μSR studies of high-T_C superconductivity in iron pnictides

Hans-Henning Klauss

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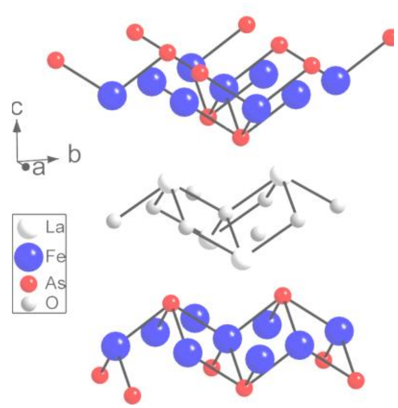
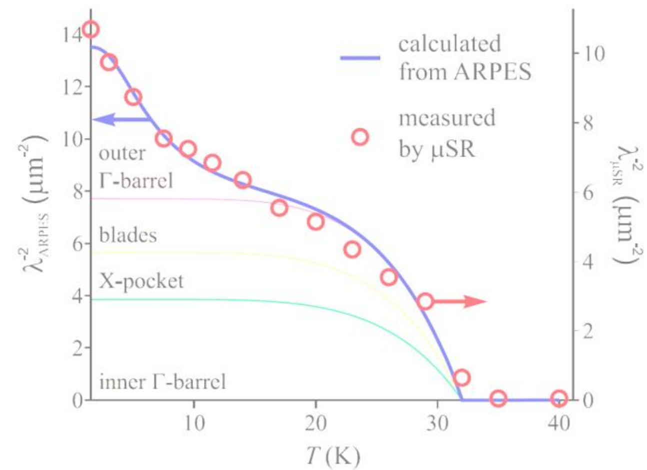
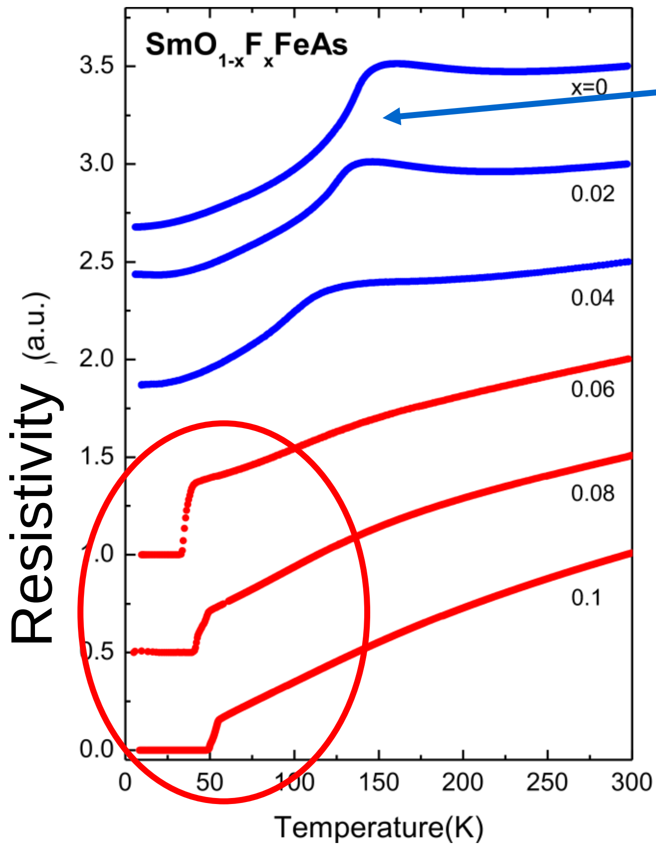


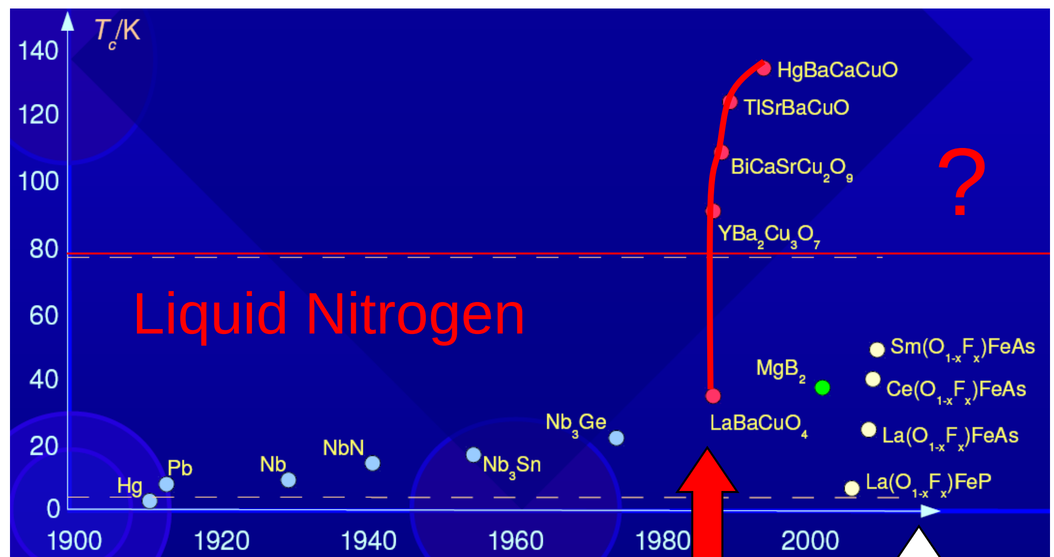


Superconductivity above 50 K



Metallic parent compounds !

Superconducting T_C



S. Glaser, U Augsburg

Cuprates

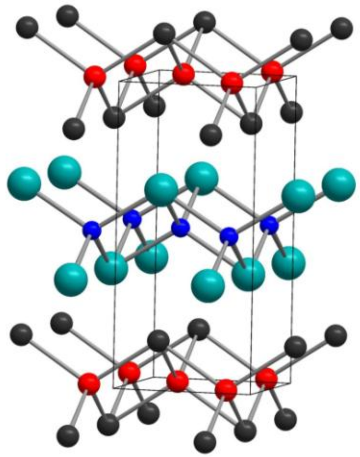
Pnictides

C. Hess et al., arxiv 0811.1651 (2008)

similar data: e.g. Ren et al. Chin Phys. Lett. 2008

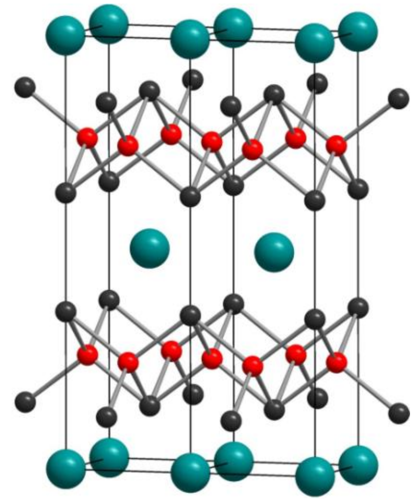
General structural motiv: FeAs layers with Fe square lattice

Y. Kamihara et al., J. Am. Chem. Soc. 130, 3296 (2008)



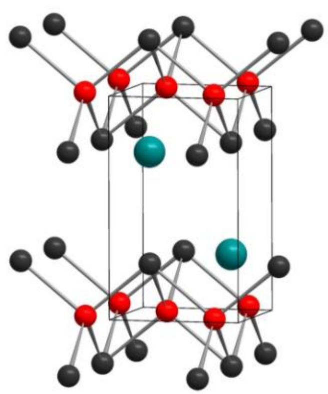
$LaO_{1-x}F_xFeAs$ „1111“

Rotter et al., Chu et al, Krellner et al. , …



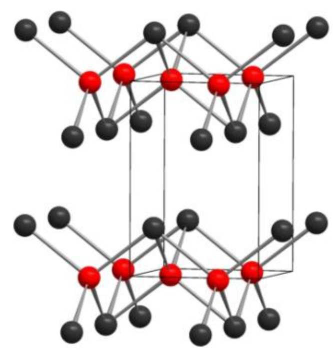
$(Sr,Ca,Ba)_{1-x}(K,Na)_xFe_{2-y}(Co,Ni)_yAs_2$ „122“

X. C. Wang et al, arXiv:0806:4688



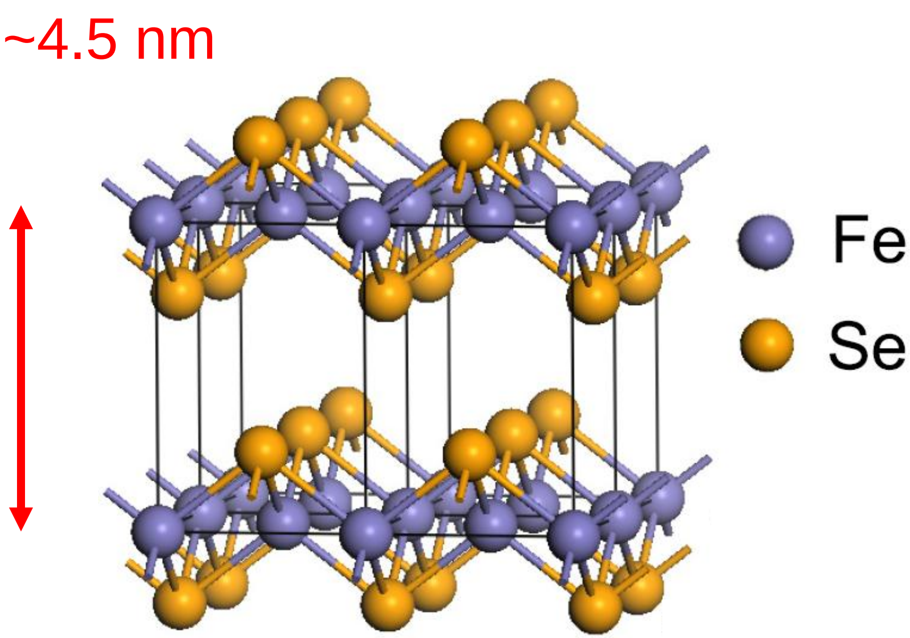
LiFeAs **„111“**

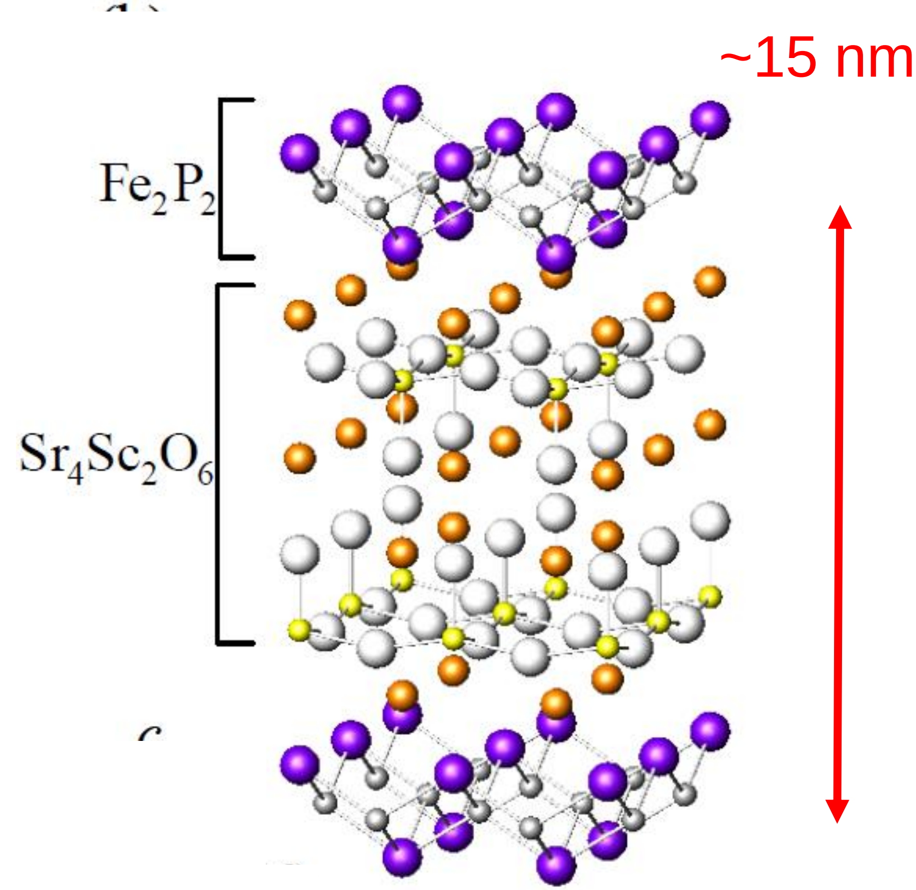
Hsu *et al.*, arXiv:0807.2369



FeSe **„011“**

Interplanar distance may differ very much!





$FeSe_{1-x}Te_x$

$T_{C,\ max}$ = 14 K

@ 9 GPa: 36,7 K !!

S. Medvedev *et al.*, Nature mat '09

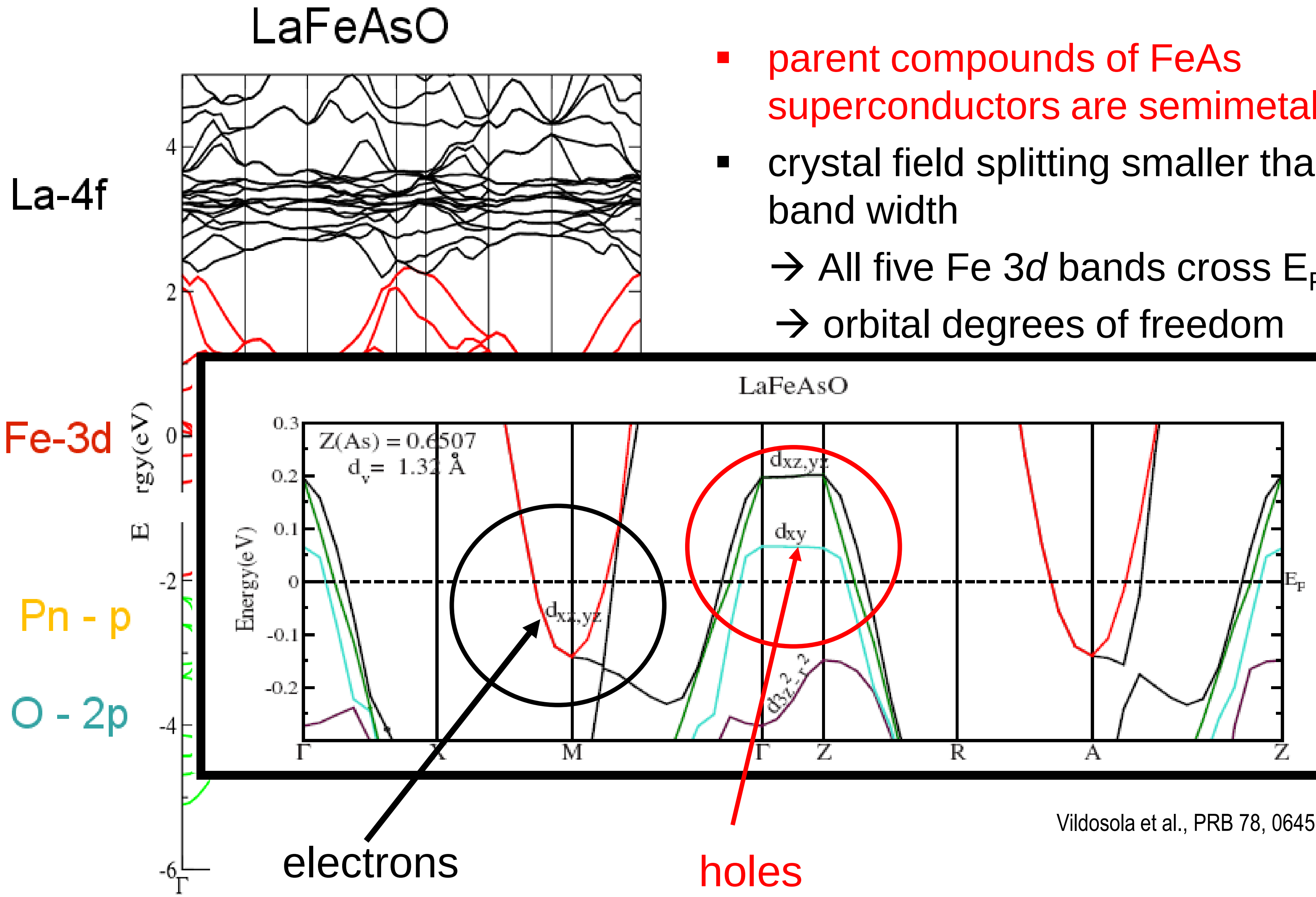
$(Fe_2P_2)(Sr_4Sc_2O_6)$

$T_{C,\ max}$ = 37 K

H. Ogino *et al.*, arXiv:0903.3314

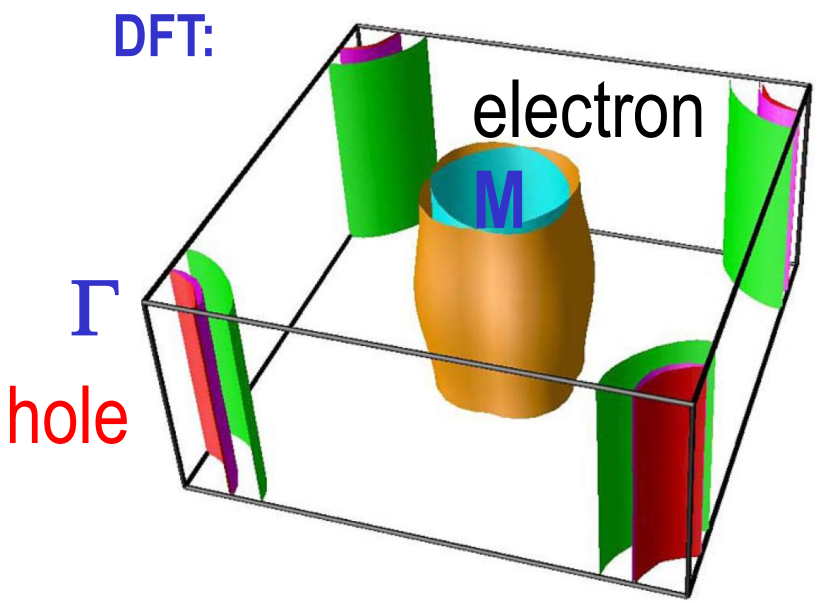
Electronic band structure

- parent compounds of FeAs superconductors are semimetals
- crystal field splitting smaller than band width
  → All five Fe 3*d* bands cross E_F
  → orbital degrees of freedom



Vildosola et al., PRB 78, 064518

Fermi surface



I. I. Mazin et al., PRB **78**, 085104 (2008)

- **parent compounds of FeAs superconductors are semimetals**
- **crystal field splitting smaller than band width**

  → all five Fe 3*d* bands cross E_F

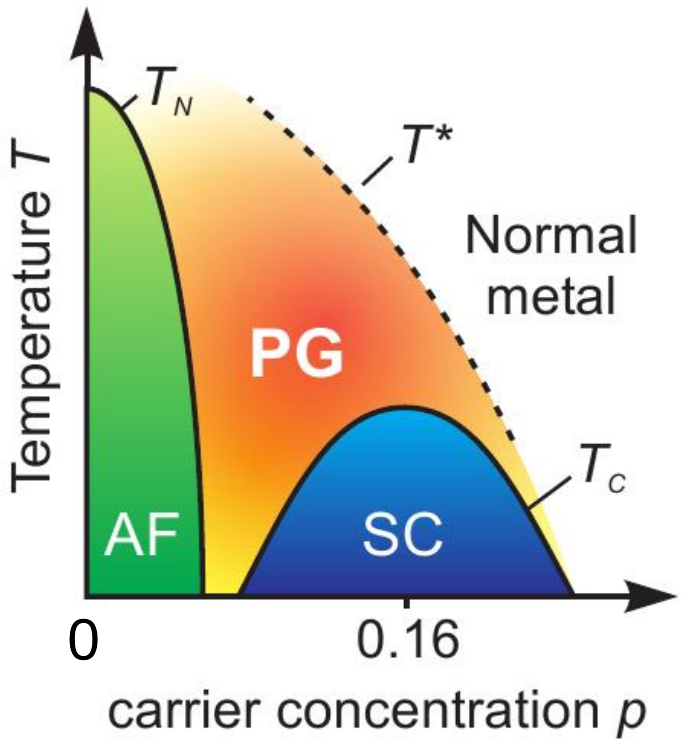
  → weak electronic correlations

  → Multi-band Fermi surface
  - **Hole like at (0,0)**
  - **Electron-like at (π,π)**
- **cylindrical shape**

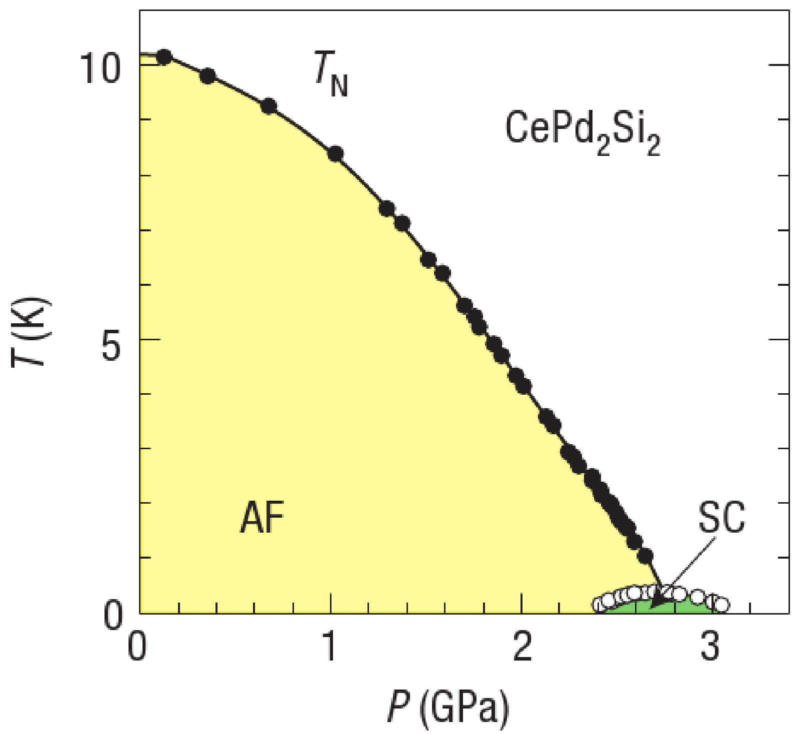
  → nearly two-dimensional electron system

Magnetism and Superconductivity

Cuprates



Heavy Fermions



Picture: Ø. Fischer et al., Rev. Mod. Phys. **79**, 353 (2005)

Mathur et al., Nature **394**, 39–43 (1998)

strong electronic correlations

→local moment AFM order (1 to 2 μ_B)

→undoped cuprates are insulators!

Outline

- **Phase Diagrams of Fe-pnictides: $RO_{1-x}F_xFeAs$ and $(Sr,Ba)Fe_{2-x}Co_xAs_2$**

  → **electronic, magnetic and superconducting properties**
  → interplay with structure, quantum criticality or phase competition

- **Interplay of R and FeAs electronic system in $R(O_{1-x}F_x)FeAs_{1-y}P_y$**
  → **non-collinear order of R and Fe spin systems**
  → afm and fm order of Ce sublattice

- **Superconductivity in $(Sr, Ba)Fe_{2-y}Co_yAs_2$ compounds**
  → multi-gap sc, nodes
  → field induced magnetism

~20 Publications (Nature mat, PRL, PRB, NJP,…) on pnictides since April 2008

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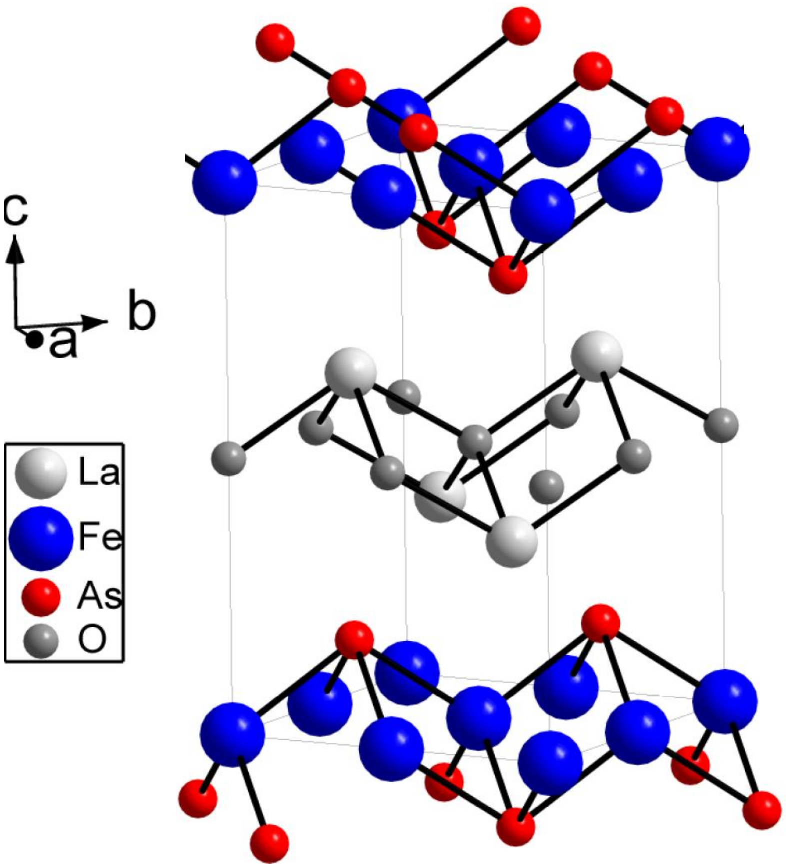
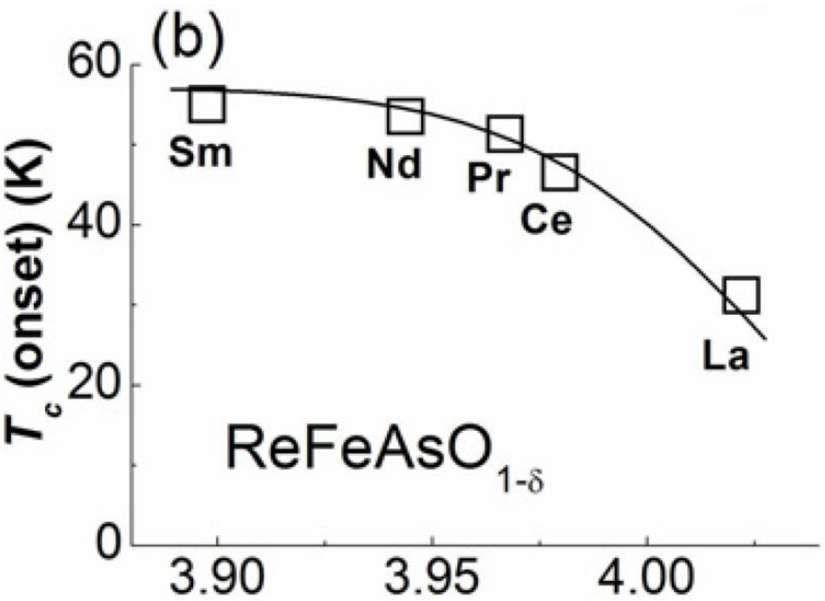
$R(O_{1-x}F_x)FeAs$





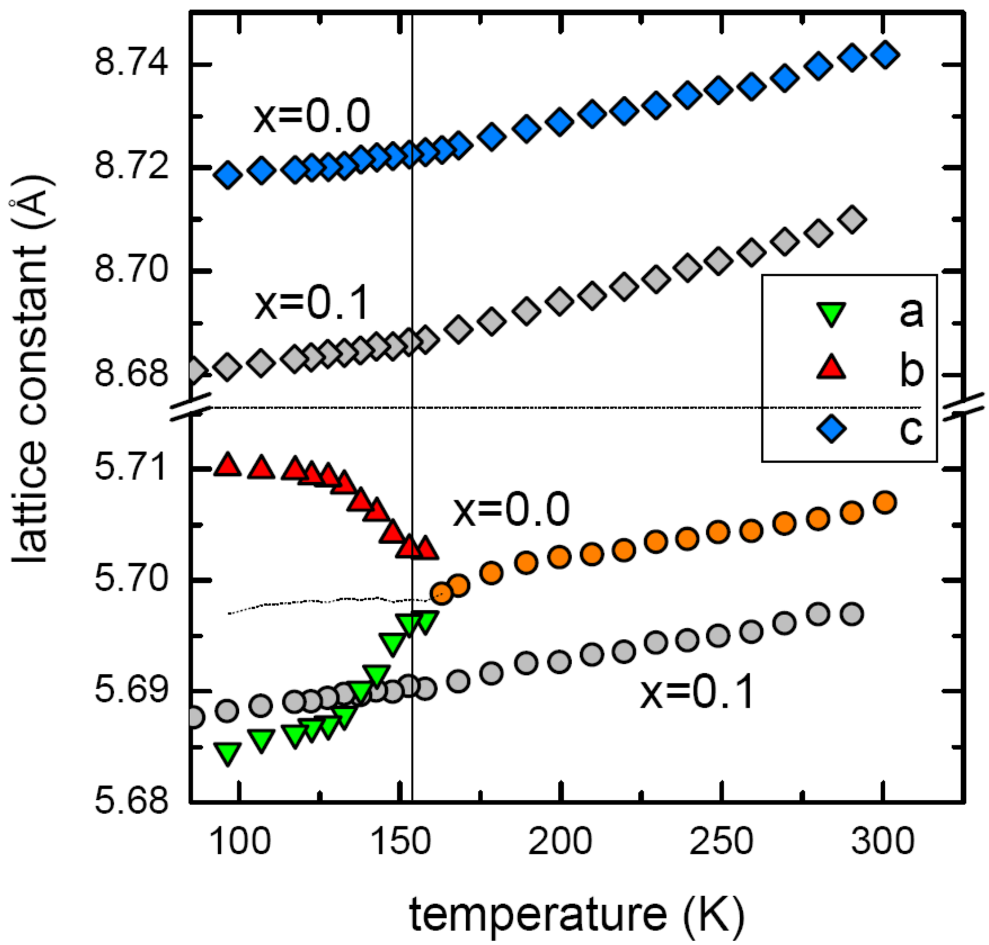
Lattice parameter a (A)

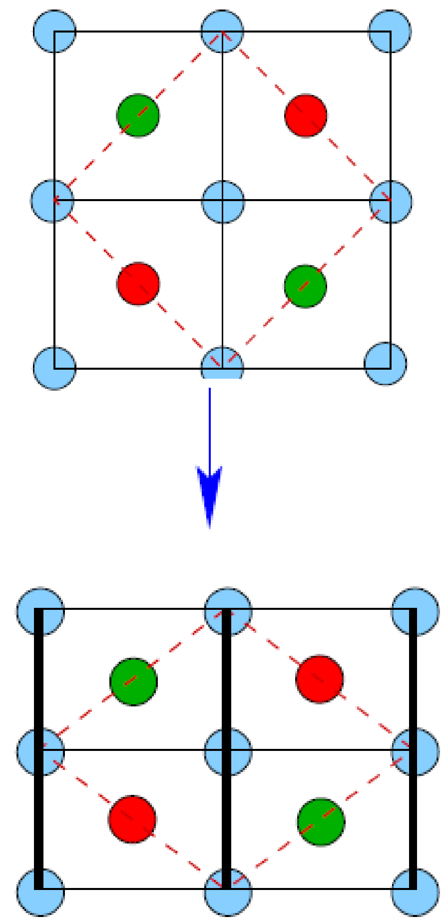
Ren et al., EPL, **83** (2008) 17002

In-plane Fe – Fe distance ~ 2.86 A only, like pure Fe!

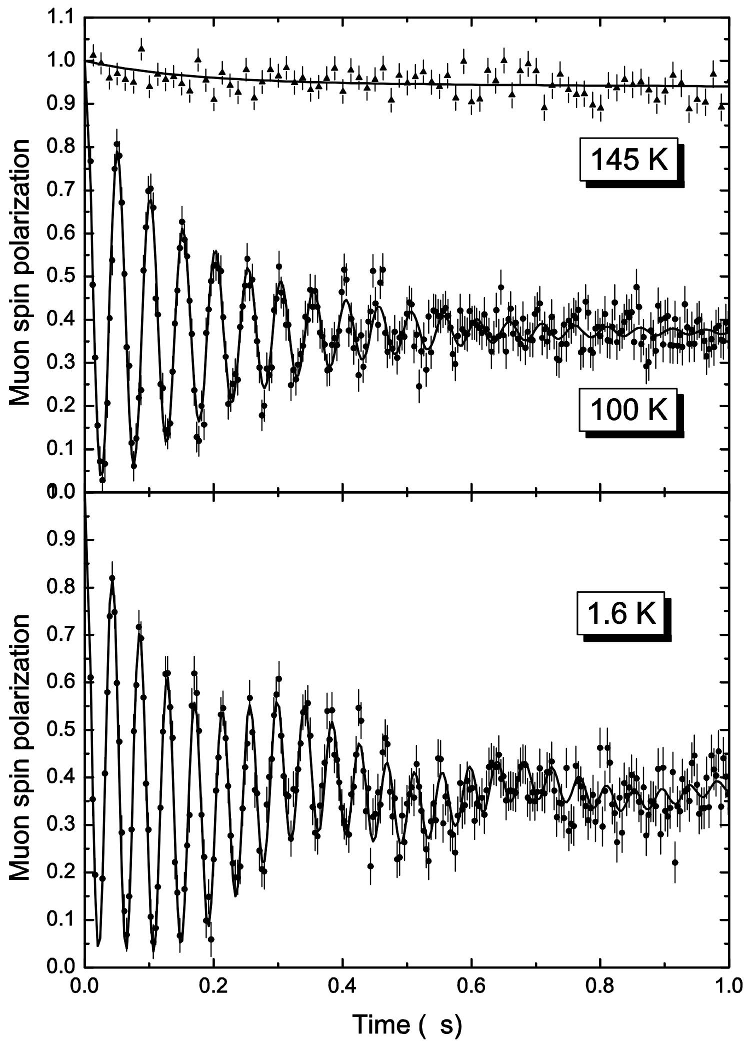
Structural Transition in undoped LaOFeAs

Tetragonal to orthorhombic distortion below 156 K in LaOFeAs





Magnetic order of LaOFeAs



μSR on LaOFeAs

- well defined local magnetic field at muon site

  $\omega = \gamma_\mu B_{local}$ **~ ordered magnetic moment**

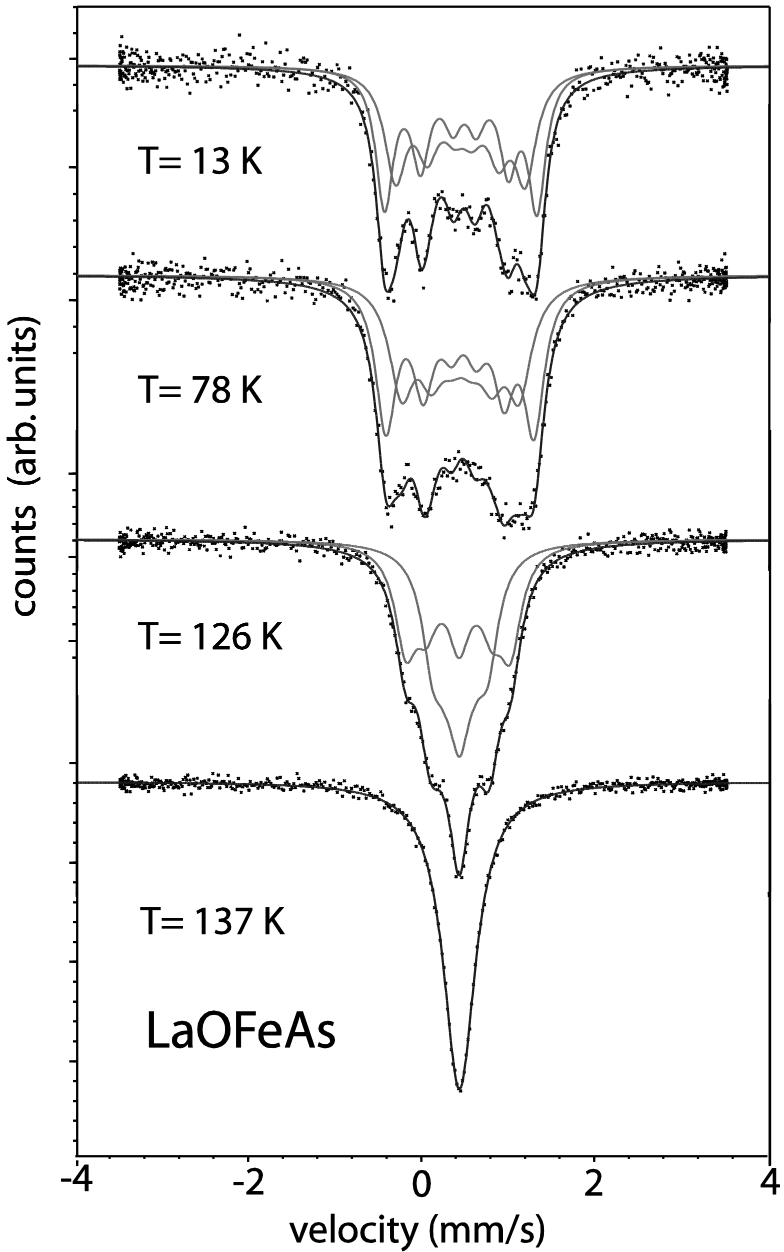
→ commensurate AFM below 138 K

- additional change below 70 K appearance of a smaller frequency

→ 2 muon sites

HHK et al., PRL 101, 077005 (2008)

Magnetic order of LaOFeAs



^{57}Fe Mössbauer spectroscopy

→ well defined magnetic hyperfine field

→ commensurate magnetic order below 138 K

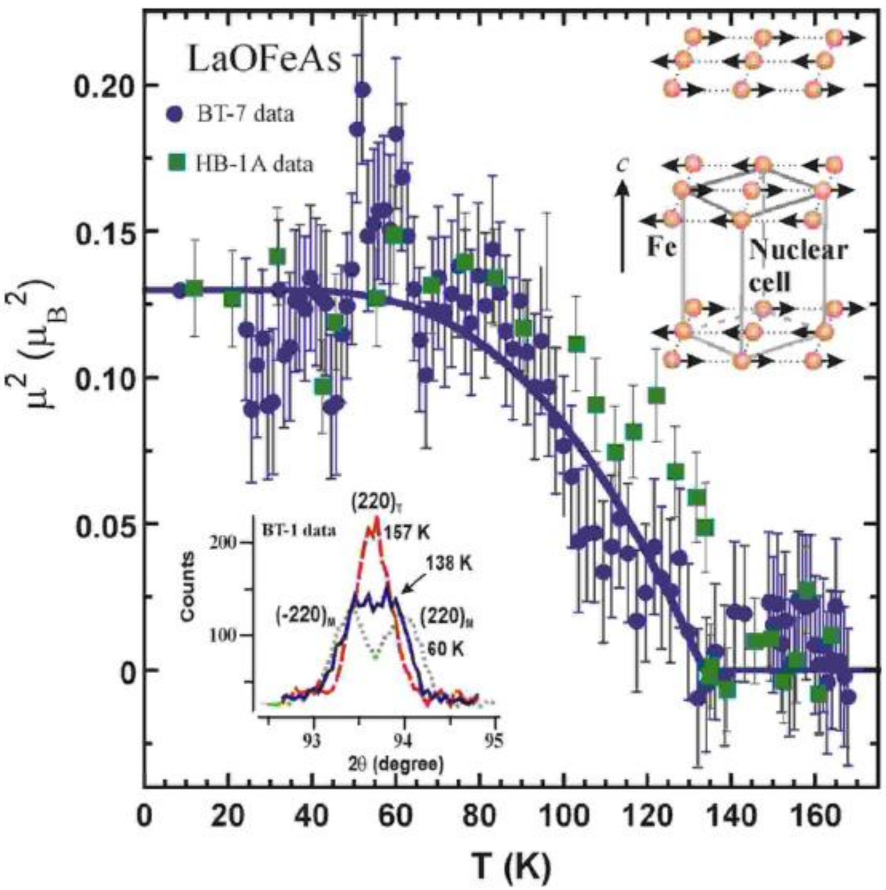
B_{hyp} (T→ 0) ~ 4.86 T

compare with bulk iron

→ ordered moment ~ 0.3 μ_B

→ itinerant magnet

Magnetic order of LaOFeAs

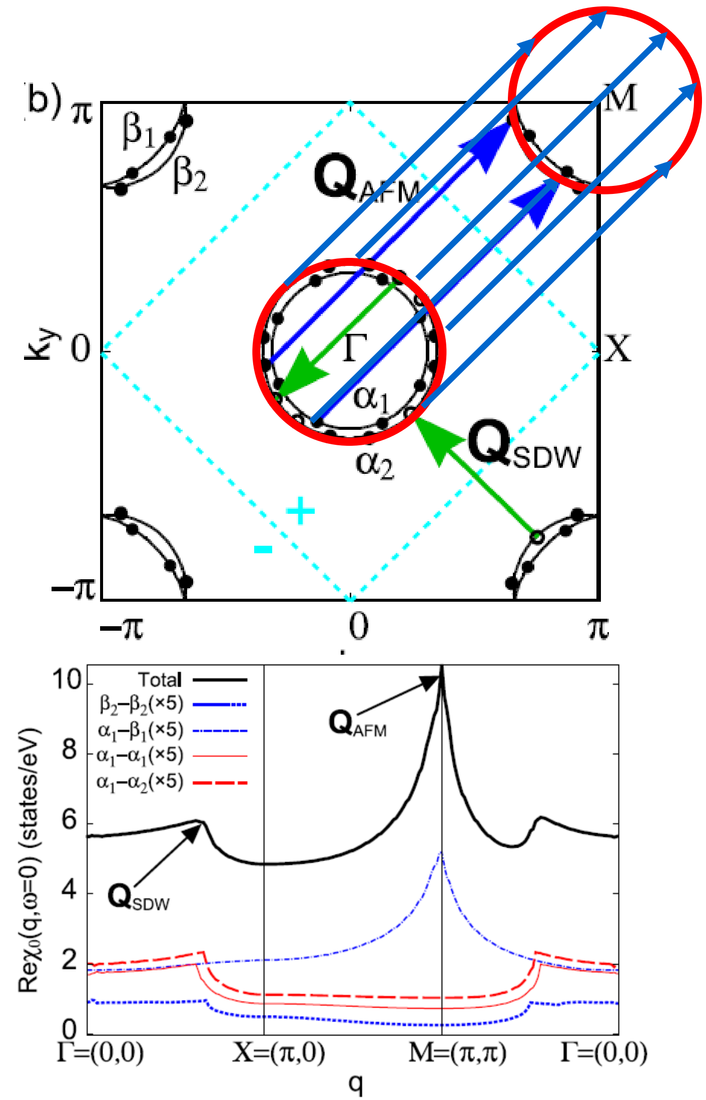


C. de la Cruz, et al., Nature 453, 899 (2008)

→ordered moment ~ 0.3 μ_B

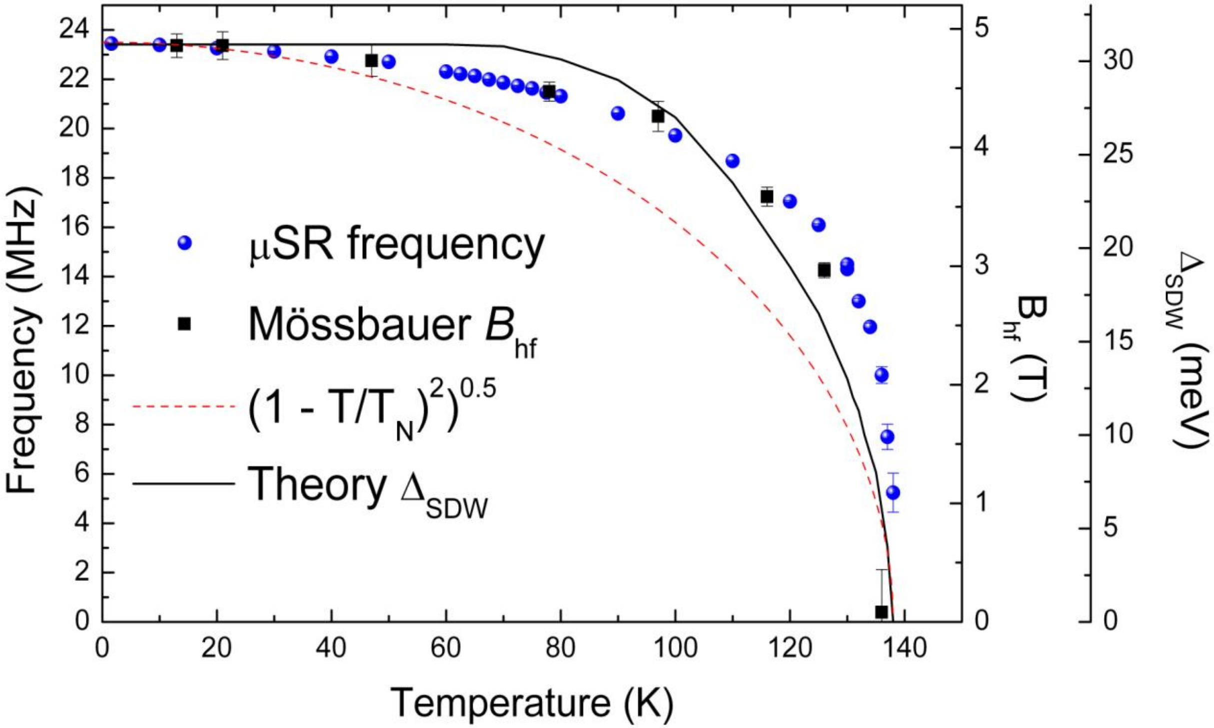
→proof of itinerant character

Spin density wave order = resonance on the Fermi Surface



M. Korshunov, I. Eremin, PRB 78, 140509(R) (2008)

Magnetic Order parameter in undoped LaOFeAs



Four band SDW theory

U=0.26eV

J=U/5

$Q_{AFM} = (\pi,\pi)$

Δ_{SDW}(0 K) = 31 meV

→ $\mu = 0.33\ \mu_B$

See:

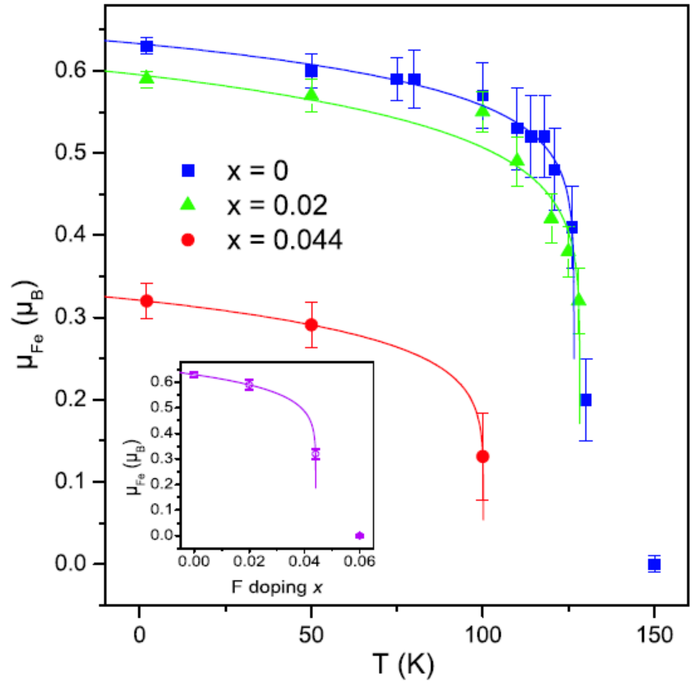
M. Korshunov and I. Eremin

arXiv:0804.1793

HHK et al., PRL08, arXiv:0805.0264

Magnetic order parameter of $LaO_{1-x}F_xFeAs$

Recent neutron scattering on the same $LaO_{1-x}F_xFeAs$ samples

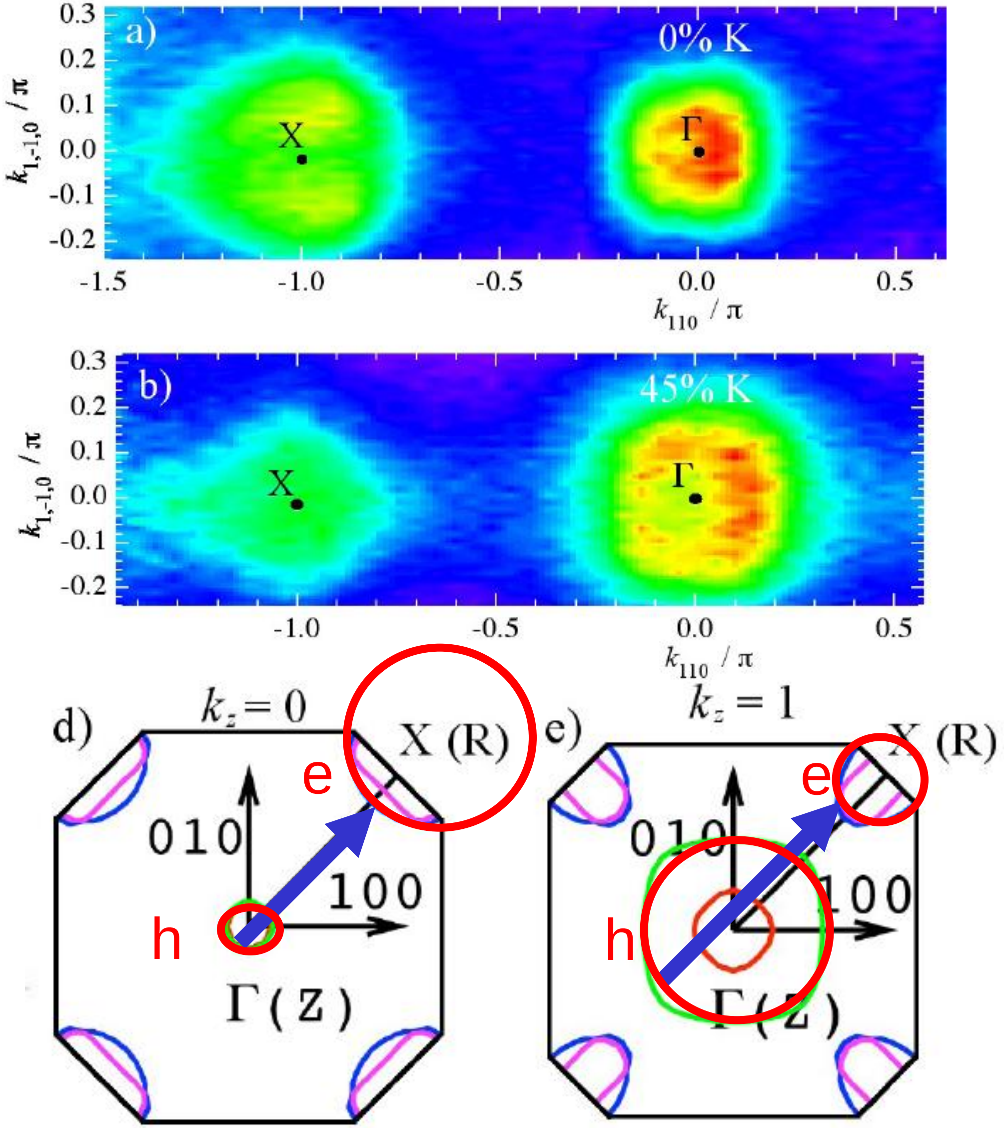


Qureshi et al., arXiv:1002.4326)

→ordered moment ~ 0.63 μ_B !

Doping electrons or holes: $Ba_{1-x}K_xFe_2As_2$

ARPES on s-xtals :Liu et al.; arXiv:0806.3453

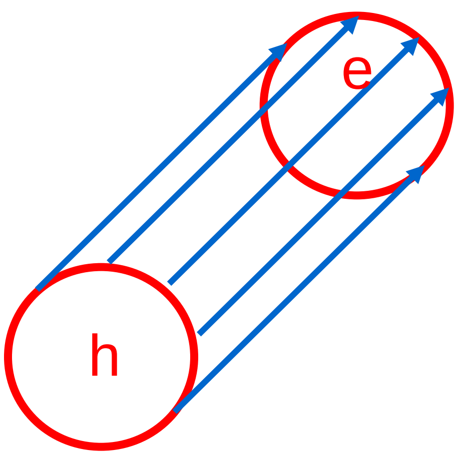


Fe ($3d^6$) → Co ($3d^7$)
= Electron doping

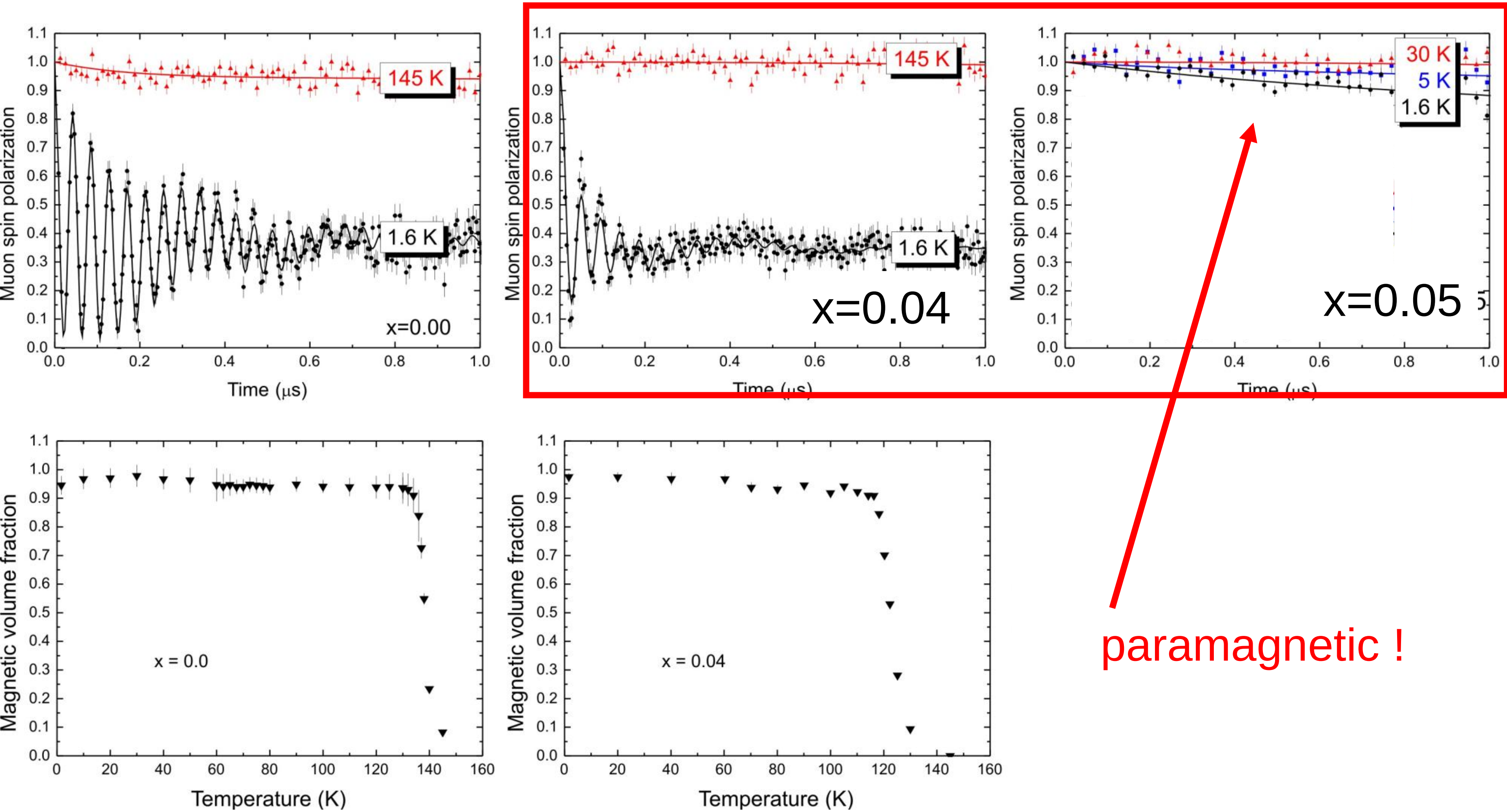
or

Ba^{2+} → K^{+}
= Hole doping

→Nesting condition on
Fermi surface destroyed

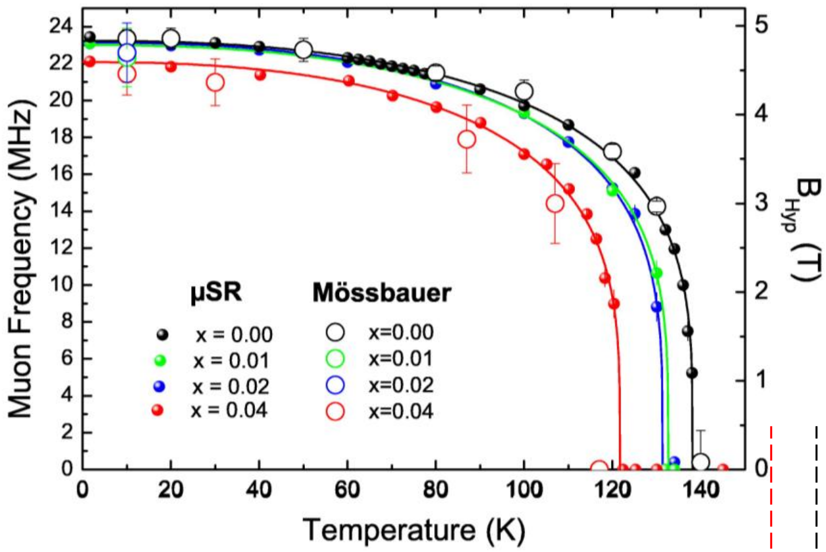


Magnetism of lightly doped $La(O_{1-x}F_x)FeAs$



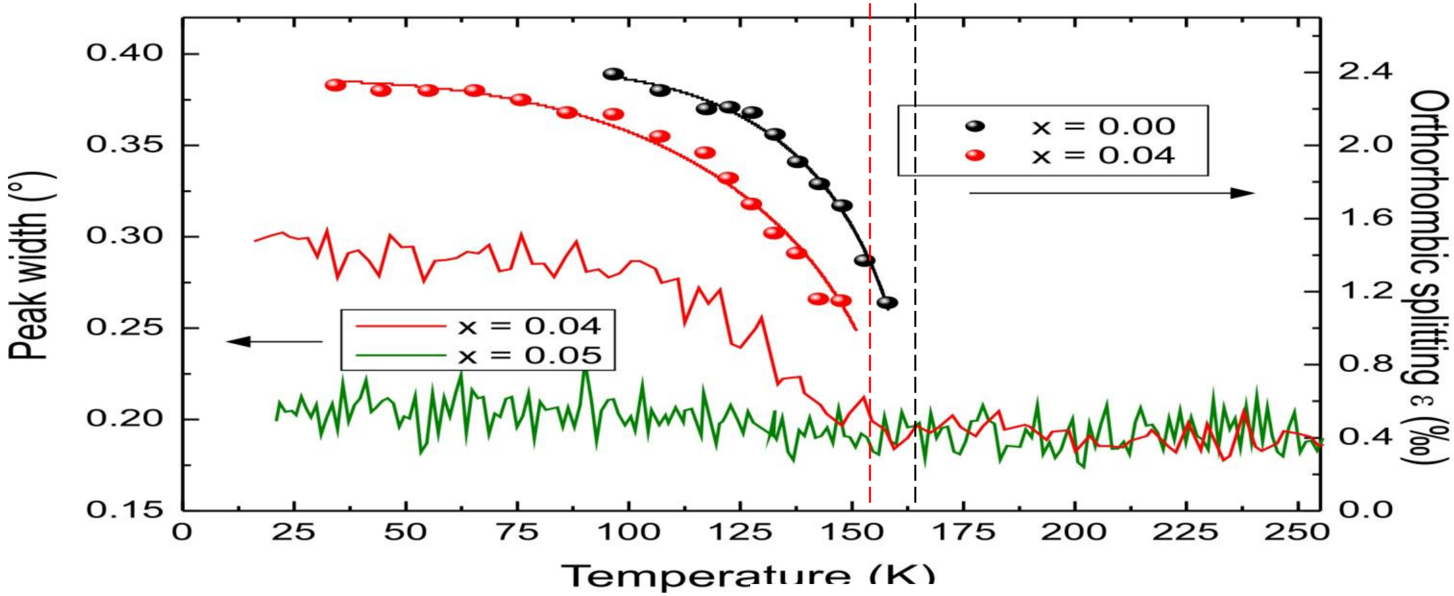
H. Luetkens et al., Nature Materials 2009

Magnetism in lightly doped $La(O_{1-x}F_x)FeAs$



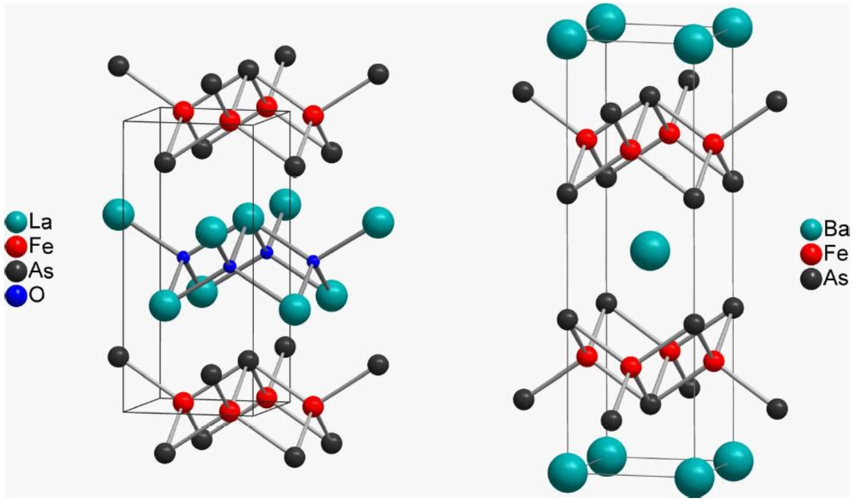
- Weak reduction of T_N and low temp order parameter for $0 \le x \le 0.04$

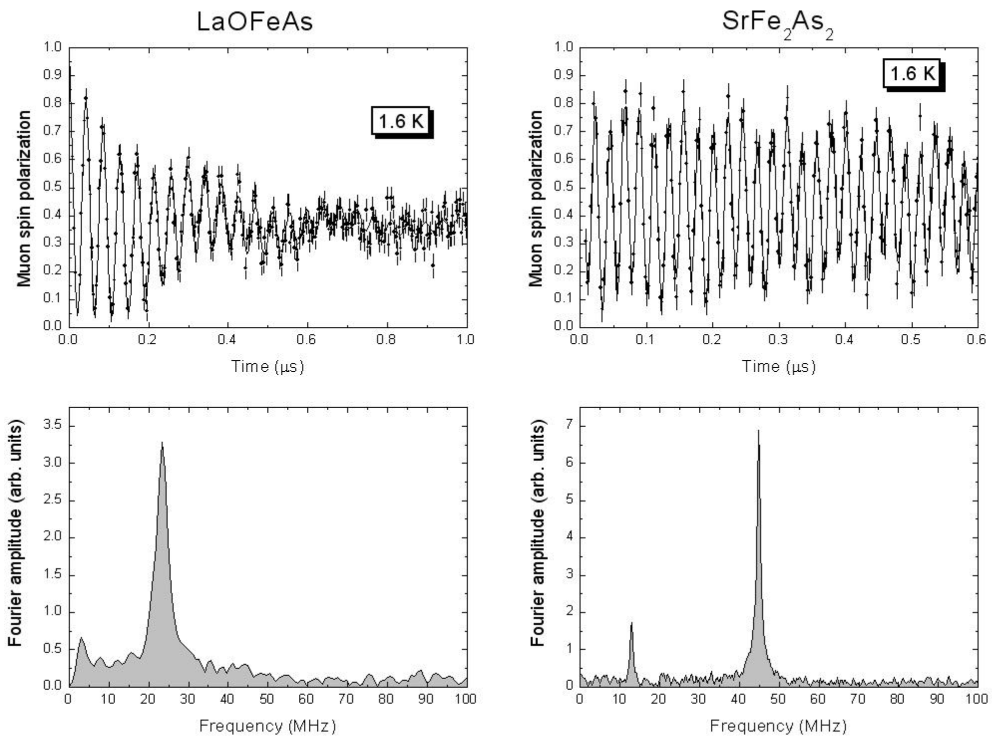
SDW magnetism correlated with orthorhombic distortion at higher temperature !



H. Luetkens et al, Nature materials 20093

SDW magnetism in $SrFe_2As_2$

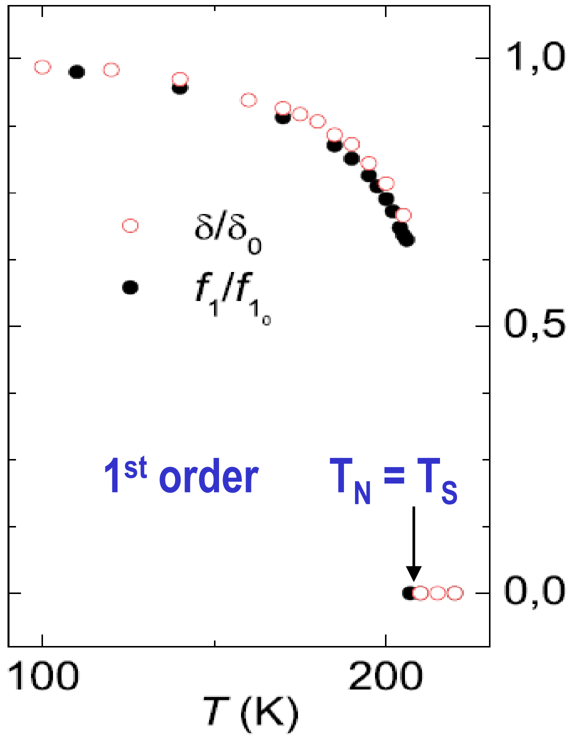


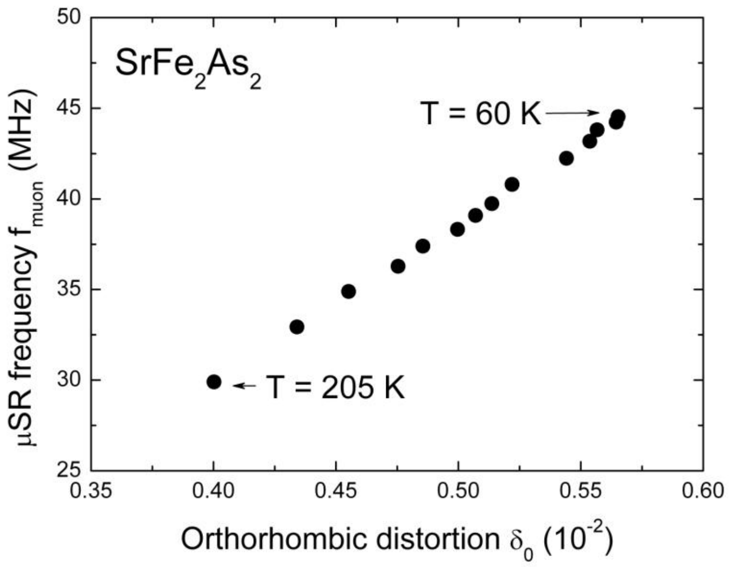


- μSR similar to LaOFeAs
- two signals same intensity ratio
- **~ 2 times larger frequency**

→2 times larger ordered moment (crf. Mössbauer, ns)

Structural and magnetic order parameter



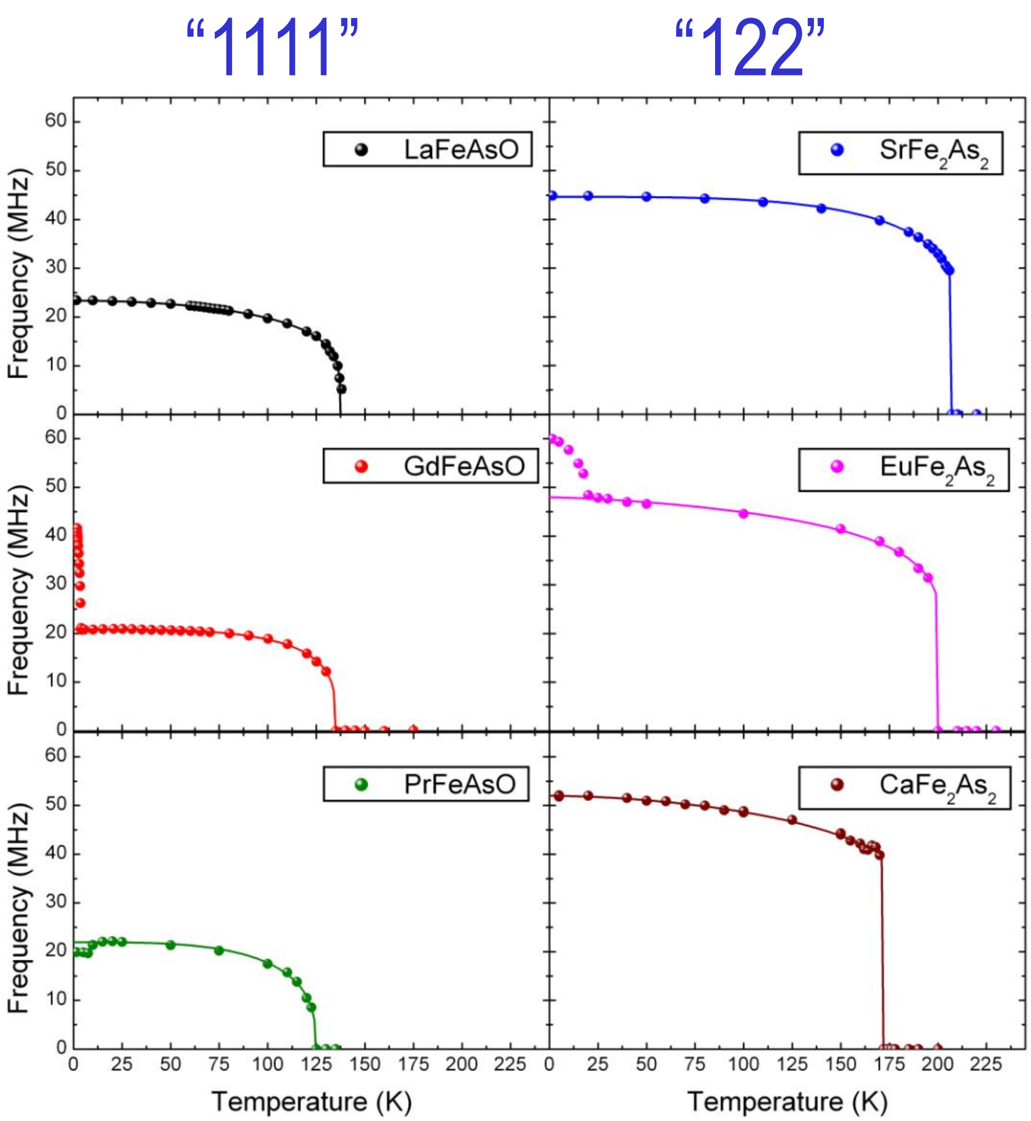


- 1st order transitions!
- identical temperature dependence of both order parameters

→Structure and magnetism are driven by the same Fermi surface instability

Jesche et al., PRB'08, arXiv:0807.0632

Comparison of "1111" and "122"



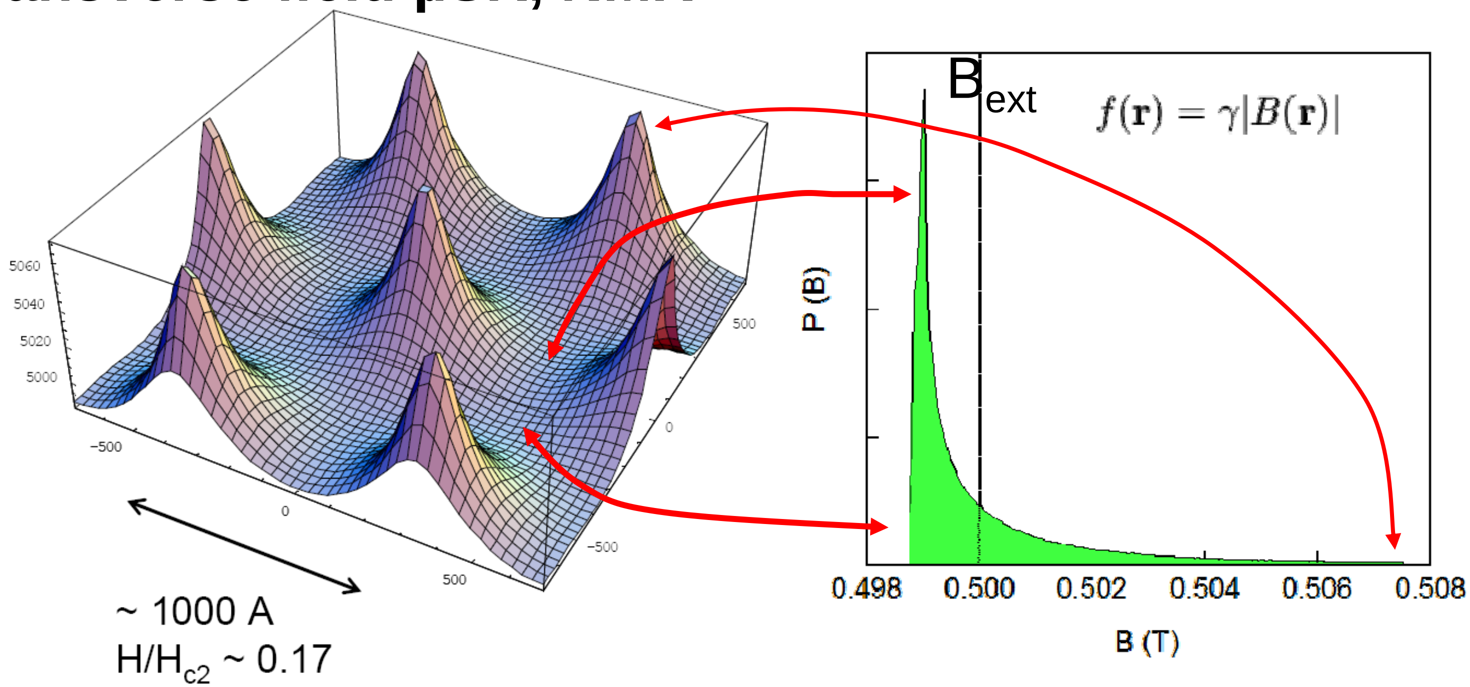
- Temperature dependence of the magnetic order parameter:
- "1111" family → second order magnetic phase transition
- "122" family → first order magnetic phase transition

How can we measure the superfluid density n_s / m^* ?

via the magnetic penetration depth λ
n_s / m^* is proportional to $1/\lambda^2$

- **measure λ in vortex state of type II superconductor via field profile p(B)**

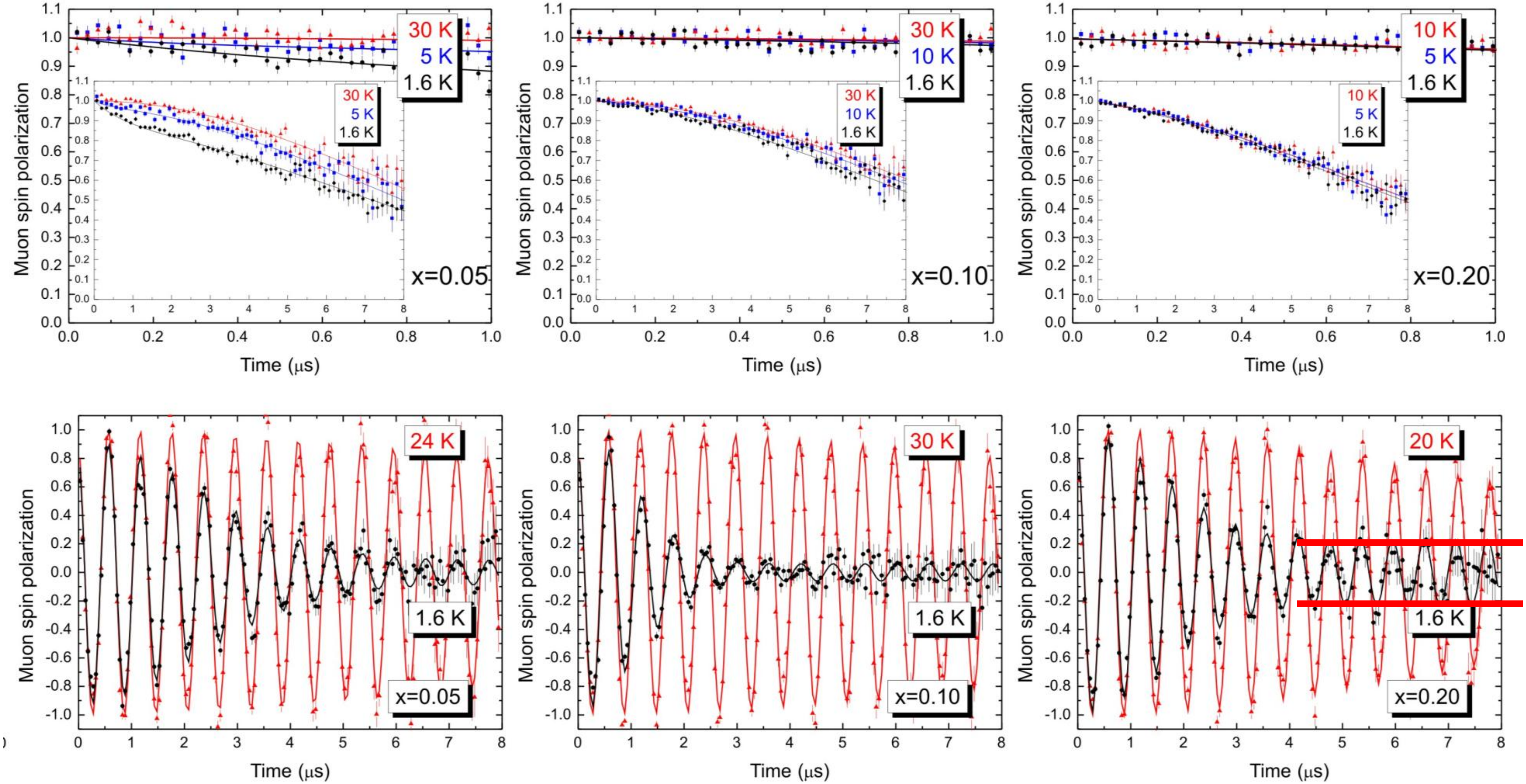
→ transverse field μSR, NMR



In powder of anisotropic superconductors
P(*B*) shows Gaussian shape

$$\langle \Delta B^2 \rangle \propto \lambda_{ab}^{-4}$$

μSR on superconducting $La(O_{1-x}F_x)FeAs$

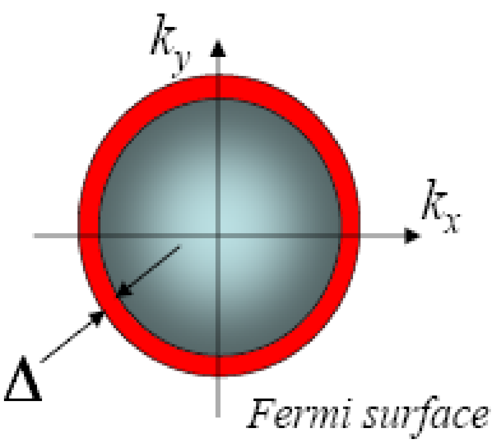


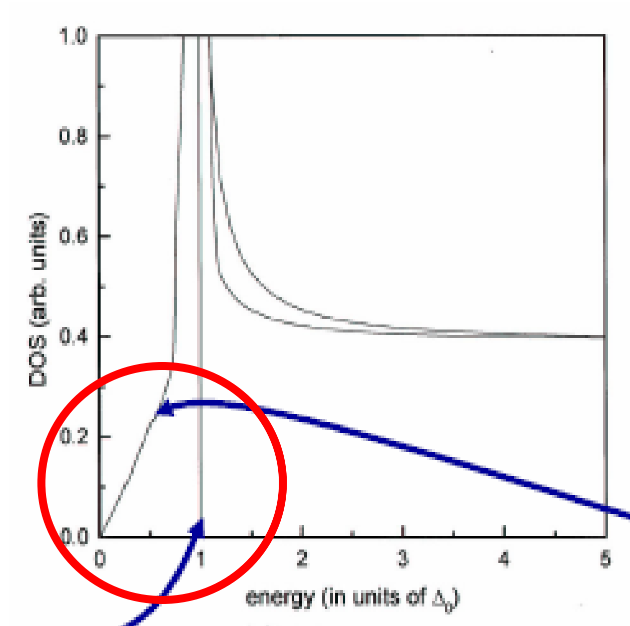
Gaussian relaxation σ_{sc} ~ $1/\lambda^2$ ~ n_s / m^* = sc order parameter

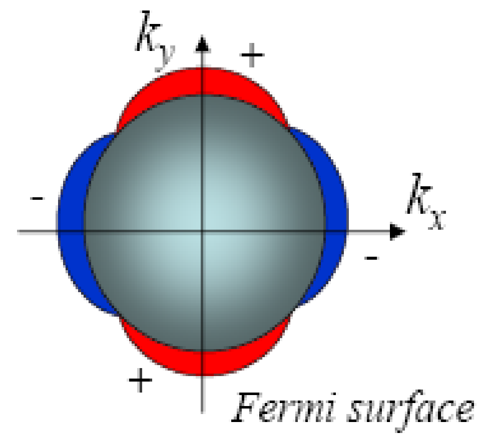
H. Luetkens et al, Nature materials 2009, arXiv:0806.3533

Superconducting Gap Function

The fundamental parameter of a superconductor is the gap $\Delta(\mathbf{k})$





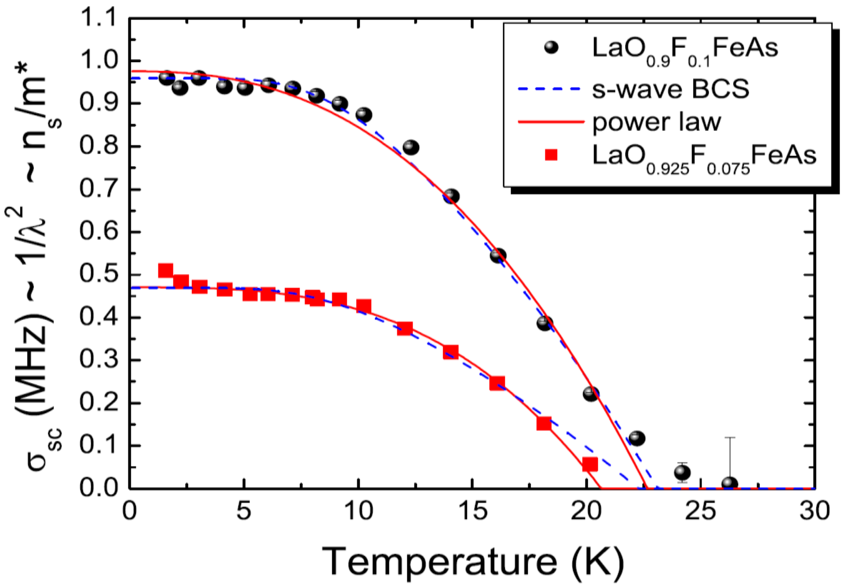


s-wave: isotropic gap

d-wave: nodes in k-space where gap vanishes

→Influence on stiffness of superconducting state

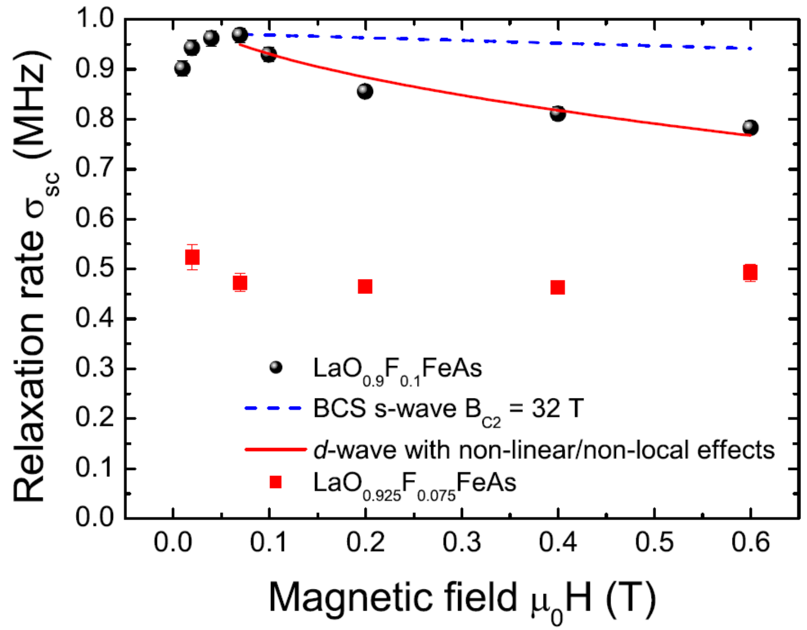
Magnetic penetration depth in $La(O_{1-x}F_x)FeAs$



H. Luetkens, HHK et al, PRL08

Temperature dependence of the relaxation rate $\sigma \propto n_s/m^*$

- Only weak temperature dependence below T_C / 3 : s-wave ?

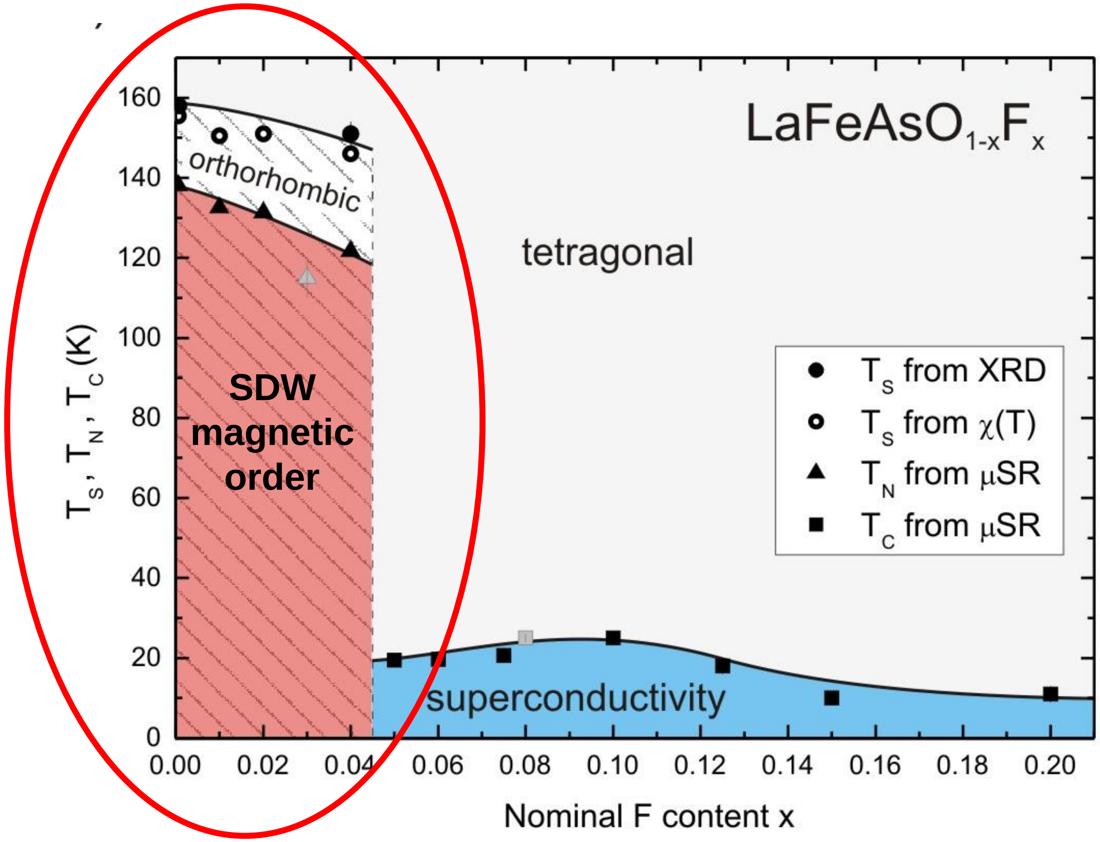


Magnetic field dependence of TF-µSR relaxation rate

- Strong field dependence: d-wave ?

- **No, extended s_{+-}-wave**
- **multi-band Fermi surface with two different gaps**

Phase Diagram of $La(O_{1-x}F_x)FeAs$



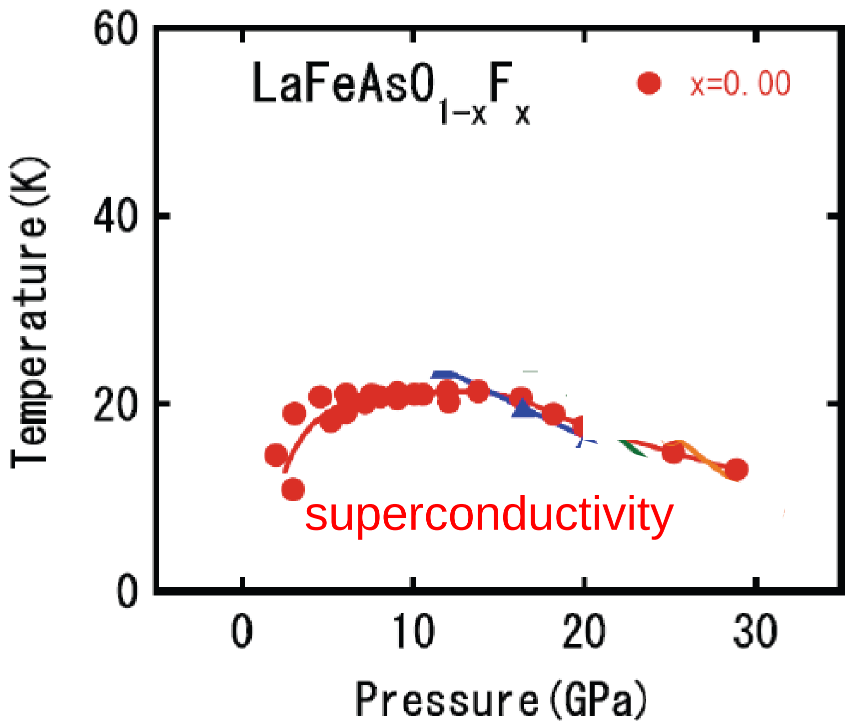
H. Luetkens, HHK et al., Nature Materials 2009

Fe pnictides are semimetals with itinerant magnetism

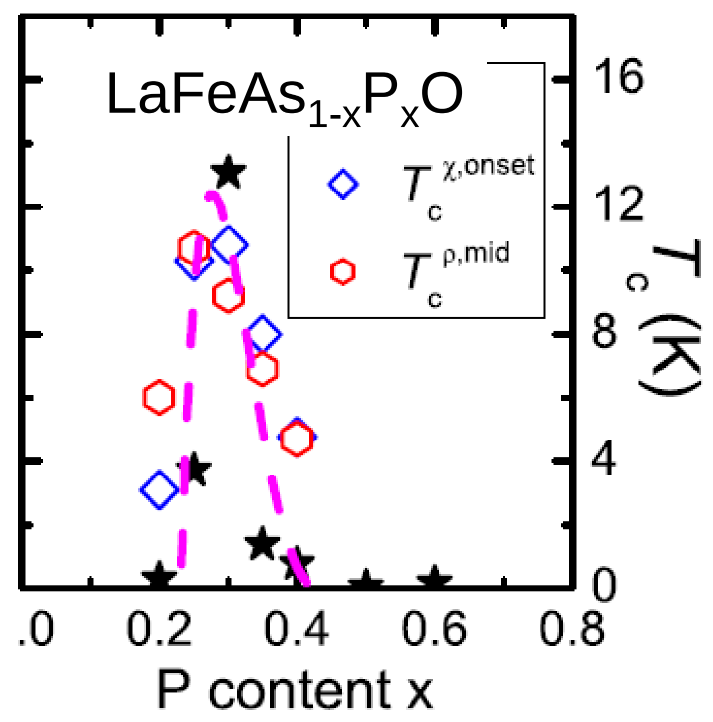
suppress magnetism by doping charge carriers, impurities or small changes of the Fermi surface (e.g. by high pressure)

→ superconductivity !

Pressure and chemical pressure

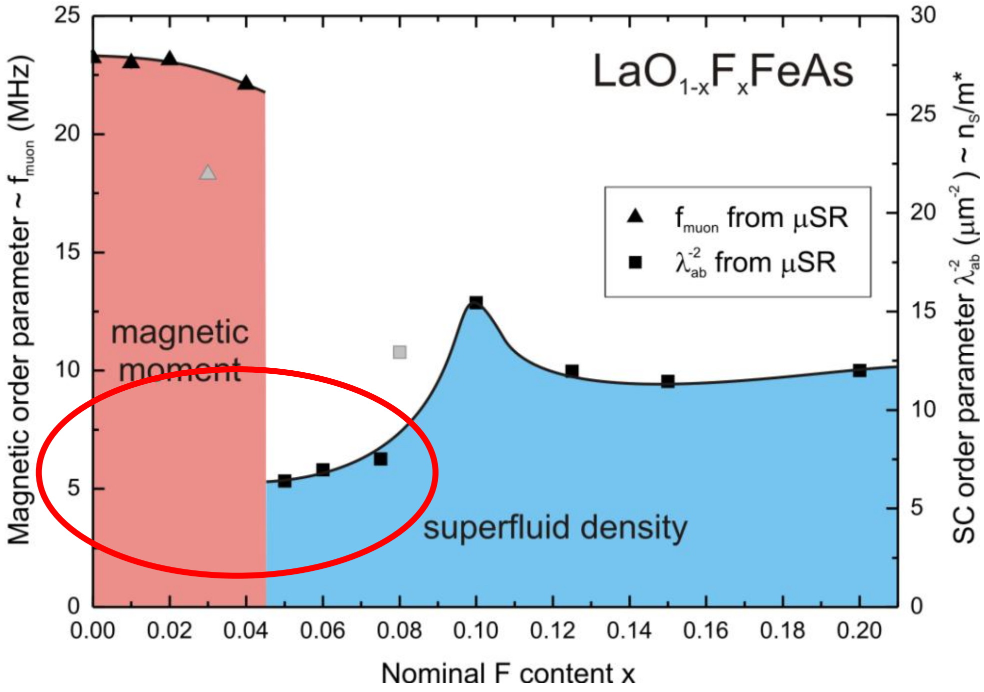


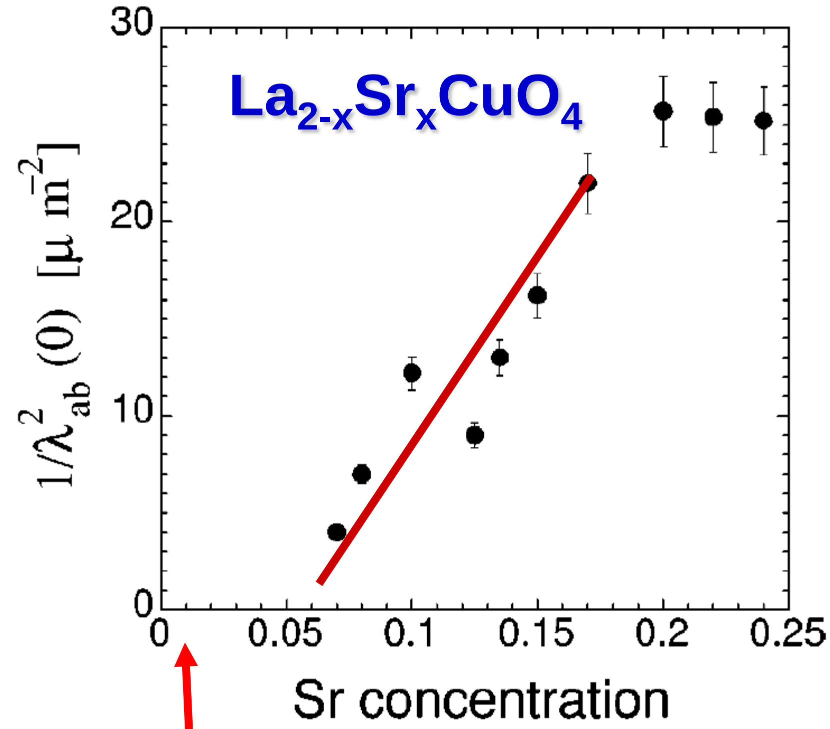
H. Takahashi et al., J. Phys. Soc. Jpn. **77**, C78 (2008)



C. Wang et al., EPL **86**, 47002 (2009)

Order Parameters in $La(O_{1-x}F_x)FeAs$





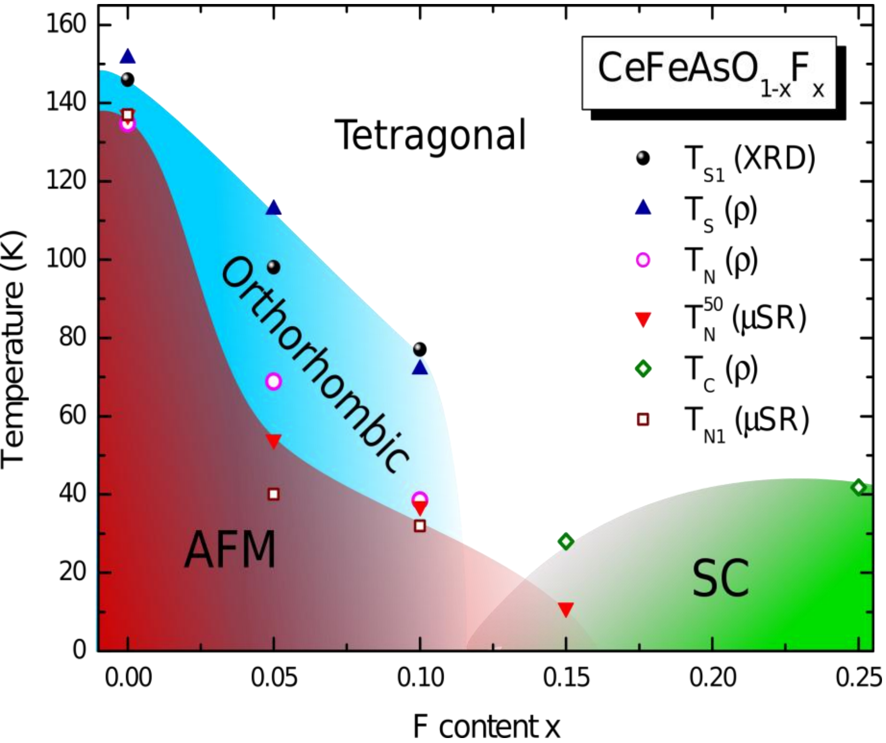
C. Panagopoulos et al.
PRB ´02

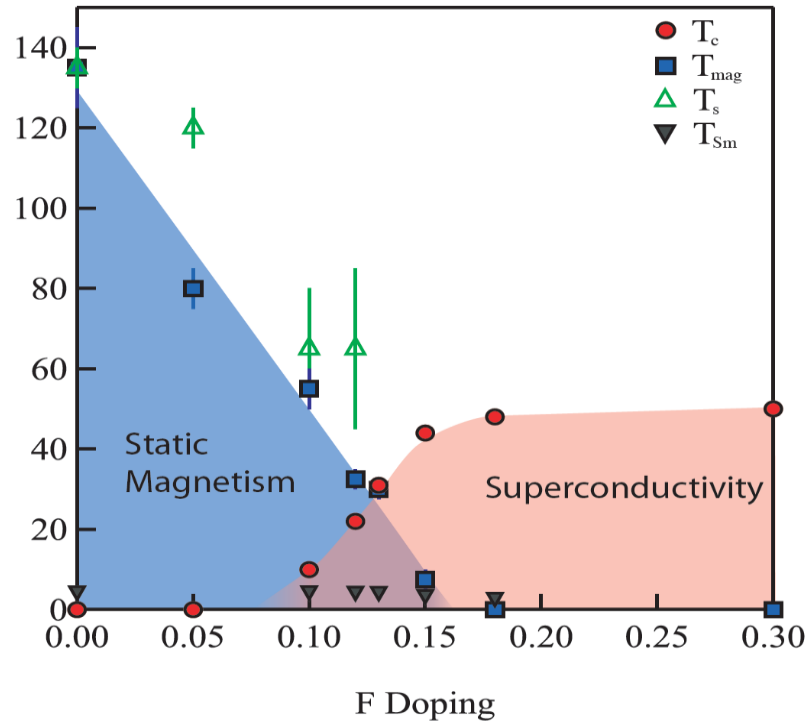
- no indications of quantum criticality in $LaO_{1-x}F_xFeAs$

no charge carriers here !

H. Luetkens et al., Nature Materials 2009

Phase Diagrams of $CeFeAsO_{1-x}F_x$ and $SmFeAsO_{1-x}F_x$





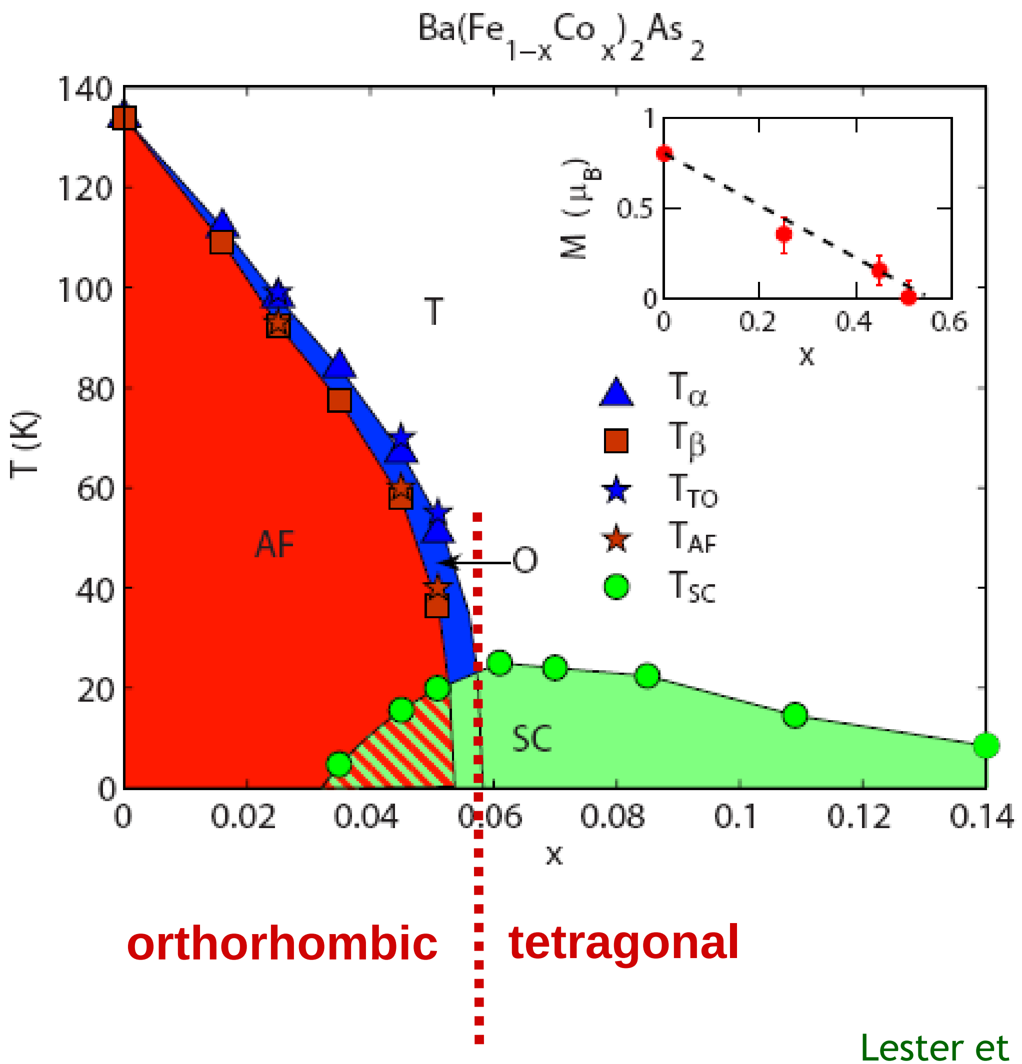
Drew et al., Nature Materials 2009

(crf. E. Baggio-Saitovich talk Tuesday)

No continuous transition between AFM and Superconductivity in the orthorhombic phase !!

Phase diagram of Co doped $BaFe_2As_2$

Single crystal neutron study: similar separation of structural and magnetic transition



Lester et al., PRB 2009

Mechanism for Superconductivity

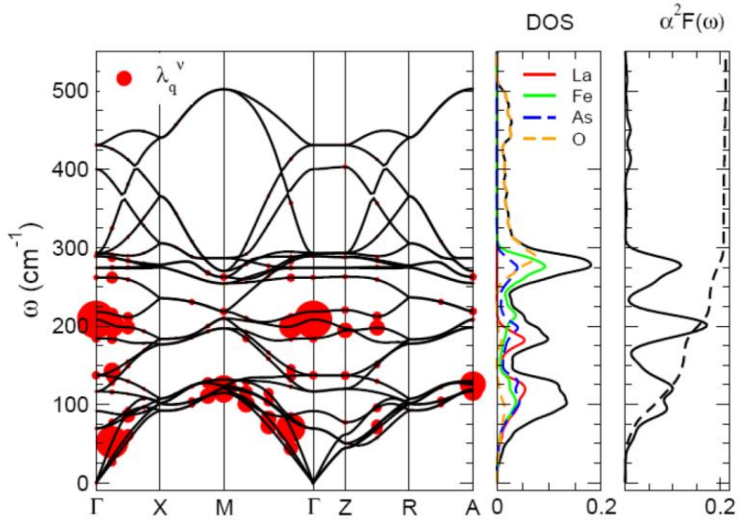
- Phonon DOS too small for T_C above *1K*

- AFM spin fluctuations result in attractive interaction in case of phase change only:
- d-wave sc in cuprates
- S_{+-} - symmetry in pnictides (Mazin et al., PRL08):

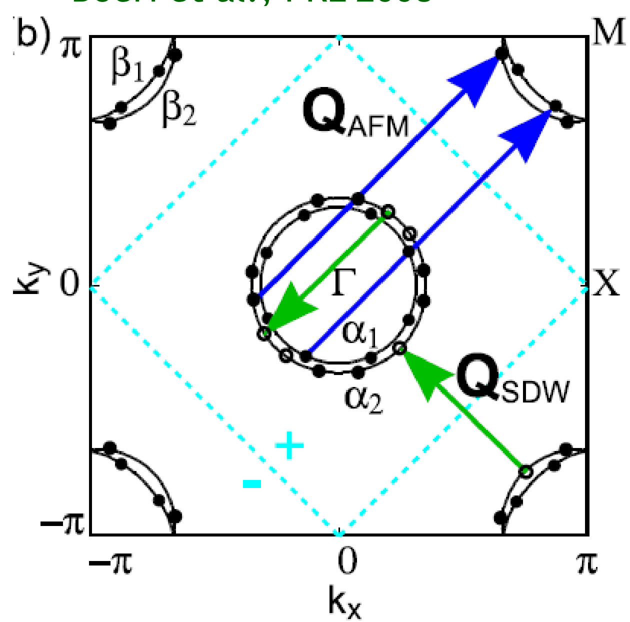
→ Full gap on each Fermi pocket
→ Phase change from scattering between hole and electron pocket

But:

d-wave and spin-triplet p-wave sc also discussed !



Boeri et al., PRL 2008



Competition of SDW and SC order

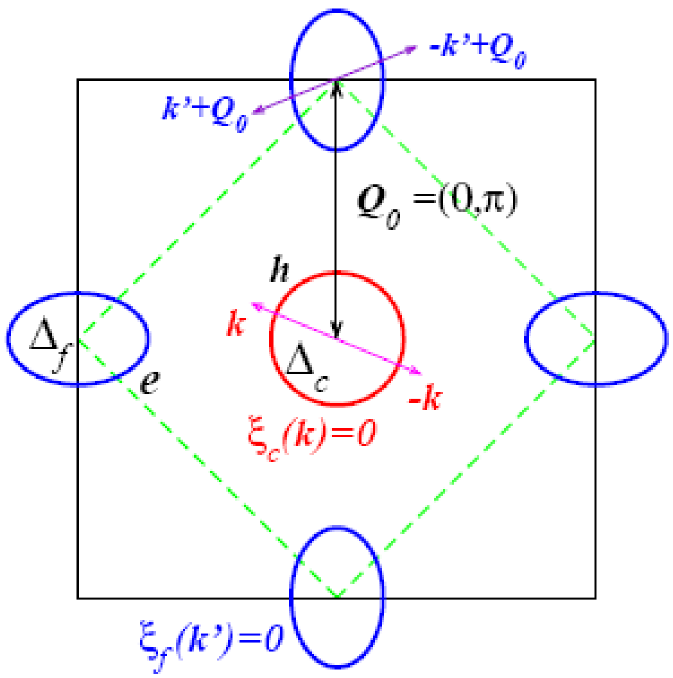
Important: Existence of nesting condition between electron and hole pockets

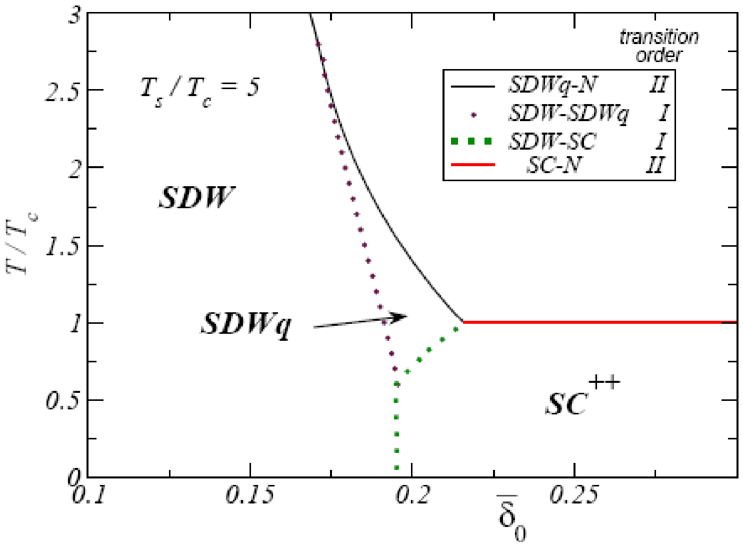
Two-band model :

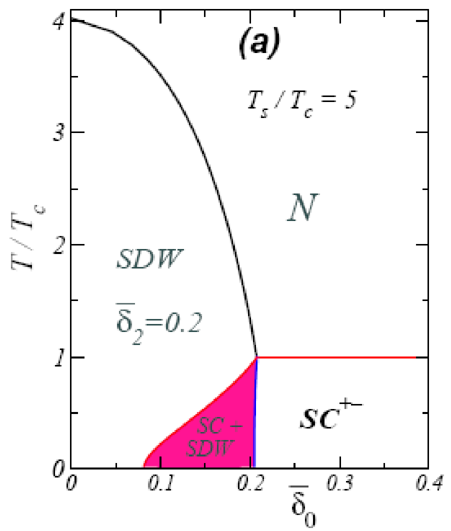
Hole and electron pockets

with different size and ellipticity

Vavilov et al., PRB 2010

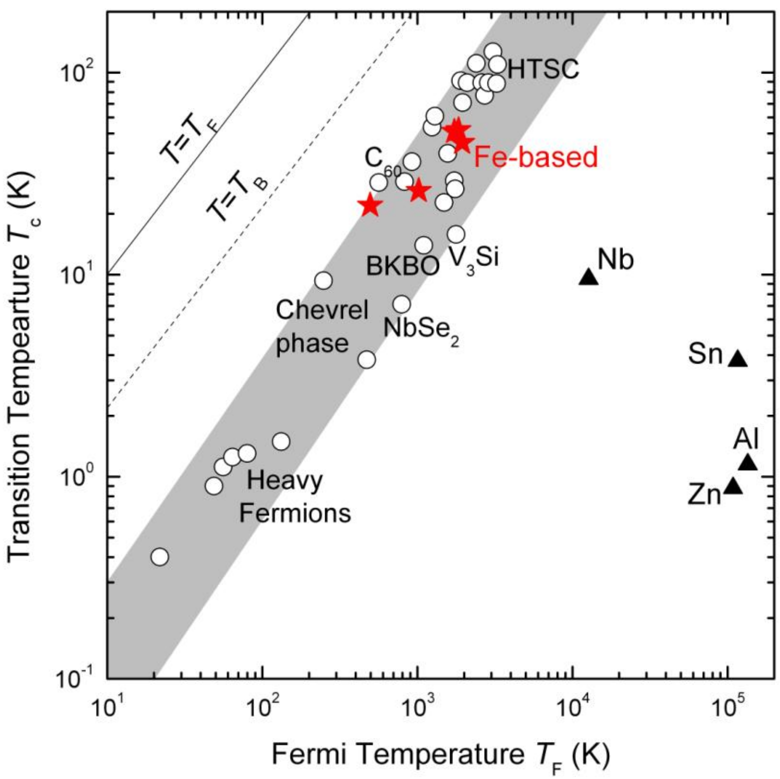






Classification of Fe-based SC

Uemura plot:



$$k_B T_F = \hbar \pi c_{int} \frac{n_s}{m^*} \propto c_{int} \sigma_{sc}$$

Y.J. Uemura *et al.*, Phys. Rev. Lett. **66**, 2665 (1991)

R. Khasanov et al., Phys. Rev. B 78, 092506 (2008)

- Conventional superconductors have low T_C and high superfluid density
- Unconventional superconductors have relatively low superfluid density ("dilute superfluid")

The Fe pnictides are unconventional superconductors

Magnetic Rare earth ions in $RO_{1-x}F_xFeAs$

Replace La with magnetic rare earth
→T_C doubles !

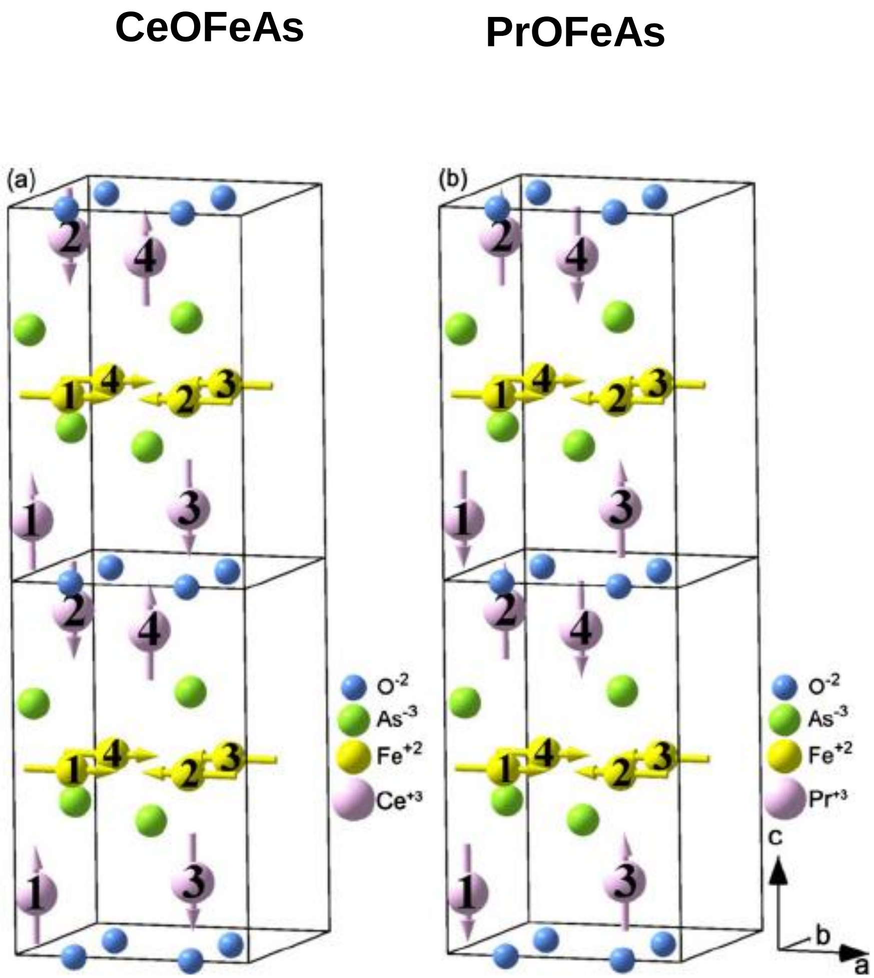
Structure: different ion size
→more favorable bond angles

regular FeAs tetrahedron has highest T_C

Magnetic interaction between rare earth ions and FeAs electronic system?

- Collinear Heisenberg interaction impossible due to frustration for planar Fe-SDW order
- **Non-collinear Heisenberg interaction possible**

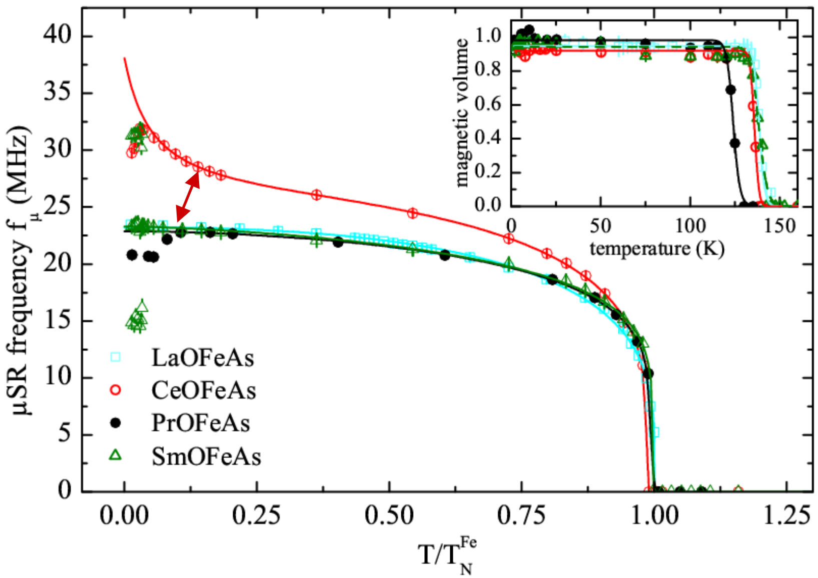
→ Non-collinear order of rare earth below T_{SDW} !



H. Maeter, HHK, *et al.*, Phys. Rev B (2009).

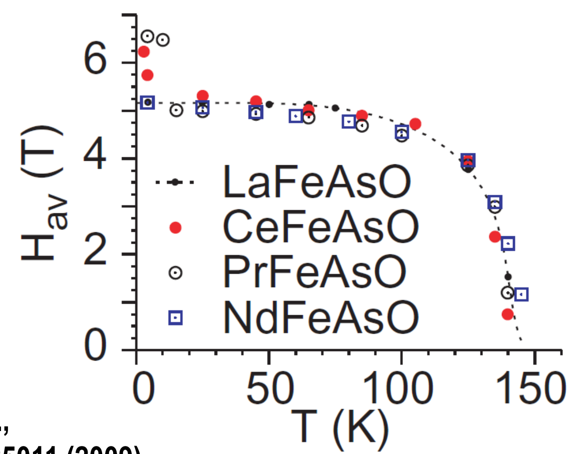
ROFeAs (R = La, Pr, Ce, Sm)

ZF-μSR:



H. Maeter, *et al.*, Phys. Rev. B (2009).

Moessbauer:

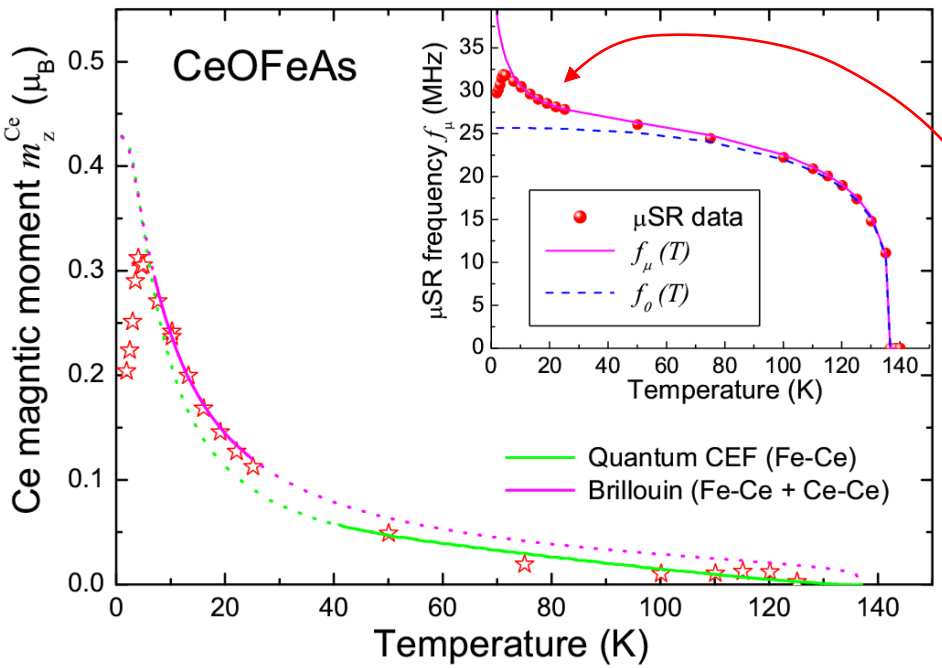


M. A .McGuire *et al.*,
New J. Phys. 11, 025011 (2009).

- **Zero Field Muon Spin Rotation**
  - Static magnetic order below T_N
  - 100% magnetic volume fraction
  - Commensurate magnetic structure
- T-dependence of μSR frequency
  - Second order transition at T_N(Fe)
  - $T_N(R)$ ~4 K
  - **Why is CeOFeAs different ?**
- **Moessbauer spectroscopy**
  - All compounds have the same ordered Fe moment !
- **Neutron scattering: 0.25 – 0.8 μ_B ?**

Ce magnetization above T_N^{Ce}

CeOFeAs

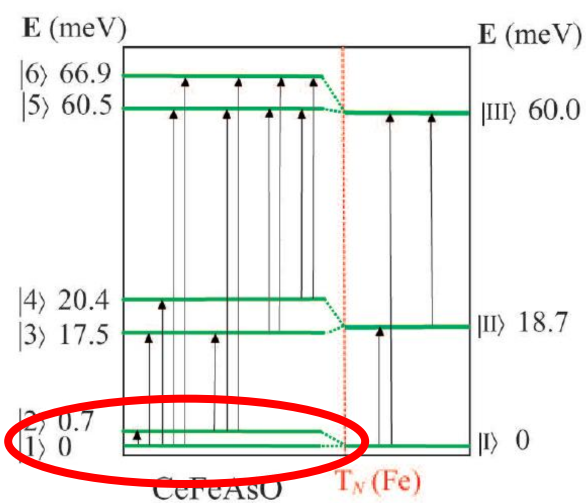


$$f(T) = \underbrace{f_0\left[1-\left(\frac{T}{T_N}\right)^{\alpha}\right]^{\gamma}}_{\text{Fe sublattice magnetization}} \cdot \left[1+\frac{\tilde{C}}{T-\Theta}\right]$$

Fe sublattice magnetization

Curie-like Ce magnetization

- **Ce-magnetization in molecular field of the Fe sublattice**
  - Contributes to same Bragg peaks as the Fe order
  - Additional field at the muon site proportional to the Ce magnetization
- **Quantitative analysis**
  - Curie-like term to the μSR frequency
  - calculation of thermal population of Ce crystal electric field (CEF) levels

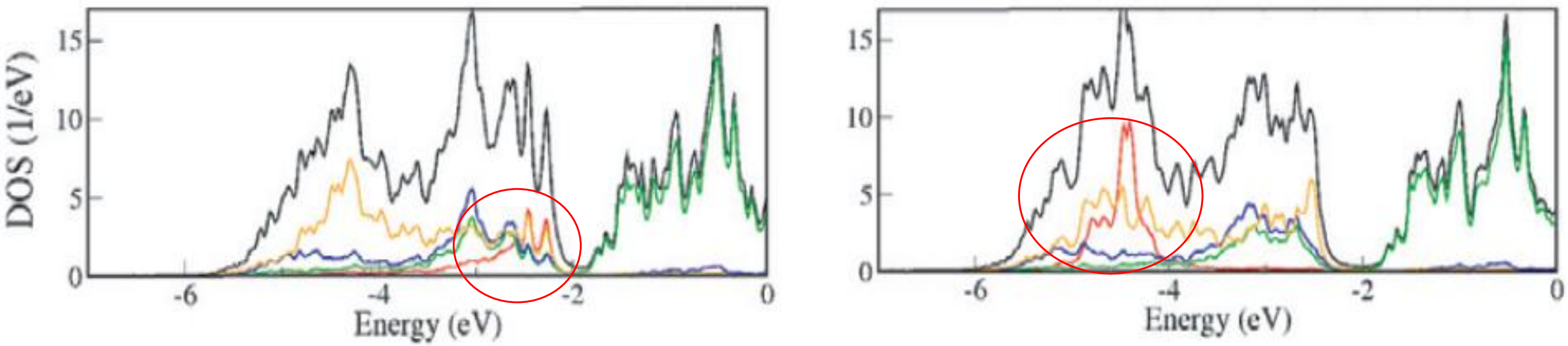


H. Maeter, *et al.*, Phys. Rev B (2009).

S. Chi *et al.*, arXiv:0807.4986 (2008).

Interplay of Rare Earth and FeAs electronic systems

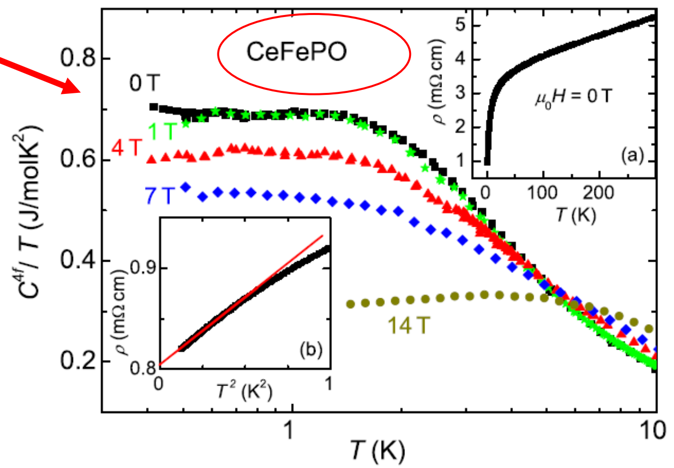
- **LDA band structure CeOFeAs** **PrOCeAs**



L. Pourovskii et al., EPL 84 37006 (2008)

- **Strong hybridization between Fe and Ce states**
- **CeOFeP is a moderate heavy fermion system**

- **Pr states shifted 2 eV downwards**

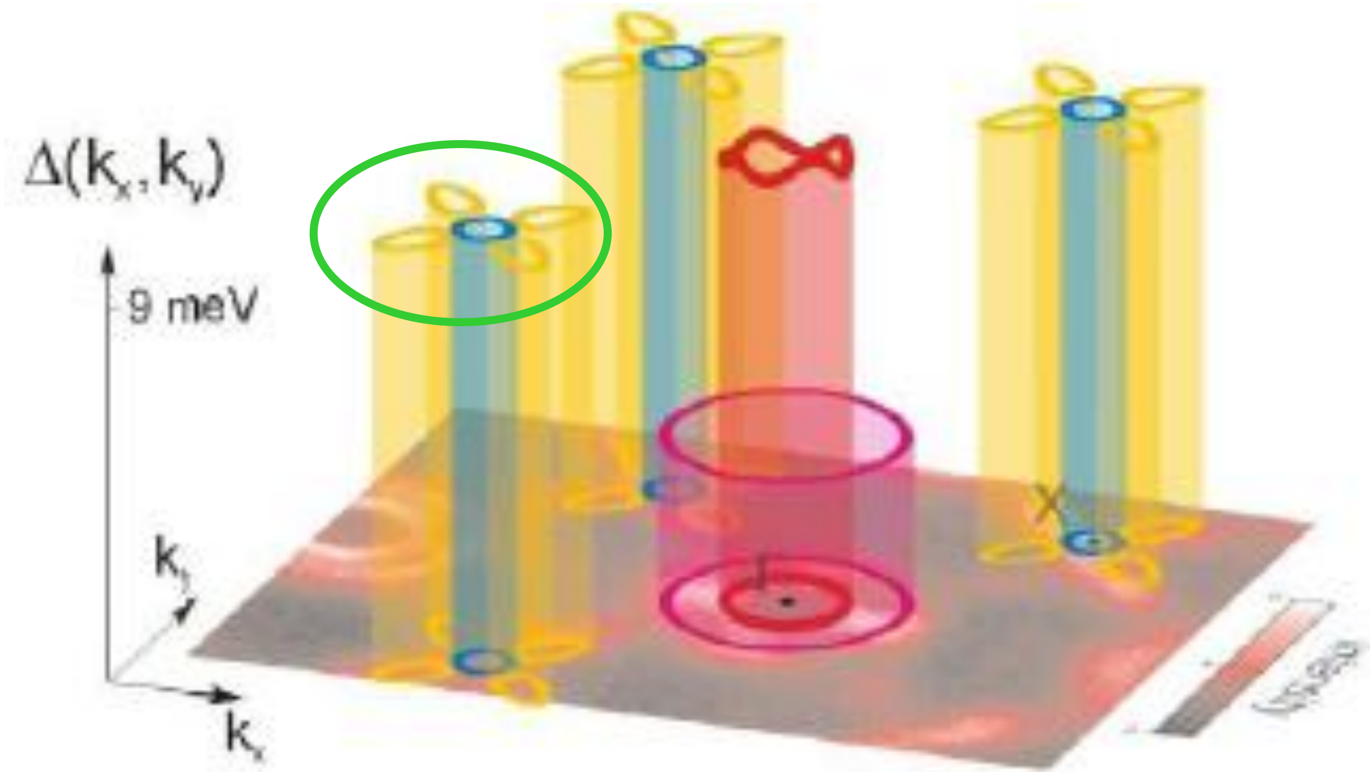


E. M. Brüning et al., Phys. Rev. Lett. 101, 117206 (2008)

Gap Anisotropy in $Ba_{1-x}K_xFe_2As_2$, T_c = 32 K

blades instead of barrels
→ correlation effect?

Coupling strength $2\Delta/k_BT_c$



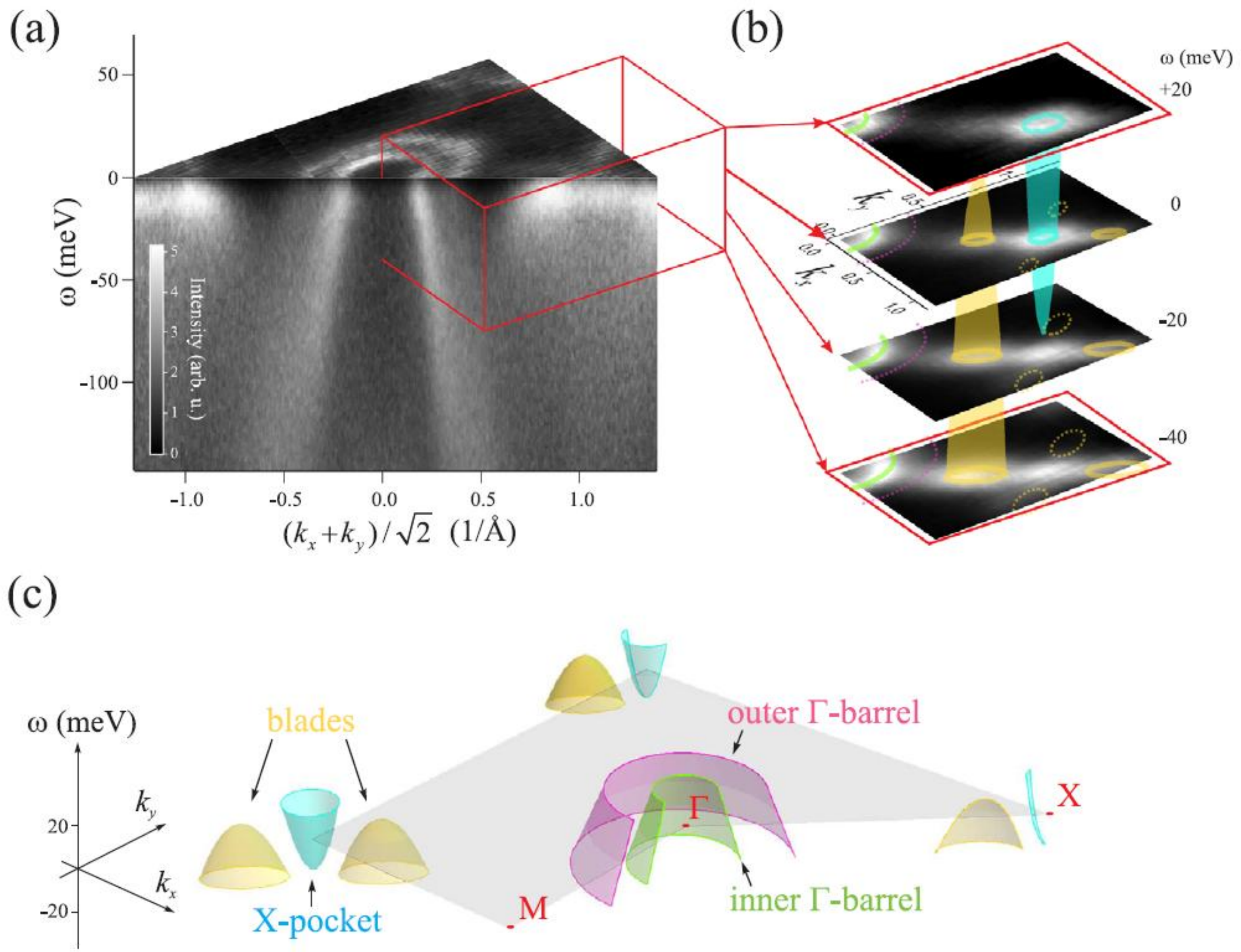
~ 7

~ 2.5

D.V. Evtushinsky et al., PRB 09, arXiv: 0809.4455

Similar results see eg. Ding et al EPL 2008

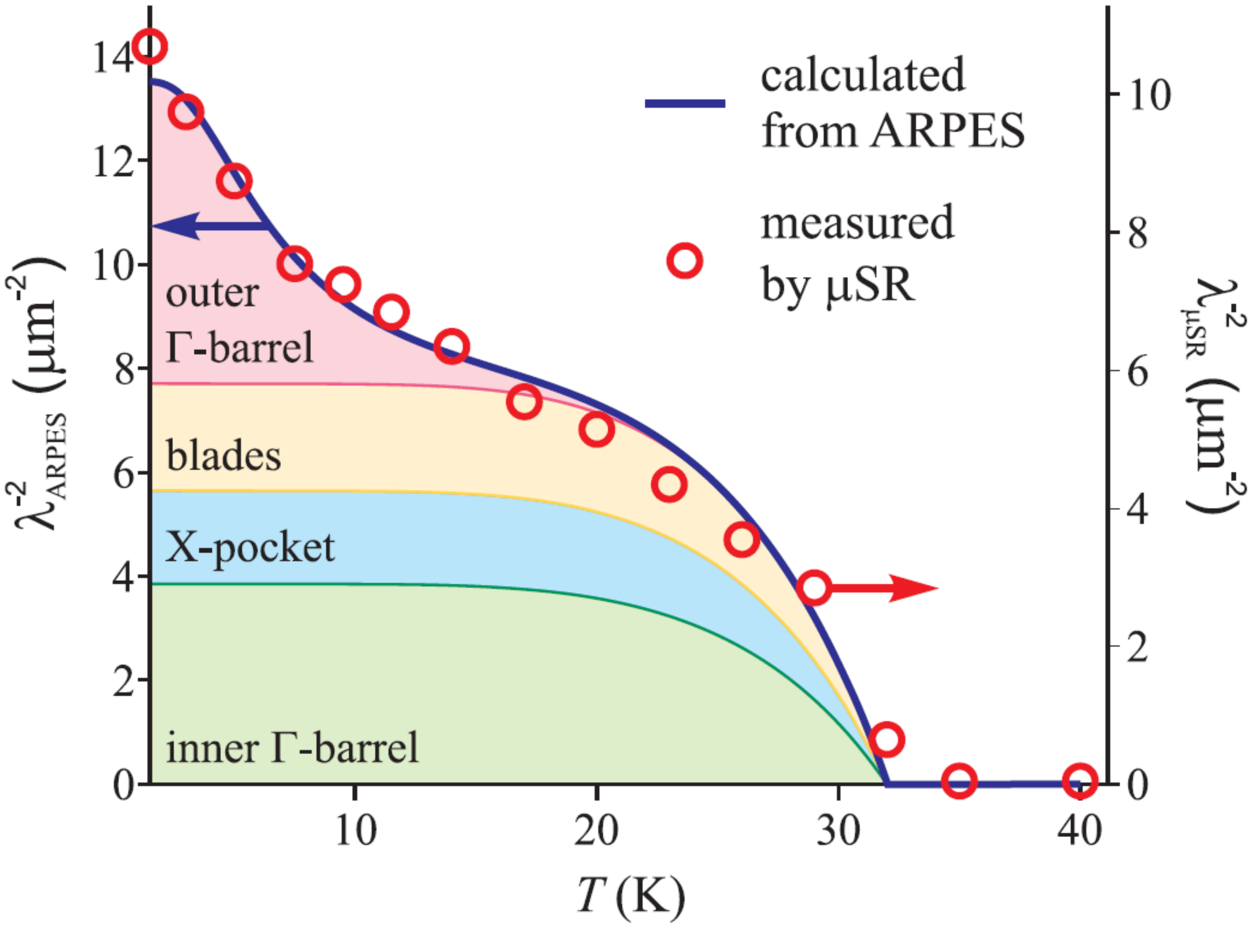
Band dispersion



D.V. Evtushinsky et al., NJP 09 in print

Band dispersion

$$\frac{1}{\lambda^2(0)} = I_1 + I_2 = \frac{e^2}{2\pi\varepsilon_0 c^2 h L_c}\left[\int_{\text{inner }\Gamma} v_F(\mathbf{k})\mathrm{d}k + \int_{\text{outer }\Gamma} v_F(\mathbf{k})\mathrm{d}k + \int_{\text{X-pocket}} v_F(\mathbf{k})\mathrm{d}k + \int_{\text{blades}} v_F(\mathbf{k})\mathrm{d}k\right]$$

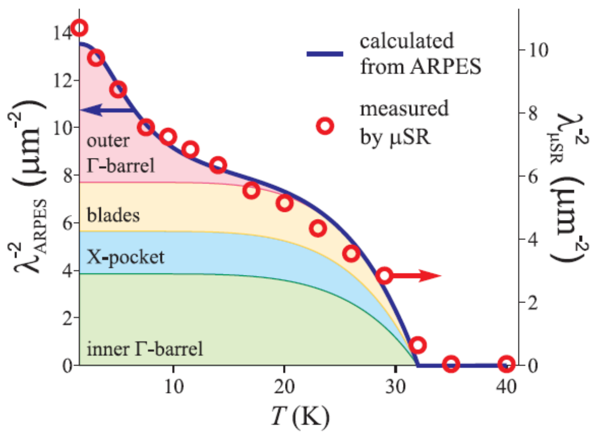


D.V. Evtushinsky et al., NJP 09 in print

R. Khasanov, PRL 09, in print

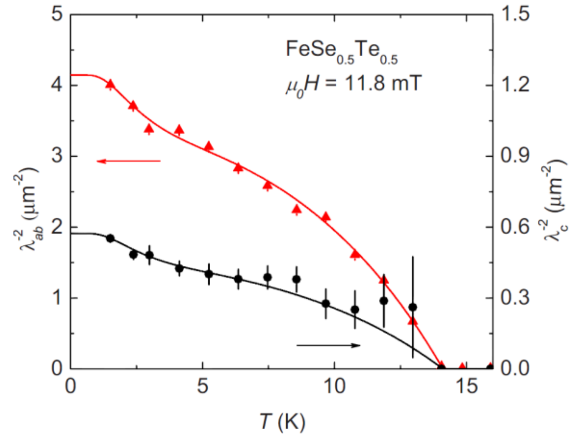
Multiband Superconductivity

$Ba_{1-x}K_xFe_2As_2$



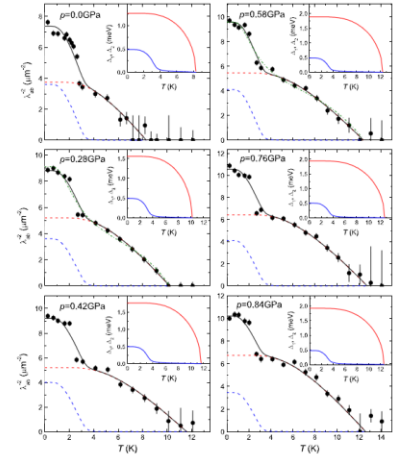
R. Khasanov *et al.*, PRL 102, 187005 (2009).

$FeSe_{1-x}Te_x$



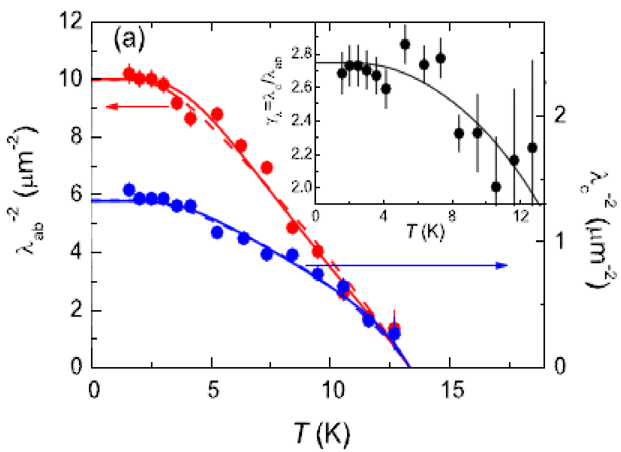
M. Bendele *et al.*, PRB 81, 224520 (2010).

$FeSe_{1-x}$



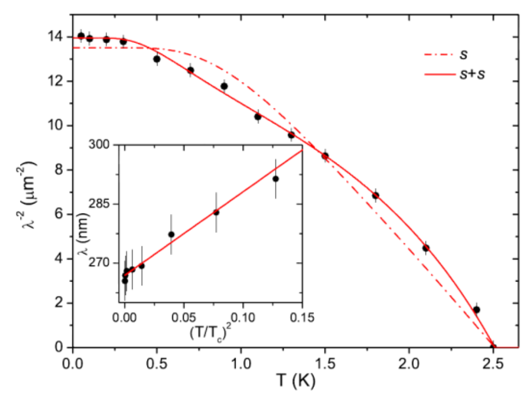
R. Khasanov *et al.*, PRL 104, 087004 (2010).

$SrFe_{2-x}Co_xAs_2$



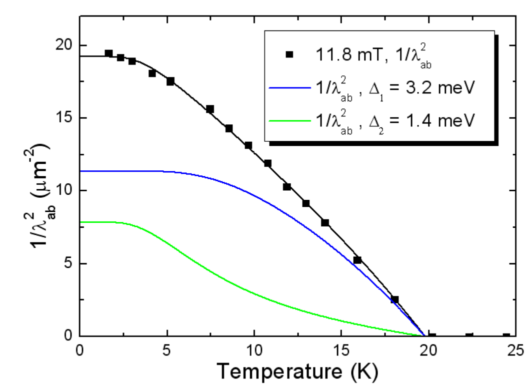
R. Khasanov *et al.*, PRL 103, 067010 (2009).

$RbFe_2As_2$



Z. Shermadini *et al.*, arXiv:1005.3989

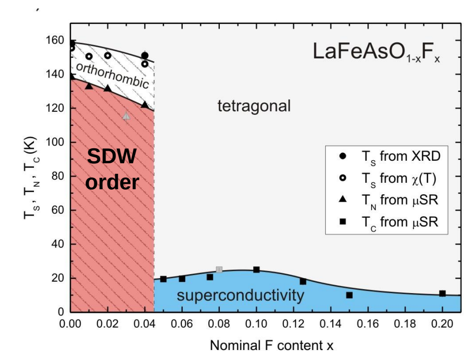
$BaFe_{2-x}Co_xAs_2$



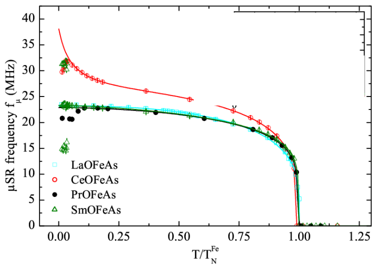
H. Luetkens *et al.*, in prep. (2010).

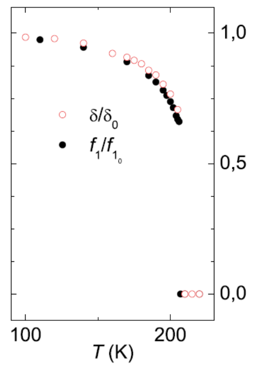
Summary

- **From spin density wave magnetism to superconductivity in $LaO_{1-x}F_xFeAs$**
  - Unconventional metal in normal state
  - SDW strongly coupled to orthorhombic phase
  - reduced moment ~ 0.3 - 0.6 μ_B
  - 1st order transition to superconductivity
  - Superfluid density finite at x= 0.05



- **$RO_{1-x}F_xFeAs$ and $ROFeAs_{1-x}P_x$**
  - no SC in othorhombic phase for R=Ce,Sm
  - independent R order below ~ 4-12 K
  - non-collinear magnetic interaction
  - between Ce and FeAs electronic systems





- **Intermetallic $(Sr,Ba)_{1-x}K_xFe_2As_2$**
  - Strong coupling of structural and magnetic order parameter
  - Phase coexistence/separation
  - under doping (and high pressure)
  - Two gap values on different FS sheets