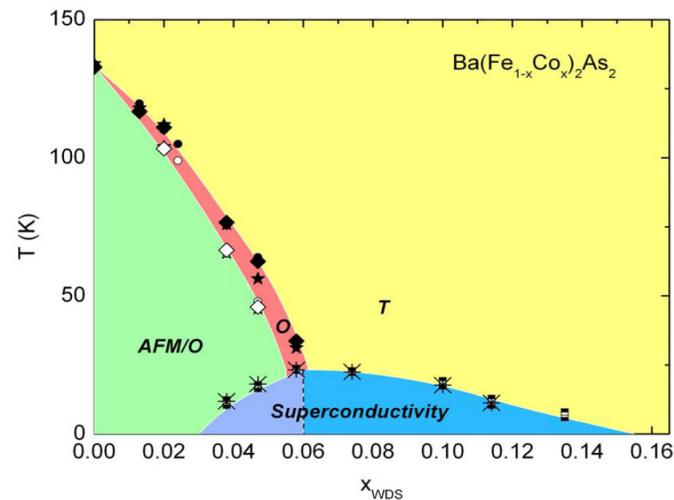


# Magnetism and superconductivity in iron-pnictides superconductors: a status report

Yann Gallais  
Université Paris Diderot

# Outline



- Iron pnictide superconductors: families and phase diagrams
- Magneto-structural coupling
- Superconducting gap structure and pairing mechanism
- Coexistence between Spin Density Wave and Superconductivity

# 2008: discovery

**JACS**  
COMMUNICATIONS

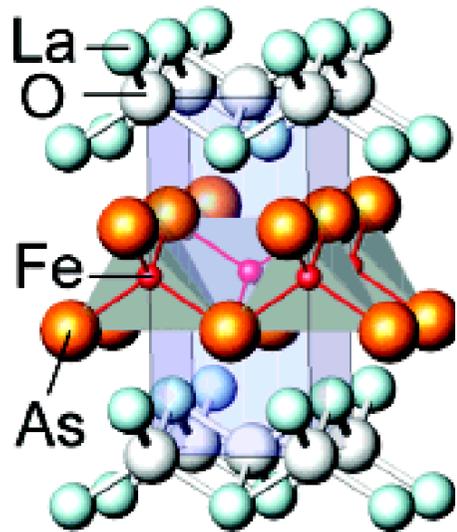
Published on Web 02/23/2008

## Iron-Based Layered Superconductor $\text{La}[\text{O}_{1-x}\text{F}_x]\text{FeAs}$ ( $x = 0.05\text{--}0.12$ ) with $T_c = 26\text{ K}$

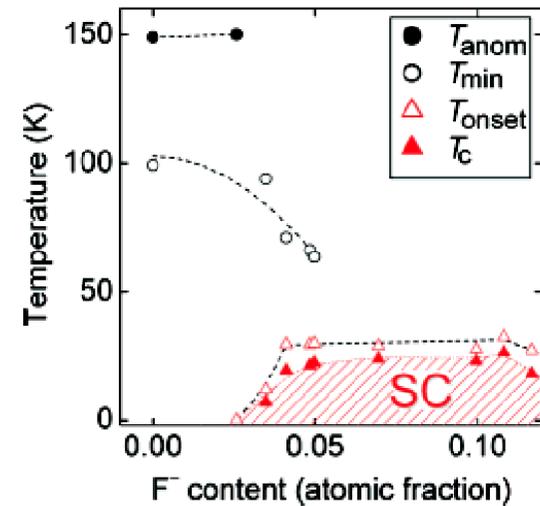
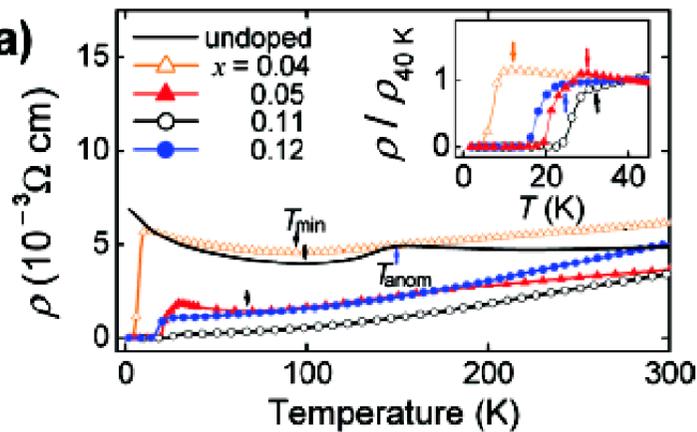
Yoichi Kamihara,<sup>\*,†</sup> Takumi Watanabe,<sup>‡</sup> Masahiro Hirano,<sup>†,§</sup> and Hideo Hosono<sup>†,‡,§</sup>

*ERATO-SORST, JST, Frontier Research Center, Tokyo Institute of Technology, Mail Box S2-13, Materials and Structures Laboratory, Tokyo Institute of Technology, Mail Box R3-1, and Frontier Research Center, Tokyo Institute of Technology, Mail Box S2-13, 4259 Nagatsuta, Midori-ku, Yokohama 226-8503, Japan*

Received January 9, 2008; E-mail: hosono@msl.titech.ac.jp

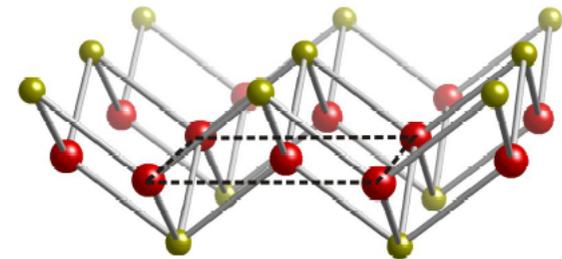
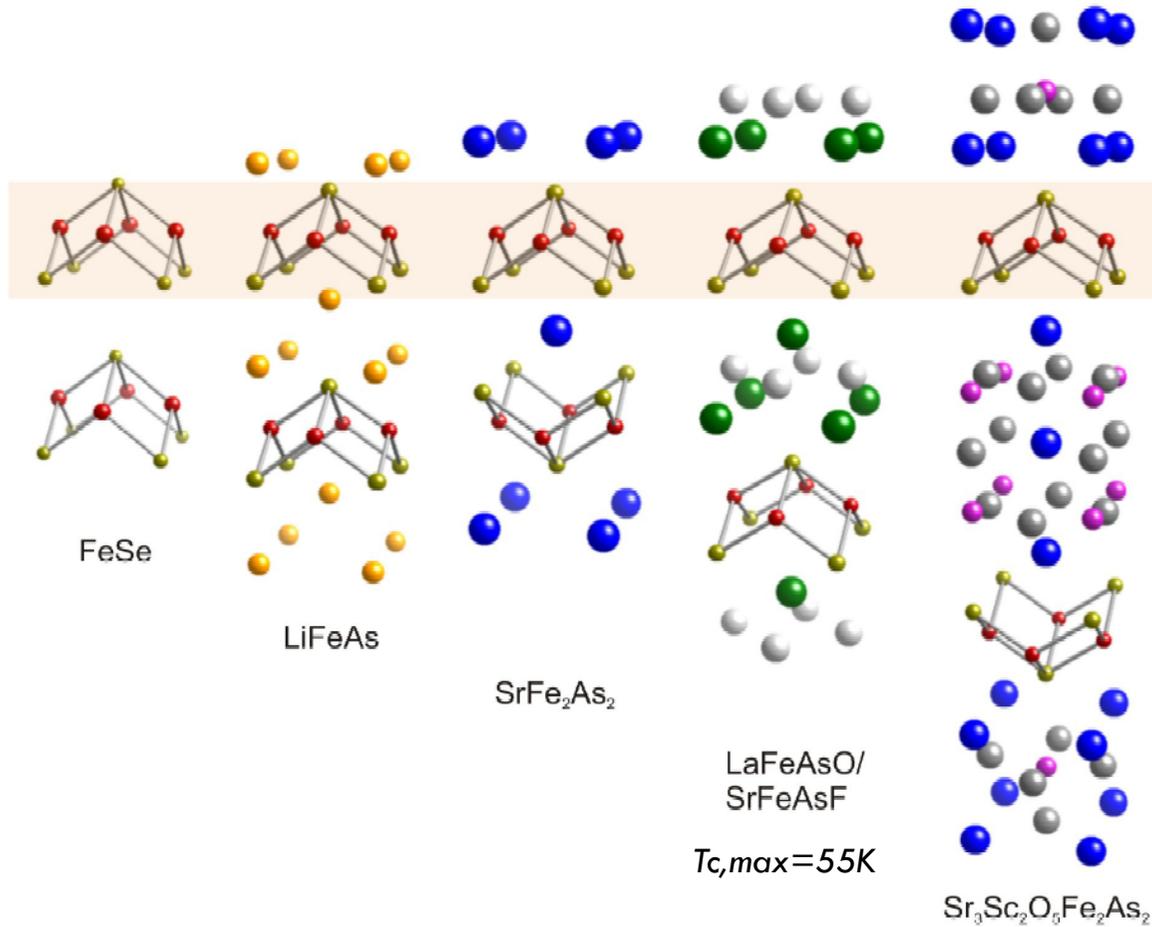


(a)



dopage électrons

# Structure and families



Common building block:  
 Fe square lattice  
 FeAs plane except FeSe

# Pnictides

pnictogen  
(P, As)

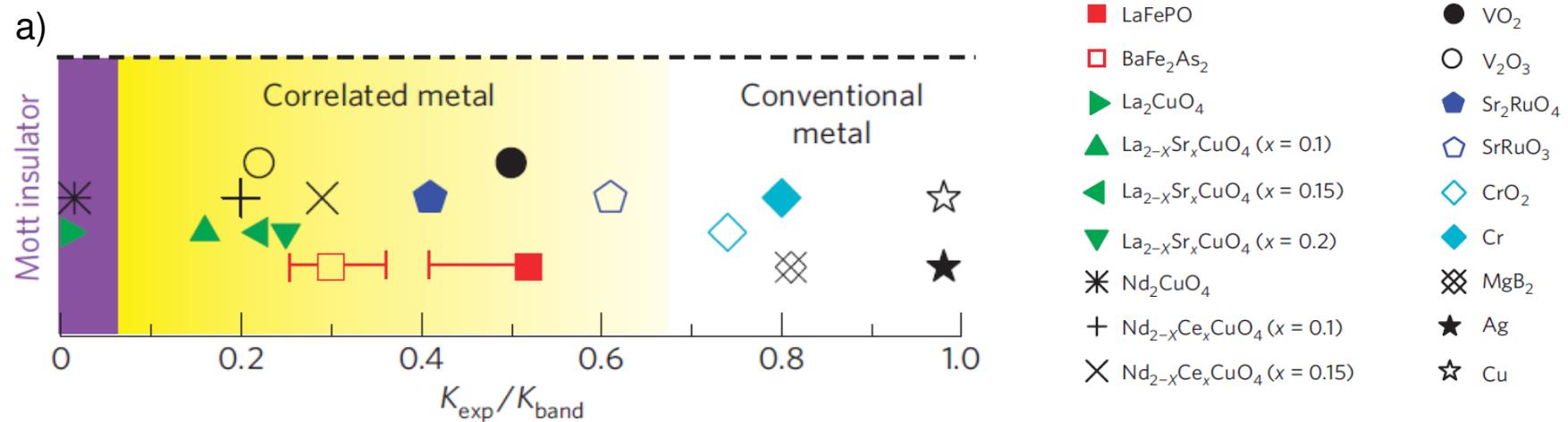
1 H Hydrogène																	2 He Hélium																														
3 Li Lithium	4 Be Béryllium											5 B Bore	6 C Carbone	7 N Azote	8 O Oxygène	9 F Fluor	10 Ne Néon																														
11 Na Sodium	12 Mg Magnésium											13 Al Aluminium	14 Si Silicium	15 P Phosphore	16 S Soufre	17 Cl Chlore	18 Ar Argon																														
19 K Potassium	20 Ca Calcium	21 Sc Scandium	22 Ti Titane	23 V Vanadium	24 Cr Chrome	25 Mn Manganèse	26 Fe Fer	27 Co Cobalt	28 Ni Nickel	29 Cu Cuivre	30 Zn Zinc	31 Ga Gallium	32 Ge Germanium	33 As Arsenic	34 Se Sélénium	35 Br Brome	36 Kr Krypton																														
37 Rb Rubidium	38 Sr Strontium	39 Y Yttrium	40 Zr Zirconium	41 Nb Niobium	42 Mo Molybdène	43 Tc Technétium	44 Ru Ruthénium	45 Rh Rhodium	46 Pd Palladium	47 Ag Argent	48 Cd Cadmium	49 In Indium	50 Sn Etain	51 Sb Antimoine	52 Te Tellure	53 I Iode	54 Xe Xénon																														
55 Cs Césium	56 Ba Baryum	57-71 Lanthanides	72 Hf Hafnium	73 Ta Tantale	74 W Tungstène	75 Re Rhénium	76 Os Osmium	77 Ir Iridium	78 Pt Platine	79 Au Or	80 Hg Mercure	81 Tl Thallium	82 Pb Plomb	83 Bi Bismuth	84 Po Polonium	85 At Astate	86 Rn Radon																														
87 Fr Francium	88 Ra Radium	89-103 Actinides																																													
<table border="1"> <tr> <td>57 La Lanthane</td> <td>58 Ce Cérium</td> <td>59 Pr Praséodyme</td> <td>60 Nd Néodyme</td> <td>61 Pm Prométhium</td> <td>62 Sm Samarium</td> <td>63 Eu Europium</td> <td>64 Gd Gadolinium</td> <td>65 Tb Terbium</td> <td>66 Dy Dyprosium</td> <td>67 Ho Holmium</td> <td>68 Er Erbium</td> <td>69 Tm Thulium</td> <td>70 Yb Ytterbium</td> <td>71 Lu Lutétium</td> </tr> <tr> <td>89 Ac Actinium</td> <td>90 Th Thorium</td> <td>91 Pa Protactinium</td> <td>92 U Uranium</td> <td>93 Np Neptunium</td> <td>94 Pu Plutonium</td> <td>95 Am Américium</td> <td>96 Cm Curium</td> <td>97 Bk Berkélium</td> <td>98 Cf Californium</td> <td>99 Es Einsteinium</td> <td>100 Fm Fermium</td> <td>101 Md Mendéléviur</td> <td>102 No Nobélium</td> <td>103 Lw Lawrencium</td> </tr> </table>																		57 La Lanthane	58 Ce Cérium	59 Pr Praséodyme	60 Nd Néodyme	61 Pm Prométhium	62 Sm Samarium	63 Eu Europium	64 Gd Gadolinium	65 Tb Terbium	66 Dy Dyprosium	67 Ho Holmium	68 Er Erbium	69 Tm Thulium	70 Yb Ytterbium	71 Lu Lutétium	89 Ac Actinium	90 Th Thorium	91 Pa Protactinium	92 U Uranium	93 Np Neptunium	94 Pu Plutonium	95 Am Américium	96 Cm Curium	97 Bk Berkélium	98 Cf Californium	99 Es Einsteinium	100 Fm Fermium	101 Md Mendéléviur	102 No Nobélium	103 Lw Lawrencium
57 La Lanthane	58 Ce Cérium	59 Pr Praséodyme	60 Nd Néodyme	61 Pm Prométhium	62 Sm Samarium	63 Eu Europium	64 Gd Gadolinium	65 Tb Terbium	66 Dy Dyprosium	67 Ho Holmium	68 Er Erbium	69 Tm Thulium	70 Yb Ytterbium	71 Lu Lutétium																																	
89 Ac Actinium	90 Th Thorium	91 Pa Protactinium	92 U Uranium	93 Np Neptunium	94 Pu Plutonium	95 Am Américium	96 Cm Curium	97 Bk Berkélium	98 Cf Californium	99 Es Einsteinium	100 Fm Fermium	101 Md Mendéléviur	102 No Nobélium	103 Lw Lawrencium																																	

exception: FeSe...



# Electron correlations?

Comparison between kinetic energy from optics and from band structure calculations



Qazilbash et al. *Nature Physics* 5, 647 (2009)

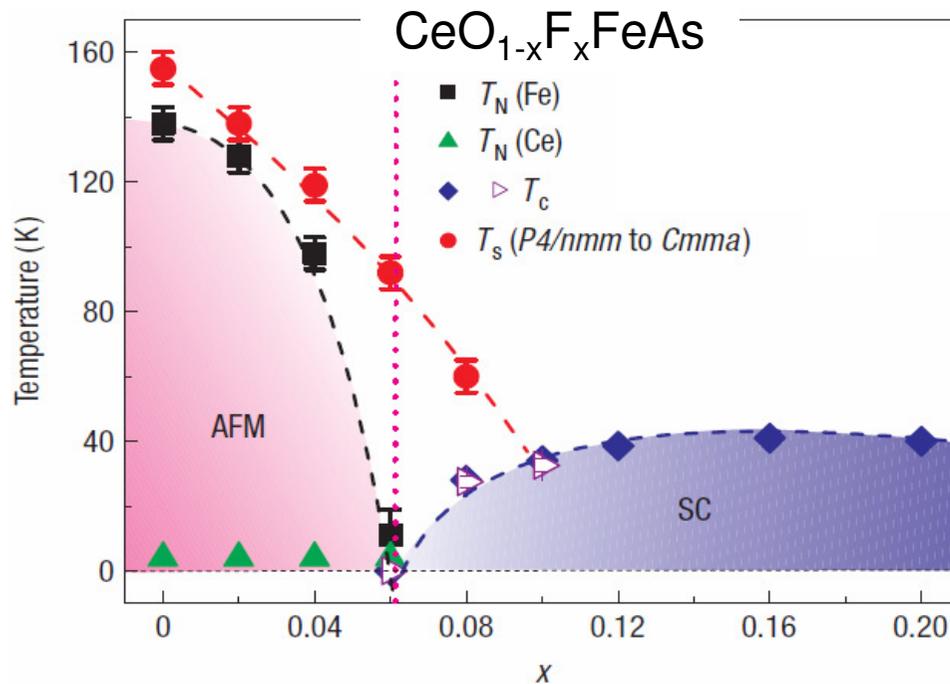
- Iron-pnictides further away from Mott insulator than cuprates (DMFT...)
- Ab-initio calculations (DFT) predict magnetism (but not the correct Fe moment) and gross features of band structure

*K. Haule et al. Phys. Rev. Lett. 100, 226402 (2008).*

*D.J. Singh, M.H. Du, Phys. Rev. Lett. 100, 237003 (2008)*

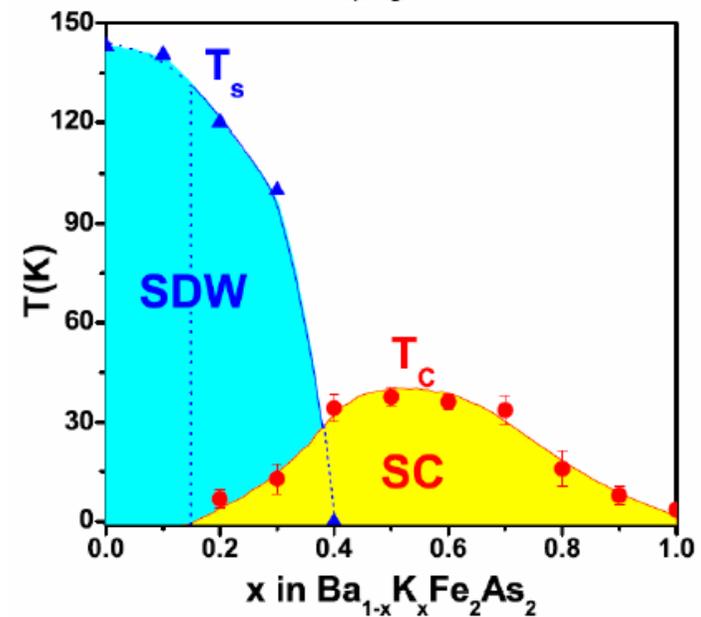
# Phase diagrams and families

1111



*J. Zhao et al. Nature Materials 7, 953-959 (2008)*

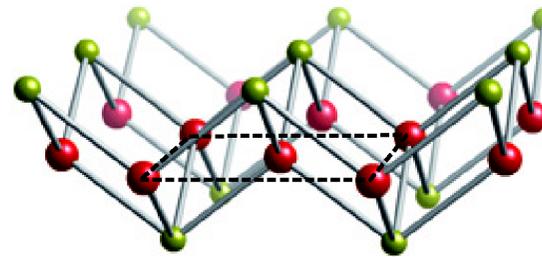
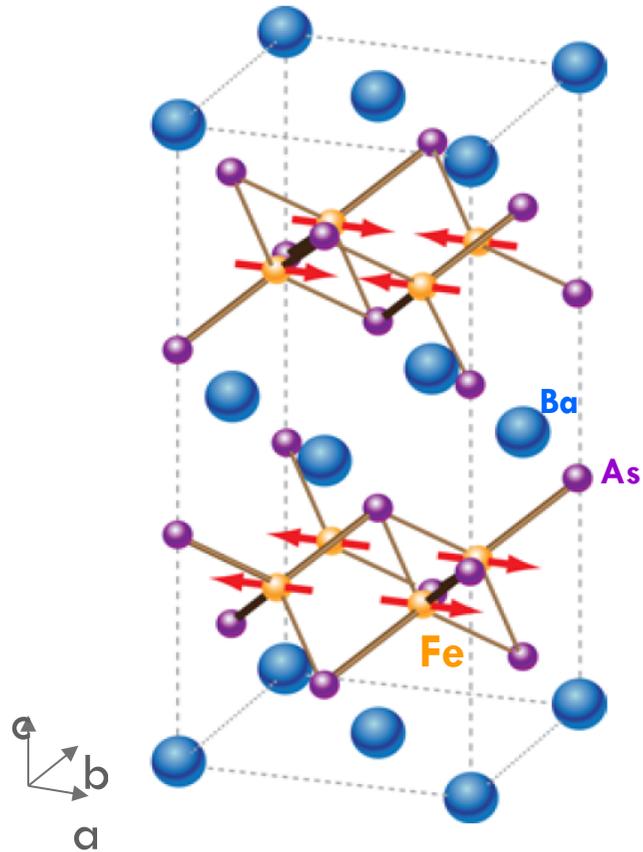
122



*H. Chen et al. Europhys. Lett. 85, 17006 (2009)*

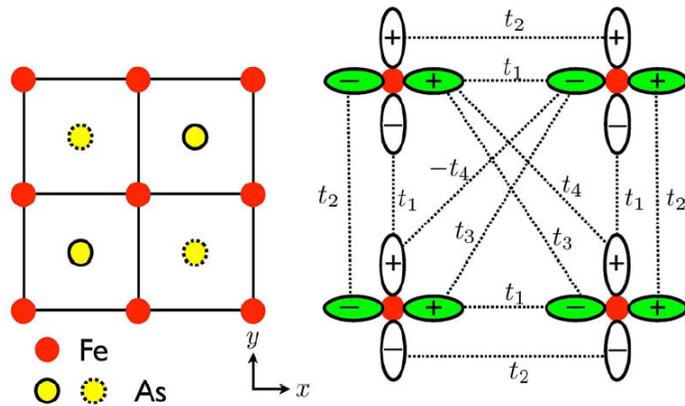
- close proximity of SC phase with magnetism (heavy fermions, cuprates)
- coexistence (or not) between magnetism and superconductivity
- magnetic and structural transitions

# Crystal structure BaFe<sub>2</sub>As<sub>2</sub>

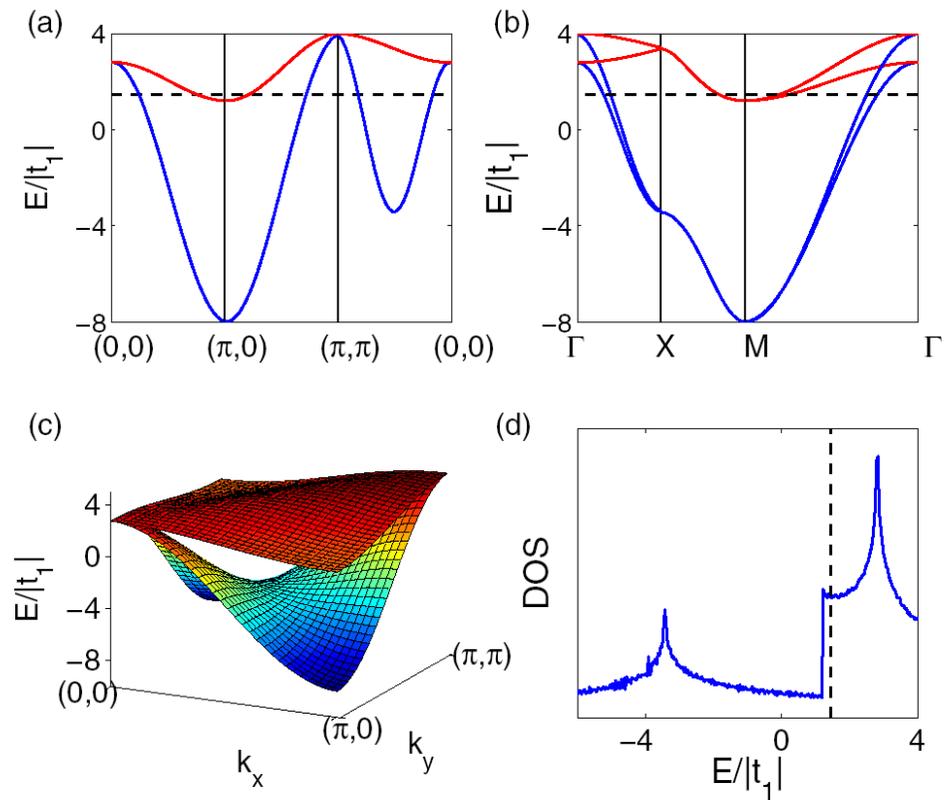


- Square plane of Fe ( $d^6$ )
- As alternating above and below Fe planes
- FeAs<sub>4</sub> tetrahedra
- Ba blocking layer
  
- FeAs plane: 2 Fe/cell
- BZ sometimes defined with 1 Fe/cell (extended BZ)

# A multi-orbital system



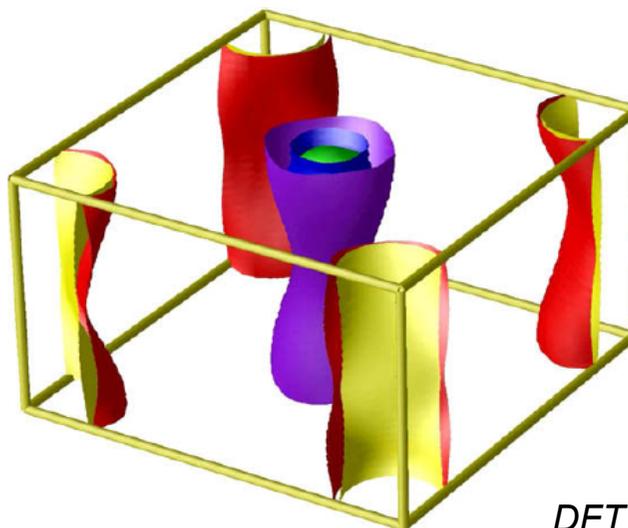
Minimal two-orbital model:  $d_{xz}$ ,  $d_{yz}$



Hole and electron Fermi surfaces

# 5 orbital models

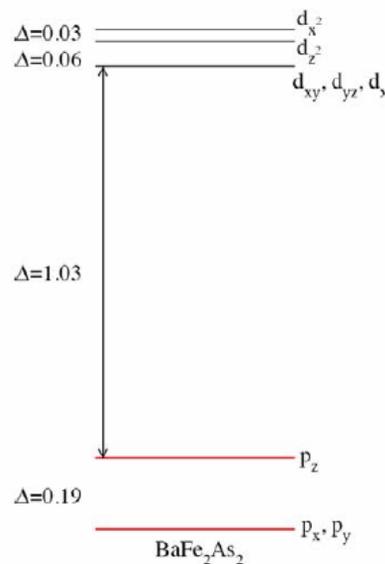
## 3D Fermi surfaces



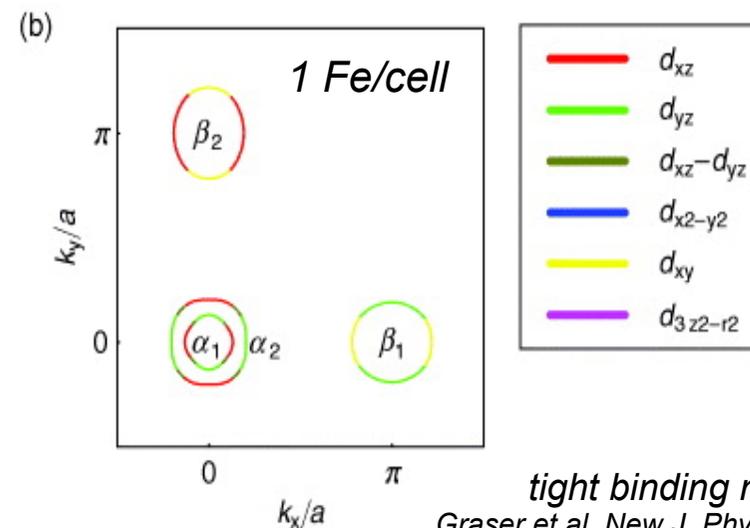
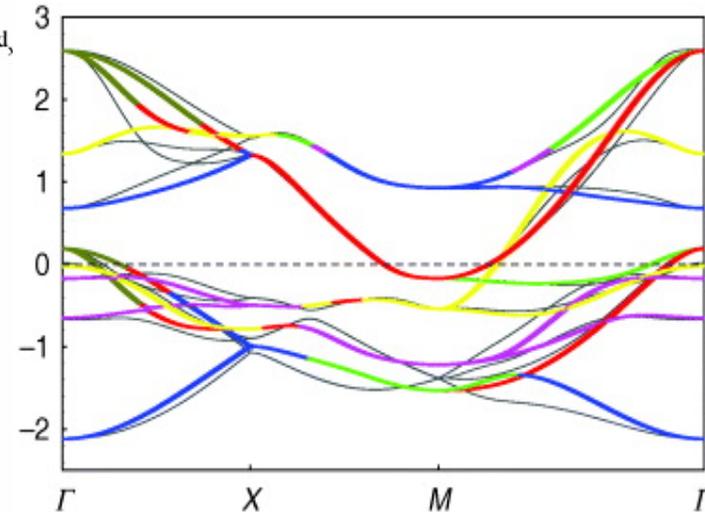
*DFT calculations*  
Mazin, *Physica C* **469**, 614 (2009)

- Up to 5 Fe derived bands cross the Fermi level: 3 hole-like and 2 electron-like
- As derived bands are 2eV below Fermi level
- relatively 2D electronic structure

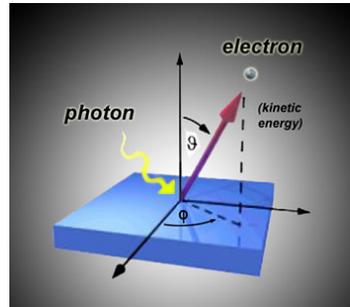
- **physics is governed by Fe orbitals**
- **importance of Fe-As-Fe hopping**
- **orbital physics: Hund coupling**



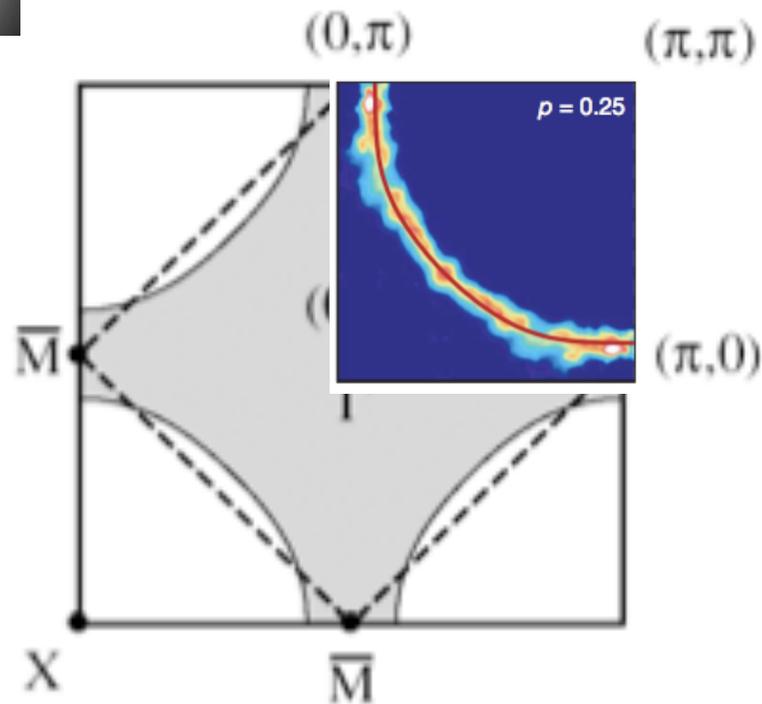
## Orbital content of Fermi surfaces



# Fermi surfaces

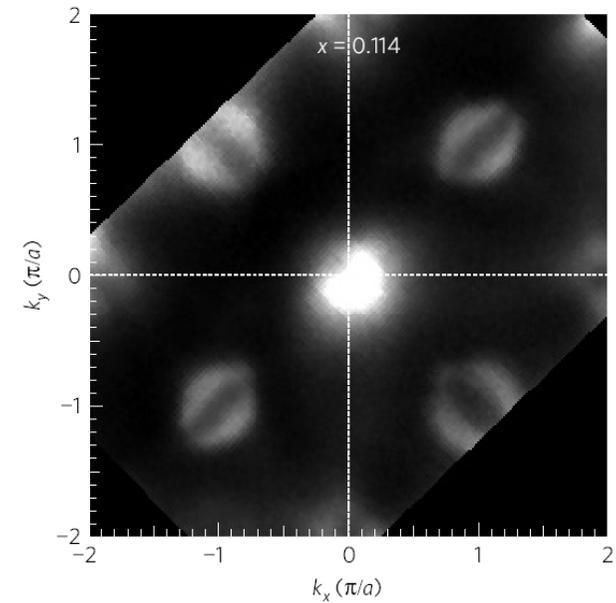


Cuprates: 1 FS



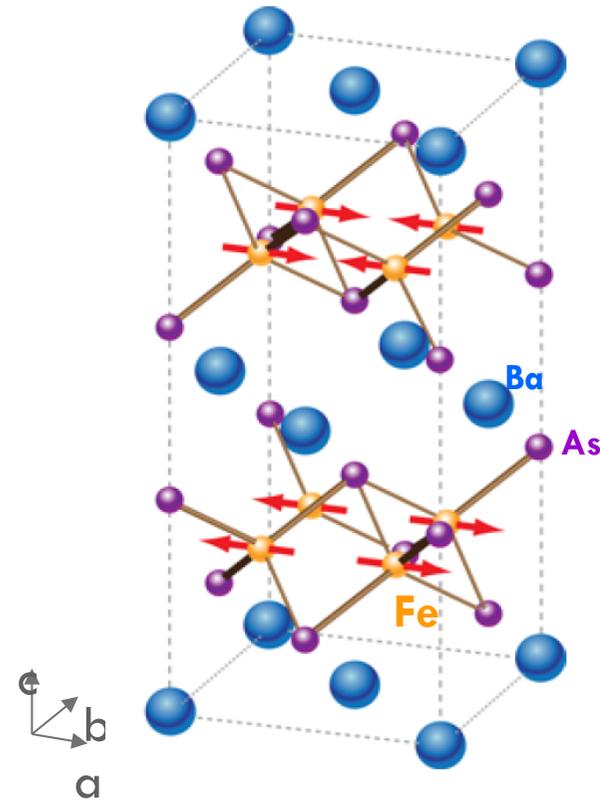
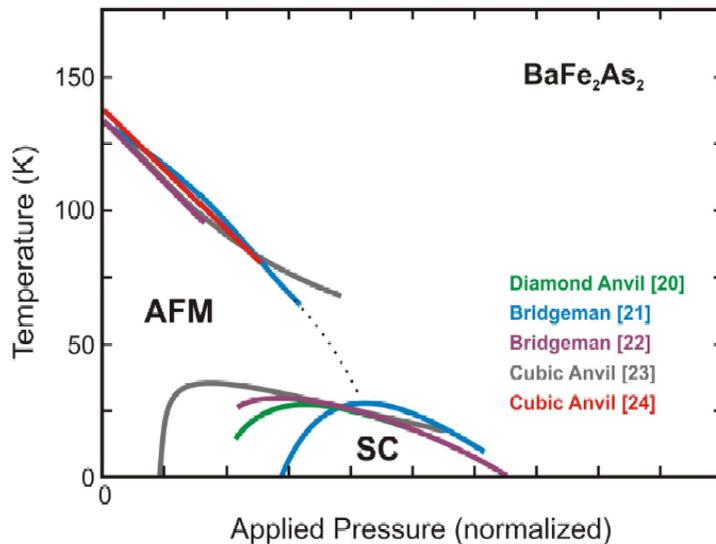
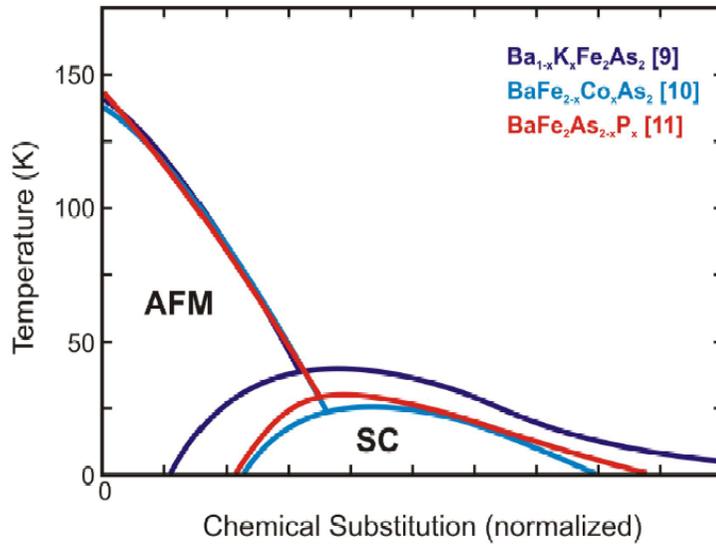
*Doiron-Leyraud et al. Nature 2007*

Pnictides: multiple FS



*Liu et al. Nature Phys. 2010*

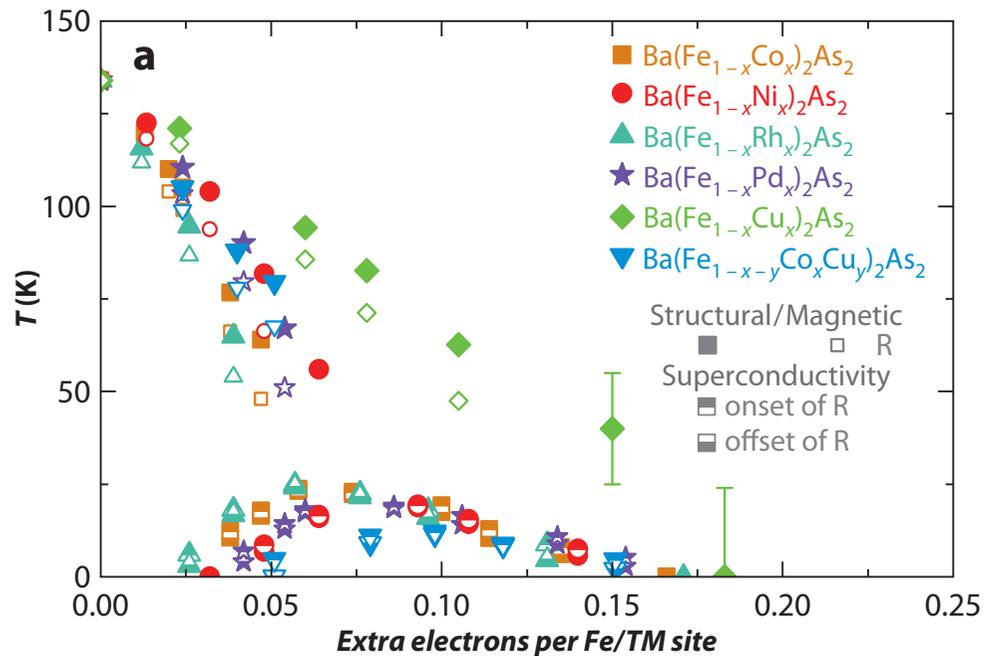
# the x parameter: tuning magnetism and superconductivity



## Different ways of tuning magnetism and SC

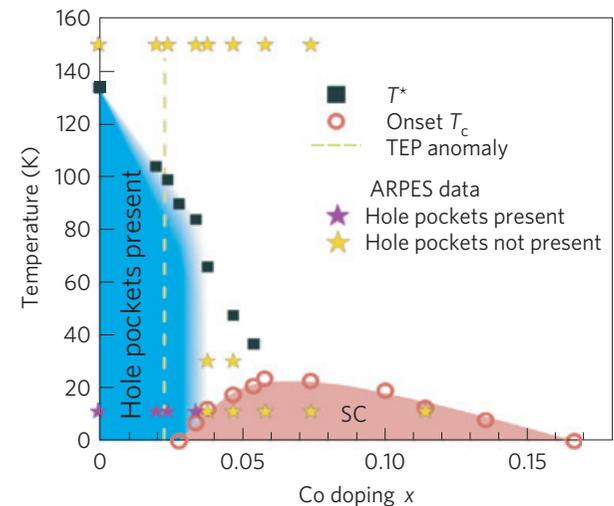
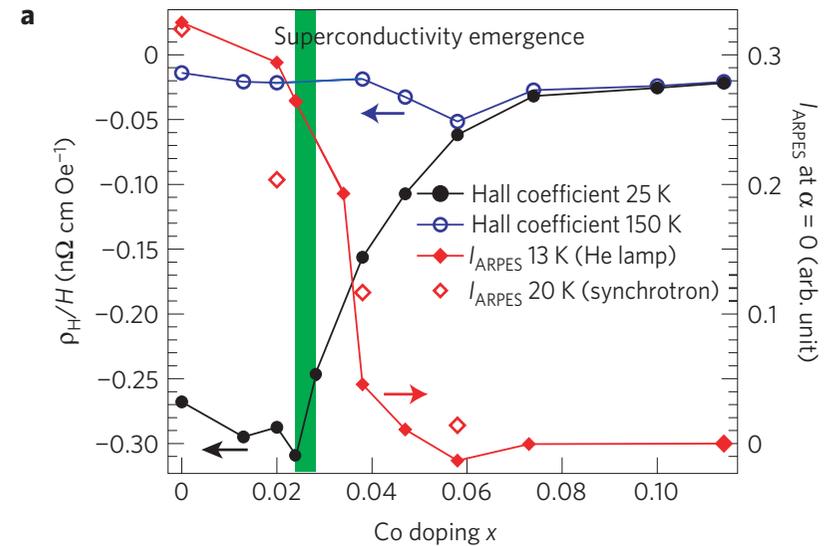
- Hole, electron, isovalent doping
- pressure
- doping in the FeAs plane is not detrimental to Tc

# the x parameter: tuning magnetism and superconductivity



Canfield and Budko, *Annu. Rev. Condens. Matter Phys.* 1, 27-50 (2010)

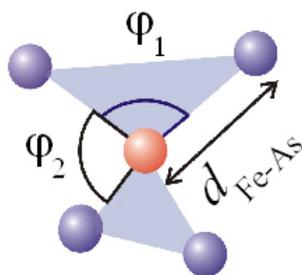
- « universal »  $T_c$  (e) phase diagram in overdoped Ba-122
- $T_c$  is correlated with  $T_{N/S}$  in underdoped Ba-122
- electronic parameter: FS topology ?



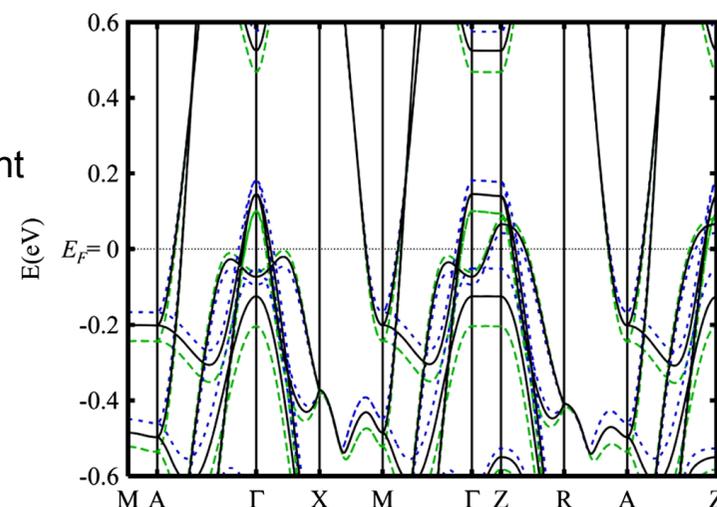
Liu et al. *Nat. Phys.* (2010)

# What is controlling $T_c$ ?

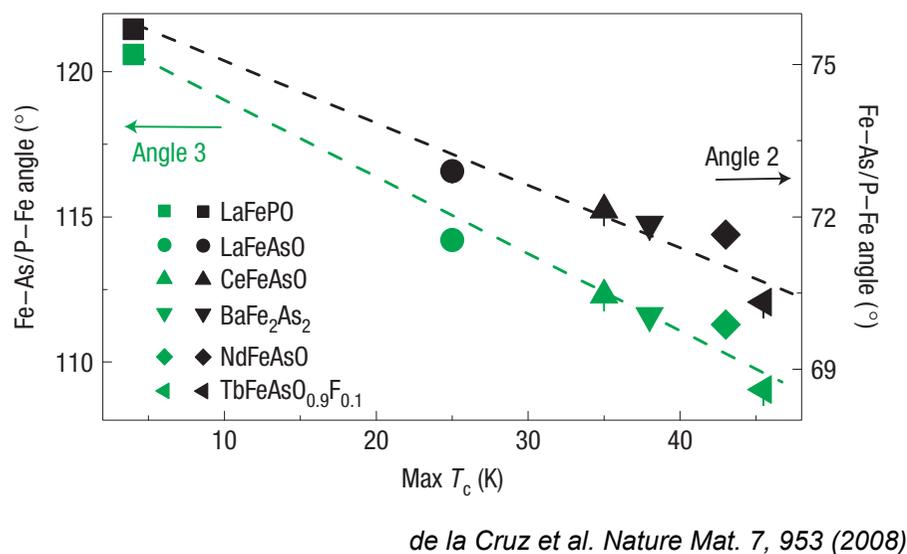
- Fe-As-Fe bond angle controls bandwidth and nesting
- Sensitivity of the band structure and calculated Fe moment with As position



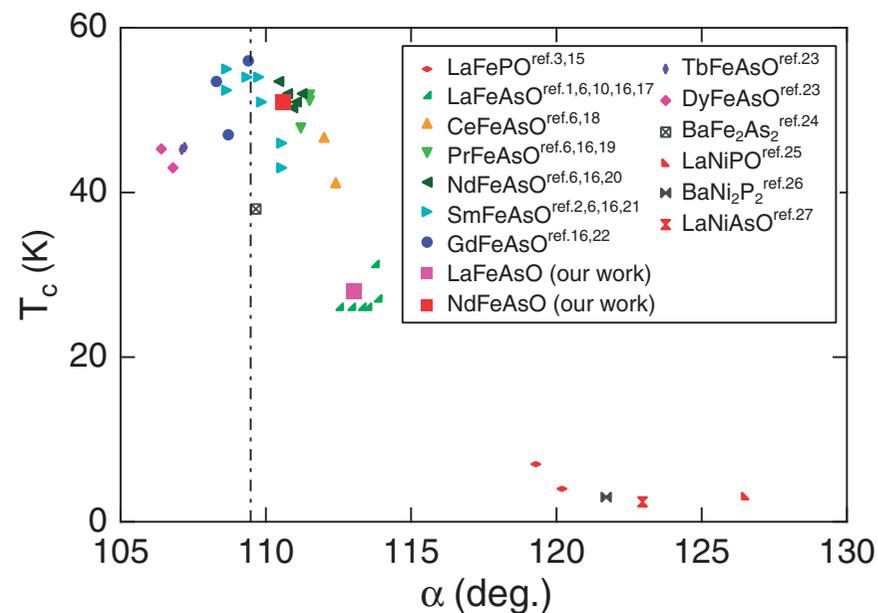
FeAs<sub>4</sub> tetrahedra



Singh et al. Phys. Rev. Lett. 100, 237003 (2008)



de la Cruz et al. Nature Mat. 7, 953 (2008)

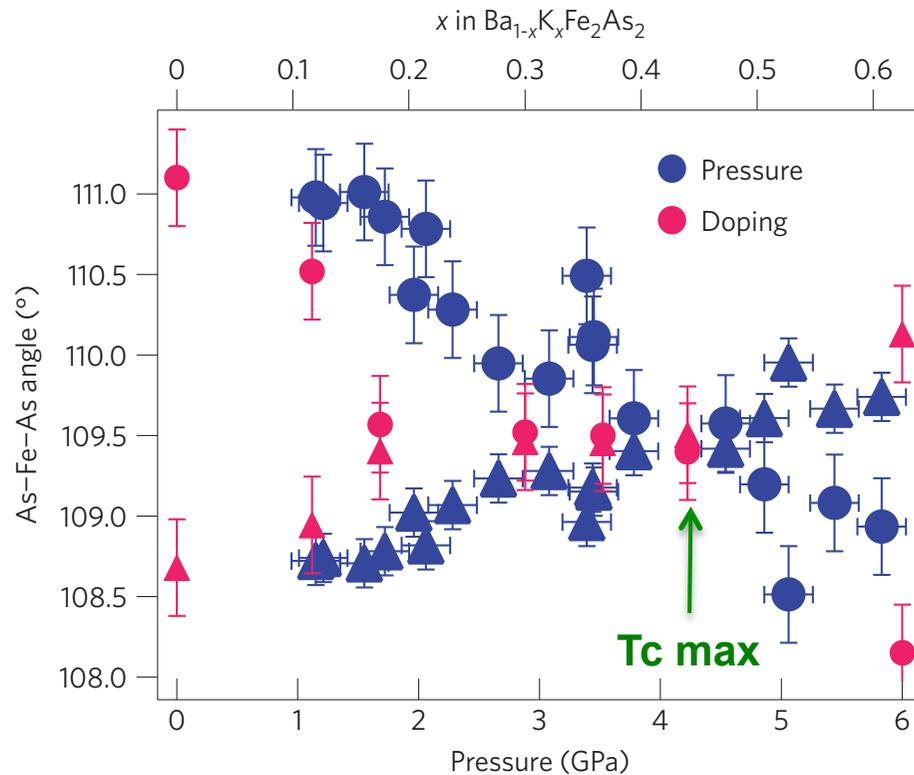


C.H. Lee et al. JPSJ 77, 083704 (2008)  
Garbarino et al. EPL 96 5 (2011) 57002

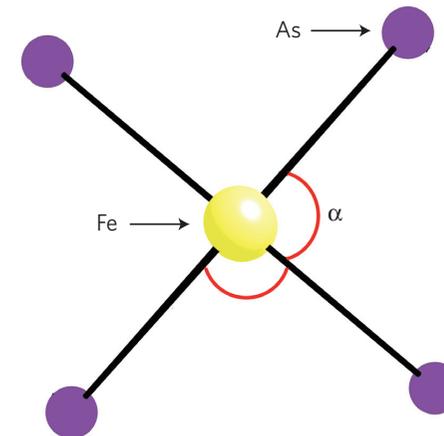
$T_c$  is max for perfect tetrahedra: « magic » angle at 109°

# x: structural tuning

K (hole) doping vs pressure



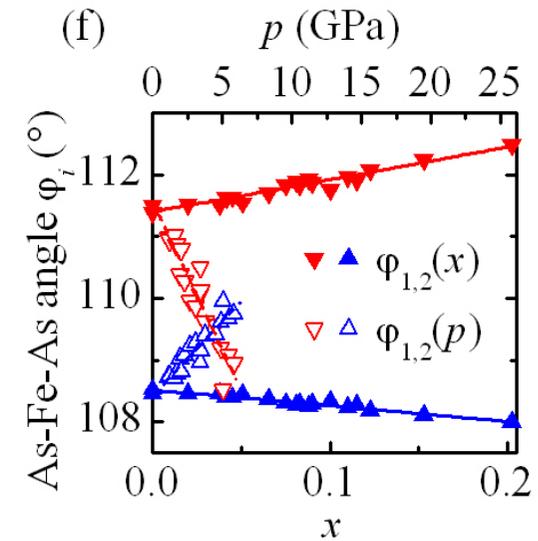
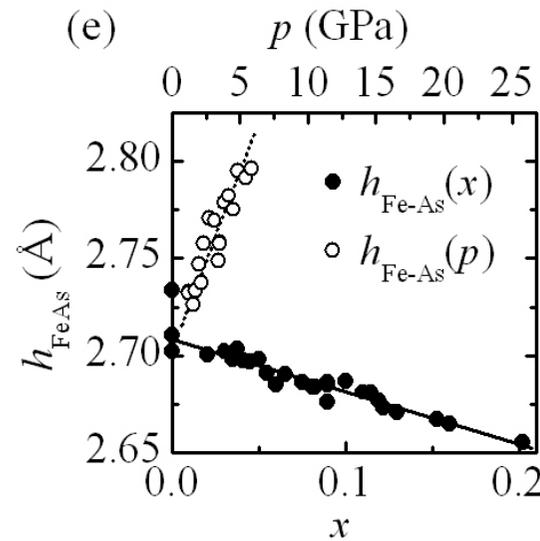
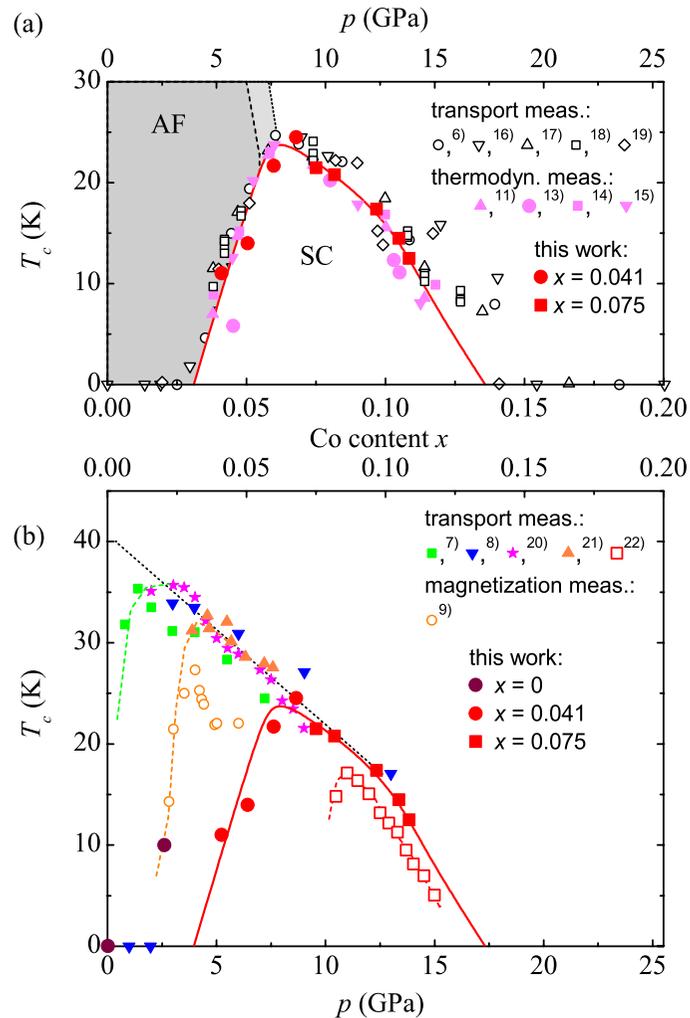
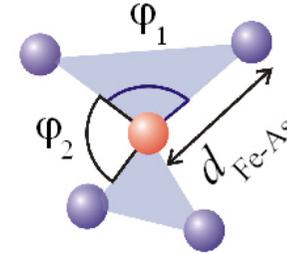
S. Kimber et al. Nature Mat. 8, 471 (2009)



- pressure and hole doping have a similar effect on bond angle (chemical vs physical pressure)
- T<sub>c</sub> is max around « magic » angle (but uncertainty in pressure dependance of T<sub>c</sub>)

# x parameter in BaFe<sub>2</sub>As<sub>2</sub> (122)

## Co doping vs pressure

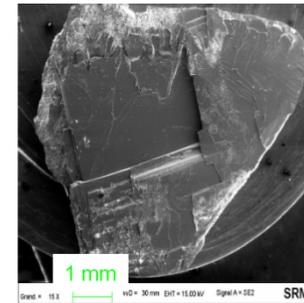
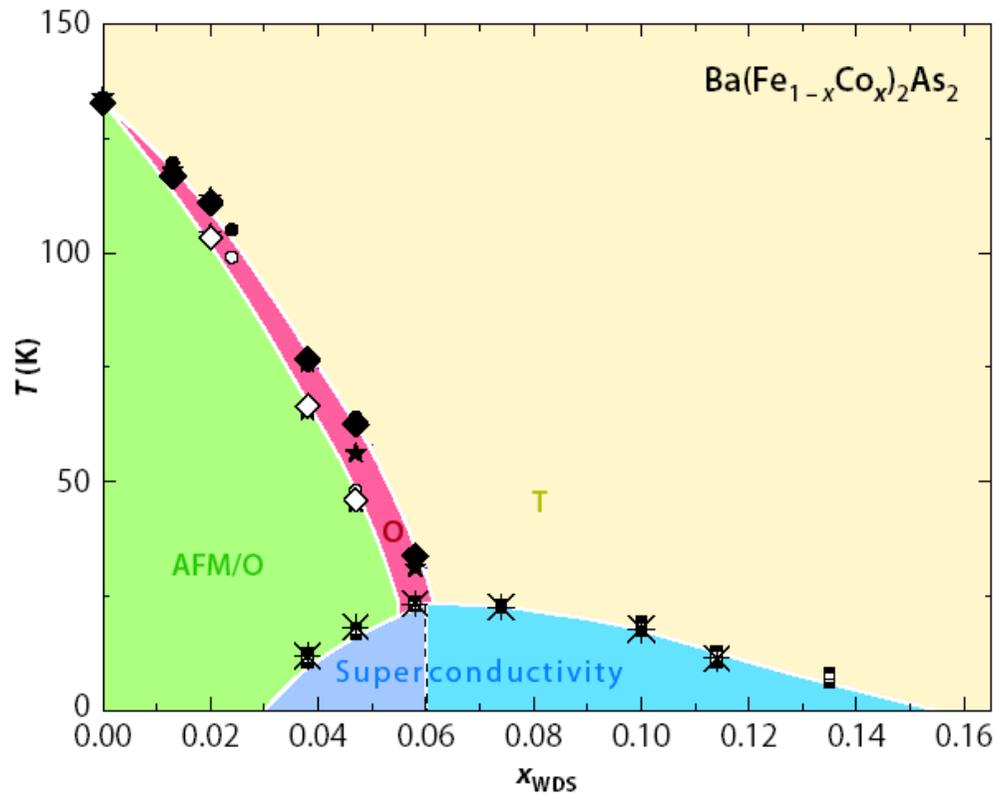


S. Drotziger et al. JPSJ. 79, 124705 (2010)

- No clear structural trends between Co and pressure
- $x$  is not just structural tuning

# Phase diagram of $\text{Ba}(\text{Fe}_{1-x}\text{Co}_x)_2\text{As}_2$

Co electron doped Ba122: most studied system

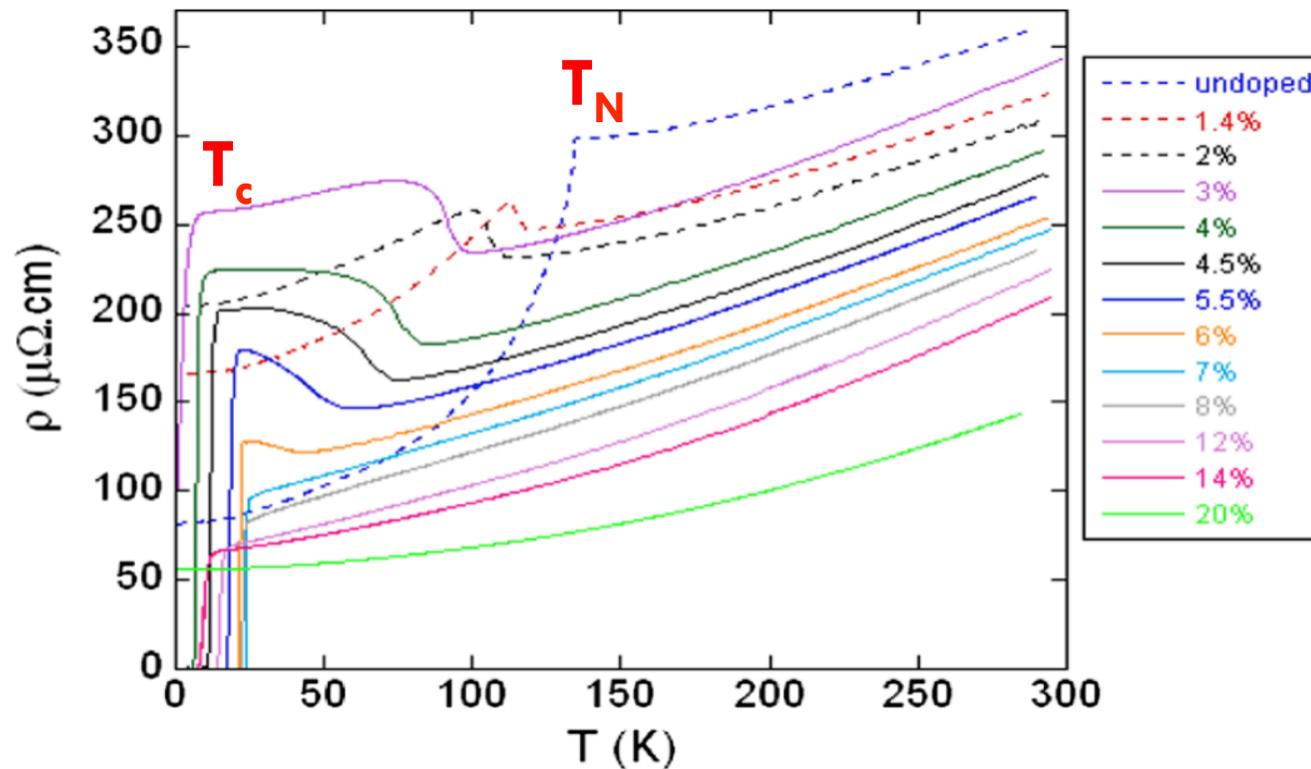


- Relatively large and good quality single crystals
- Homogeneous Co doping (no segregation)
- Fine control of Co

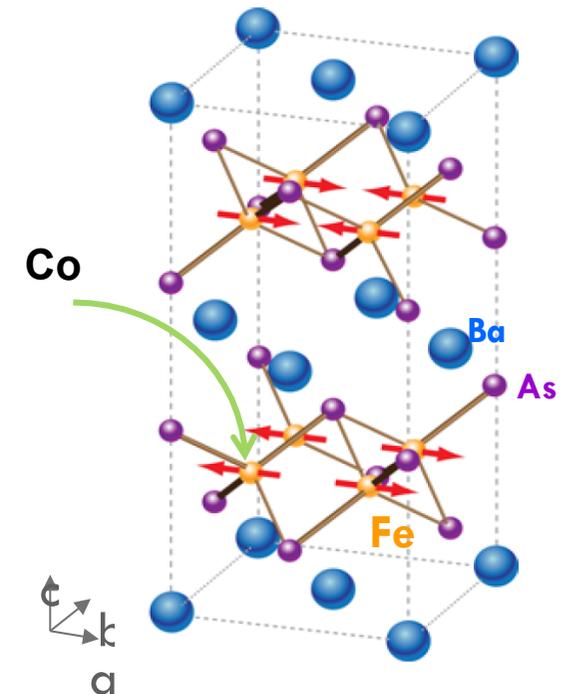
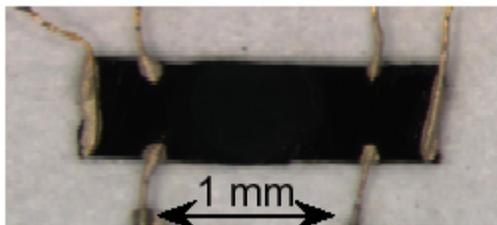
Canfield and Budko, *Annu. Rev. Condens. Matter Phys.* 1, 27-50 (2010)

F. Rullier-Albenque & al, *Phys. Rev. Lett.* **103**, 057001 (2009)

# Transport in $\text{Ba}(\text{Fe}_{1-x}\text{Co}_x)_2\text{As}_2$

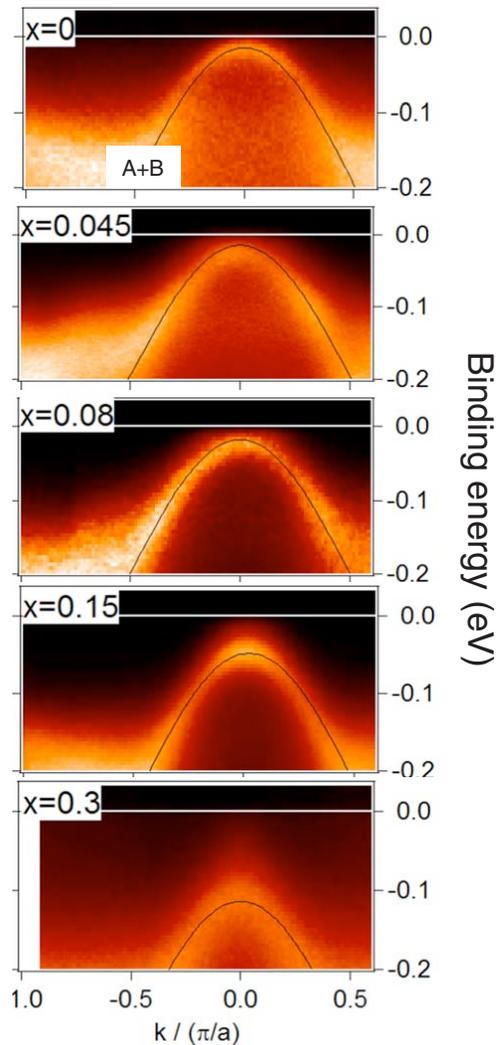


F. Rullier-Albenque & al, *Phys. Rev. Lett.* **103**, 057001 (2009)



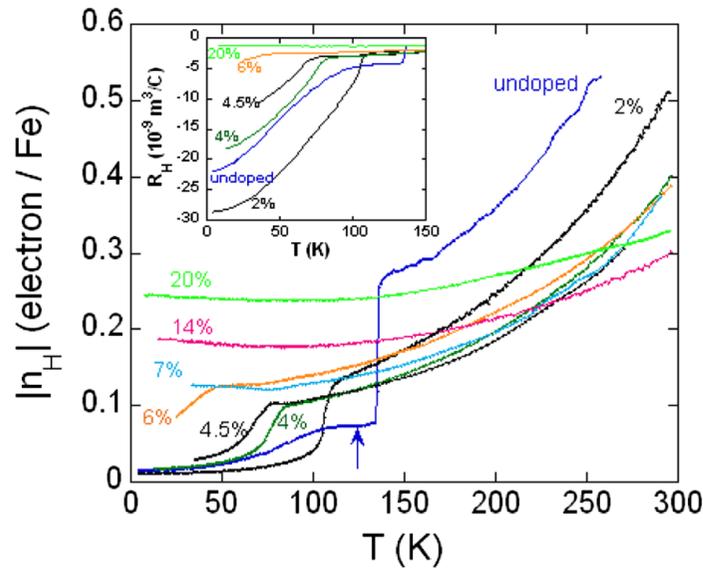
Electron doping:  $\text{Co}^{3+}$  replaces  $\text{Fe}^{2+}$

# Electron doping in $\text{Ba}(\text{Fe}_{1-x}\text{Co}_x)_2\text{As}_2$



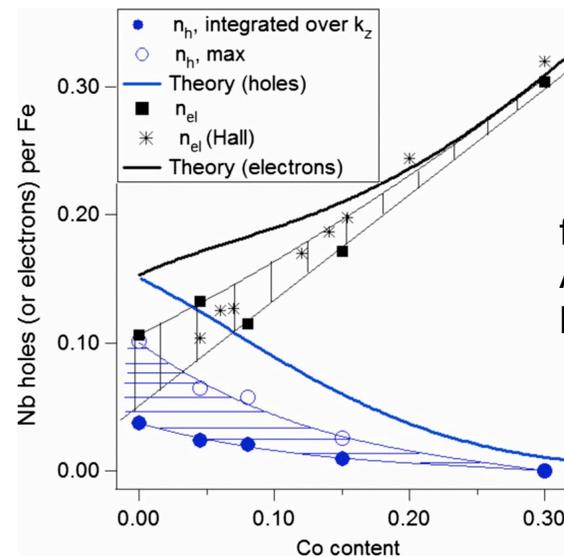
V. Brouet et al, *Phys. Rev. B* **80**, 165115 (2009)

ARPES: hole band sinks below  $E_F$



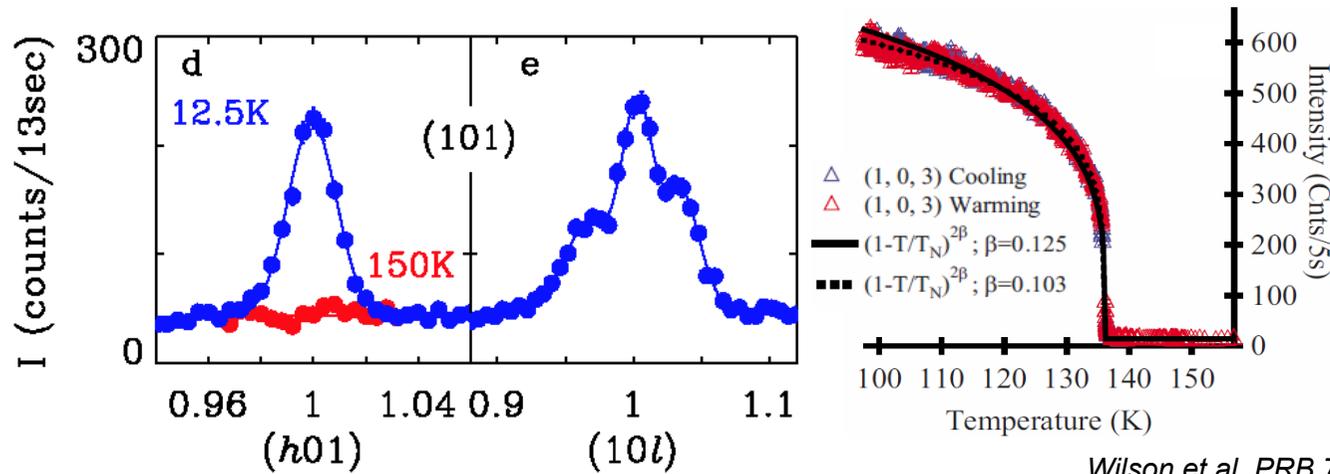
Hall effect: increase in electron-like carrier

F. Rullier-Albenque & al, *Phys. Rev. Lett.* **103**, 057001 (2009)



fair agreement between Hall and ARPES (Luttinger theorem): rigid band picture

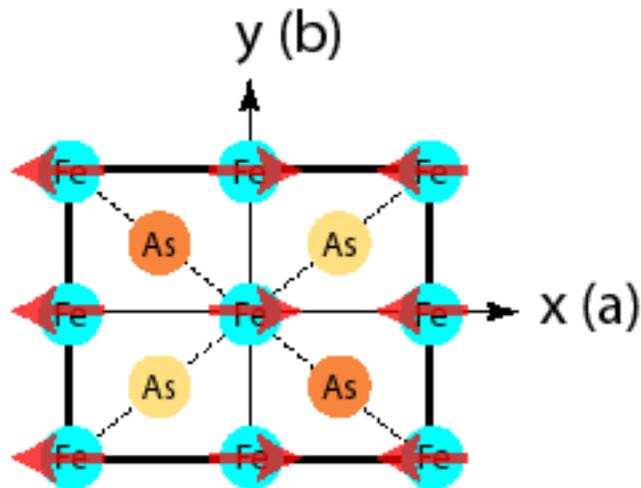
# BaFe<sub>2</sub>As<sub>2</sub> : magnetic transition



Neutron diffraction: new Bragg peaks below 135K

*Wilson et al. PRB 79, 184519 (2009)*

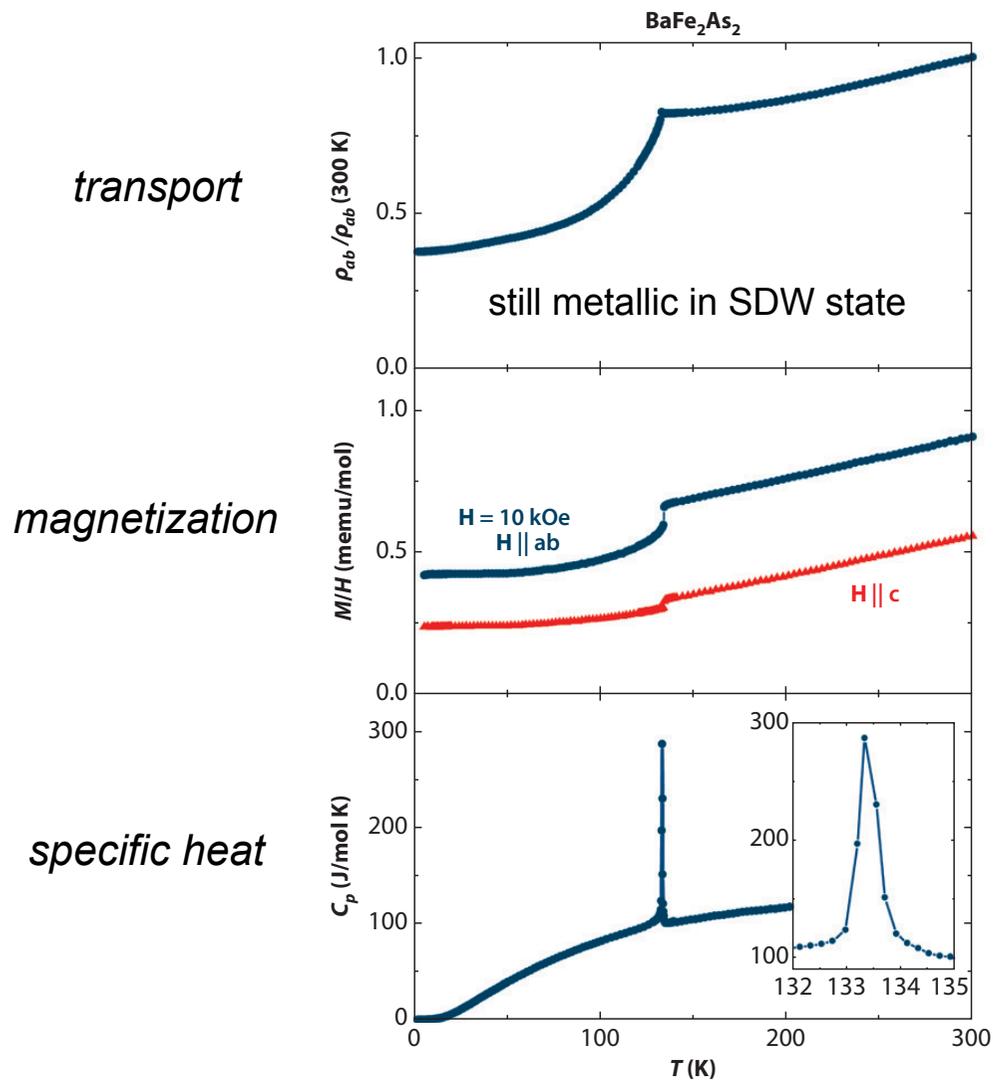
*Huang et PRL 2008*



- transition second (Ba-122) or first (Ca-122) order
- stripe-like AF order: in-plane magnetic anisotropy

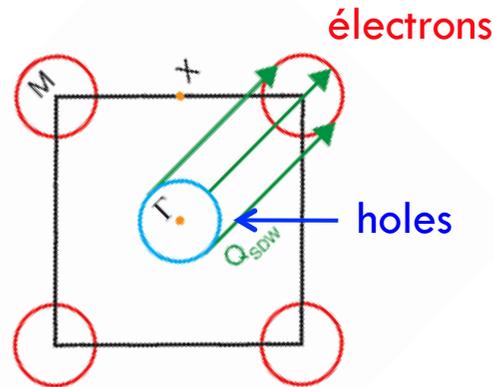
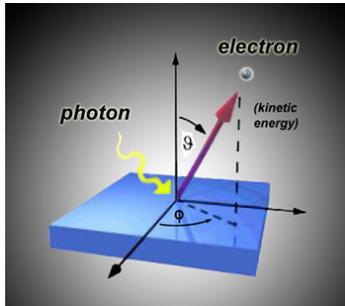
**itinerant magnetism, not Mott magnetism**

# Spin Density Wave transition

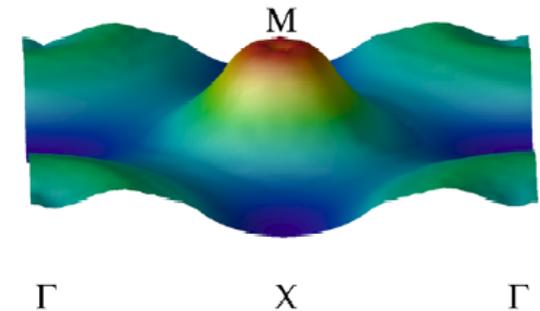


itinerant magnet: SDW transition

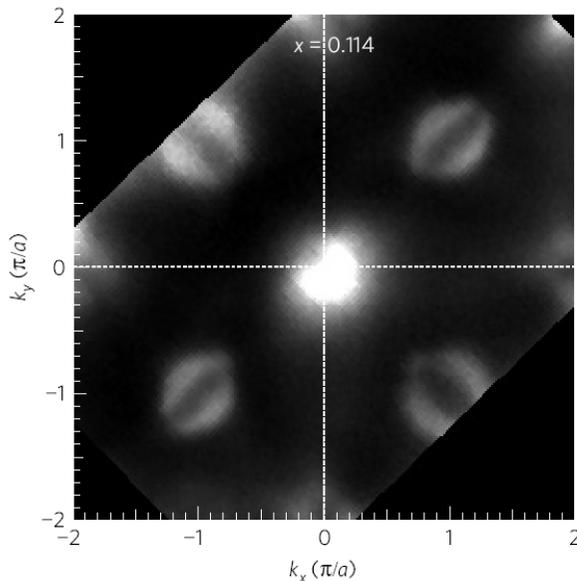
# SDW and Fermi surface nesting



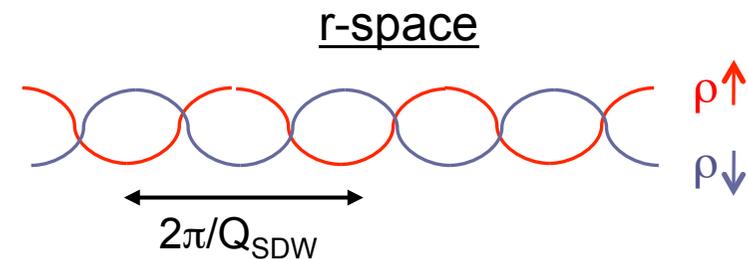
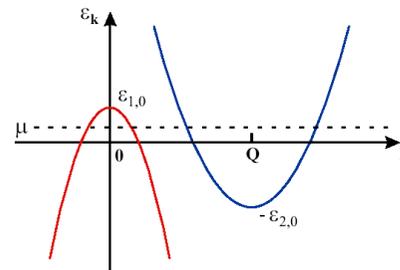
k-space susceptibility



Mazin et al. PRL 2008

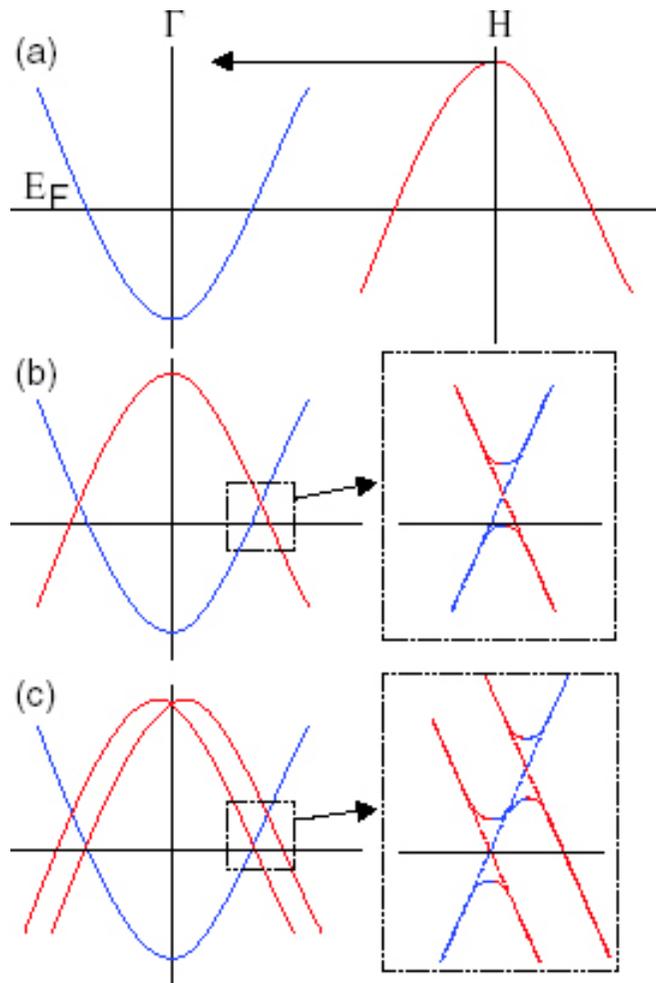


ARPES: Liu et al. Nature Phys. 2010



- approximate Fermi surface nesting  $\mathbf{Q}_{SDW}$  between **holes** and **electrons** pockets
- enhancement of susceptibility at  $\mathbf{Q}_{SDW}=(\pi,\pi)$ : instability
- DFT correctly predicts magnetism but over-estimate magnetic moment

# Fermi surface reconstruction in the SDW state

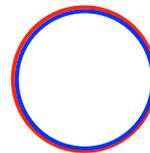


- Backfolding of the band
- Spin density wave gap at  $E_F$  (anticrossing)

- Perfect nesting: insulator
- Imperfect nesting: SDW metal

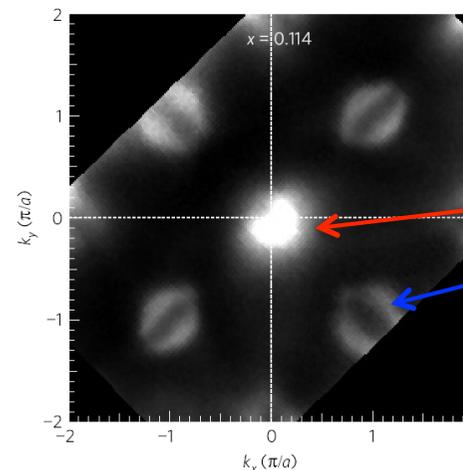
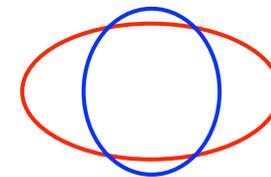
perfect nesting

$$m = m_x = m_y$$



ellipticity

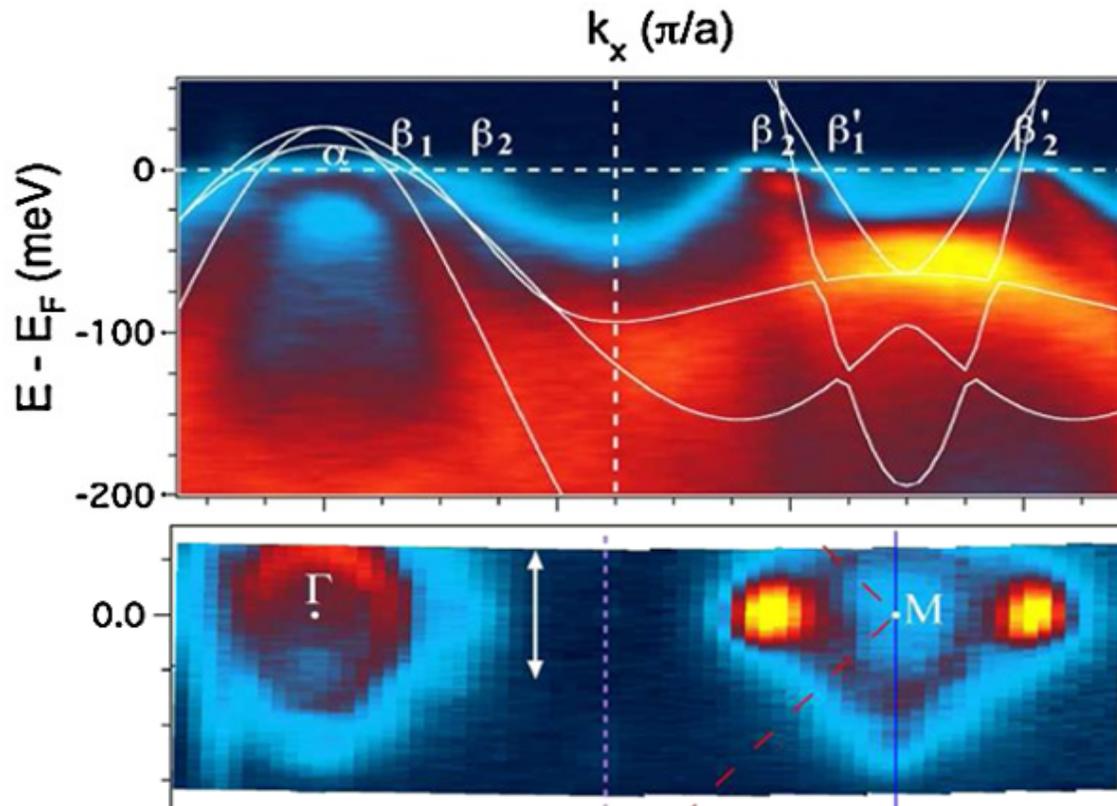
$$m \neq m_x \neq m_y$$



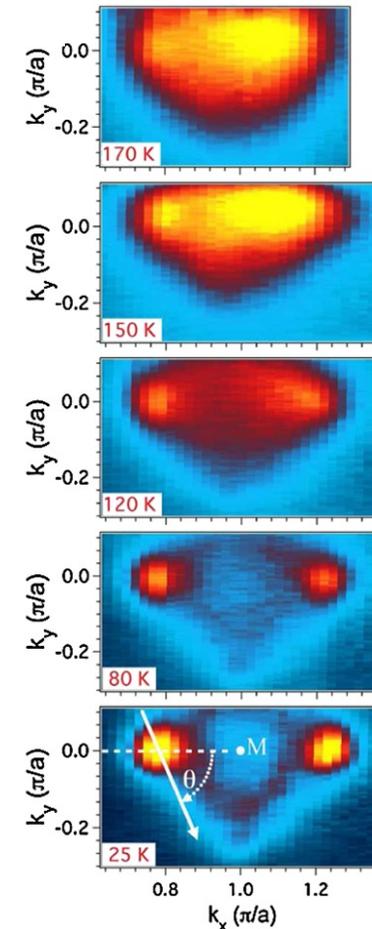
hole FS: circular  
electron FS: elliptic

ARPES: Liu et al. Nature Phys. 2010

# Fermi surface reconstruction



- imperfect nesting: residual Fermi surfaces
- Not all the bands are clearly resolved
- SDW gaps unclear
- More than simple band folding ?

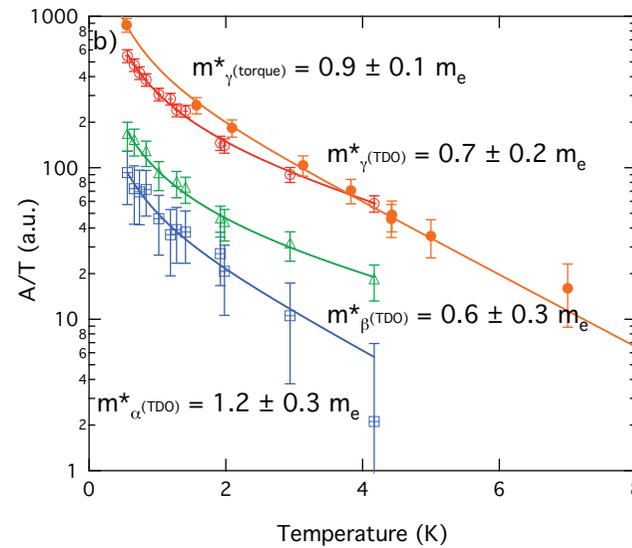
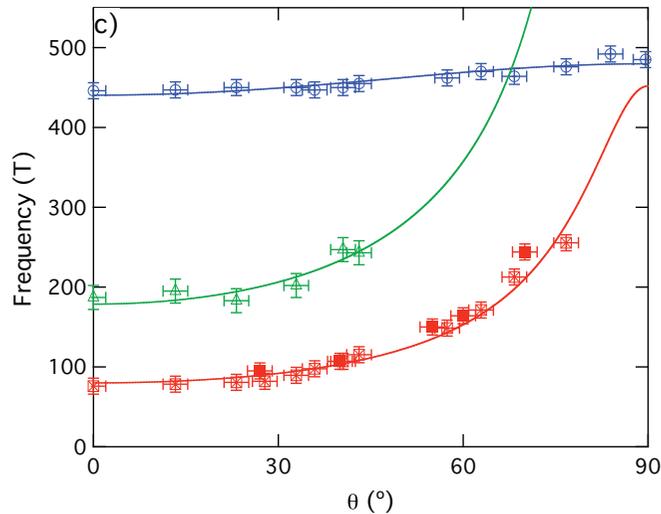
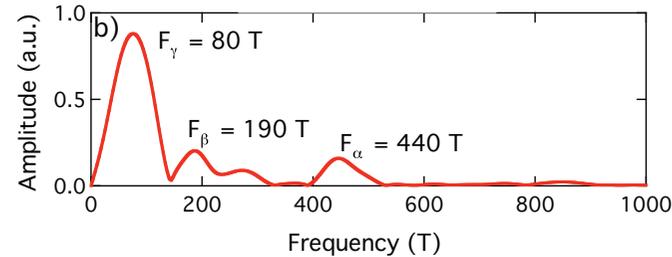


Richard et al. , *Phys. Rev Lett.* 104, 137001 (2010)

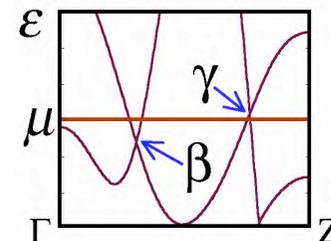
Liu et al. *Nature Phys.* 6, 419 (2010)

Ran et al. *Phys. Rev. B* 79, 014505 (2009)

# Fermi surface reconstruction: quantum oscillations (SdH)



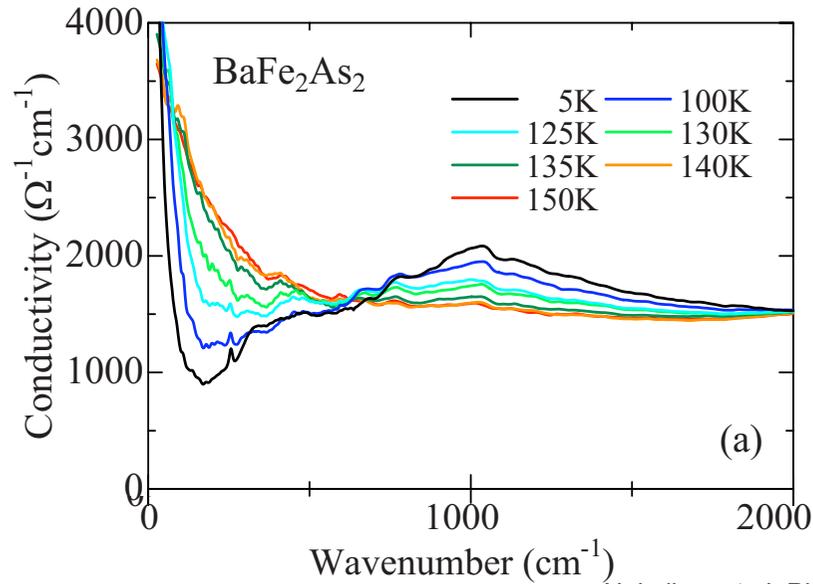
Analytis et al. Phys. Rev. B 80, 064507 (2009)



- very small FS area in the SDW phase (1.7%, 0.7% et 0.3% de ZB para): FS reconstruction
- one FS is isotropic and the other 2 anisotropic (cigar-shaped: Dirac point)

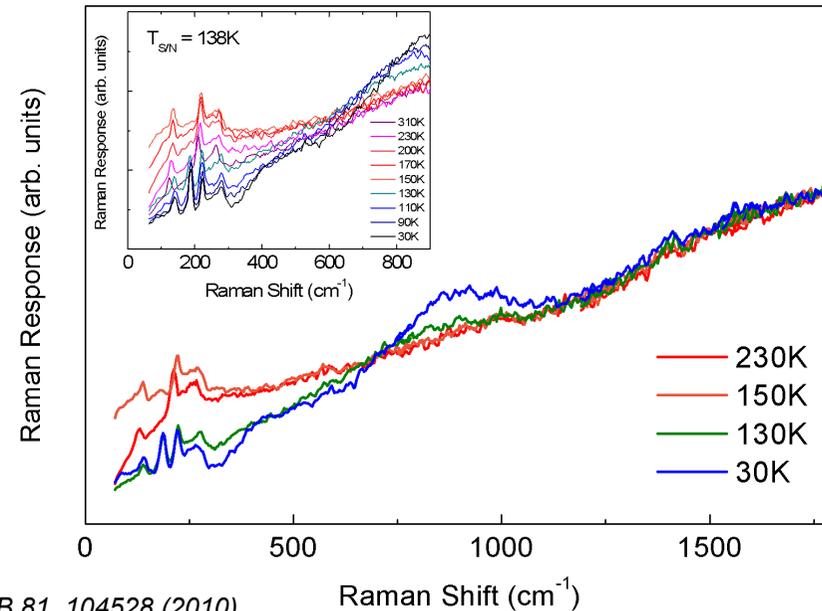
# Spin density wave gaps

## optical conductivity



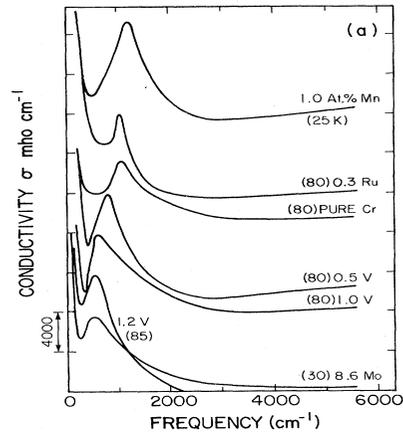
Nakajima et al. *Phys. Rev. B* 81, 104528 (2010)

## Raman scattering

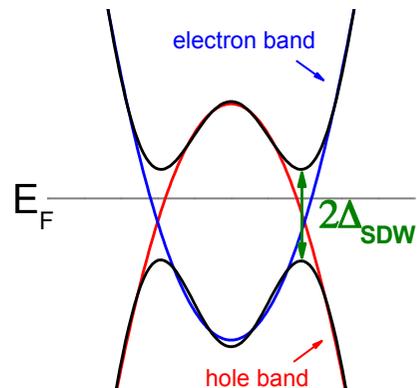


Chauvière et al. *Phys. Rev. B* 84, 104508 (2011)

## Cr alloys

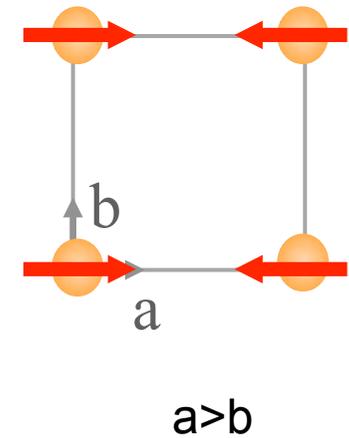
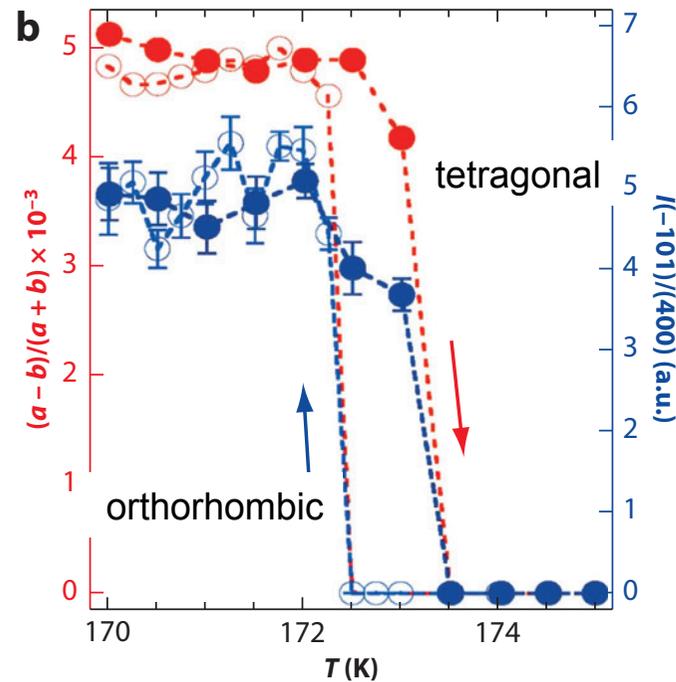
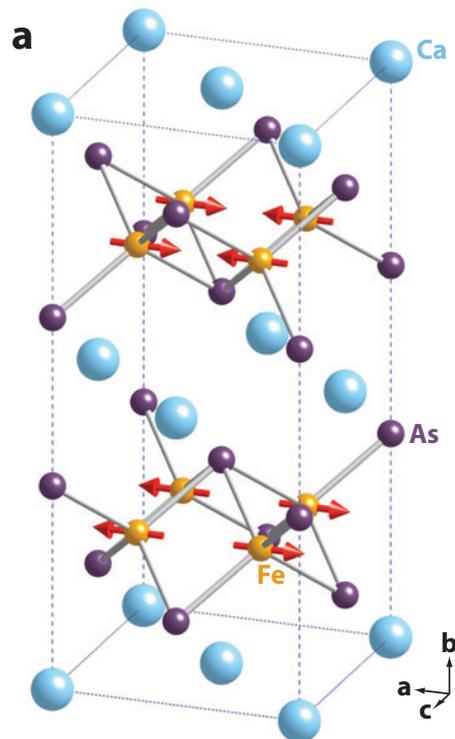


Barker et al. *Phys. Rev B* 1, 4378 (1970)



- opening of SDW gaps consistent with band folding
- residual Drude weight in the SDW state: incomplete gap

# Magneto-structural transition

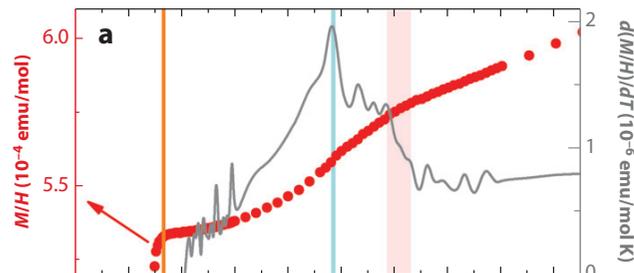


- first order in (Ca,Sr)-112 but second order in Ba-122
- orthorhombic distortion is less than 0.5%
- Spin driven structural transition ?

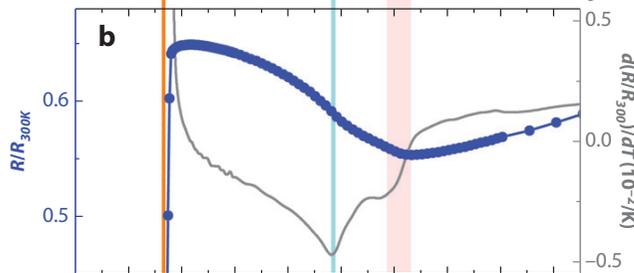
# Splitting of the transition in $\text{Ba}(\text{Fe}_{1-x}\text{Co}_x)_2\text{As}_2$

$x=0.047$

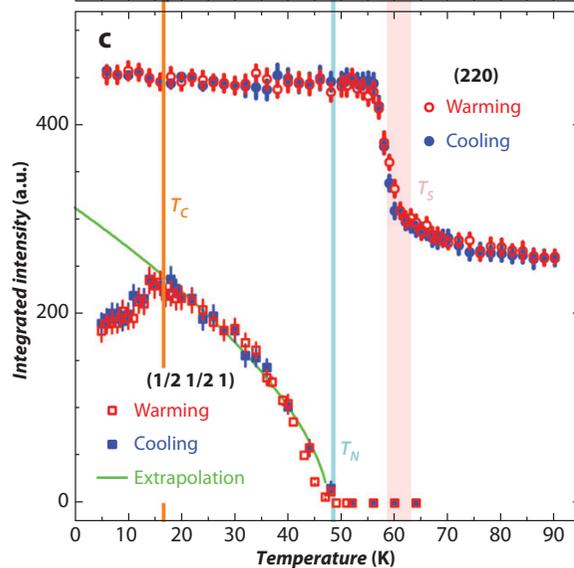
magnetization



transport

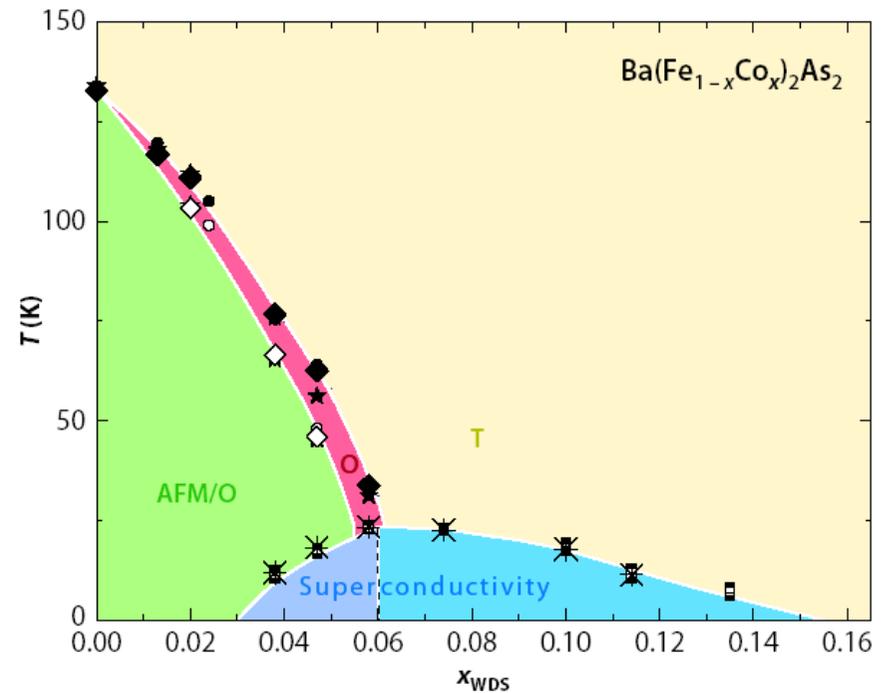
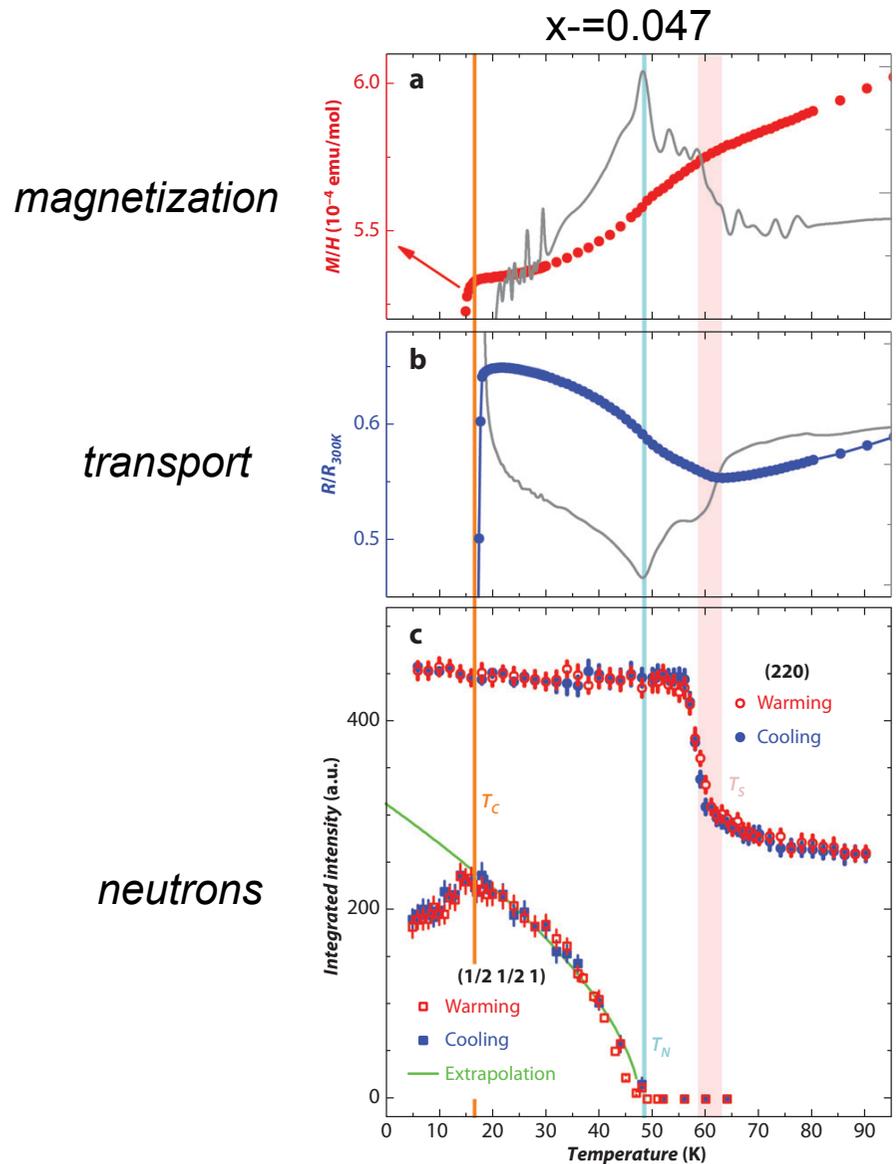


neutrons

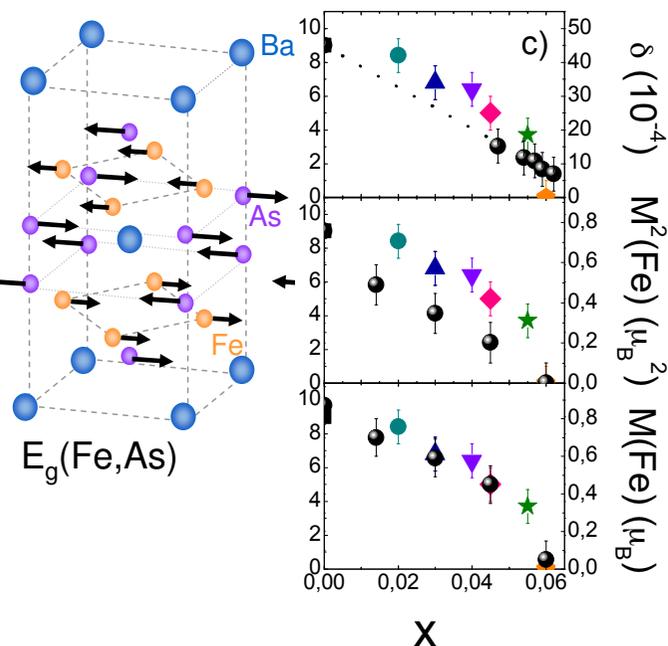
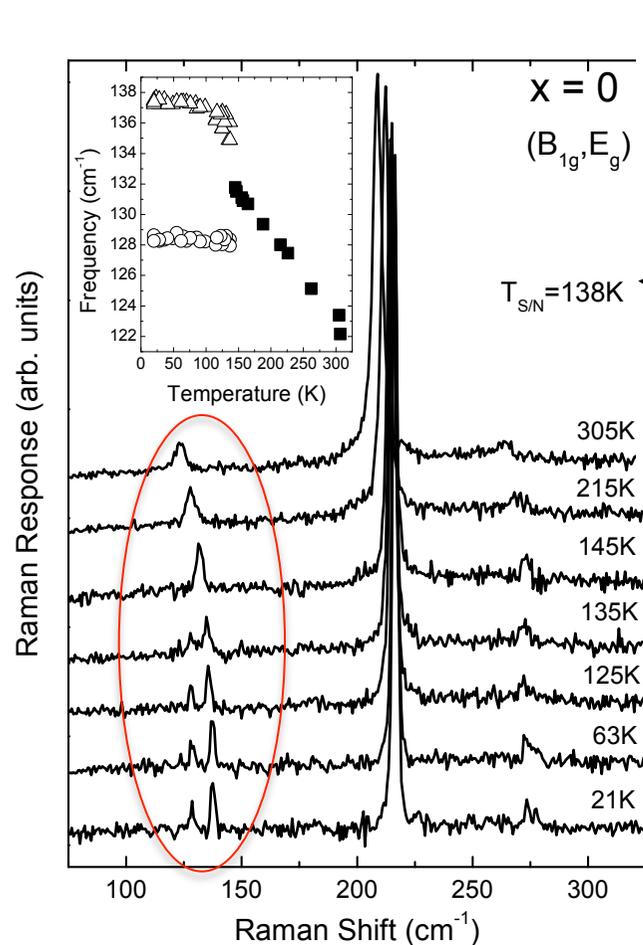


- magnetic and structural transitions split upon Co doping
- not observed in all systems (disorder?)
- fluctuating magnetic domains ?

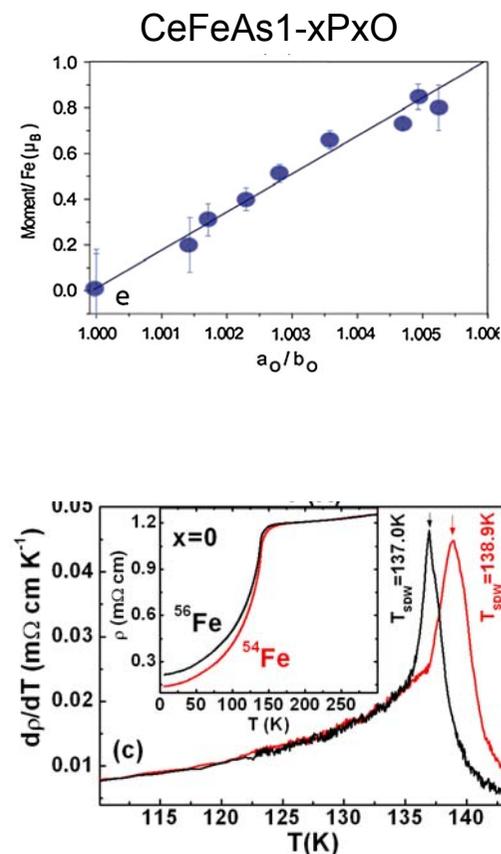
# Splitting of the transition in $\text{Ba}(\text{Fe}_{1-x}\text{Co}_x)_2\text{As}_2$



# Spin-lattice coupling



Chauvière et al. *Phys. Rev. B* 80, 094504 (2009)  
 de la Cruz et al., *Phys. Rev. Lett.* 104, 017204 (2010)  
 Liu et al. *Nature* 459, 64-67 (2009)

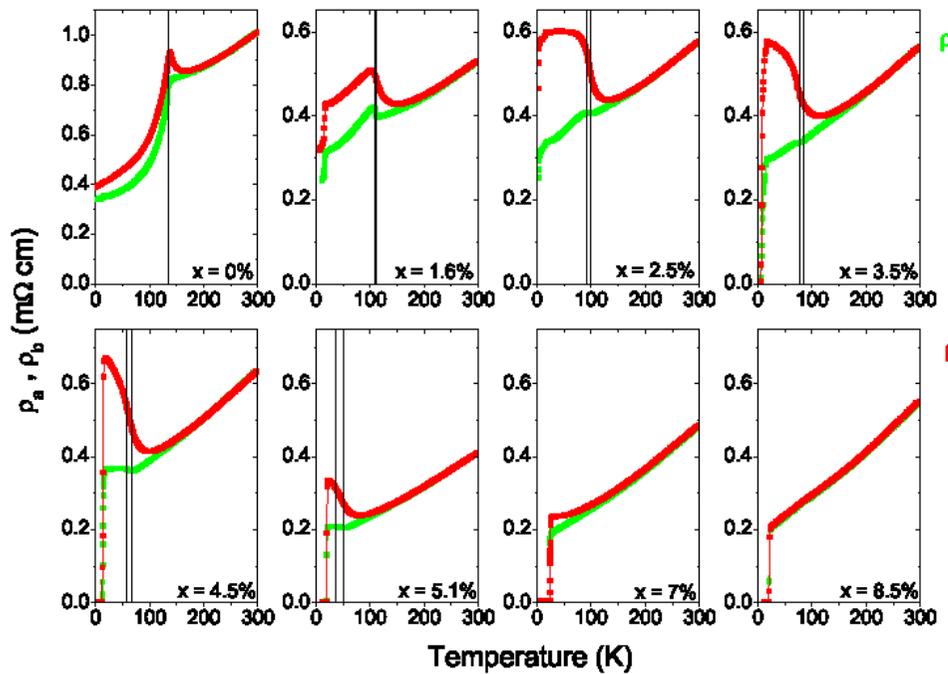


isotope effect on  $T_N$

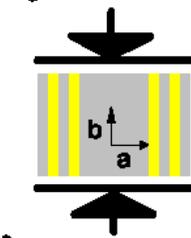
- phonon splitting much larger than expected from lattice distortion alone
- strong spin-phonon coupling: modulation of the exchange constant by atomic motion
- linear relation between lattice distortion, phonon splitting and magnetic moment

# Anisotropic transport

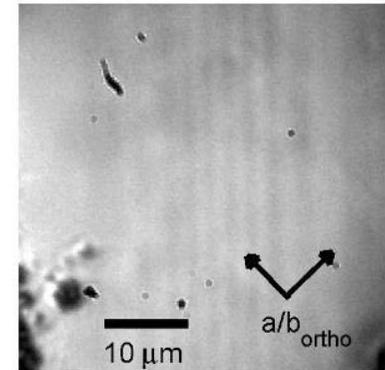
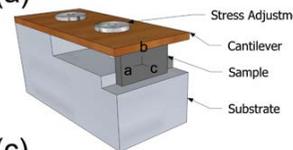
transport in mechanically detwinned crystals



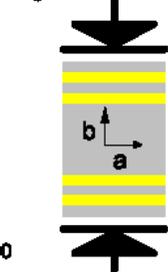
$\rho_a$  Configuration



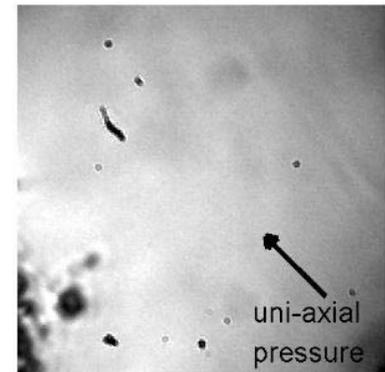
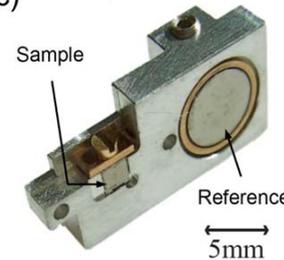
(a)



$\rho_b$  Configuration



(c)

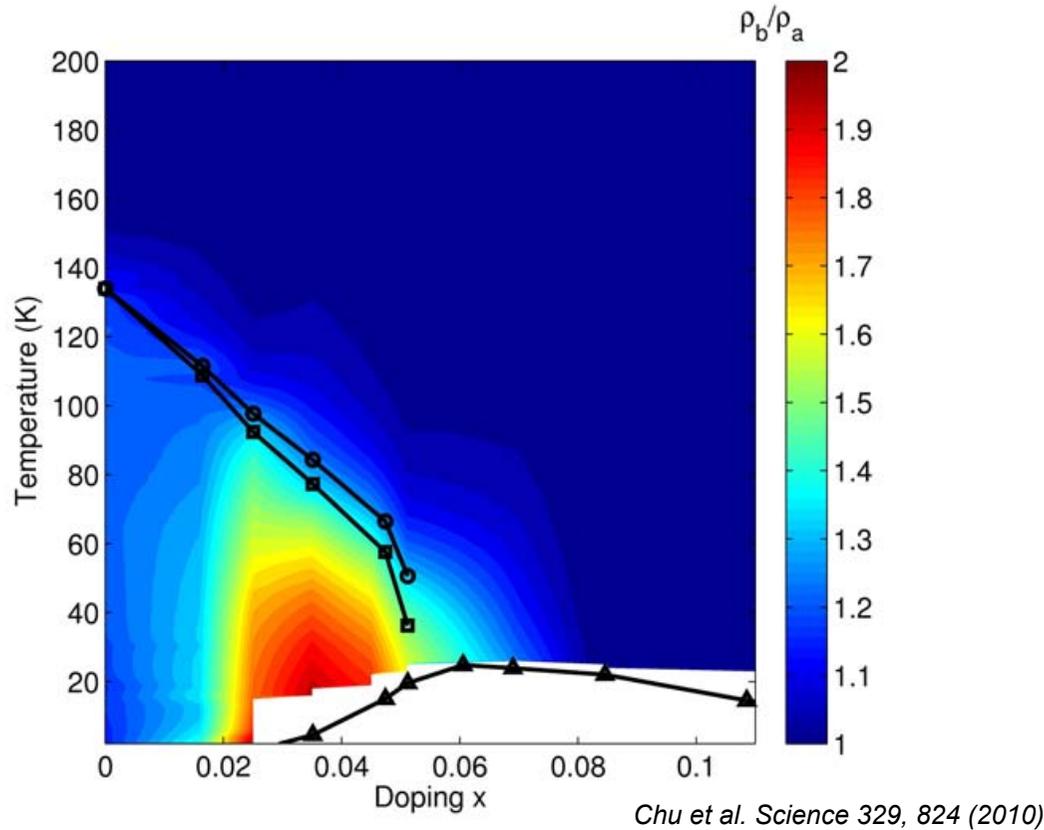


Chu et al. Science 329, 824 (2010)

- very large transport anisotropy at low temperature
- extremely strong sensitivity of properties to stress above  $T_S$ : nematic susceptibility

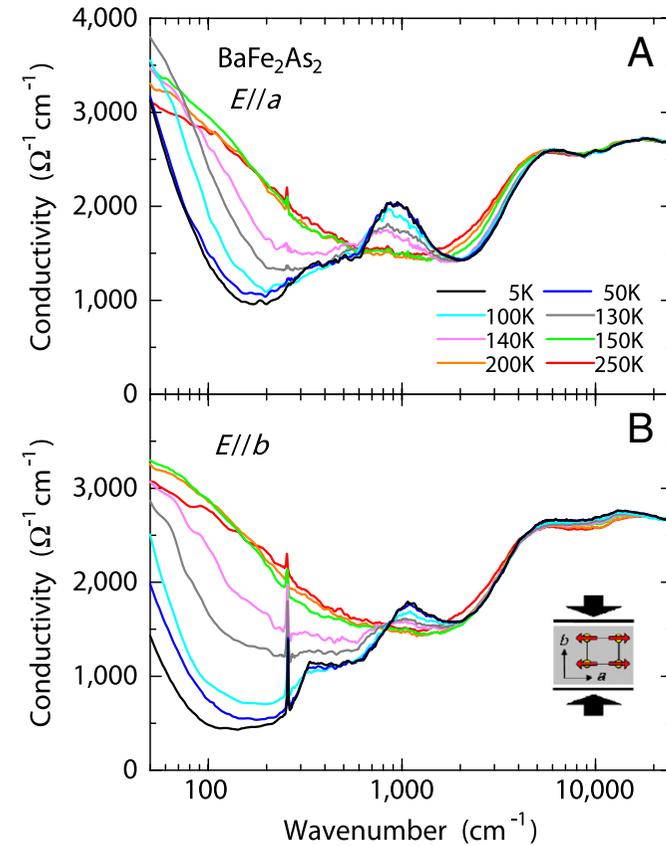
# Nematic order ?

## transport in mechanically detwinned crystals



anisotropy (or nematic susceptibility?) is maximum around onset of SC order

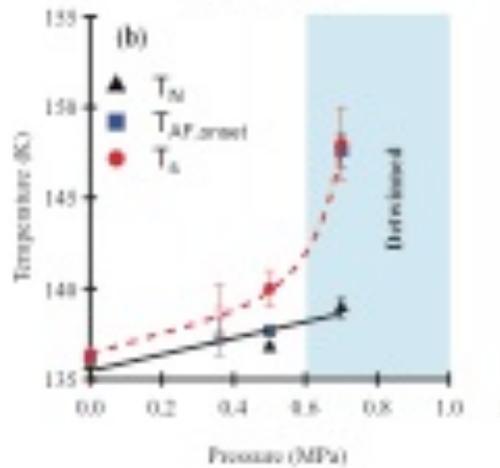
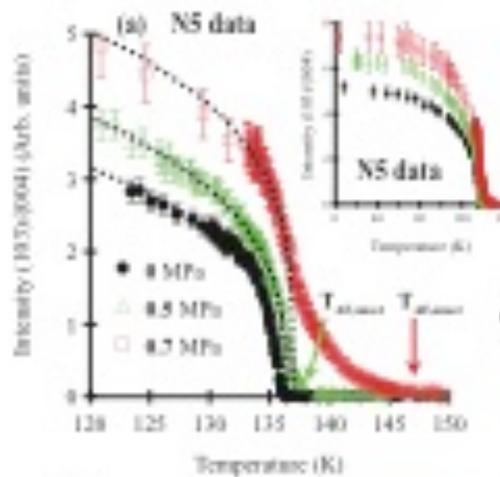
## optical conductivity



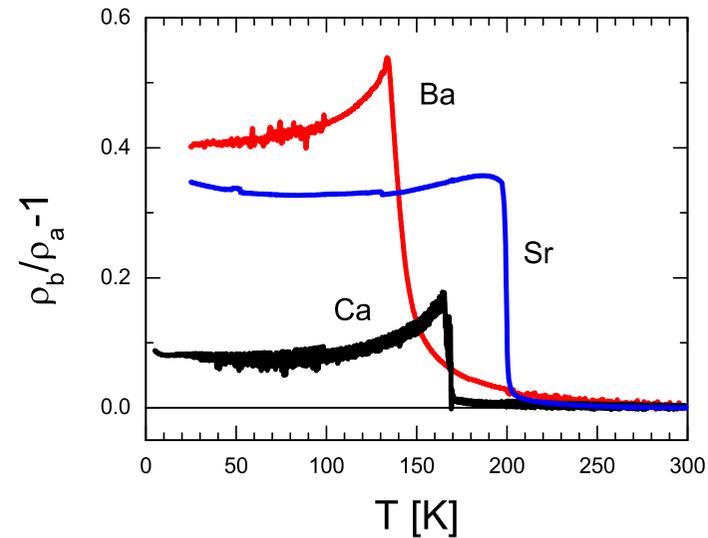
strong reduction of Drude weight along b-direction only

**strong in-plane anisotropy of the electronic properties**

# Nematic order ?



Dimai et al. arXiv (2011)



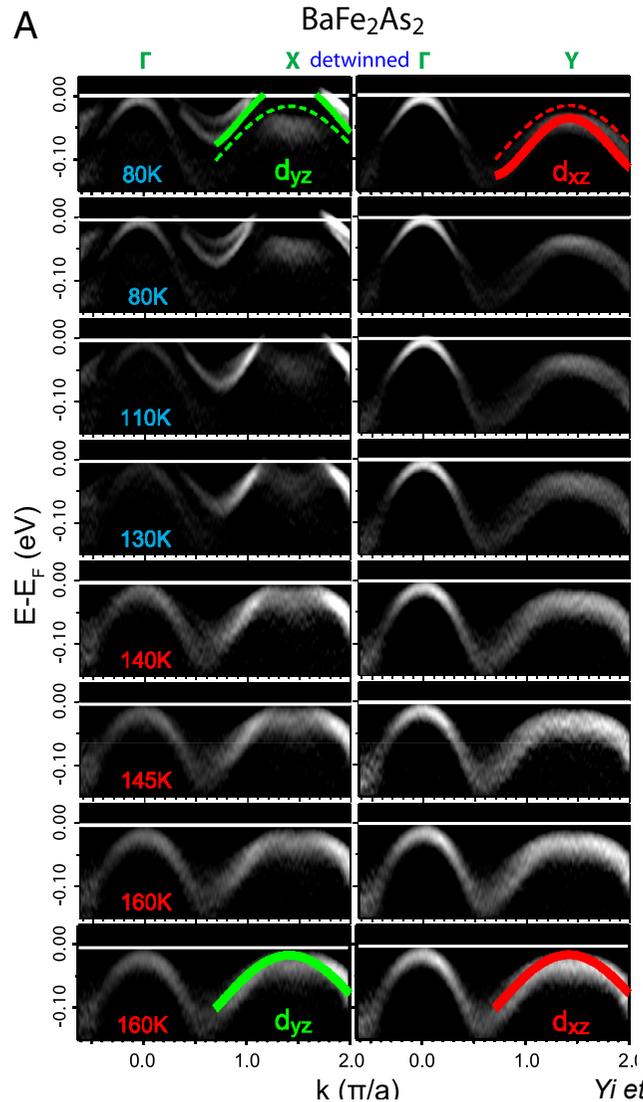
Blomberg et al. Phys. Rev. B 83, 134505 (2011)

- no anisotropy above  $T_S$  for Ca122 and Sr122
- first order vs second order transition
- nematic phase above  $T_S$  is not generic
- Fluctuating magnetic domain

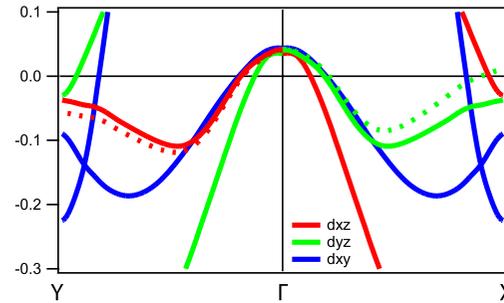
small stress induced large shift of  $T_{S,N}$

# Orbital dependent band splitting

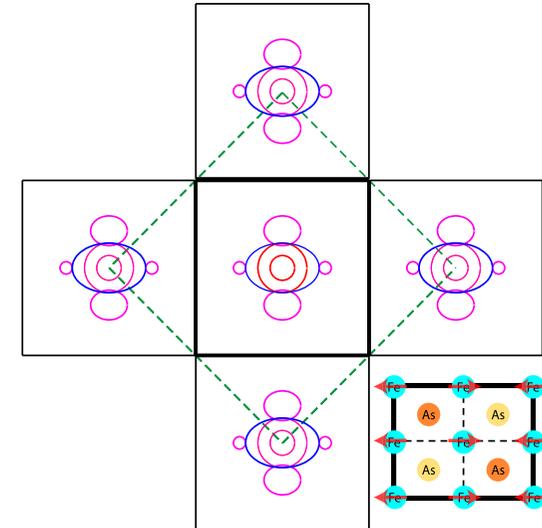
ARPES on detwinned crystals



Orbital-Dependent Symmetry Breaking



Orthorhombic/SDW



- $C_4$  symmetry is broken
- splitting larger than expected from structural distortion
- orbital degrees of freedom may play a role in the magneto-structural transition

# Magneto-structural coupling

what is the driving force behind the M/S transition? a chicken and egg problem

- Magnetic driven structural distortion:** magnetic fluctuations drive the distortion via magneto-elastic coupling or via Ising nematic fluctuations that break  $C_4$  symmetry above  $T_S$  ( $\varphi = \mathbf{m}_1 \cdot \mathbf{m}_2$ ) (« nemato-elastic » coupling)

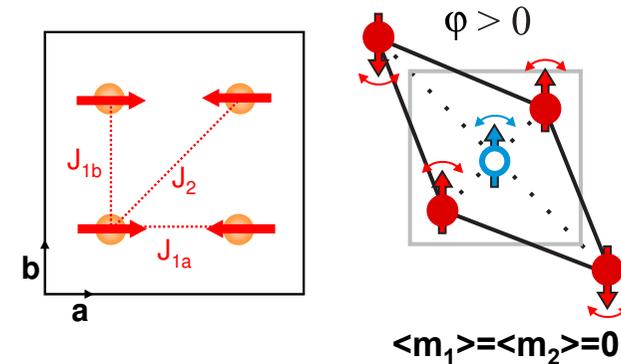
*T. Yildirim, Phys. Rev. Lett. 101, 057010 (2008)*

*Fernandes et al., Phys. Rev. Lett. 105, 157003 (2010)*

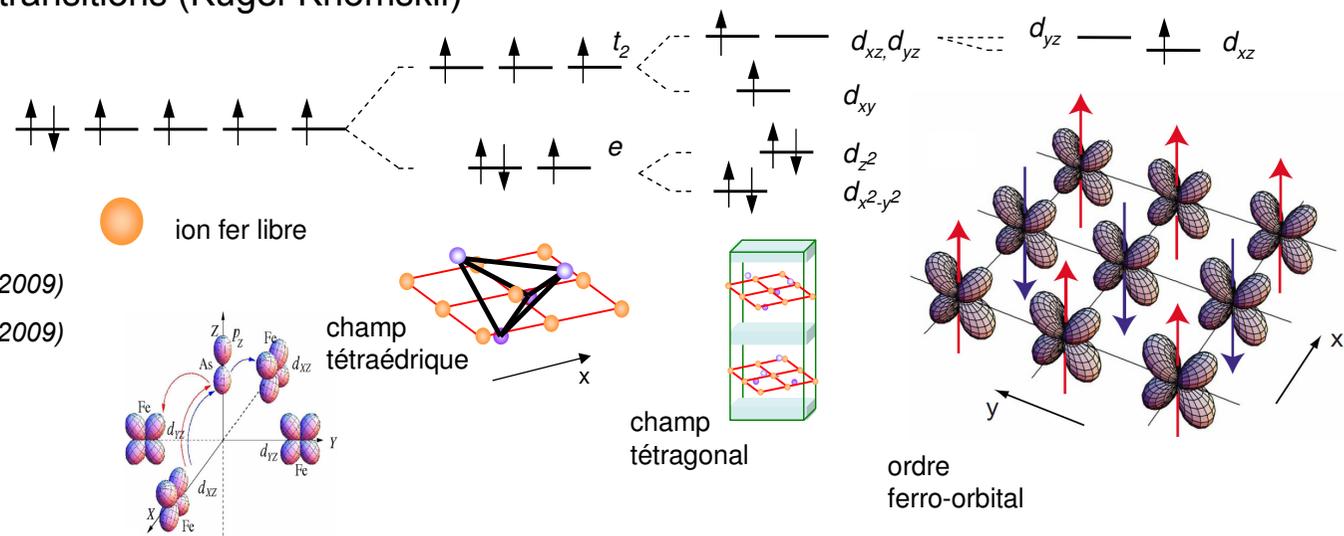
*Chandra et al., Phys. Rev. Lett. 64, 88 (1990)*

*A. Cano et al., Phys. Rev. B 82, 020408(R) (2010)*

*I. Paul, Phys. Rev. Lett. 107, 047004 (2011)*



- Orbital ordering:** difference in  $d_{xz}$  and  $d_{yz}$  occupation drives both magnetic and structural transitions (Kugel-Khomskii)

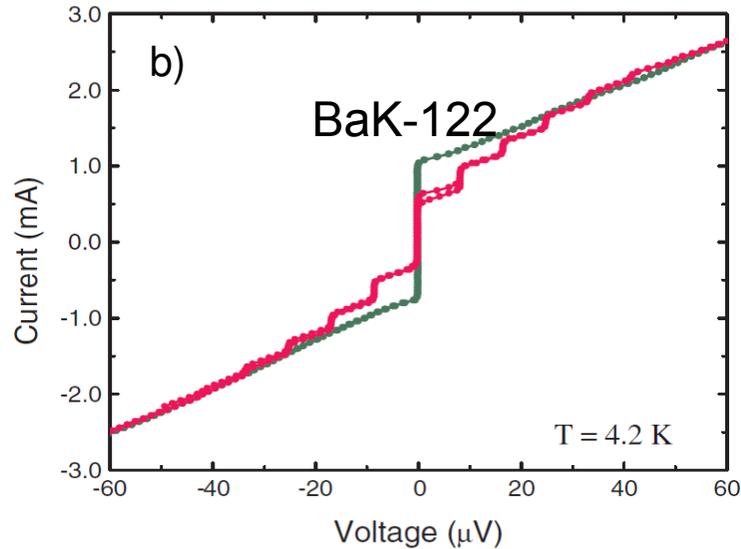


*Kruger et al. Phys. Rev. B 79, 054504 (2009)*

*Lv et al. Phys. Rev. B 80, 224506 (2009)*

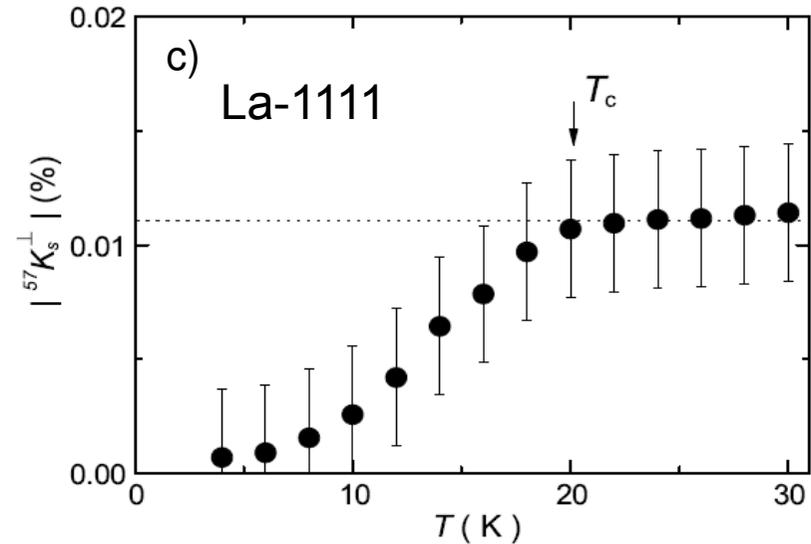
# Superconducting state

AC Josephson effect: charge  $2e$



Zhang et al. Phys. Rev. Lett. 102, 147002 (2008)

NMR: spin-singlet



Teresaki et al. JPSJ 78, 13701 (2008)

Electron-phonon coupling too weak to explain  $T_c > 10\text{K}$

Boeri et al. Physica C 469, 628-634 (2009)

# Gap structure and spin fluctuation pairing

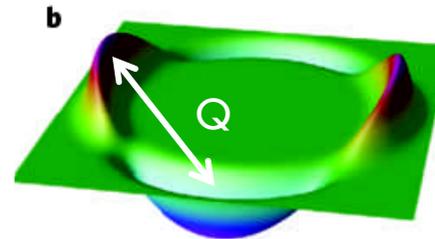
- weak electron-phonon coupling
- proximity of AF order suggests spin fluctuation pairing

$$\Gamma_s(\mathbf{k}, \mathbf{k}') = \frac{3}{2}U^2 \frac{\chi_0(\mathbf{q})}{1 - U\chi_0(\mathbf{q})} \quad \text{singlet repulsive interaction (Stoner-Hubbard)}$$

$$\Delta_{\mathbf{k}} = - \sum_{\mathbf{k}'} \Gamma_s(\mathbf{k}, \mathbf{k}') \frac{\Delta_{\mathbf{k}'}}{2E_{\mathbf{k}'}} \tanh \frac{E_{\mathbf{k}'}}{2T}, \quad \text{solution allowed if } \Delta \text{ changes sign}$$

Berk and Schrieffer. *Phys.Rev.Lett.* 17, 433 (1966)  
 Scalapino et al., *Phys. Rev. B* 34, 8190 (1986)

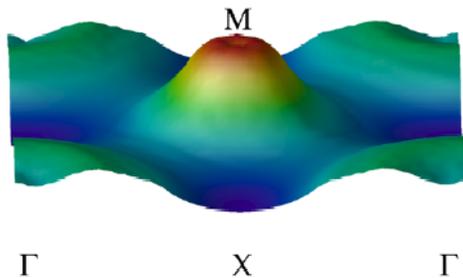
**In cuprates:** susceptibility is peaked at  $Q=(\pi,\pi)$



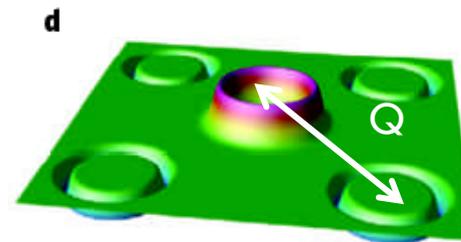
d-wave gap

Scalapino. *Phys. Rep.* 250, 329 (1995)

**In pnictides:** susceptibility is peaked at  $Q=(\pi,0)$



$$\Delta_i = \sum_j \Lambda_{ij} \Delta_j F(\Delta_j, T)$$



$s^{+-}$  gap

Suhl et al. *Phys. Rev. Lett.* 3, 552 (1959)  
 Kuroki et al. *Phys.Rev.Lett.* 101, 087004 (2008)  
 Mazin et al. *Phys. Rev. Lett.* 101, 057003 (2008)

**alternative model:** orbital fluctuations theory predicts  $s^{++}$

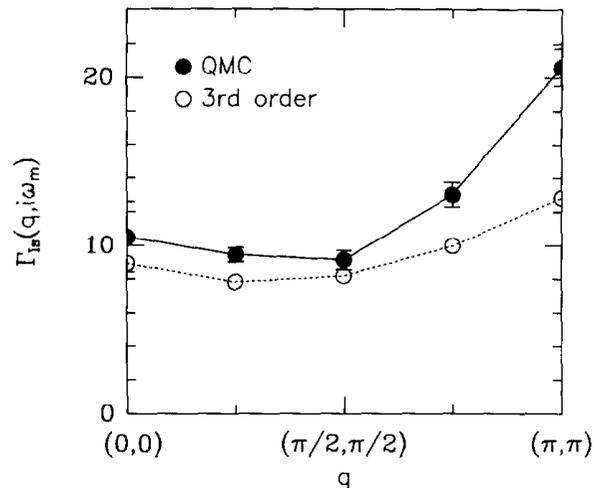
Saito et al. *Phys.Rev. B* 82, 144510 (2010)

# Gap structure and spin fluctuation pairing

- weak electron-phonon coupling
- proximity of AF order suggests spin fluctuation pairing

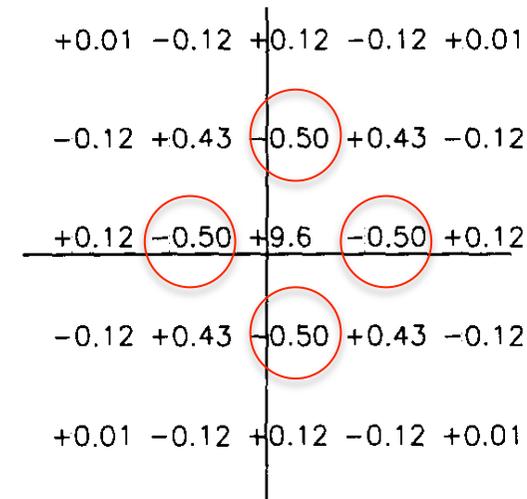
$$\Gamma_s(\mathbf{k}, \mathbf{k}') = \frac{3}{2}U^2 \frac{\chi_0(\mathbf{q})}{1 - U\chi_0(\mathbf{q})} \quad \text{singlet repulsive interaction (Stoner-Hubbard)}$$

*Berk and Schrieffer. Phys.Rev.Lett. 17, 433 (1966)*  
*Scalapino et al., Phys. Rev. B 34, 8190 (1986)*



Pairing interaction for cuprates  
 (Monte Carlo and 3<sup>rd</sup> order perturbation theory)  
 Repulsive!

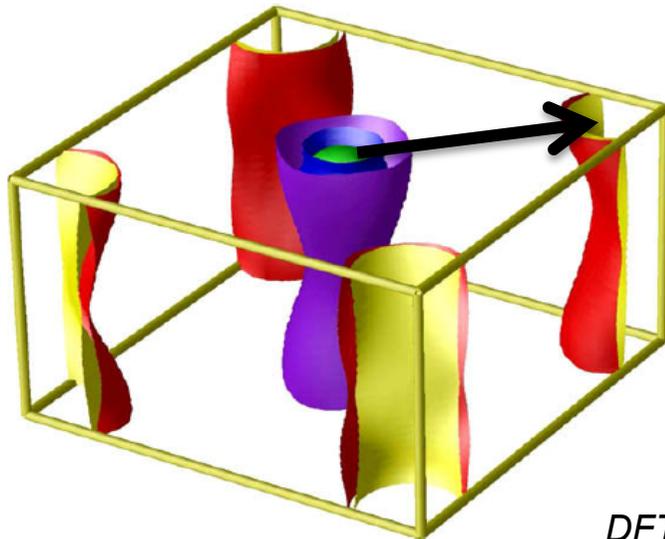
$$\Gamma_{Is}(\mathbf{l}) = \frac{1}{N} \sum e^{i\mathbf{q}\cdot\mathbf{l}} \Gamma_{Is}(\mathbf{q}).$$



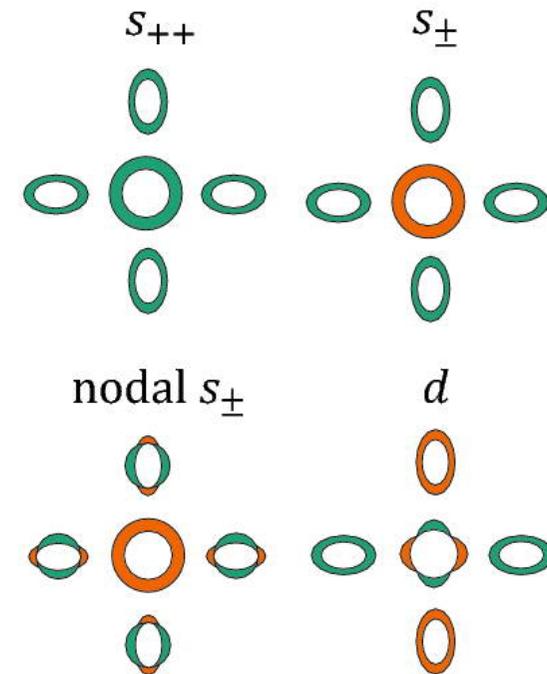
Pairing interaction is attractive for specific regions  
 in real space

# Gap symmetry vs gap structure

- spin fluctuation pairing naturally leads to  $s^+$  symmetry in pnictide
- Coulomb interband interaction is responsible for both SDW and SC phase
- gap symmetry does not tell much about presence of nodes



*DFT calculations*  
Mazin, *Physica C* **469**, 614 (2009)

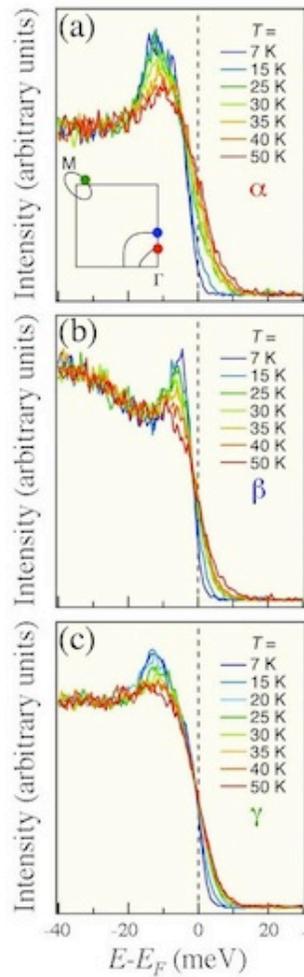


**same symmetry but different gap structure!**

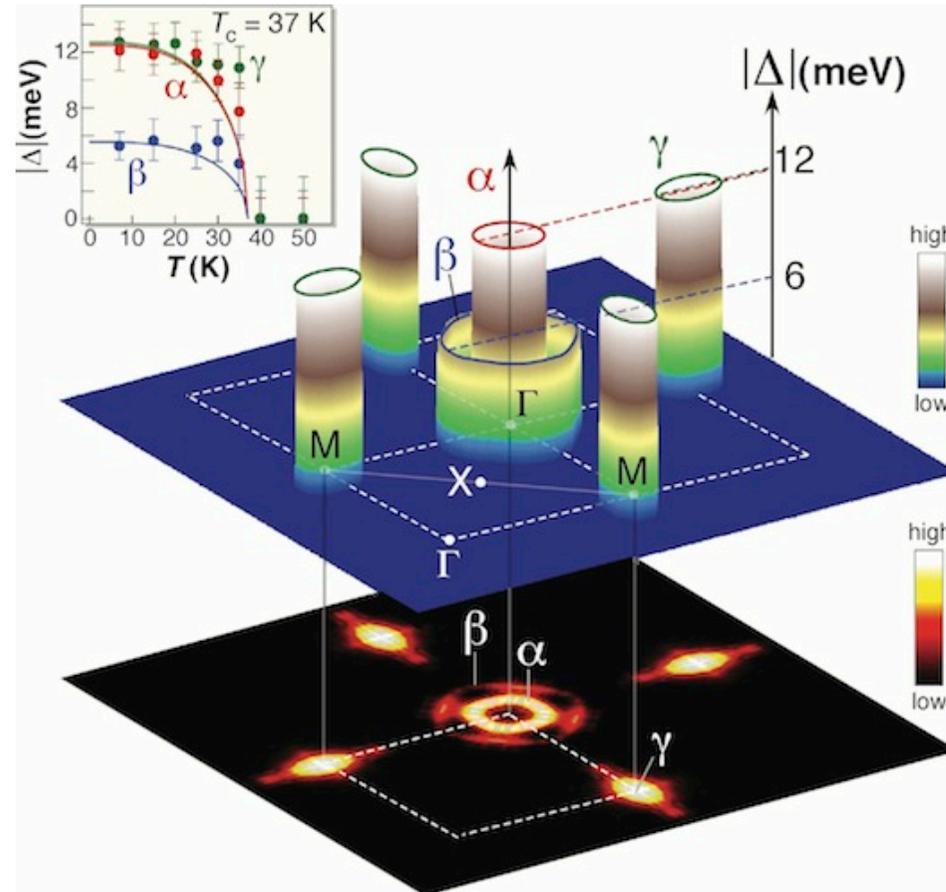
- possible source of anisotropy around FS: orbital content, intraband interaction, FS topology
- crucial role of nesting properties

*Maier et al. Phys.Rev. B* **79**, 224510 (2009)  
*Kuroki et al. Phys. Rev. B* **79**, 224511 (2009)

# Multiple gaps in optimally-doped K-Ba122



$T_c = 37\text{K}$

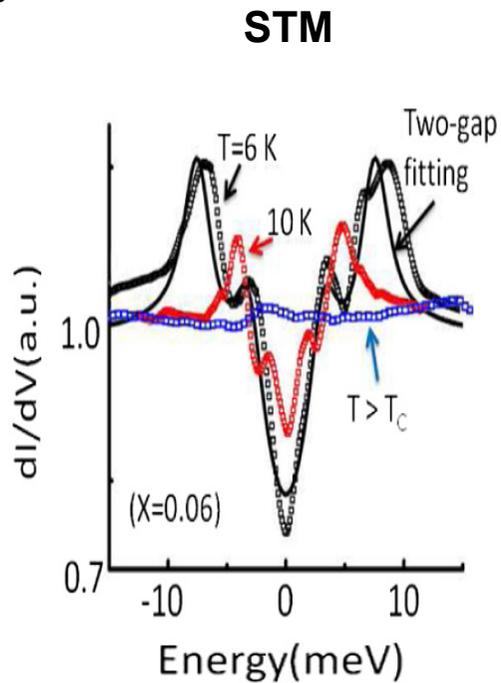


Ding et al. *Europhys. Lett.* 83, 47001 (2008)

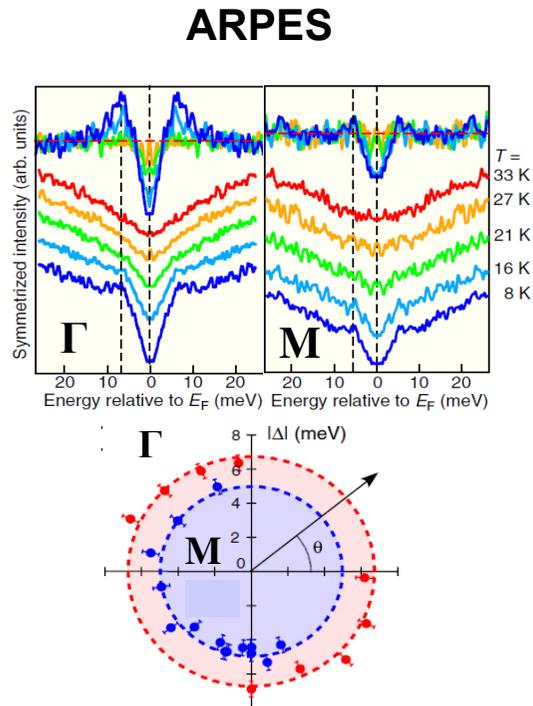
**FS dependent pairing strength ( $3.5 - 7 k_B T_c$ )**

# Multiple gaps in optimally-doped Co-Ba122

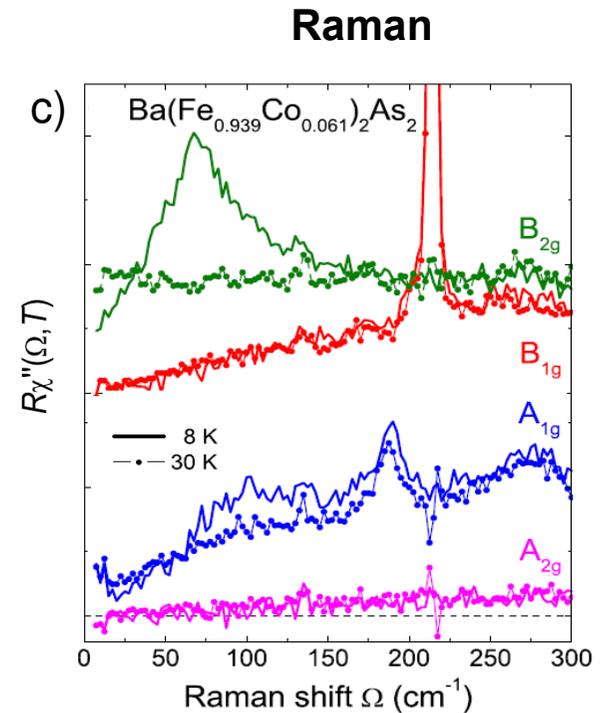
$T_c = 25\text{K}$



Teague et al. Phys. Rev. Lett. 106, 087004 (2011)



Terashima et al. PNAS 106, 7330 (2009)

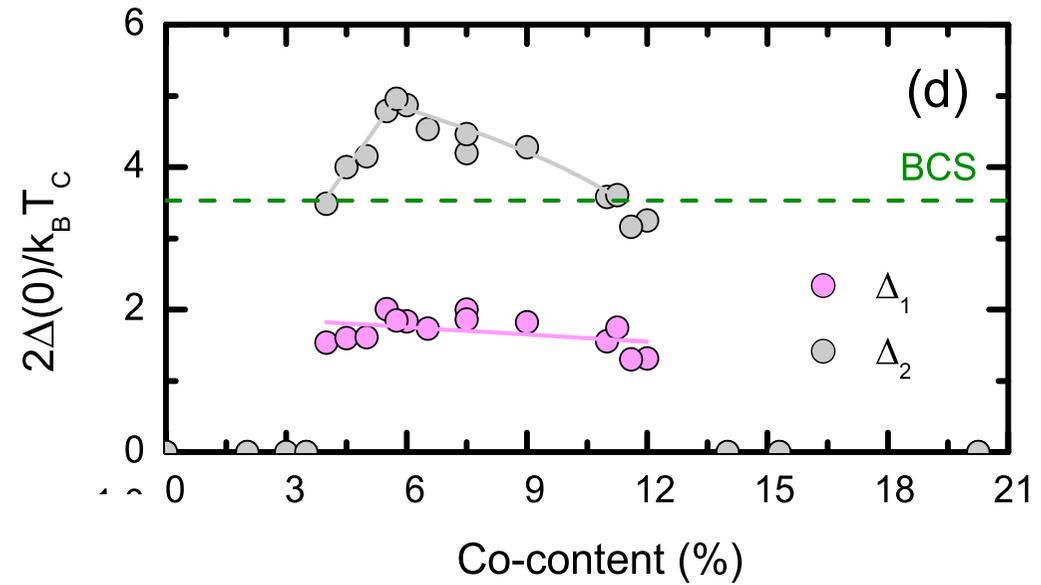
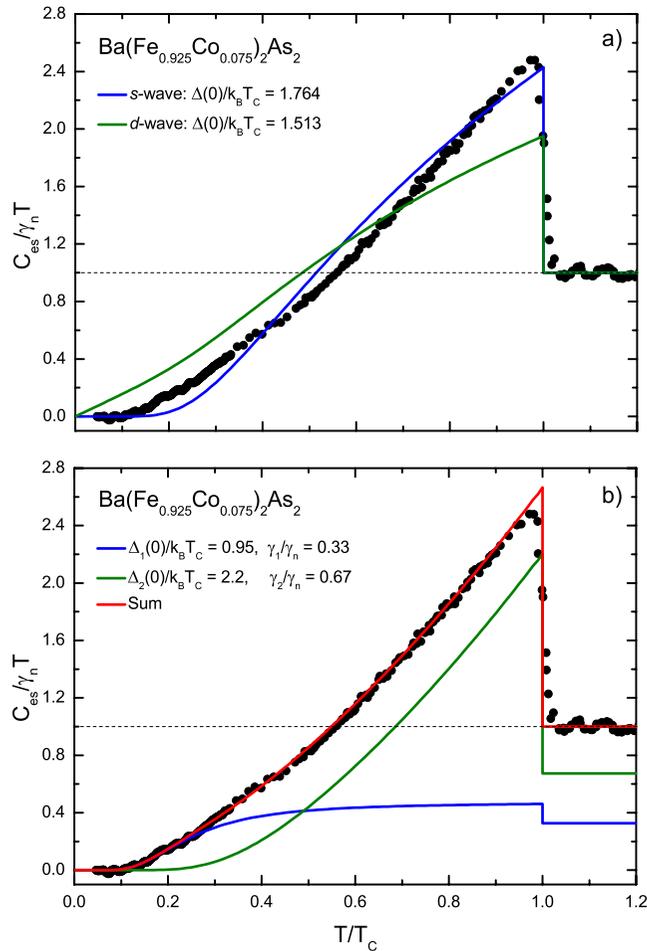


Muschler et al. Phys. Rev. B 80, 180510 (2009)

- at least 2 gaps around electron and hole pockets
- up to three different gaps have been reported

$$\frac{2\Delta_e}{k_B T_c} \approx 4 \quad \frac{2\Delta_h}{k_B T_c} \approx 6$$

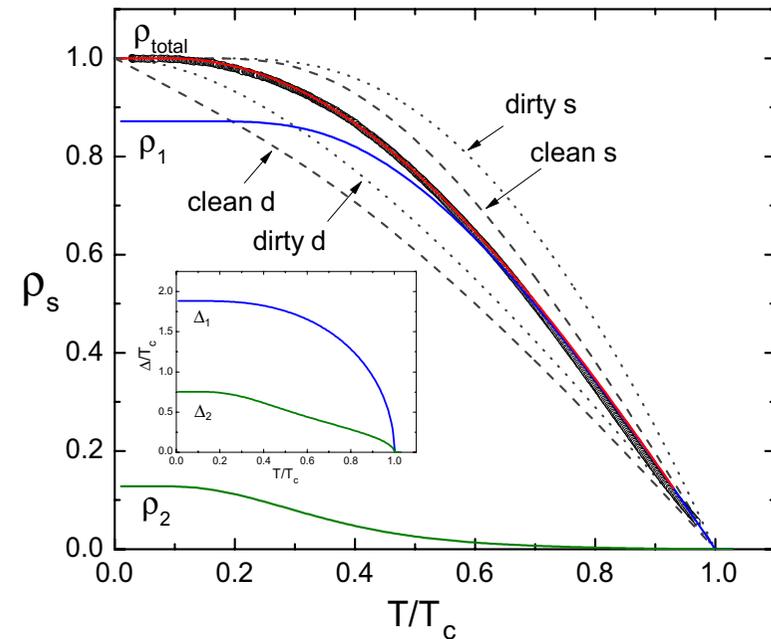
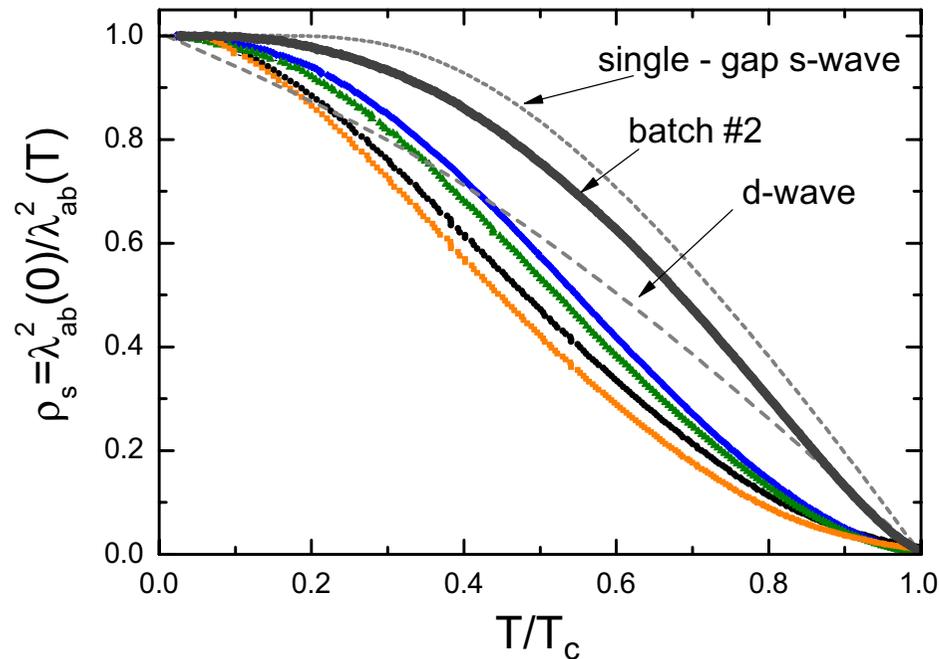
# Specific Heat in Co-Ba122



Hardy et al. Phys. Rev. B 81, 060501 (2010)  
 Hardy et al. Europhys. Lett. 91, 47008 (2010)

- significantly smaller gaps: one smaller than BCS weak coupling ratio one bigger
- role of anisotropy?

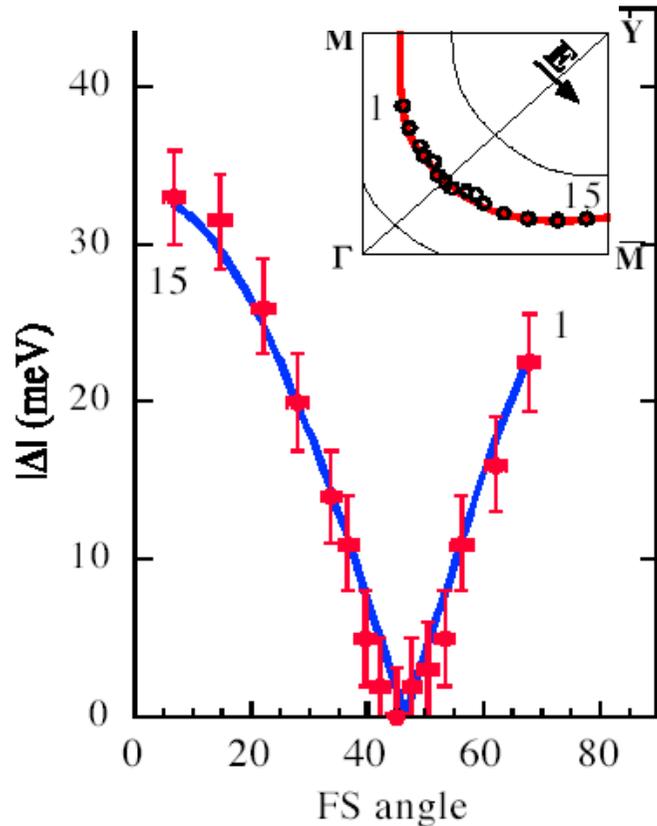
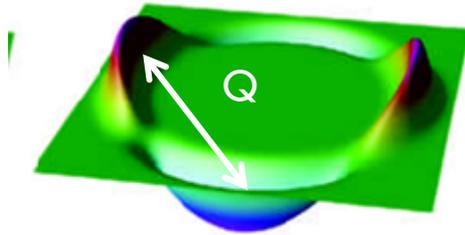
# London penetration depth in Co-Ba122



Prozorov et al. Rep. Prog. Phys.. 74, 124505 (2011)

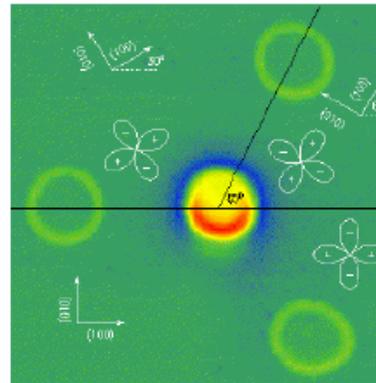
- significantly smaller gaps: one smaller than BCS weak coupling ratio one bigger
- fit must be done self-consistently: one cannot assume two independent BCS  $T$  dependences
- different techniques may be sensitive to different FS (effective mass, Fermi velocity....)

# Probing the phase - Cuprates: reminder



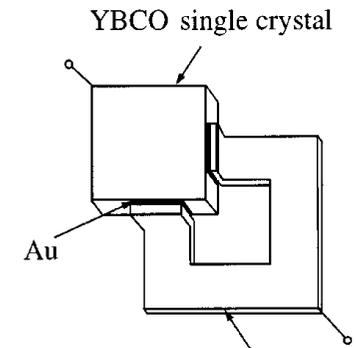
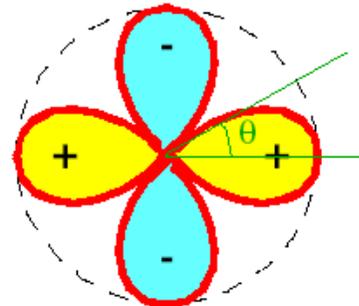
tricristal experiment

Half-Integer Flux Quantum Effect



crystal orientations:  $\pi$  ring

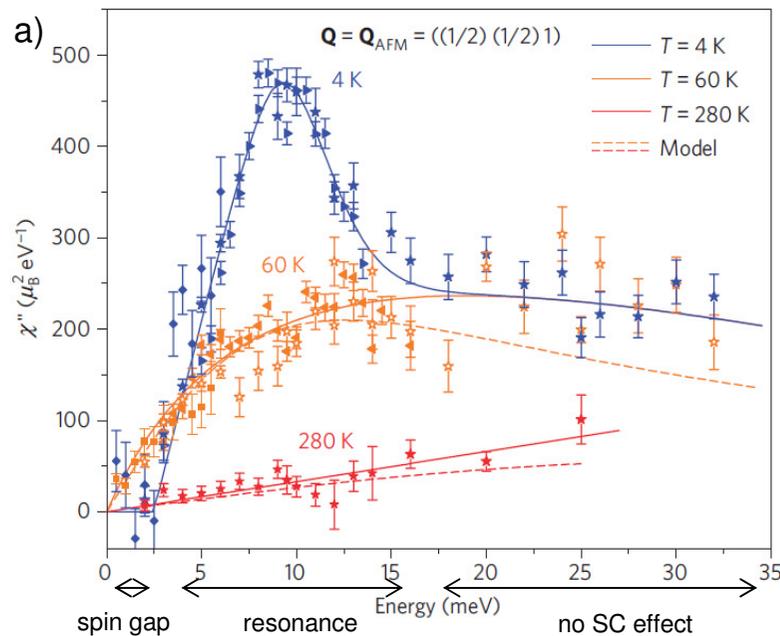
$d_{x^2-y^2}$



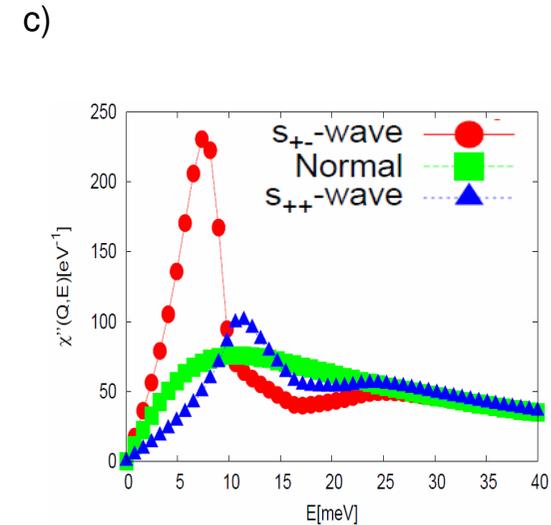
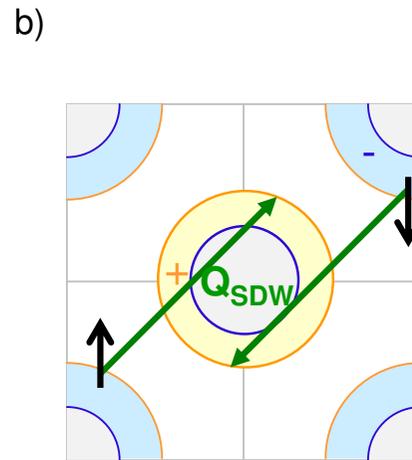
# Neutron resonance in Co-Ba122

$T_c = 25\text{K}$

## Spin excitation spectrum in SC state



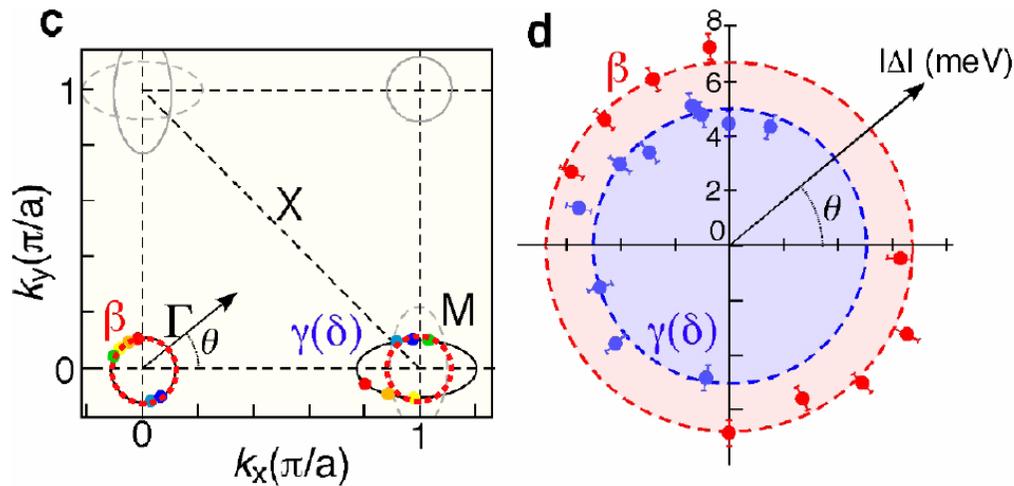
Christianson et al. *Nature* 456, 930 (2008)  
 Isonov et al. *Nature Phys.* 6, 178 (2010)



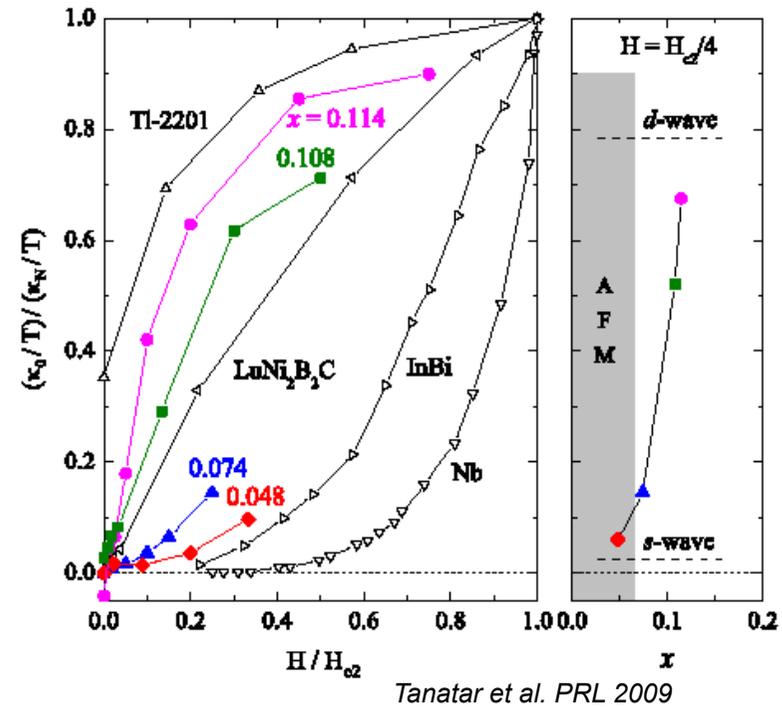
Korshunov et al. *Phys.Rev.B* 81, 024511 (2009)  
 Mazin et al. *Phys. Rev. Lett.* 101, 057003 (2008)

- collective spin excitation below  $2\Delta$  at  $Q_{AF}$
- fingerprint of a sign changing gap and residual AF fluctuations
- observed in various families (11, 122, 1111...) and other SC: cuprates; heavy fermions...
- no truly conclusive phase sensitive test up to now (phase shift in Josephson loops, qp interferences...)

# Gap anisotropy in Co-Ba122



Terashima et al. PNAS 2009



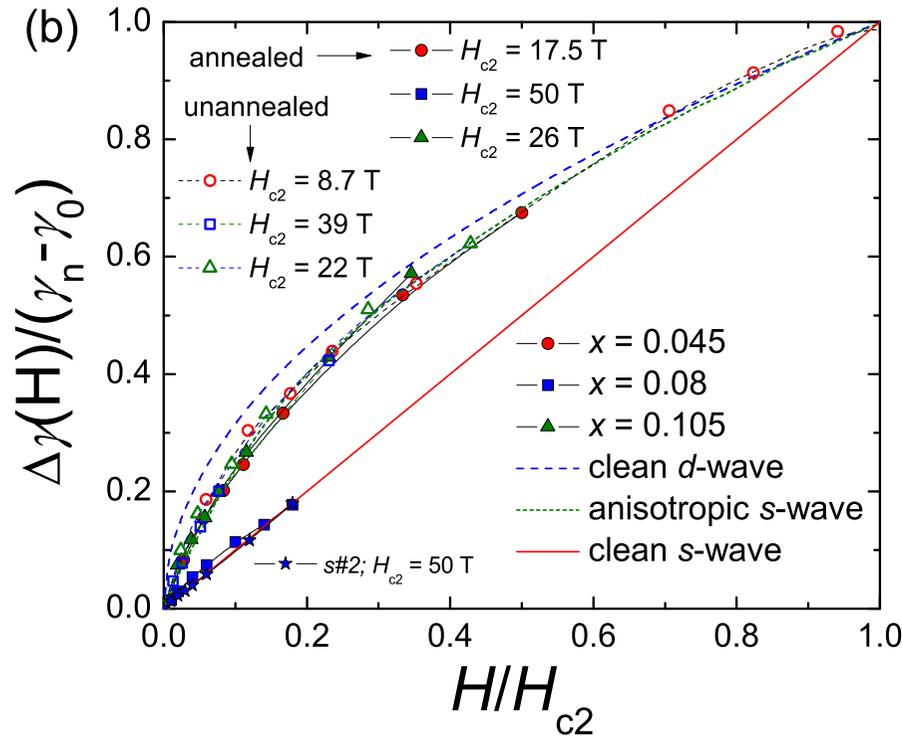
Tanatar et al. PRL 2009

ARPES sees isotropic and large gaps

Thermal conductivity: anisotropic gap or very small gap (but no nodes)

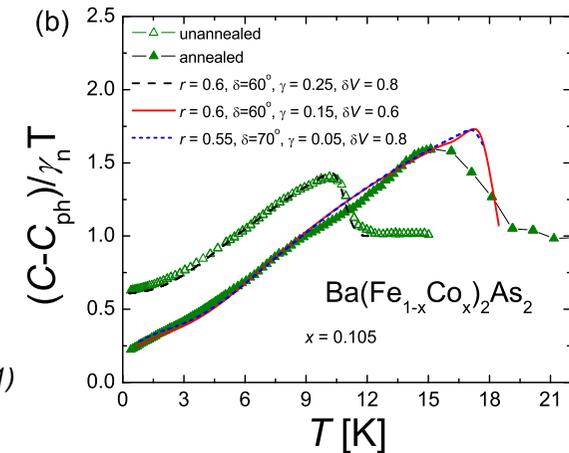
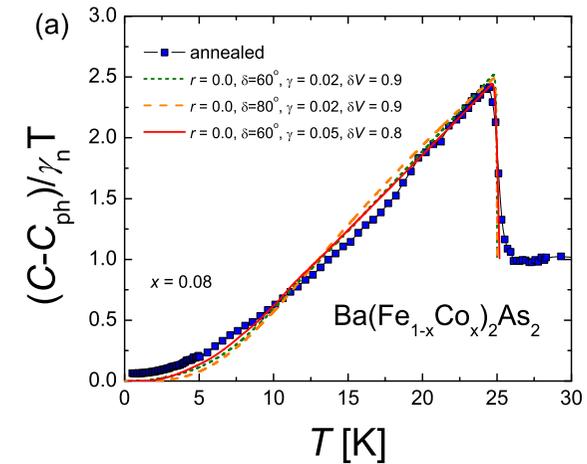
- Surface vs bulk issue?
- ARPES resolution?

# Gap anisotropy in Co-Ba122



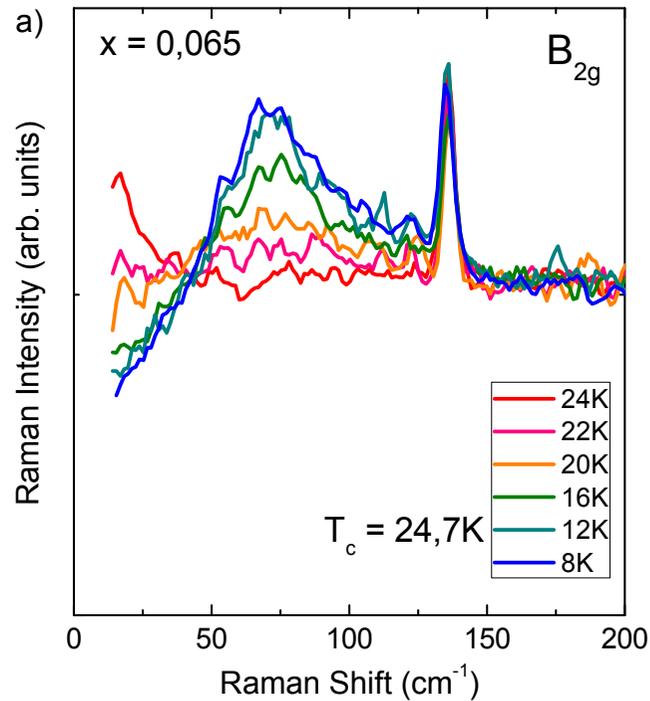
Gofryk et al. Phys. Rev. B 83, 064513 (2011)

- Field dependence of the low temperature residual term of electronic specific heat: anisotropic gap but doping dependent!
- Optimal doping: full gaps
- Under and overdoped: significant anisotropy

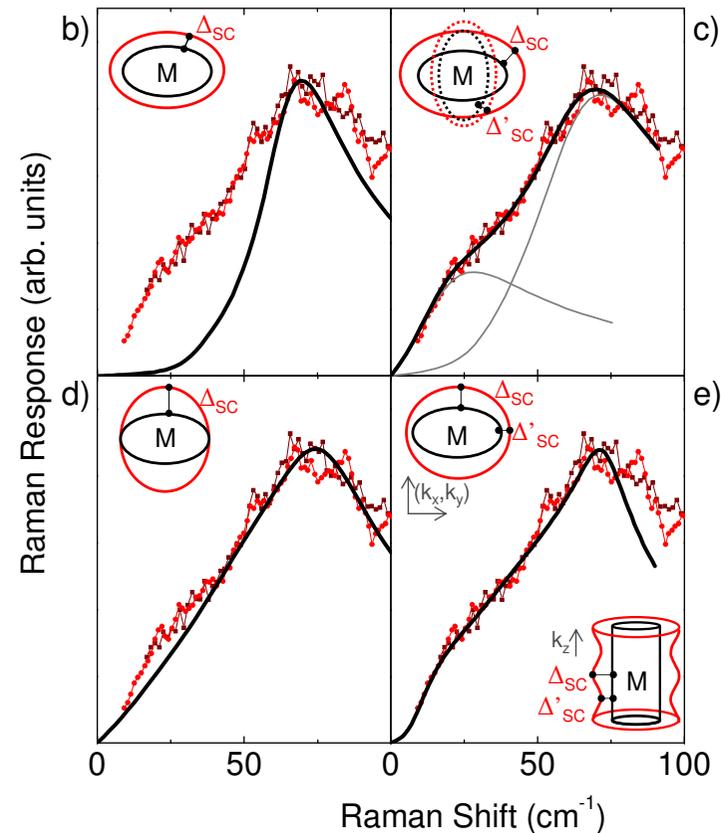


# Gap anisotropy in Co-Ba122

## Raman pair-breaking peak



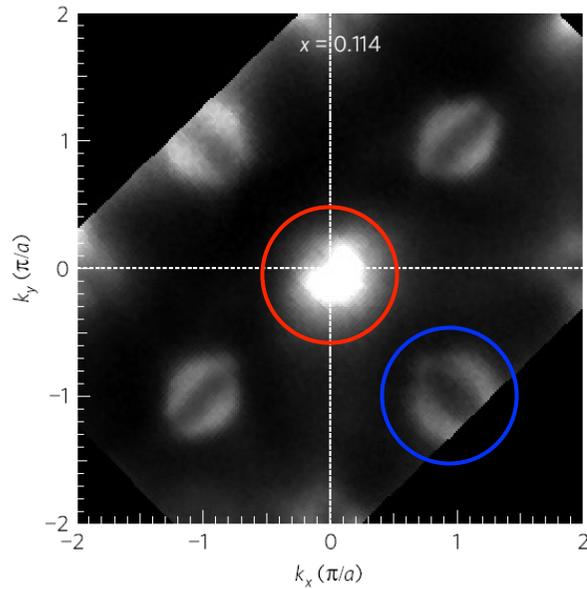
*L. Chauvière et al. Phys. Rev. B 82, 180521 (2010)*



- significant anisotropy around electron pocket:  $\Delta_{\max} = 6-7 \Delta_{\min}$
- in-plane or out of plane anisotropy

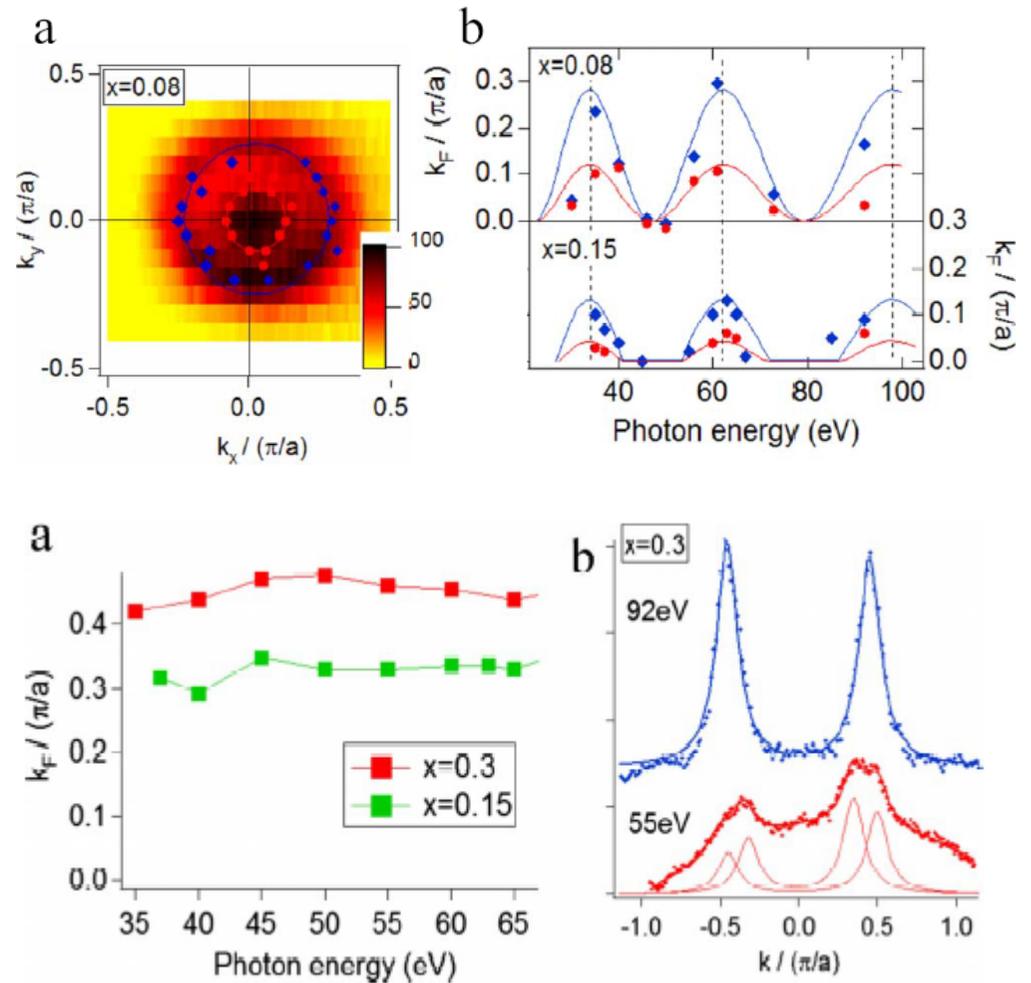
# 2D vs 3D Fermi surfaces

$k_z$  is tuned via incident photon energy



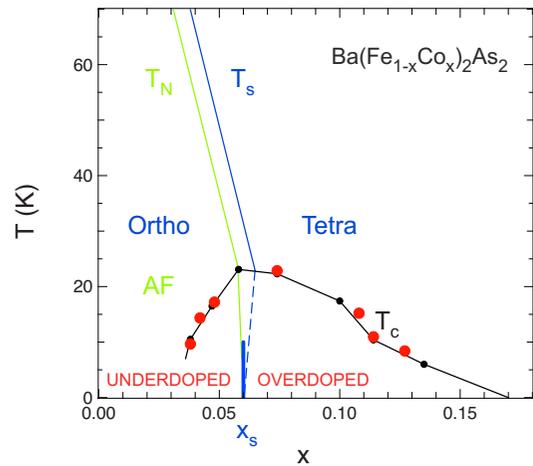
Hole FS

Electron FS

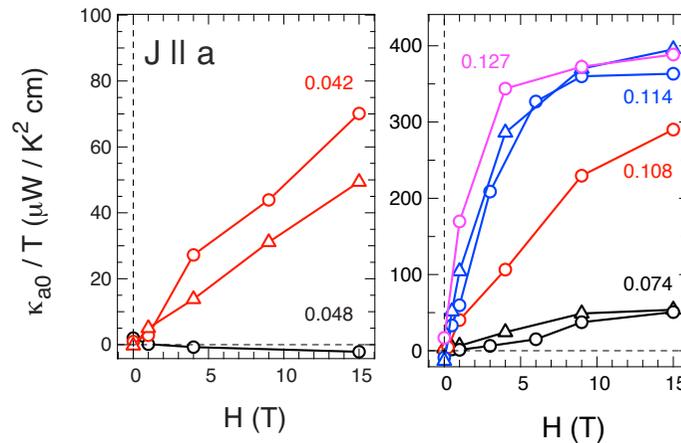


Note: 11 and 1111 families are more 2D

# Directional thermal conductivity in Co-Ba122

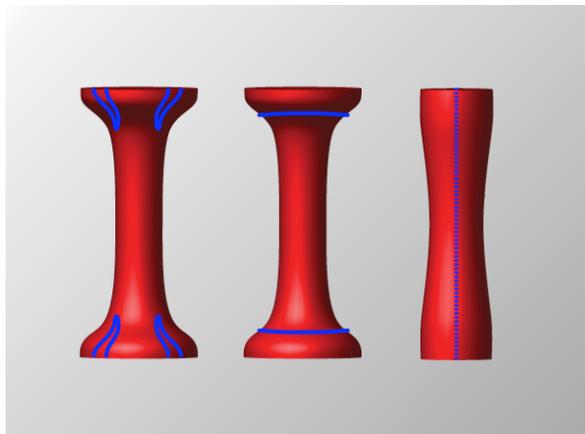
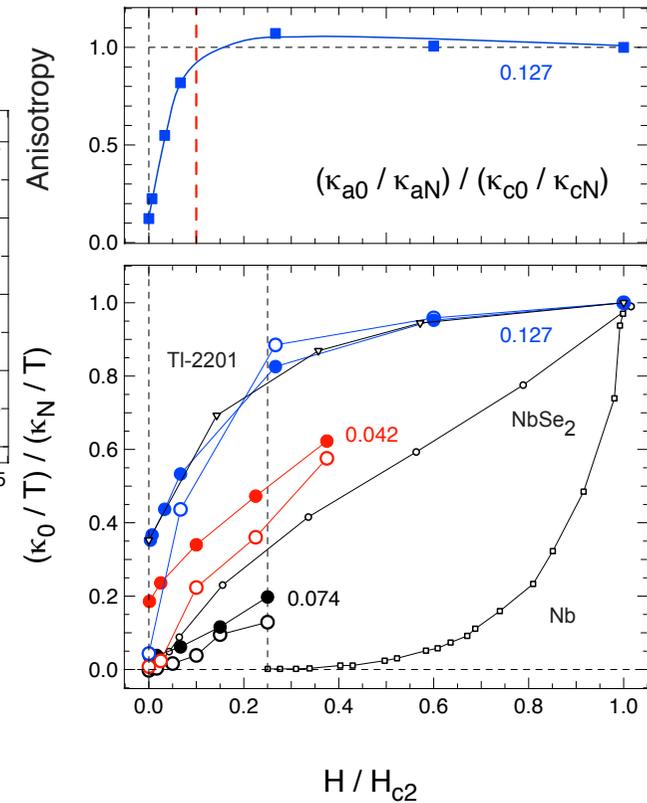


**a-axis: no residual linear term**



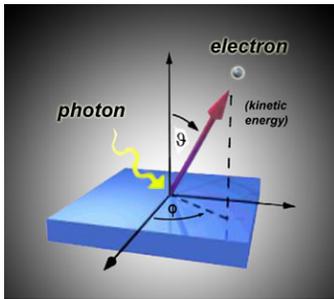
Reid et al, Phys. Rev. B 82, 064501 (2010)

**c-axis: residual linear term**

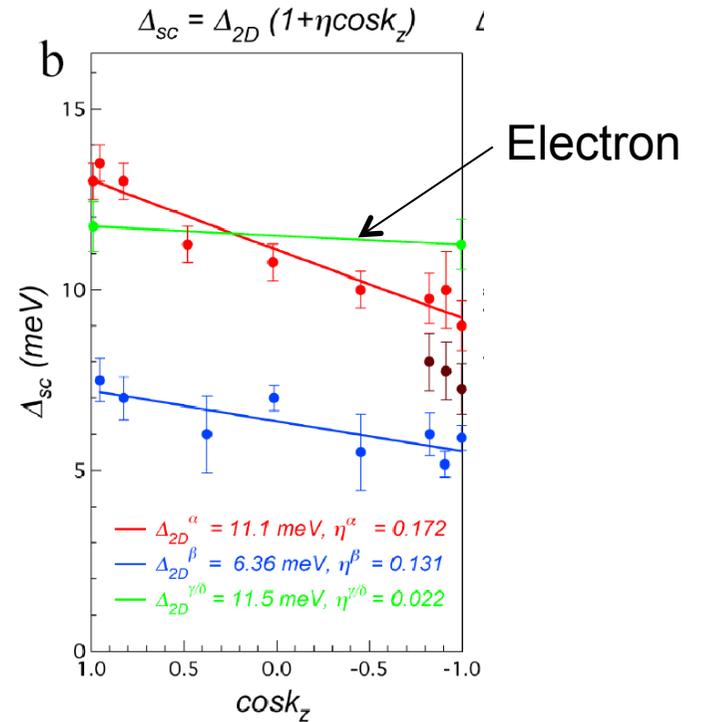
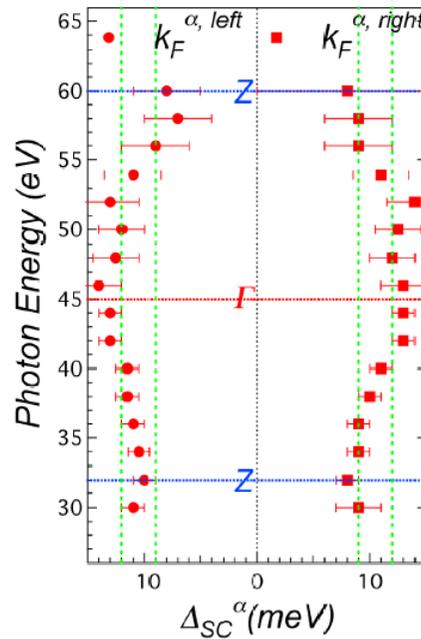
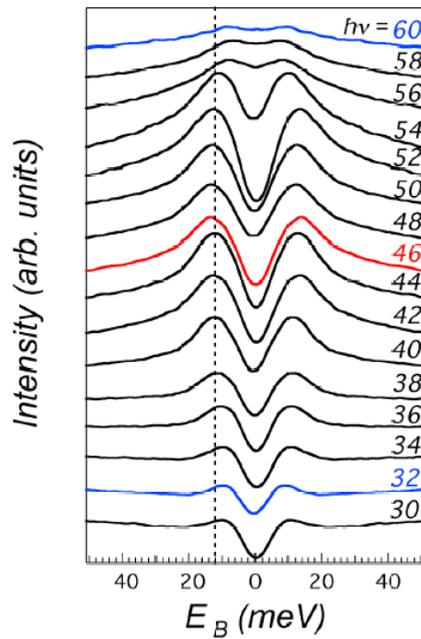


- nodes on FS part with high  $v_F$  along c-axis
- penetration depth shows similar behavior
- strong doping dependence

# $k_z$ dependence of the gap via ARPES



(BaK)Fe<sub>2</sub>As<sub>2</sub> (hole doped)

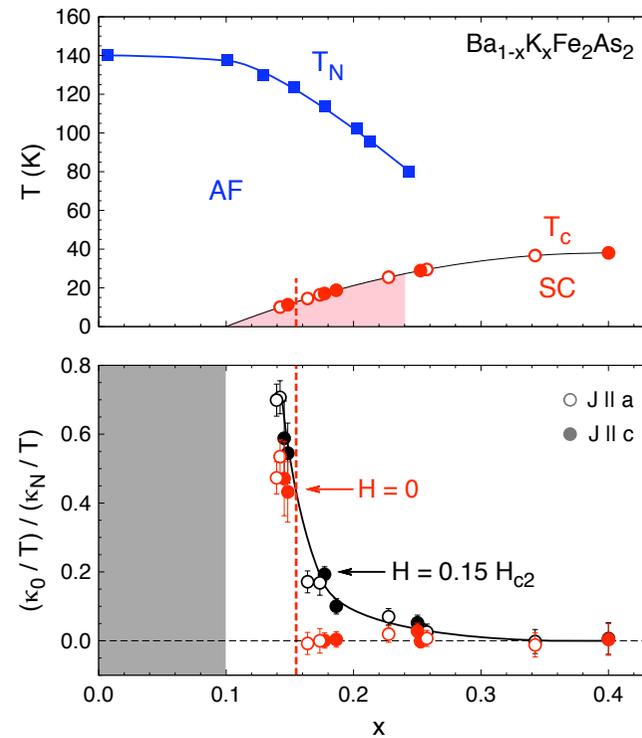
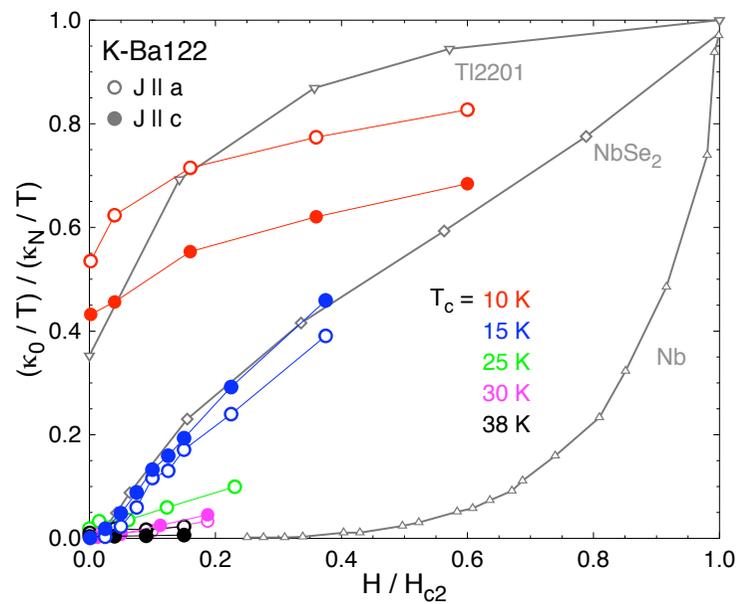


Xu et al. [arXiv:1006.3958](https://arxiv.org/abs/1006.3958) (2010)

$k_z$  is tuned via incident photon energy

- Hole FS strong  $k_z$  dependence (3D): **c** axis  $\kappa_{th}$
- Electron FS weak  $k_z$  dependence (2D): **Raman**

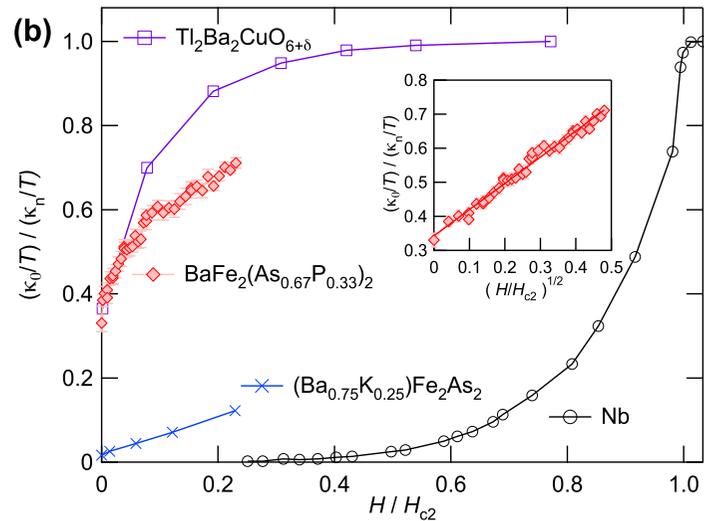
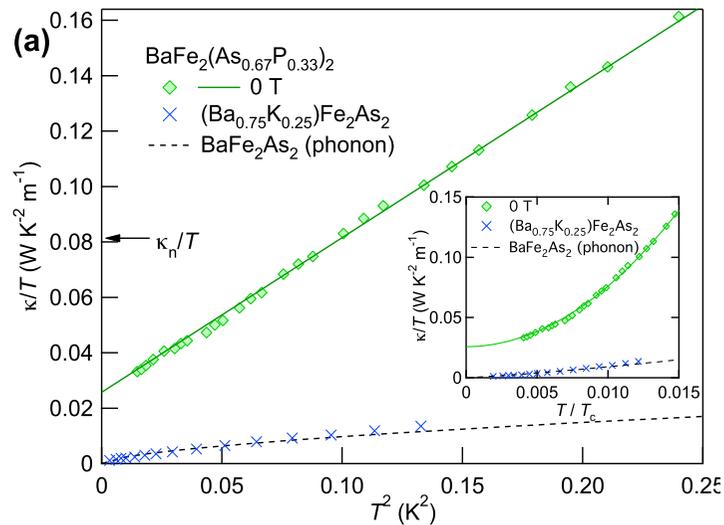
# Directional thermal conductivity in K-Ba122



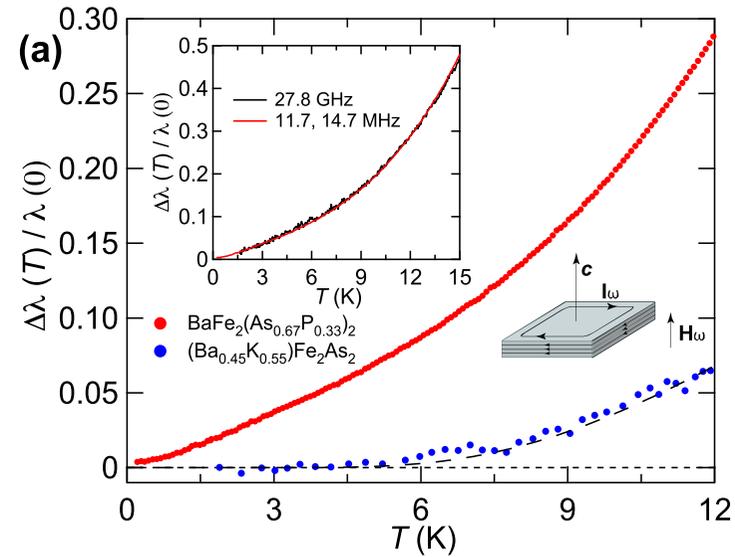
the structure of the gap is strongly doping dependent

# Substitution dependence of the gap anisotropy

$\kappa_{th}$ : isovalent versus hole doping



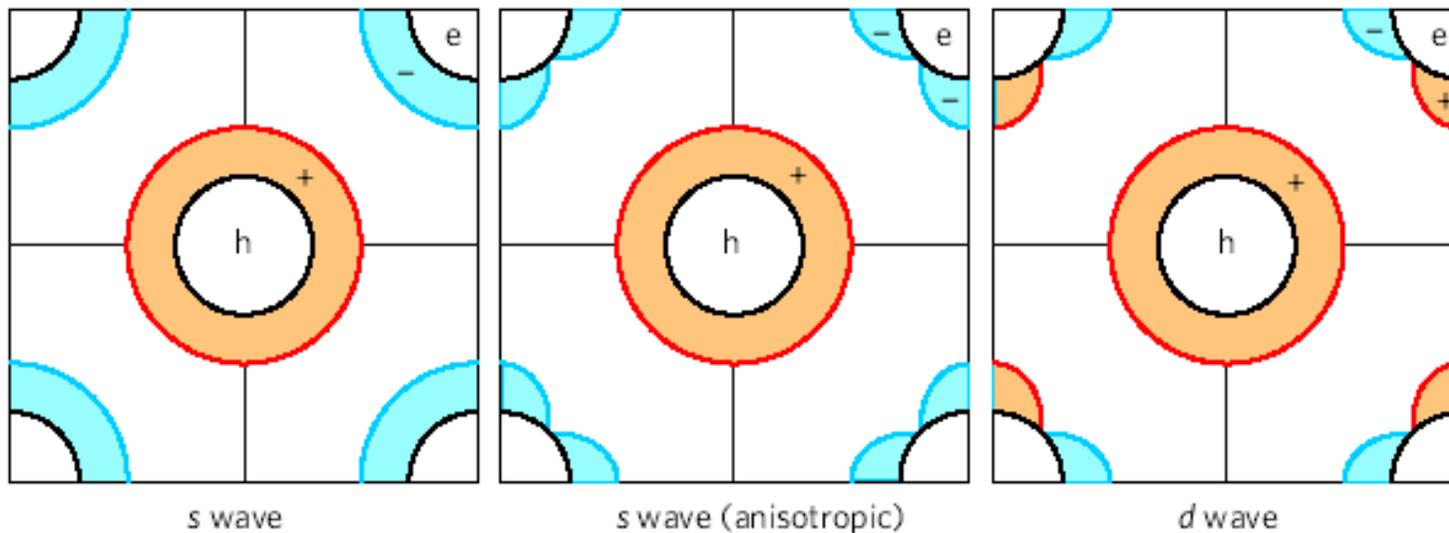
London penetration depth: isovalent vs hole doping



Hashimoto et al, Phys. Rev. B 81, 220501(R) (2010)

- $BaFe_2(As_{1-x}P_x)_2$  shows clear indication of nodes
- gap structure is not universal

# Gap structure in Ba122



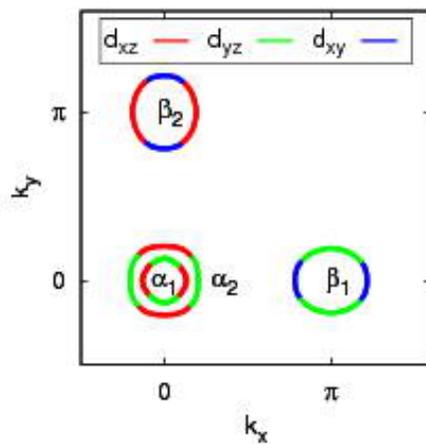
Interband pair interaction  $\longrightarrow$  Intra and interband pair interaction

- **plus** k-dependence of interaction (nesting) + orbital dependence
- doping dependent ! fine tuning

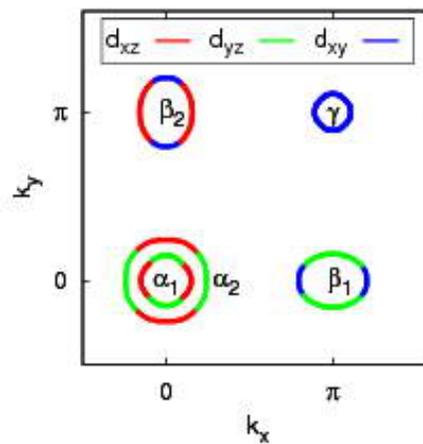
# Role of orbital content

## Fermi surfaces

Electron doping



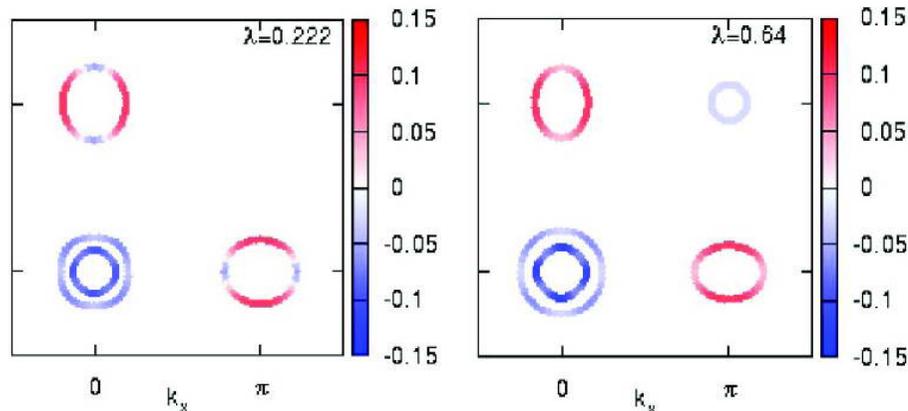
Hole doping



- orbital dependent FS leads to modulation of interband interaction matrix: intra-orbital scattering dominates
- $d_{yz}/d_{xz}$  scattering between electron and hole pocket lead to  $s^{+-}$  pairing
- $d_{xy}$  scattering between electron pocket frustrates  $s^{+-}$  pairing: anisotropy
- additional hole pocket stabilizes isotropic  $s^{+-}$

## gap structures

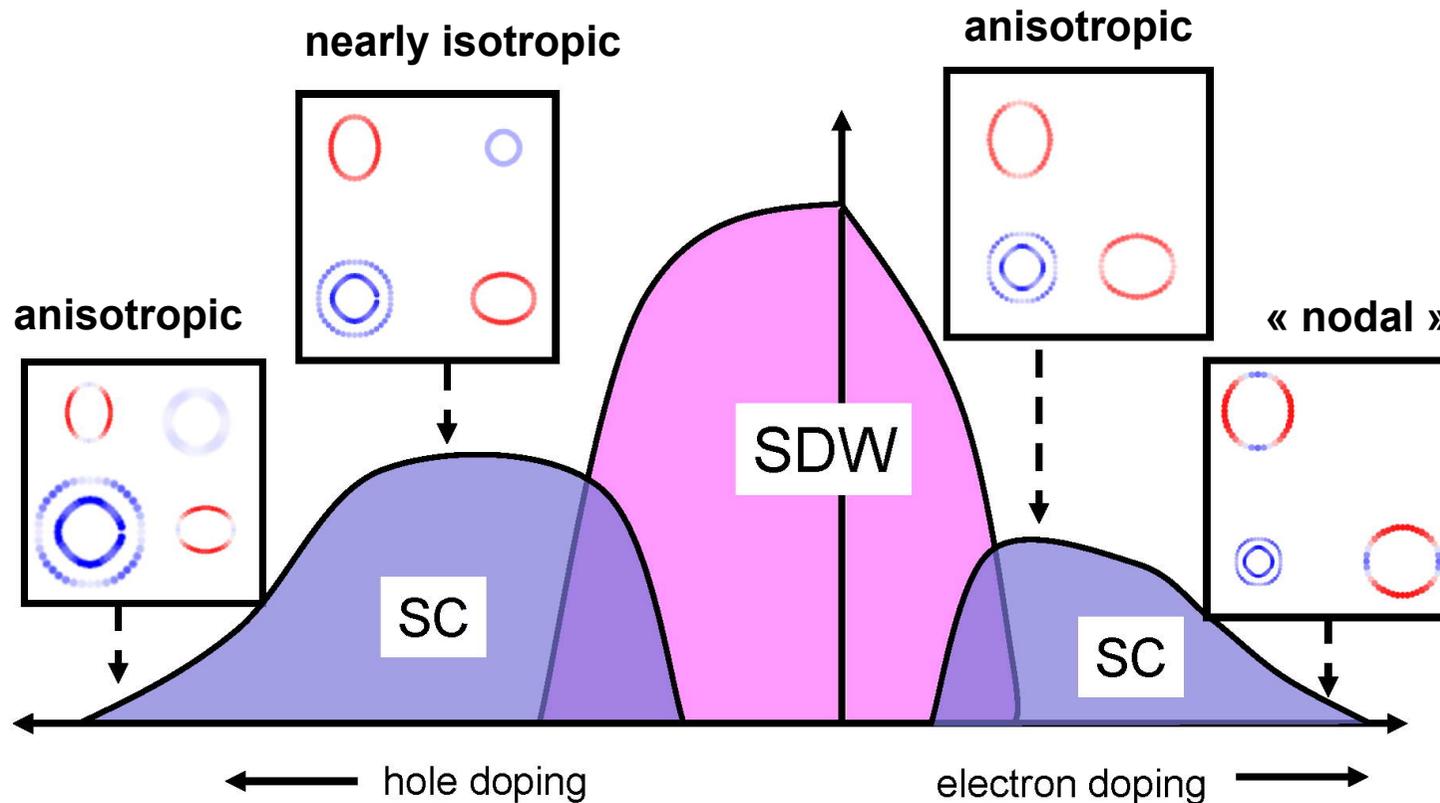
$n=6.03, U=1.3, J=0.2$



*Kuroki et al. PRB 79, 224511 (2009)*  
*Maier et al. PRB 79, 224510 (2010)*

**Strong sensitivity to FS topology  
(doping, As height...)**

# Doping dependant gap and interband spin fluctuations

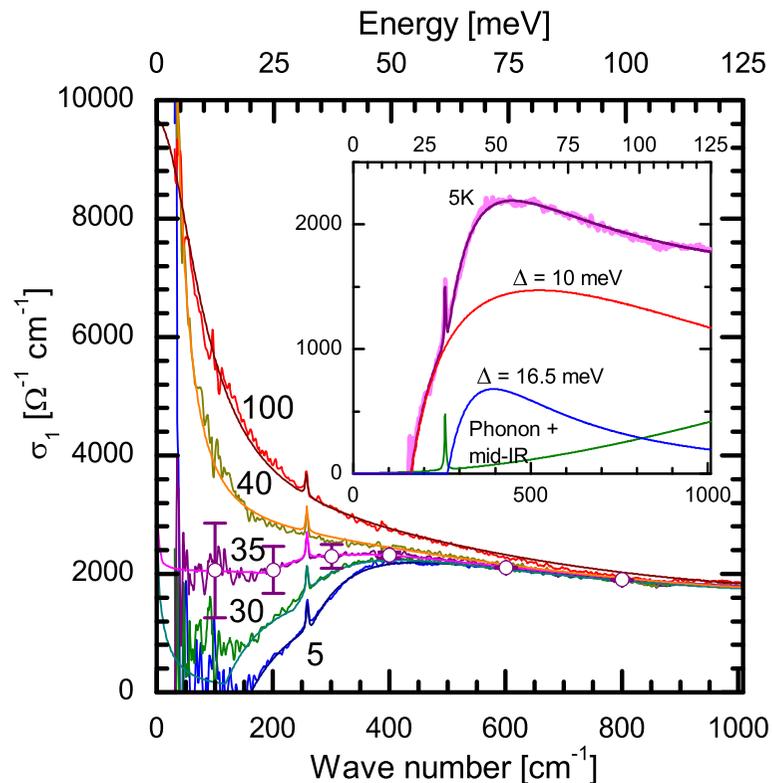


Hirschfeld et al. arXiv:1106.3712 (2011)

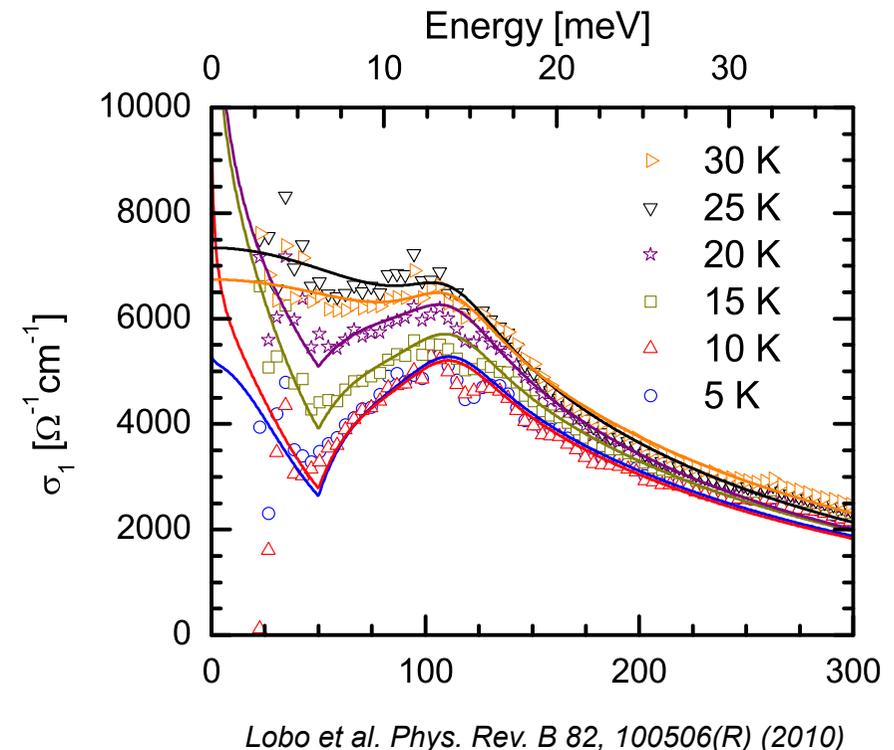
**Phase diagram of the gap structure in Ba122 from spin fluctuation theory**

# Role of disorder: optical conductivity

K-Ba122: out of plane substitution

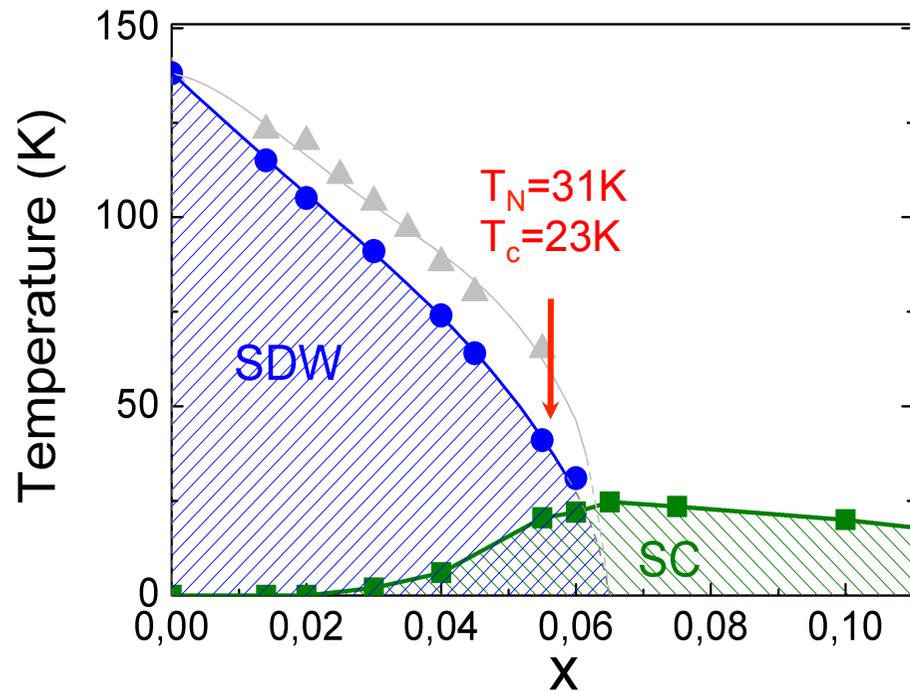


Co-Ba122: in plane substitution

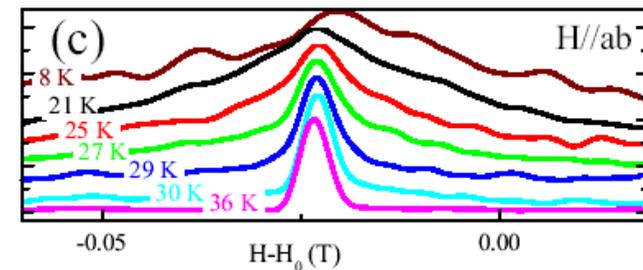
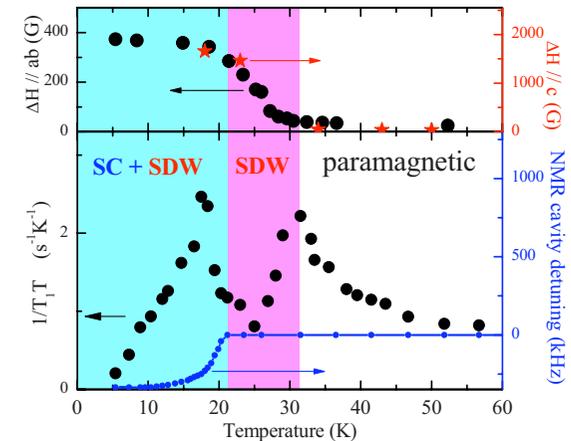


- subgap absorption in Co-Ba122: anisotropy or pair-breaking?
- interband impurity scattering is pair-breaking for  $s^{+-}$
- importance of interband versus intraband impurity scattering ?

# SDW + SC orders



## $^{75}\text{As}$ NMR



Laplace et al. PRB **80**, 140501 (2009)  
Julien et al. EPL **87**, 37001 (2009)

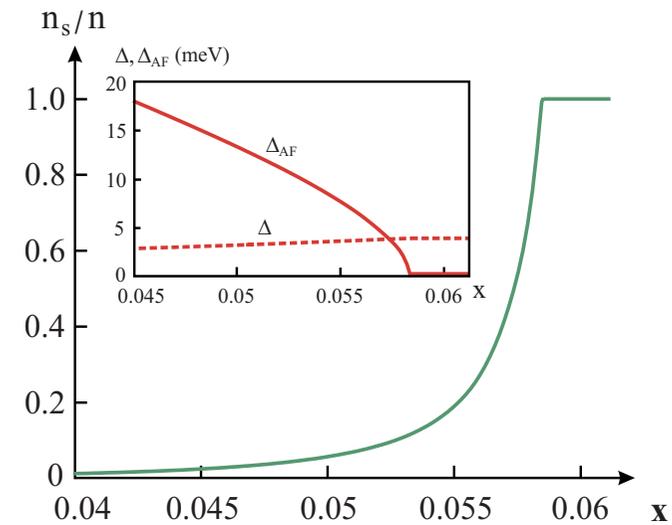
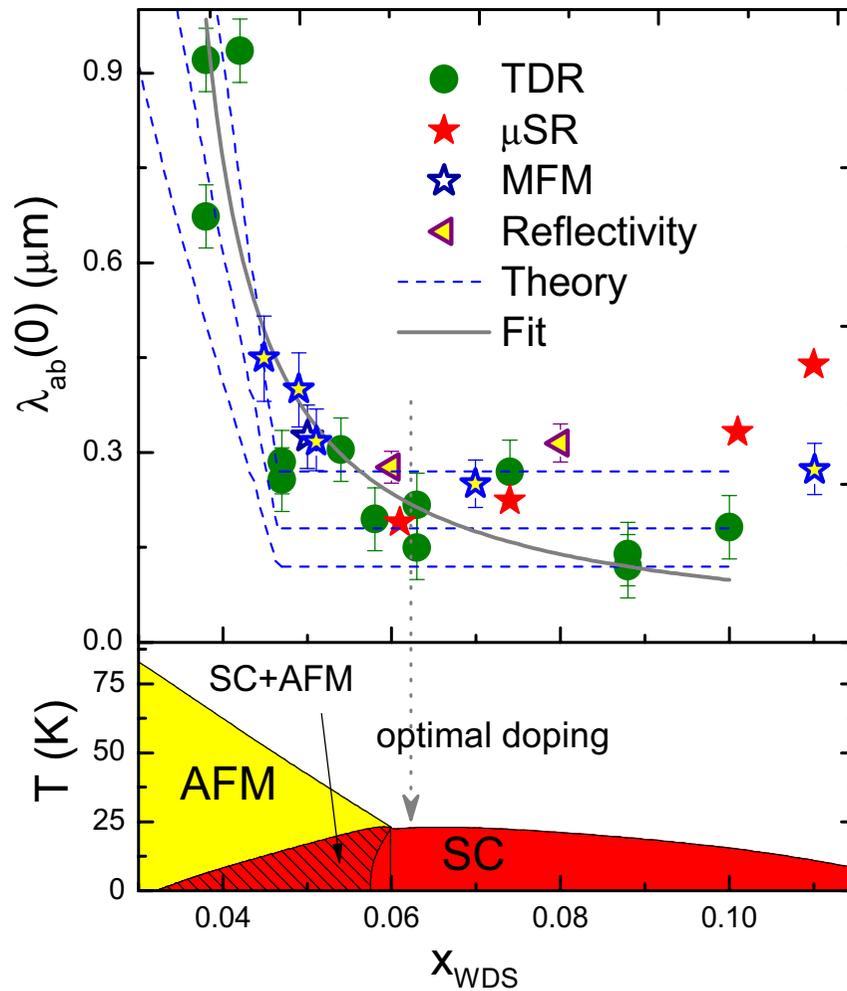
NMR spectra homogeneously broadened  
All Fe involved in SDW order

- SDW+SC: atomic coexistence (NMR,  $\mu\text{Sr}$ ...) for Co-Ba122: situation less clear in other systems
- Fe conduction electrons are involved in both orders: competition
- $s^+$  gap and incommensurability favor coexistence

Vorontsov and Chubukov Phys. Rev. B **81**, 174538 (2010)  
Fernandes and Schmalian Phys. Rev. B **82**, 014521 (2010)



# SDW vs SC



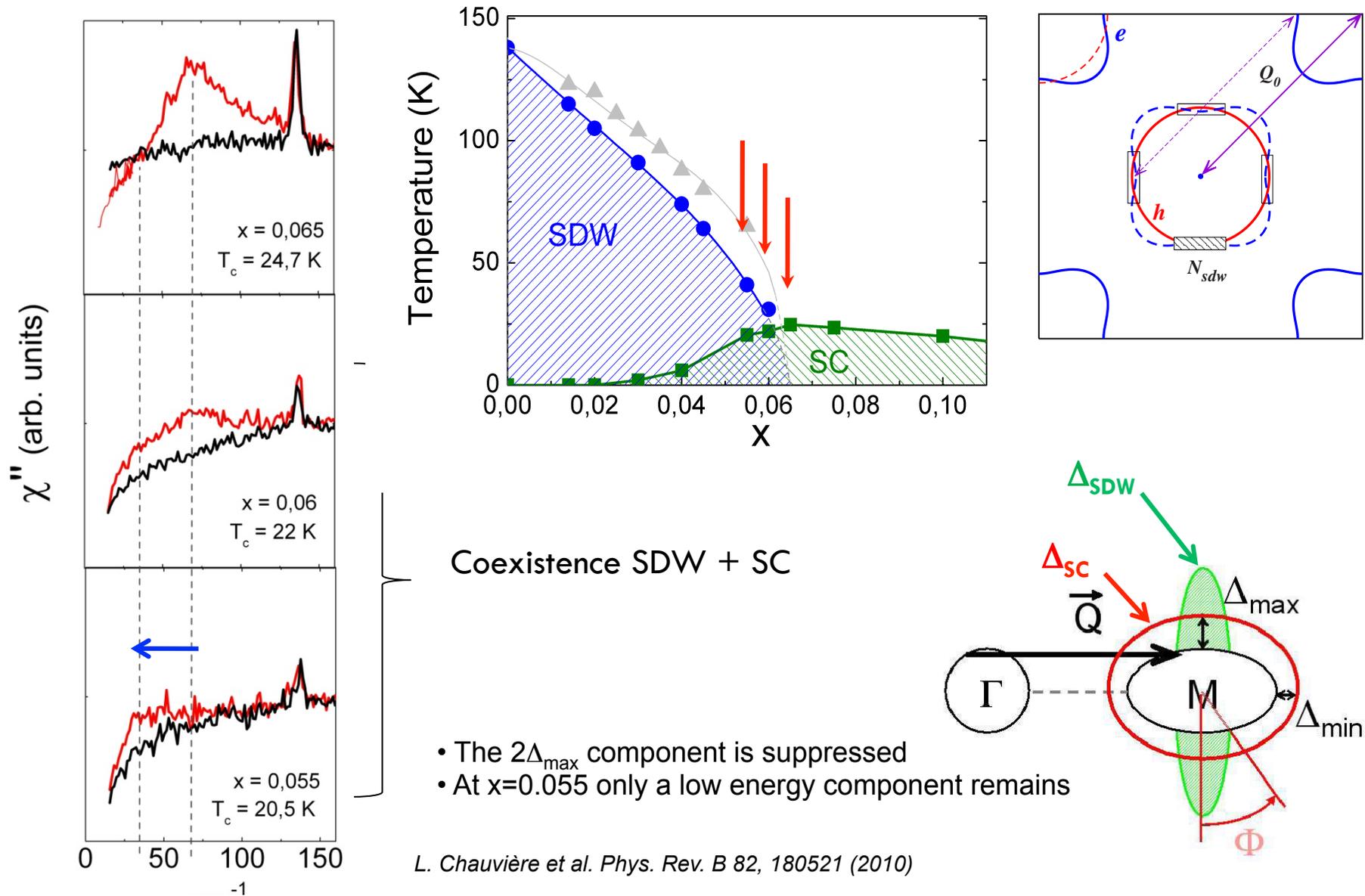
$$\lambda_{ab}^{\text{SC+SDW}}(0) = \lambda_{ab}^0(0) \sqrt{1 + \frac{\Delta_{\text{AF}}^2}{\Delta_0^2}}$$

Prozorov et al. *Rep. Prog. Phys.* 74, 124505 (2011)  
 Fernandes et al. *Phys. Rev. B* 82, 014520 (2010)

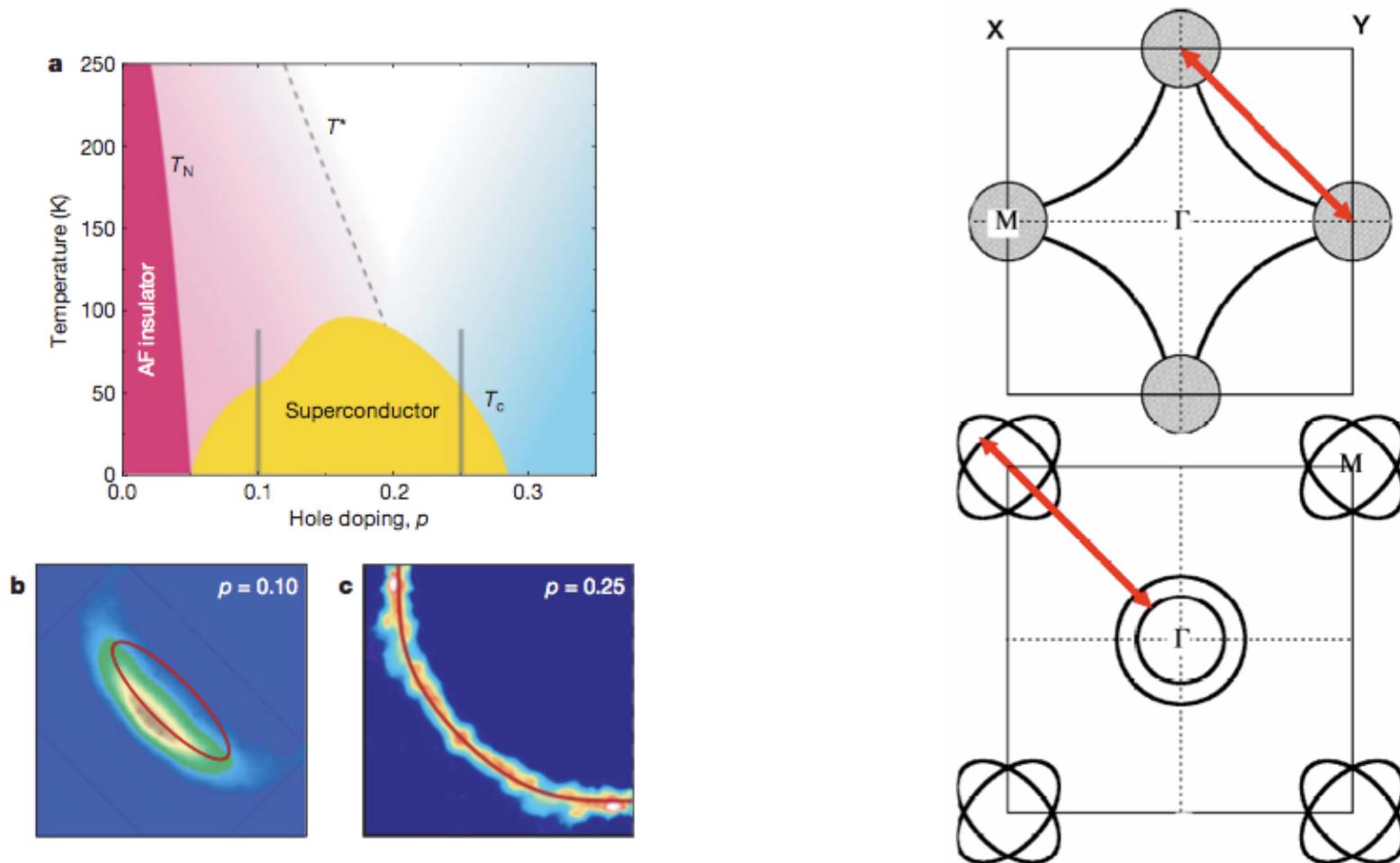
- **drastic increase of penetration depth in the coexistence regime**
- **drop in the superfluid density**

# SDW vs SC: Raman

Vorontsov and Chubukov Phys. Rev. B 81, 174538 (2010)



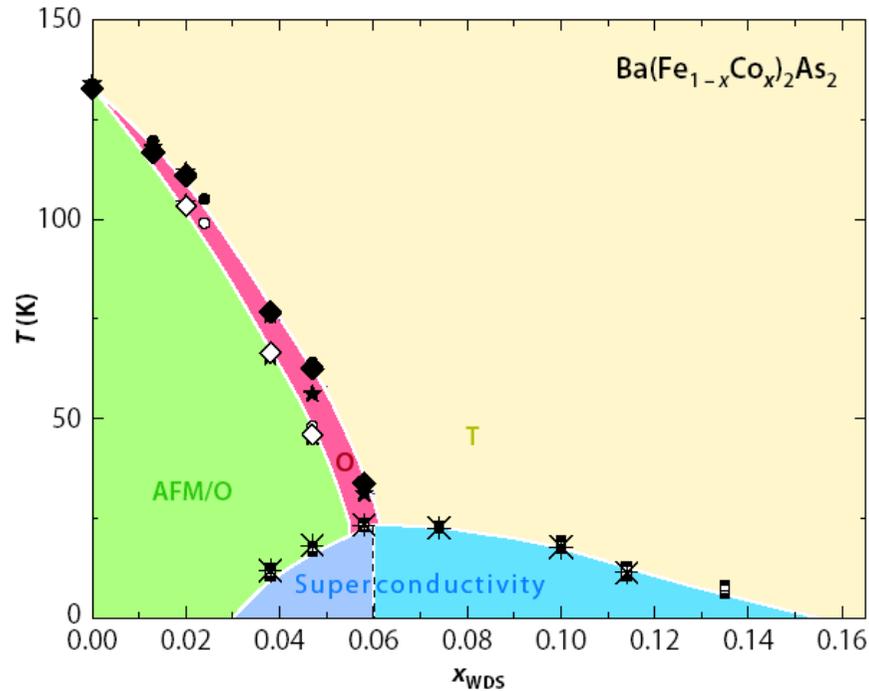
# Hot spots in underdoped cuprates and pnictides



Doiron-Leyraud et al. Nature 2007

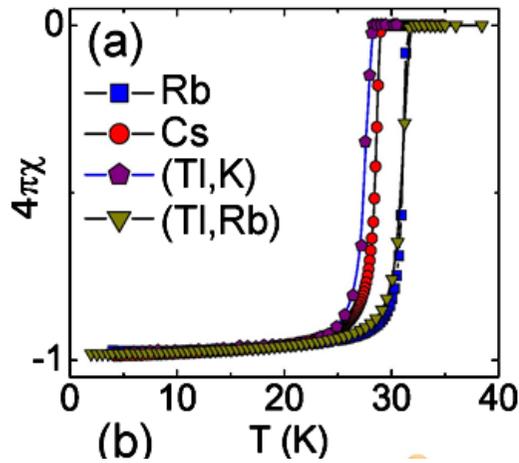
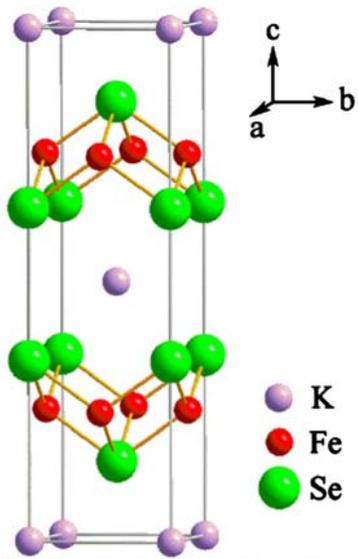
Superconductivity is confined in k-space in both systems close to competing order

# Summary

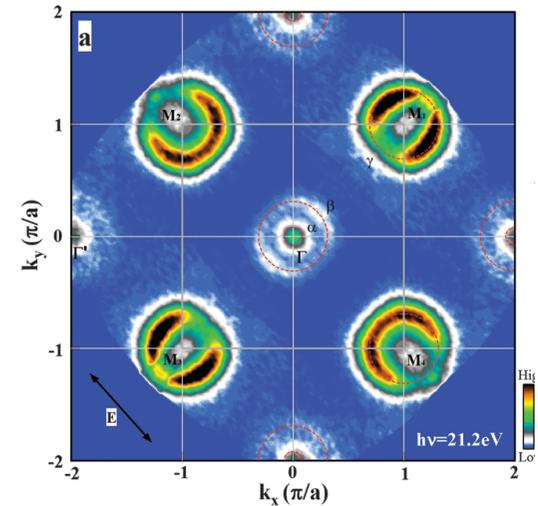


- key role of magnetic fluctuations
- interband Coulomb interaction drive both SC and SDW
- gap structure is not universal (but gap symmetry is s-wave)
- maximum  $T_c$ : optimum nesting without magnetism
  
- need to confirm s+- gap !
- is their a role for structural degrees of freedom ?

# The case of $A_2Fe_4Se_5$

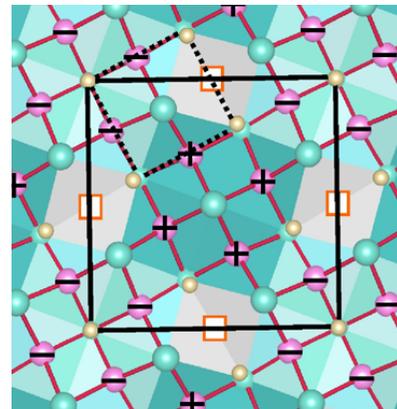
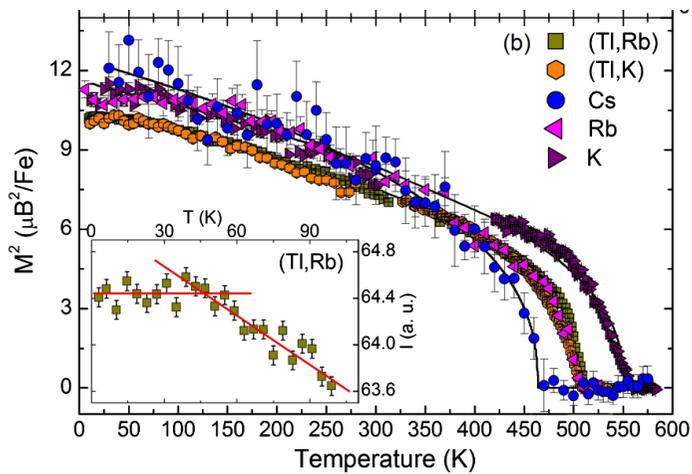


*J. Guo et al., Phys. Rev. B 82, 180520(R) (2010)*



*D. Mou et al., Phys. Rev. Lett. 106, 107001 (2011)*

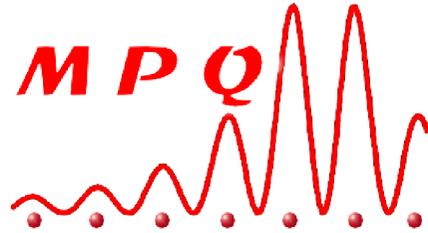
absence of electron-hole nesting



$T_N=560K$  !!! (Fe ordered vacancies)  
local magnetism?

coexistence or phase separation?

*F. Ye et al., Phys. Rev. Lett. 107, 137003 (2011)*



Ludivine Chauvière, Marie-Aude Méasson, Maximilien Cazayous  
Alain Sacuto, **MPQ Paris Diderot**

D. Colson, A. Forget, **SPEC CEA Saclay**