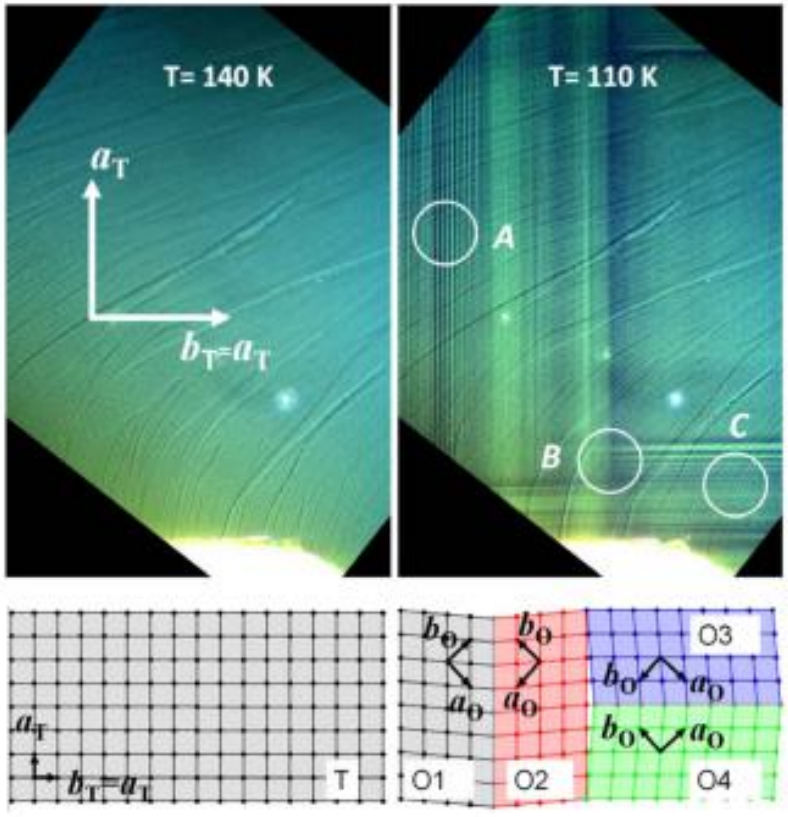
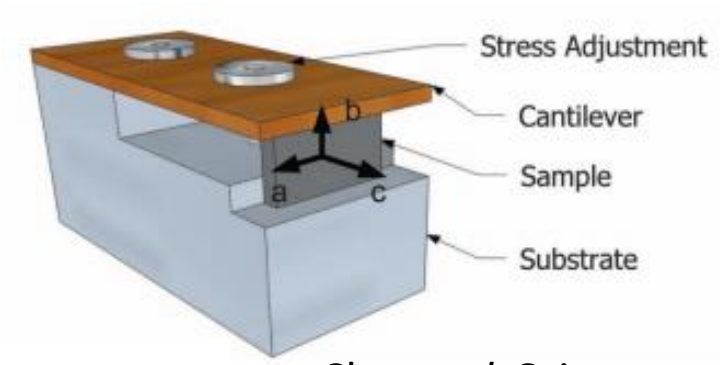


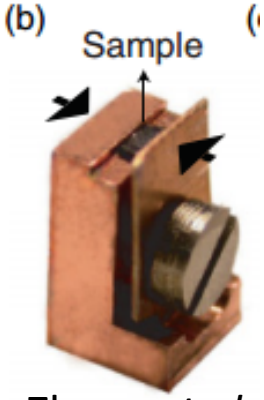
Image size is several hundred microns and characteristic domain size is 10-50 microns

Tanatar *et al.* PRB **79**, 180508R (2009)

Solution 1: mechanical de-twinning

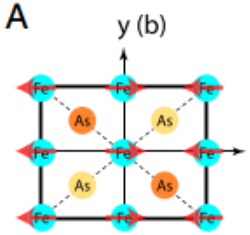


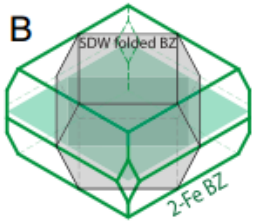
Chu *et al,* Science **329** p824 (2010)

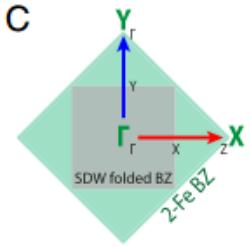


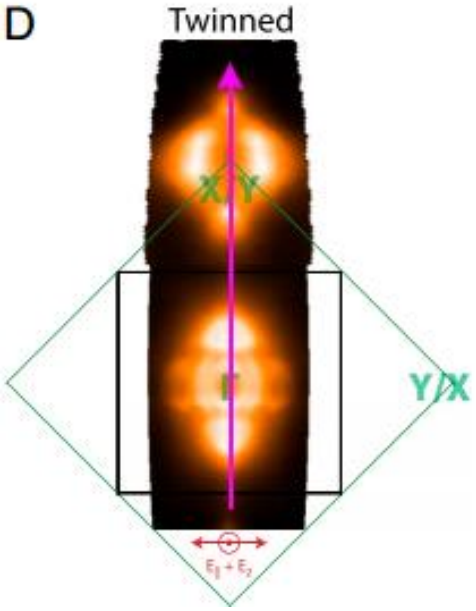
Zhang *et al,* PRB **85**, 085121 (2012)

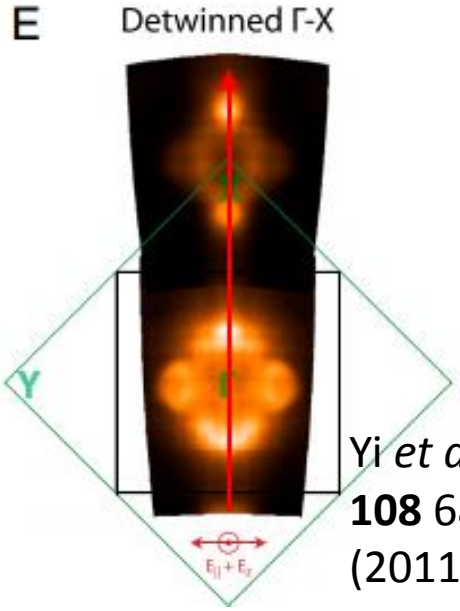
Material: $BaFe_2As_2$

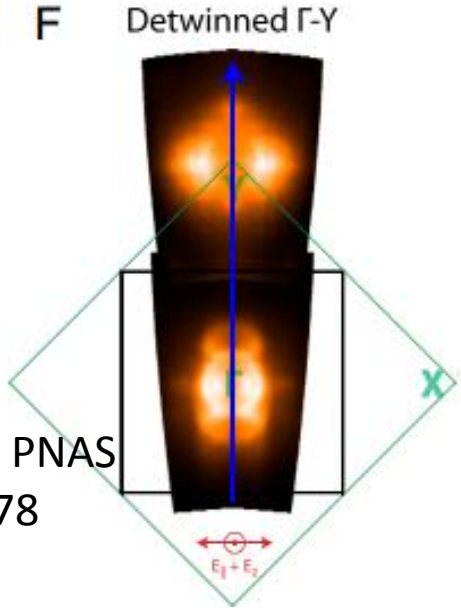










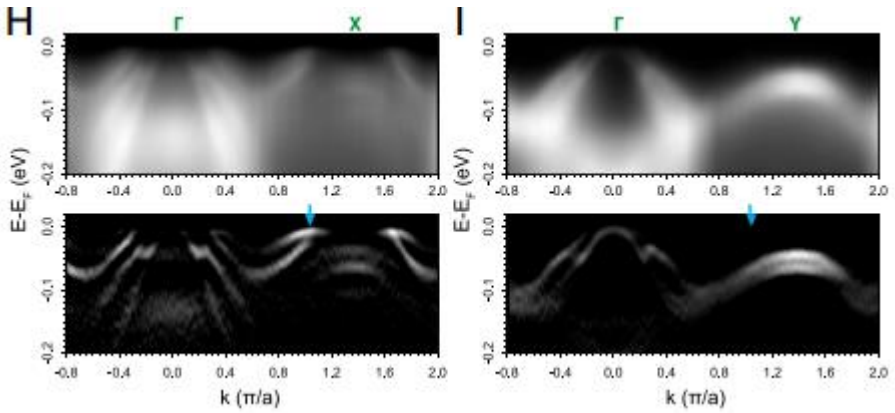


Yi *et al.* PNAS **108** 6878 (2011)

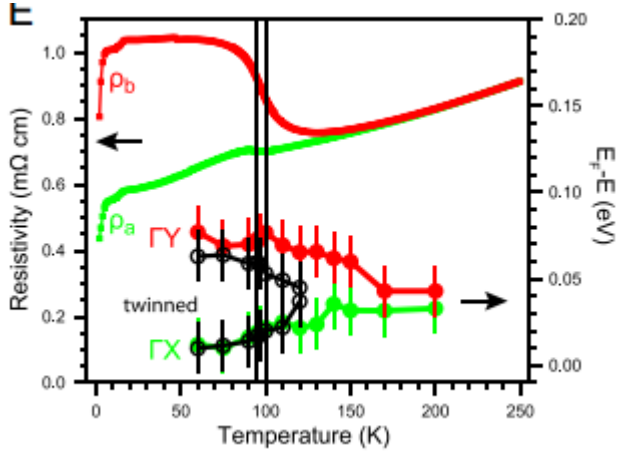
Signatures of band folding: extra bands

Material: $BaFe_2As_2$

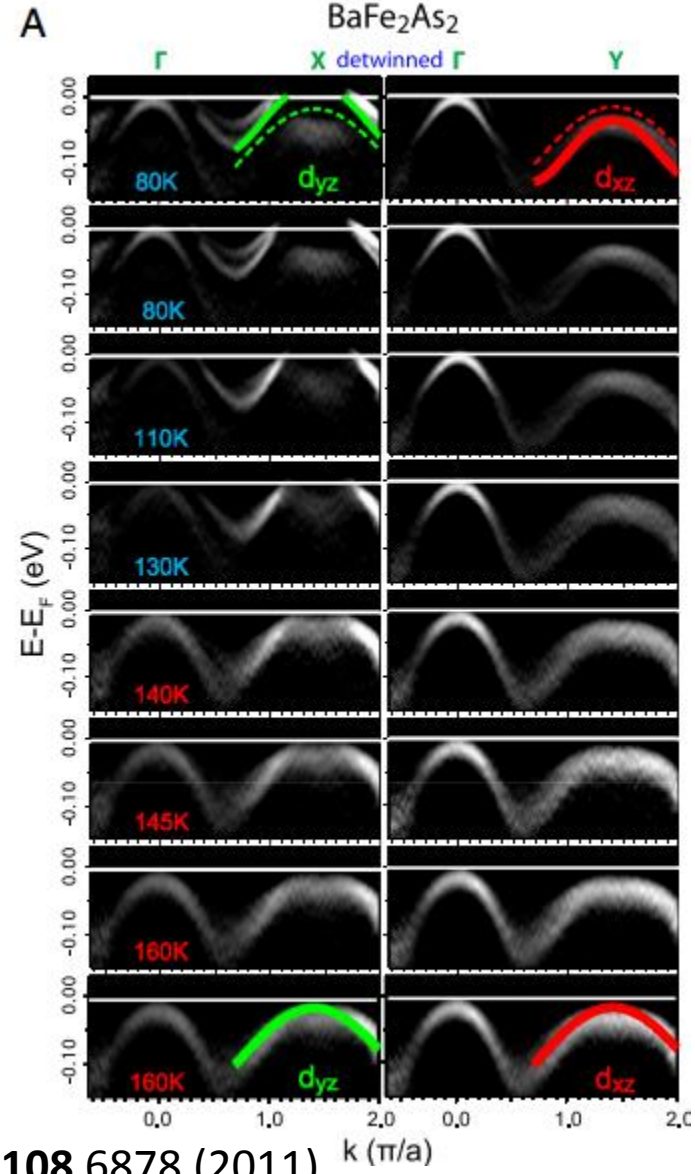
Raw data



2nd derivative



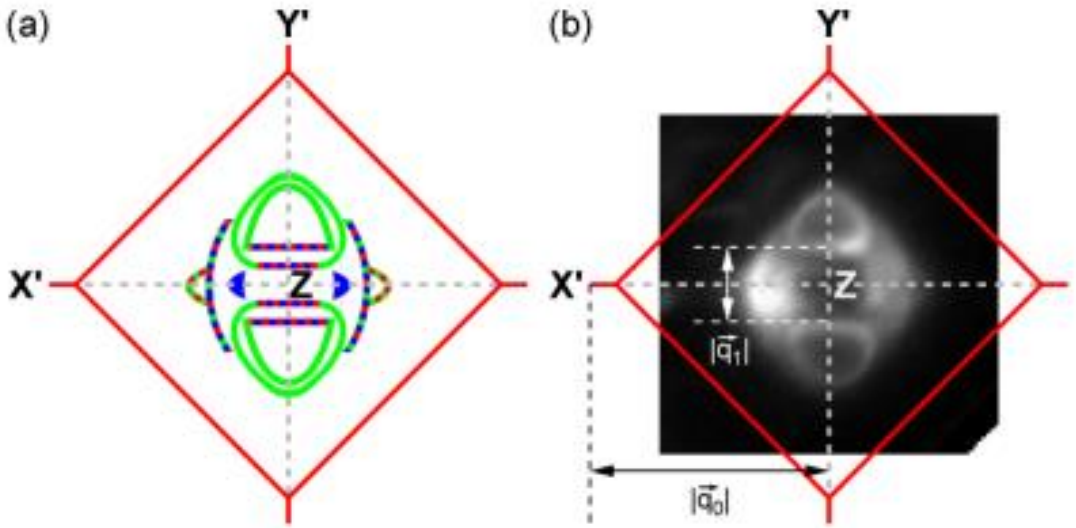
Next lecture: nematicity



Yi *et al.* PNAS **108** 6878 (2011)

Solution 2: micro-ARPES

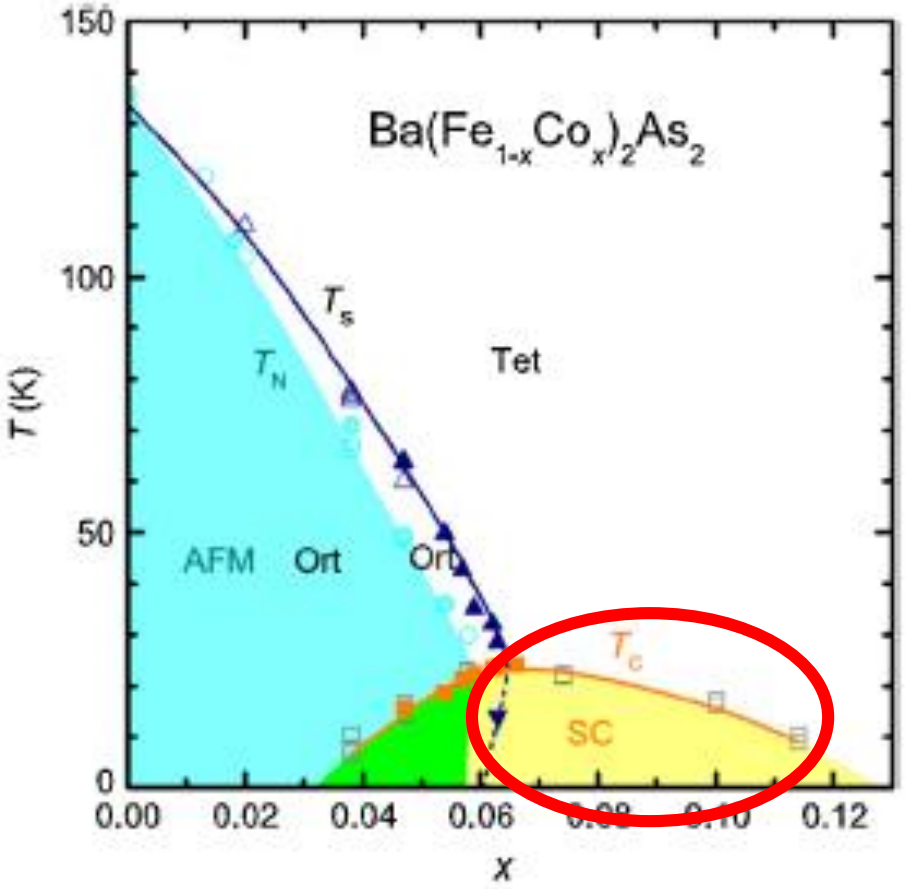
Material: $CaFe_2As_2$



Wang *et al, PRB* **88**, 235125 (2013)

- Spot size ~50 μm (usually synchrotron beams used for ARPES are ~150-200μm)
- Now, beamlines with good energy/momentum resolution and ~10μm spot size are available, or beamlines where resolution is sacrificed to get ~100nm spot
- This paper also used matrix elements in quantitative way to discern orbital character of bands

Summary of SDW



- Magnetic order *inferred* from ARPES because of its effect on band structure and Fermi surface
- Modifications of ARPES technique needed to deal with twinning
- Relevant to discussion of nematicity (next lecture)

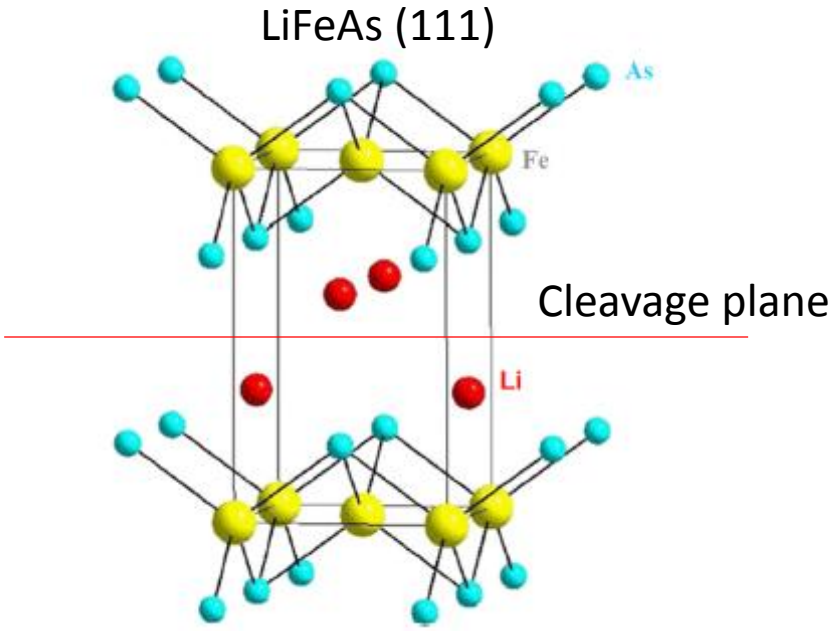
Next: superconductivity

ARPES measurements of superconducting gaps in Fe-SCs

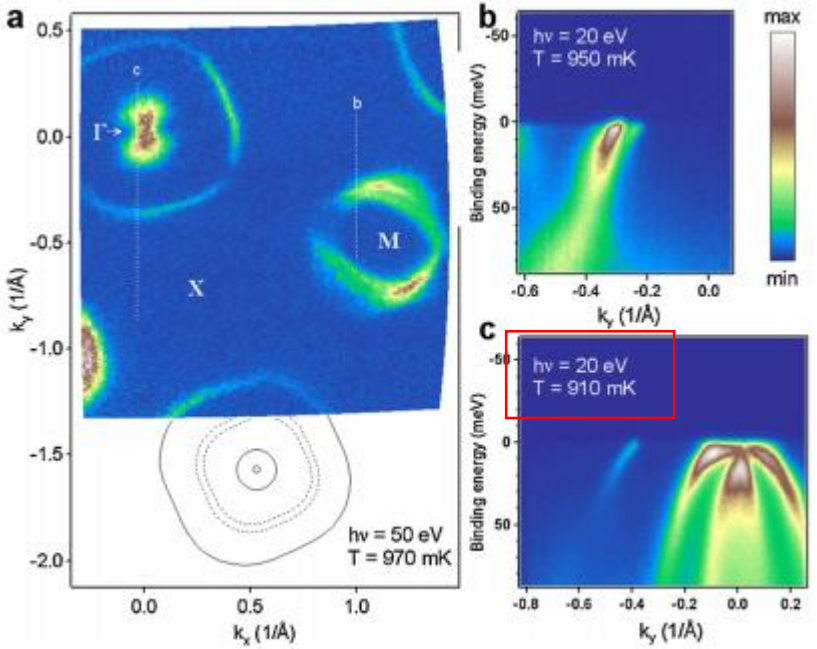
- Much more difficult than cuprates because:
  - Tc is lower (100K vs 25K)
  - Gaps are smaller (~30 meV vs 3 meV)
  - Multiple Fermi surfaces (1 vs 5)

Material 1: LiFeAs (111)

- DFT calculations showed that LiFeAs is not expected to have surface states, giving cleaner ARPES signal (Lankau *et al* PRB **82**, 184518 (2010))

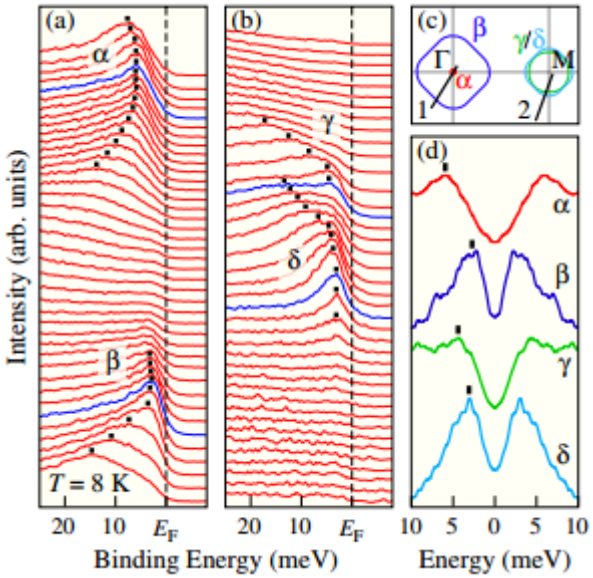


Deng *et al,* EPL (2009)

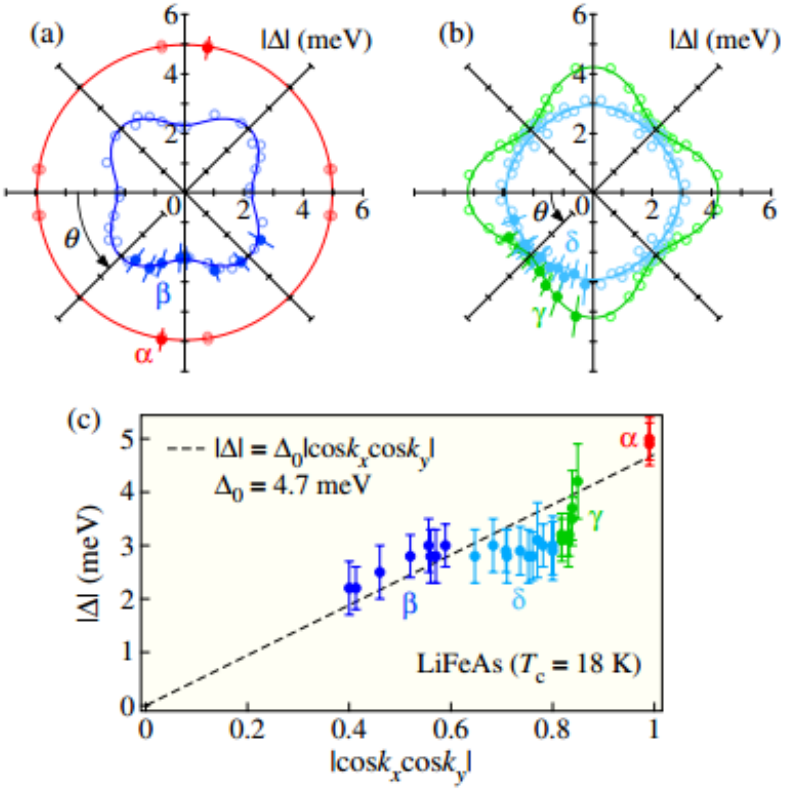


Borisenko *et al,* PRL 105, 067002 (2010)

Superconducting gap in LiFeAs (T_c=18K)

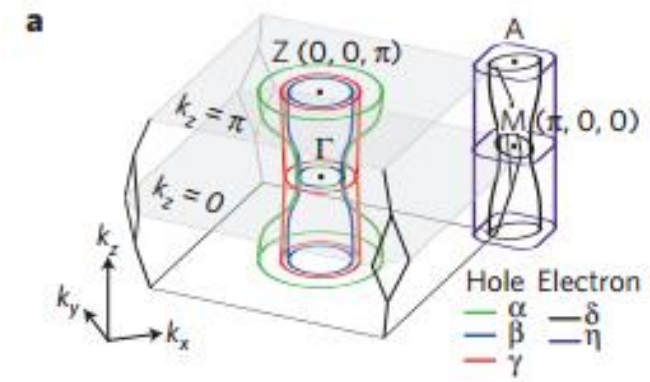


K. Umezawa *et al,* PRL **108**, 037002 (2012)



- Gaps are anisotropic but there are no nodes
- Consistent with $s_{\pm}$ pairing

Superconducting gap in $BaFe_2(As_{0.7}P_{0.3})_2$ (T_c=30K)

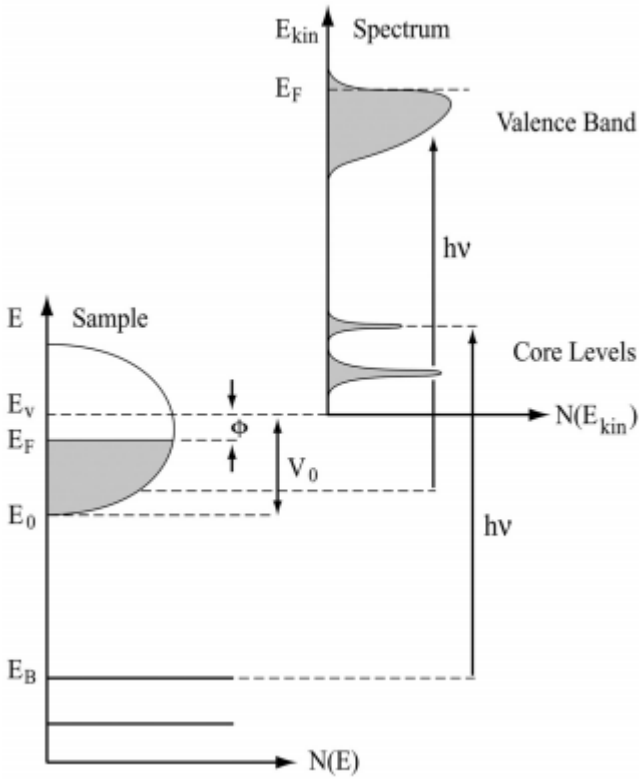


FS is 3D, so you need to access different kz to fully map out superconducting gap

Zhang *et al,* Nat. Phys. **8** 371 (2012)

k_z ($k_\perp$) in ARPES

Final state dispersion assumed to be free-electron-like: $E_f(\boldsymbol{k}) = \frac{\hbar^2 k^2}{2m} - |E_0| = \frac{\hbar^2(k_\parallel^2 + k_\perp^2)}{2m} - |E_0|$



$E_{kin} = E_f - \Phi$

$\hbar k_\parallel = \sqrt{2mE_{kin}} sin\vartheta$

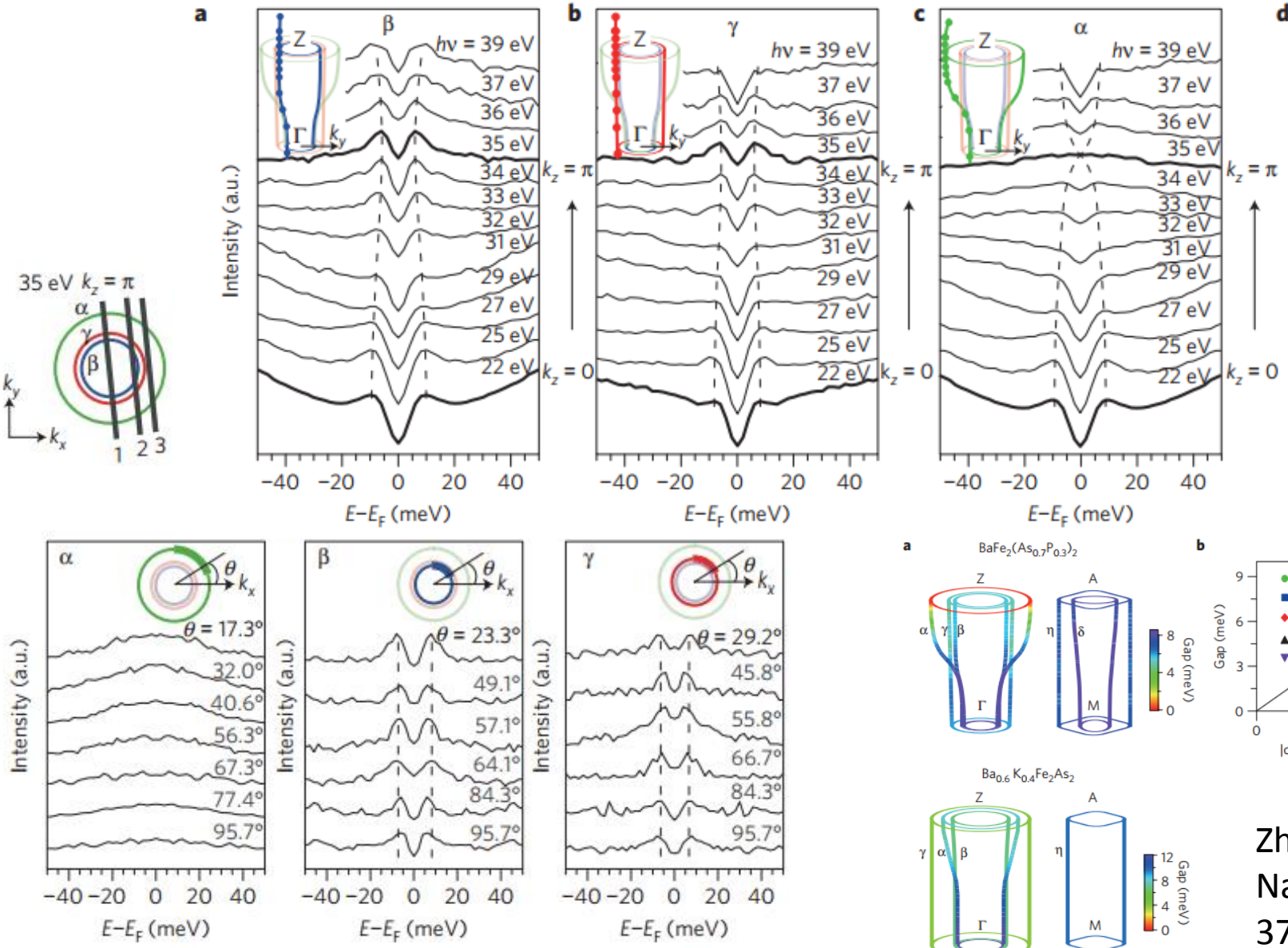
$$k_\perp = \frac{1}{\hbar}\sqrt{2m(E_{kin}\cos^2\vartheta + V_0)}$$

V_0=inner potential=bottom of valence band
Determined by:

- Comparison to band structure calculations
- Experimentally observed periodicity of $E_f(\boldsymbol{k})$, measured by varying photon energy

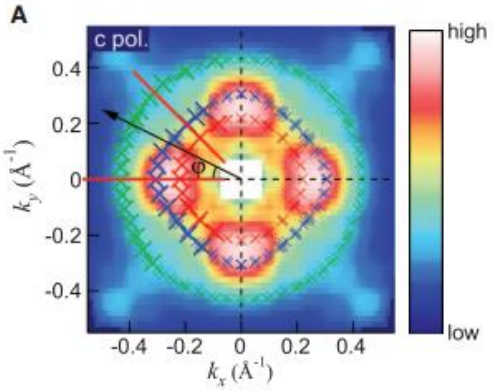
A. Damascelli,
https://www.cuso.ch/fileadmin/physique/document/Damascelli_ARPES_CUSO_2011_Lecture_Notes.pdf

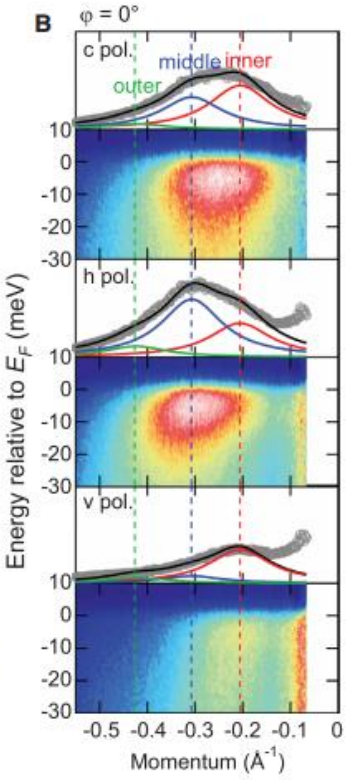
SC gap in $BaFe_2(As_{0.7}P_{0.3})_2$ (T_c=30K)



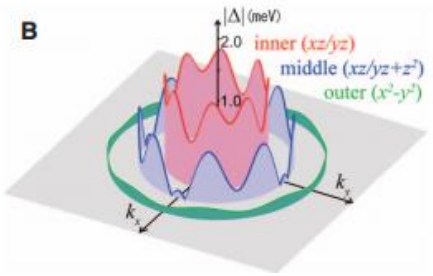
Zhang *et al*, Nat. Phys. **8** 371 (2012)

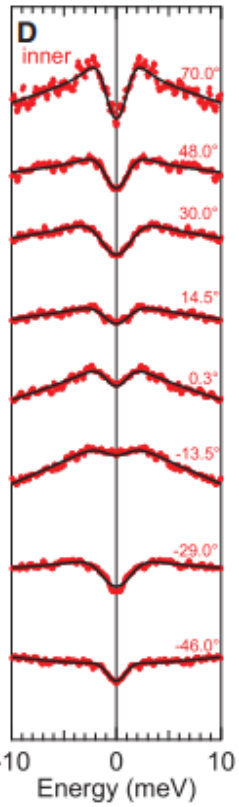
SC gap in KFe_2As_2 (T_c=3.4K)

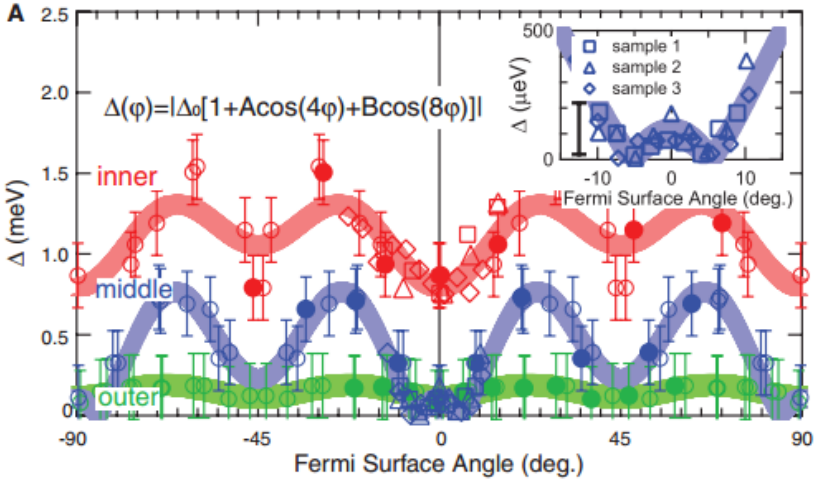




- Measurement temperature=2K
- Usually, ARPES can only measure down to ~8K





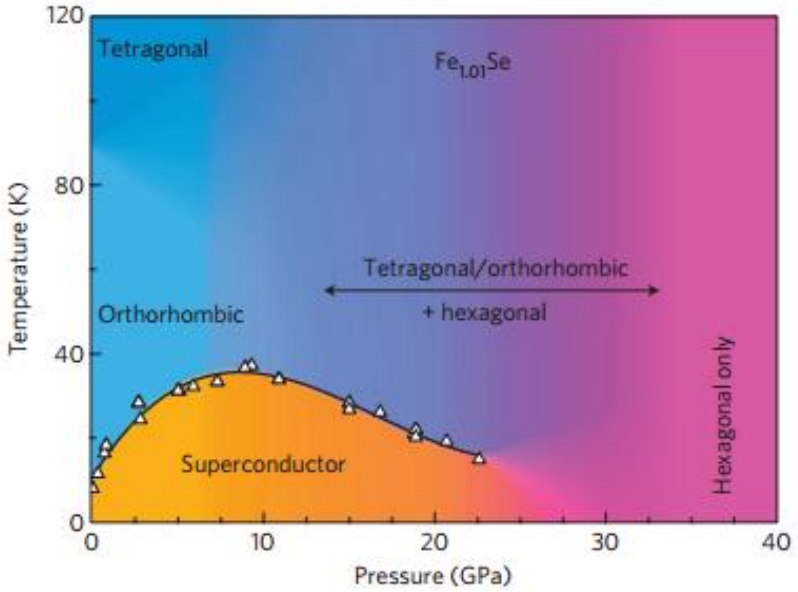


Okazaki *et al,* Science **337** p1314 (2012)

Summary: superconducting gap in Fe-SCs

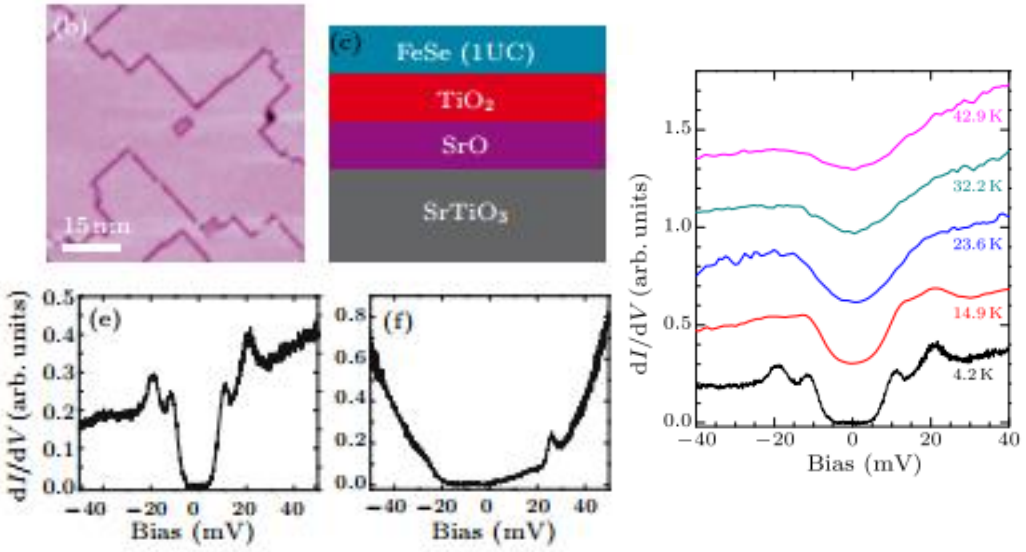
- Different materials and different experiments yield different gap structure
- This ambiguity holds if one considers other techniques for assessing gap structure (e.g. specific heat, thermal conductivity)

Monolayer FeSe



Bulk FeSe

- T_c=9K at ambient pressure
- T_c can be increased to 37K with pressure



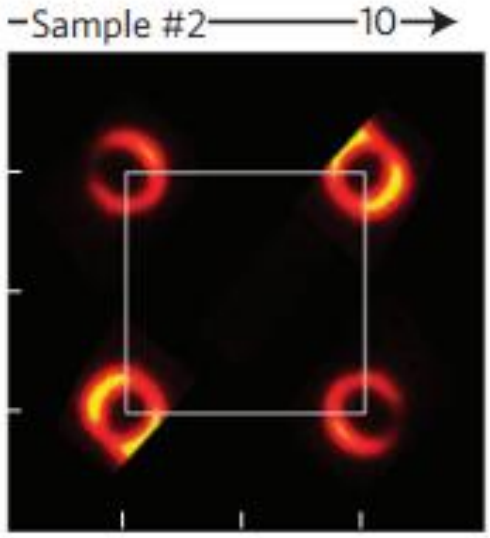
Monolayer (1 unit cell) FeSe on $SrTiO_3$ (TiO_2 terminated)

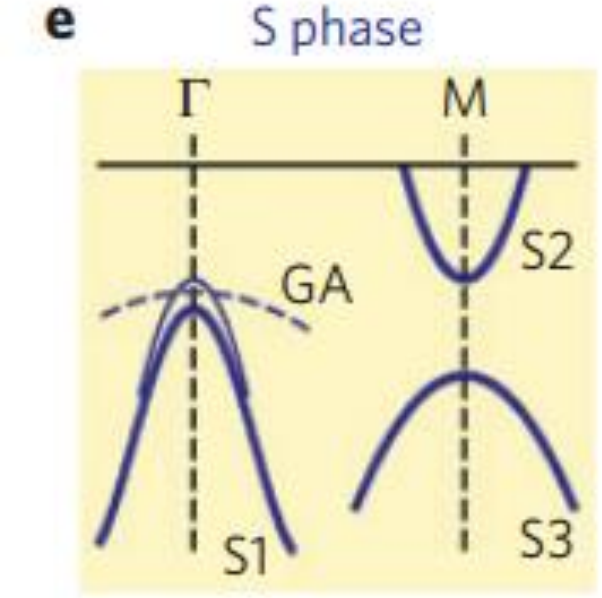
- Gap ~20 meV→suggests high Tc
- Gap persists to >50K
- Highest reported Tc=109K, highest accepted Tc=65K

Medvedev *et al,* Nat. Mater **8** 630 (2009)

Wang *et al,* Chin. Phys. Lett. **29** 037402 (2012)

Monolayer FeSe: Fermiology

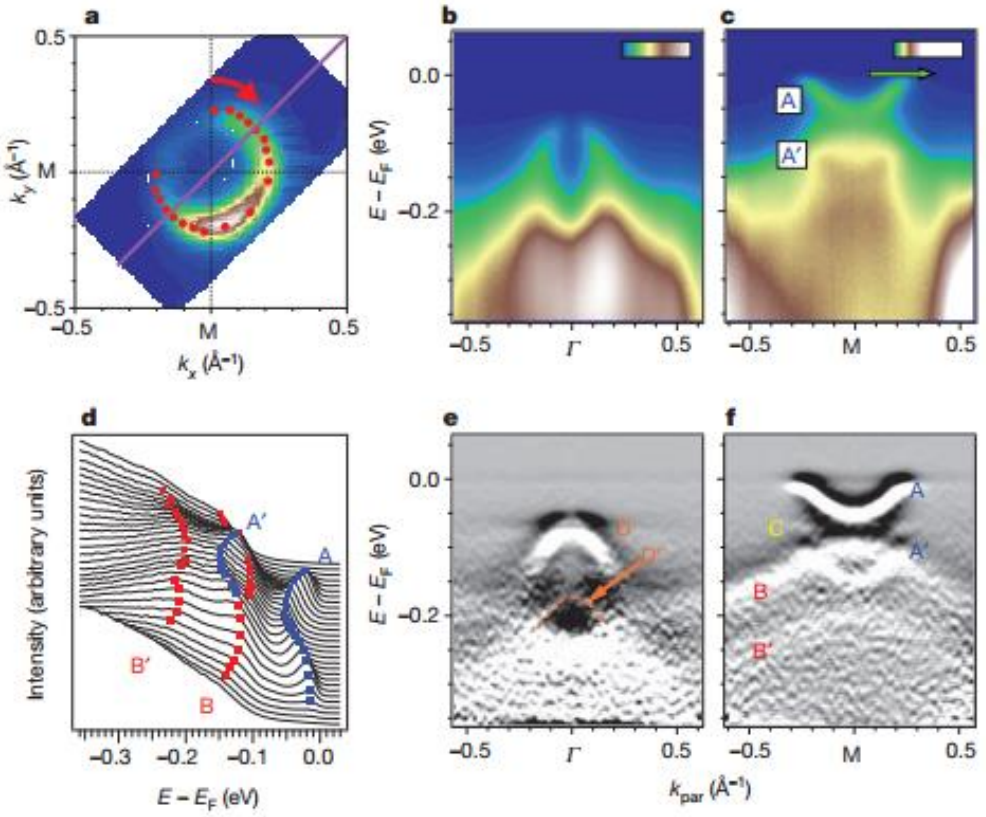




High-Tc FeSe monolayer does not have FS at Γ, unline bulk FeSe and most other Fe-SCs

He *et al.* Nat. Mater. **12** 605 (2013)

Monolayer FeSe: possible mechanism of T_c enhancement



- Observation: 'copies' of band structure in a way which is not consistent with quantum well state
- Interpretation: strong coupling to phonon mode in STO at q=0
- Consequence: interface e-ph coupling is responsible for Tc enhancement

Lee *et al.* Nature **515** 245 (2014)

Summary 1: Fe-SCs vs cuprates

Property	Cuprates	Fe-SCs
Number of compounds	Many	Many++
Building blocks	CuO_2 plane or CuO_6 octahedral	FeAs or FeSe layers
Dimensionality	Almost 2D	Almost 2D, but 3D effects are important too
Number of bands crossing E_F	1 per CuO2 plane, derived from Cu $3d_{x^2-y^2}$ orbitals	Usually 5, originating from Fe $3d_{xy,yz,xz}$ orbitals
Tuning phase diagram	Electron or hole doping; most materials cannot be tuned over entire superconducting dome	Electron, hole, isovalent doping; pressure; most materials can be tuned over entire superconducting dome
Proximity to magnetism	Yes, but overlap only (potentially) on electron-doped side; **q**=(½, ½)	Yes, likely microscopic coexistence; **q**=(0, ½)
SC gap symmetry	d-wave with line nodes on electron and hole-doped side	Symmetry and presence of nodes debated and may be materials dependent
SC mechanism	Debated	Debated

Summary 2: ARPES measurements on Fe-SCs

- Technological advancements of the technique that Fe-SCs have fostered or utilized
  - In-situ uniaxial pressure
  - Small beam spot size
  - Ultra low temperature (<4 K)
  - 2nd derivative band visualization
  - $k_{\perp}$ mapping
  - Quantitative analysis of matrix elements to discern orbital character of bands
- Contributions to our understanding of Fe-SCs
  - Fermiology
  - Band folding in ortho/SDW phase
  - Band-dependent superconducting gaps in some materials

Resources

- Q. Si, R. Yu, E. Abrahams, *High temperature superconductivity in iron pnictides and chalcogenides,* Nat. Rev. Mater. **1** 1 (2016)
- G. R. Stewart, *Superconductivity in iron compounds,* Rev. Mod. Phys. **83** 1589 (2011)
- Hosono and Kuroki, *Iron-based superconductors: Current status of materials and pairing mechanism*, Physica C **514** 399–422 (2015)
- A. Chubukov and P. Hirschfeld, *Iron-based superconductors, seven years later*, Physics Today **68**, 46 (2015)