Electronic Properties of Pnictide Superconductors

Leibniz-Institut
für Festkörper- und
Werkstoffforschung
Dresden

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Dresden

High Temperature Superconductivity in FeAs Compounds

OUTLINE

Monday

- **Introduction**
- **Phase Diagram of $LaFeAsO_{1-x}F_x$ (and other pnictides)**
  Structural, magnetic, and superconducting transitions
- **Superconducting State**
  Gap, penetration depth, relaxation rate

- **Normal State Properties**
  Electronic Structure (XAS, PES, ARPES)
  „Pseudogap“ (NMR, χ)
  Electronic transport and spin fluctuations
  Charge inhomogeneity (NQR)

Some of the people @ IFW involved in the research on FeAs …

Synthesis:	G. Behr, J. Werner, S. Singh, C. Nacke, S.Wurmehl et al.
M, Thermodynamics:	N. Leps, L. Wang, R. Klingeler et al.
NMR, ESR:	H. Grafe, G. Lang. F. Hammerath, V. Kataev et al.
Transport :	A. Kondrat, G. Friemel, C. Hess et al.
X-ray diffraction:	J. Hamann-Borrero
Spectroscopy:	S. Borysenko, D.V. Evtushinsky, A. Koitzsch, J. Geck A. Kordyuk, V.B. Zabolotnyy, T. Kroll, M. Knupfer et al.

Cooperations

μSR, Mößbauer	**H.H.Klauss, H. Maeter et al.**	**TU Dresden**
μSR	H. Luetkens, R. Khasanov et al.	PSI Villingen
Crystals	C.T. Lin, D. Inosov, V. Hinkov, B. Keimer et al.	MPI FKF Stuttgart
NMR	N. Curro	UC Davis
X-ray/neutron diffraction	M. Braden et al.	U Köln
X-ray/neutron diffraction	R. Feyerherm, D. Argyriou et al.	HZ Berlin

DFG-Research Unit FOR538

Doping Dependence of Phase Transitions and Ordering Phenomena in Copper-Oxygen Superconductors

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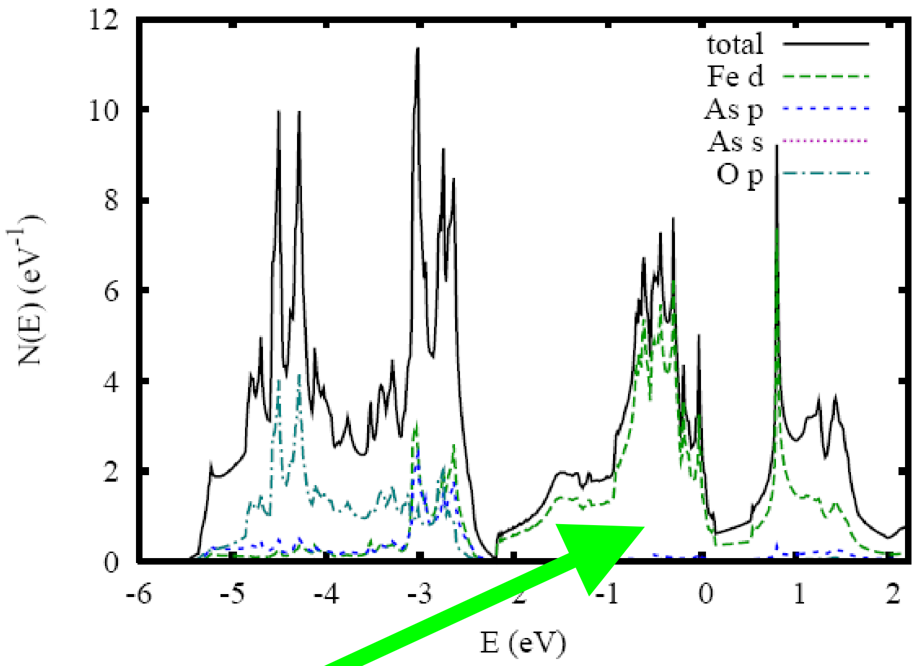
Electronic Properties of Pnictide Superconductors

OUTLINE

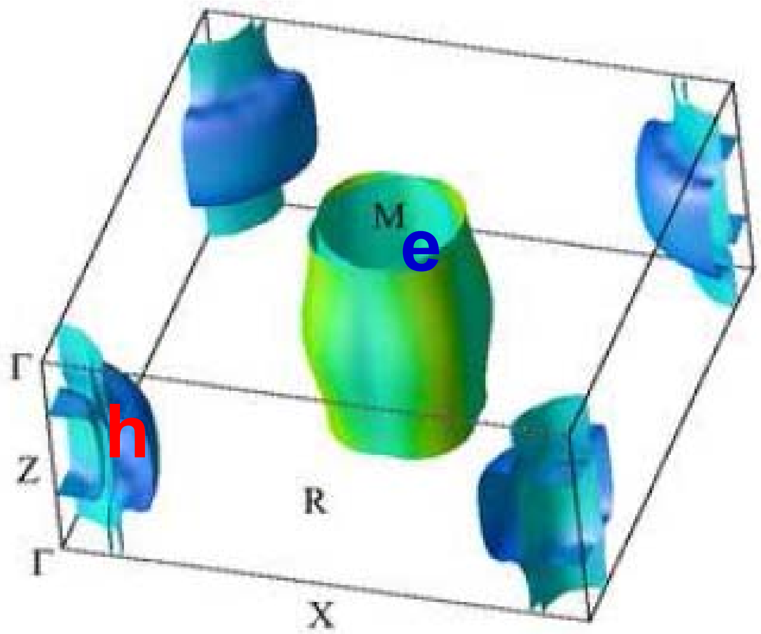
- „Local physics“, Hubbard U etc.
- ARPES, Fermi surface etc.
- „Pseudogap“, Strange T dependencies
- Normal state resistivity
- Charge inhomogeneity (NQR)

Magnetic order of LaOFeAs

Electronic Structure: LAPW LDA



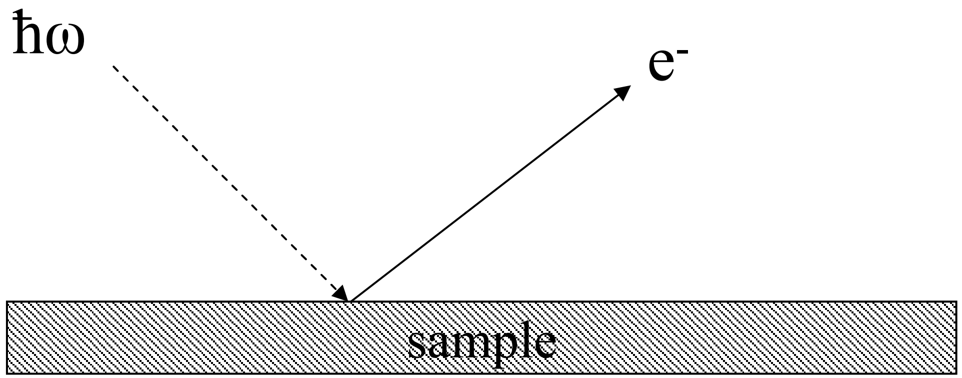
Fe^{2+} 3d^6-states

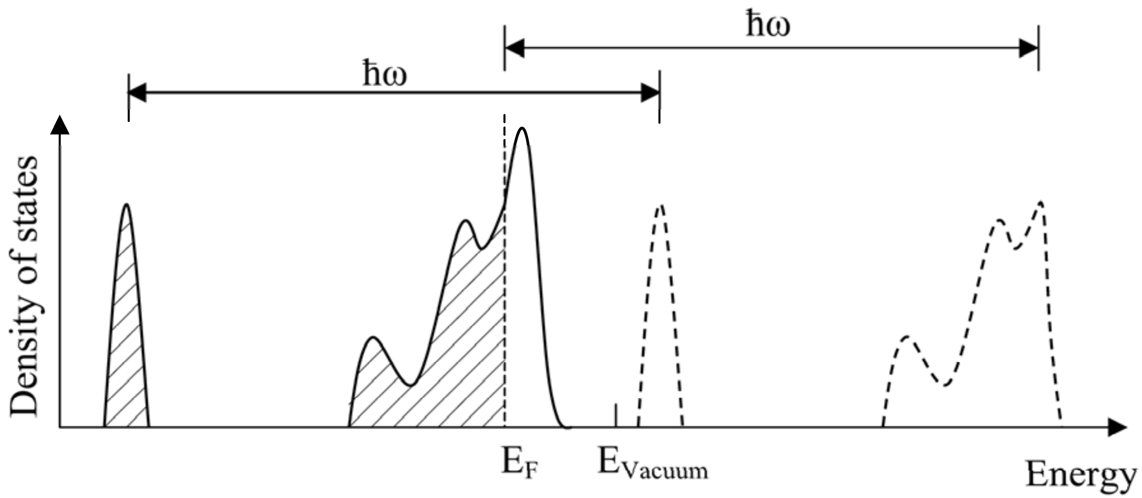


Weak CEF splitting: all 5 orbitals are crossing the Fermi level

Normal Photoemission

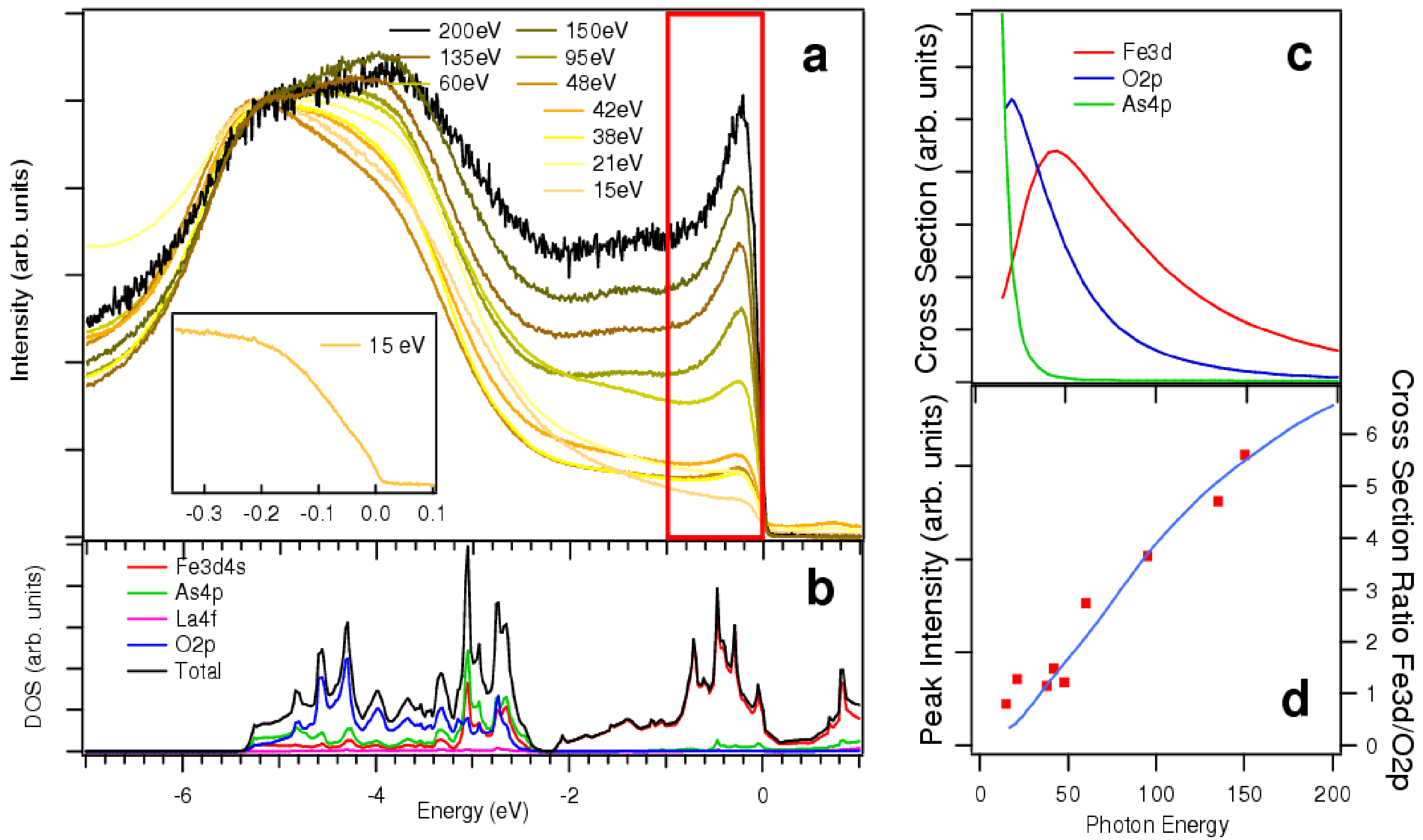
Principle





Results

Photoemission

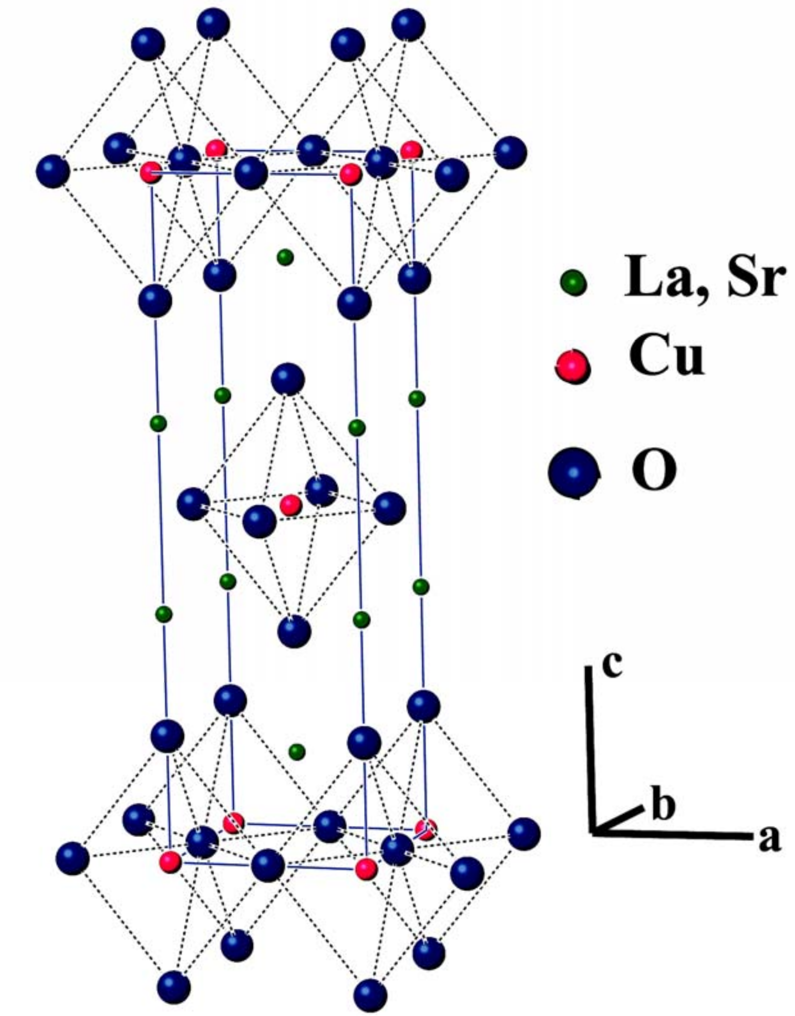


- Low energy states purely Fe derived
- Valence band agrees with LDA, but small differences
  $\Rightarrow$ Introduction of (small) *U*

A. Koitzsch *et al.*, PRB 2008

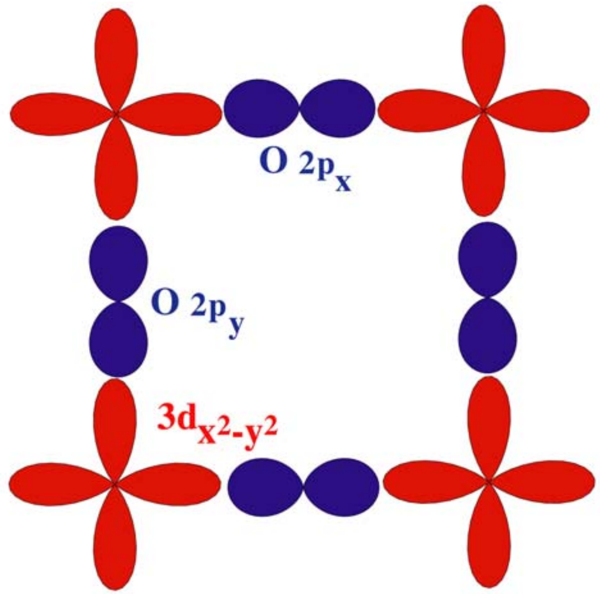
Transition Metal Oxides: complex electronic properties due to electronic and magnetic correlations

Prominent examples: High T_c superconductors, e. g. **$La_{2-x}Sr_xCuO_4$**



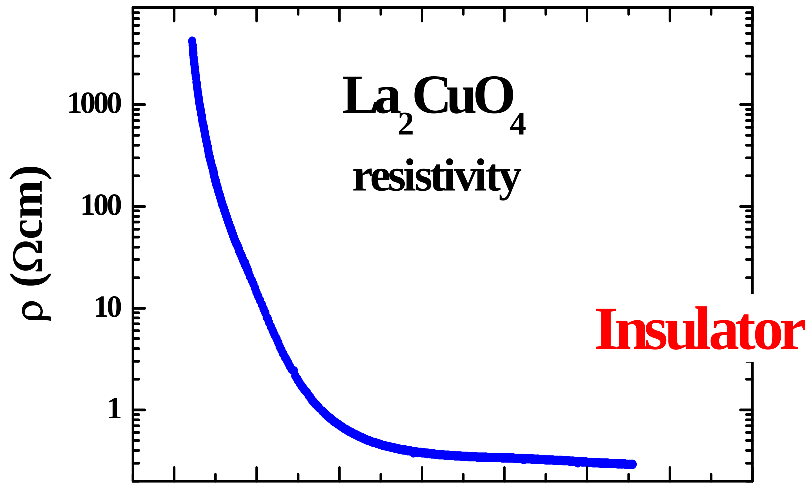
• mother compound: **La_2CuO_4**, **Cu^{2+} ($3d^9$)**

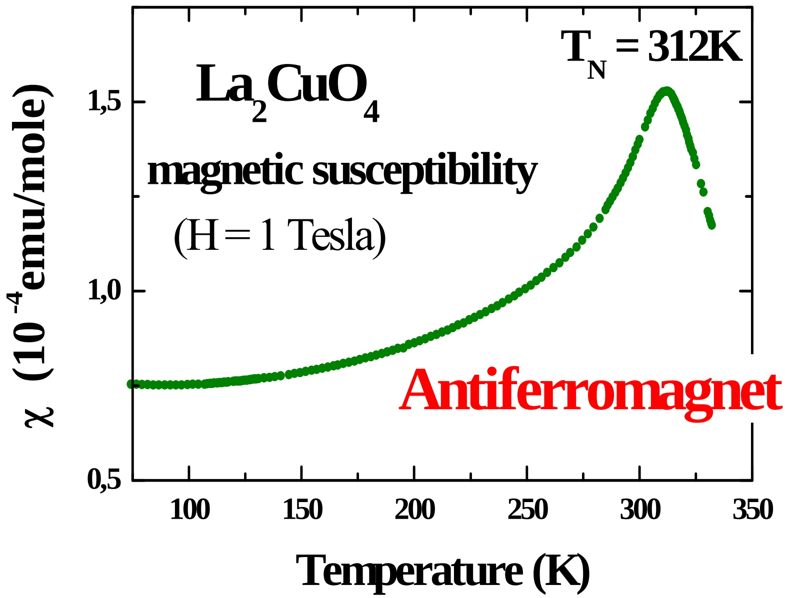
CuO_2-layers



LDA band structure: La_2CuO_4 metal

Electronic Correlations and Antiferromagnetism



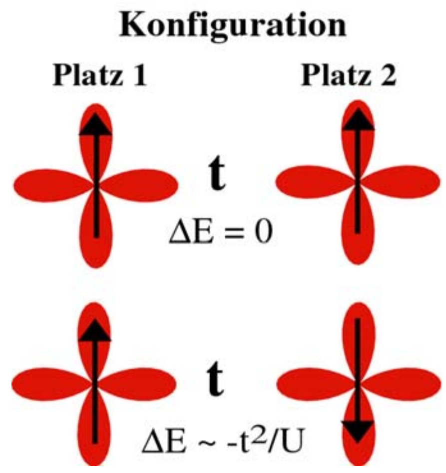


- Coulomb repulsion U

  Insulator

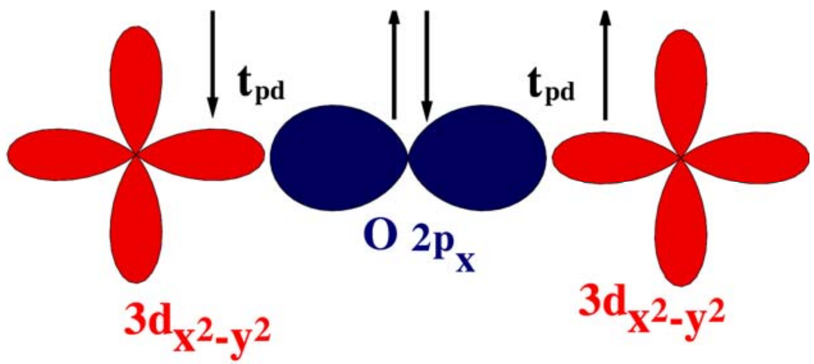
- Hybridisation t

  Antiferromagnet

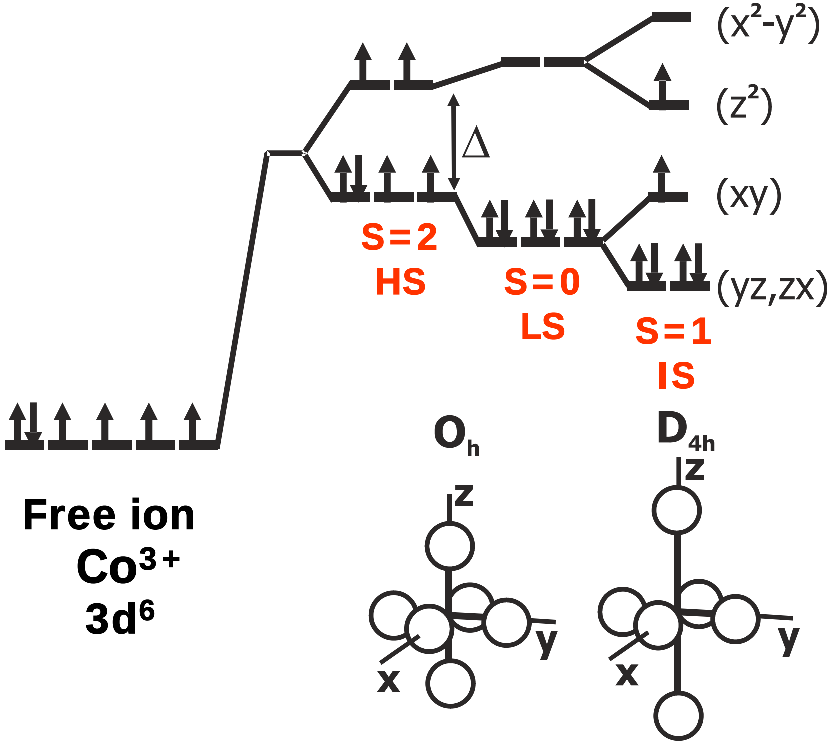


2d-antiferromagnet, $J/k_B \sim 1500K$

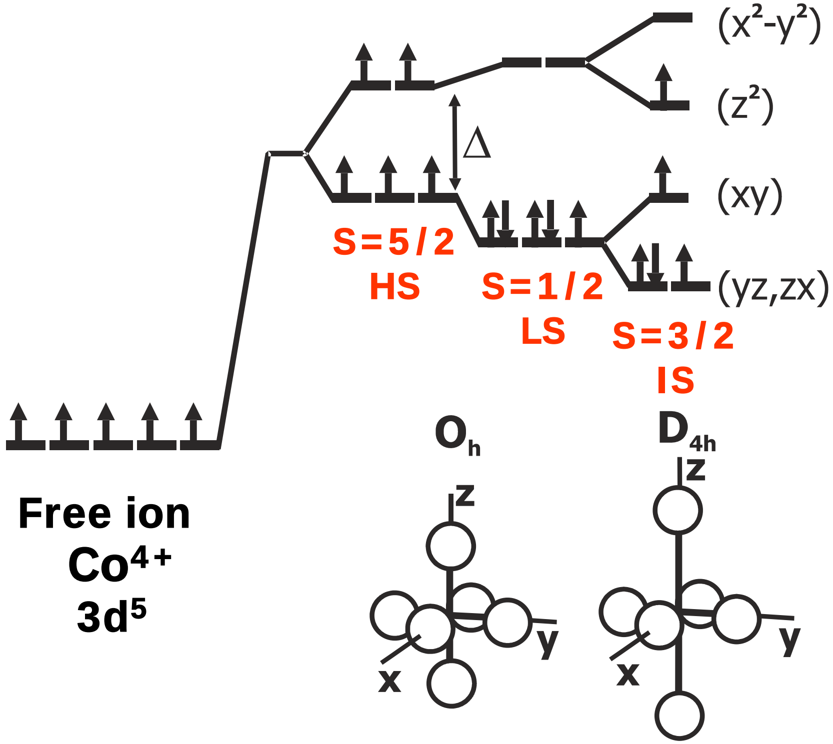
Cu-O-Cu super exchange



Co^{3+} and Co^{4+} spin states in perovskite oxides



Possible electronic configurations of Co^{3+} ions

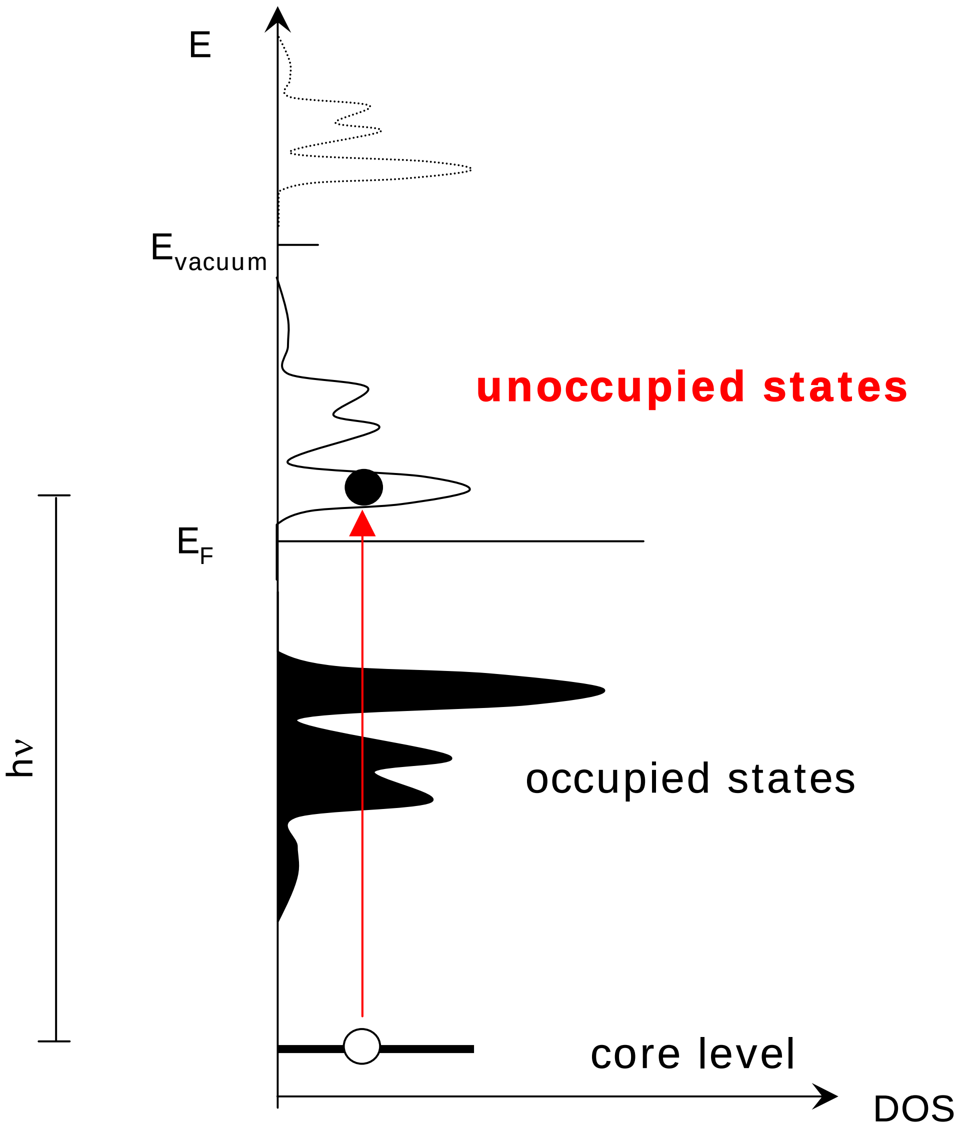


Possible electronic configurations of Co^{4+} ions

$LaCoO_3$: S = 0 low spin state

Doped Co^{4+}: 1/2 < S < 5/2

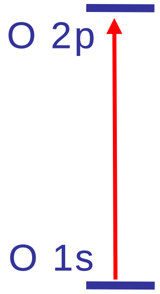
X-ray absorption spectroscopy

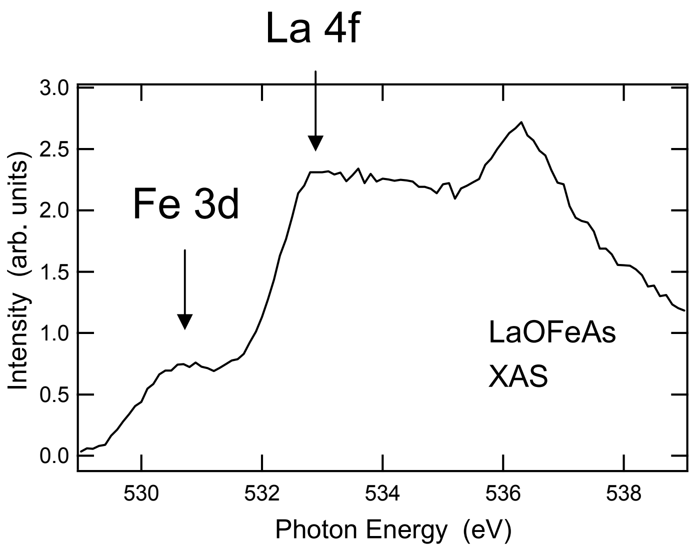


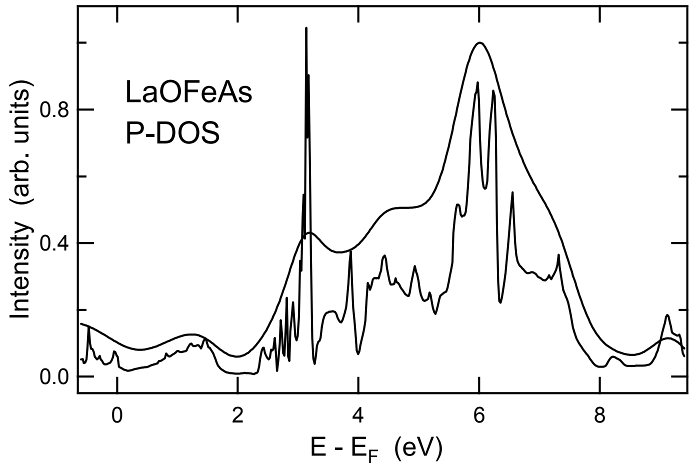
- XAS probes the DOS of the unoccupied states
- element specific
- Detection of fluorescence and/or Auger decay

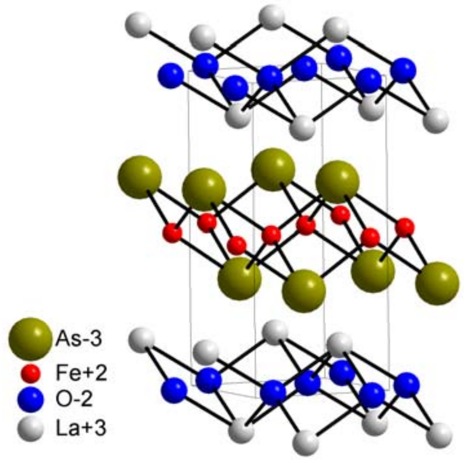
T. Kroll *et al.*, Phys. Rev. B 78, 220502(R) (2008)
T. Kroll *et al.*, New Jour. Phys. 11 (2009) 025019

Results: X-ray absorption: Oxygen 1s → 2p fluorescence signal









LaOFeAs

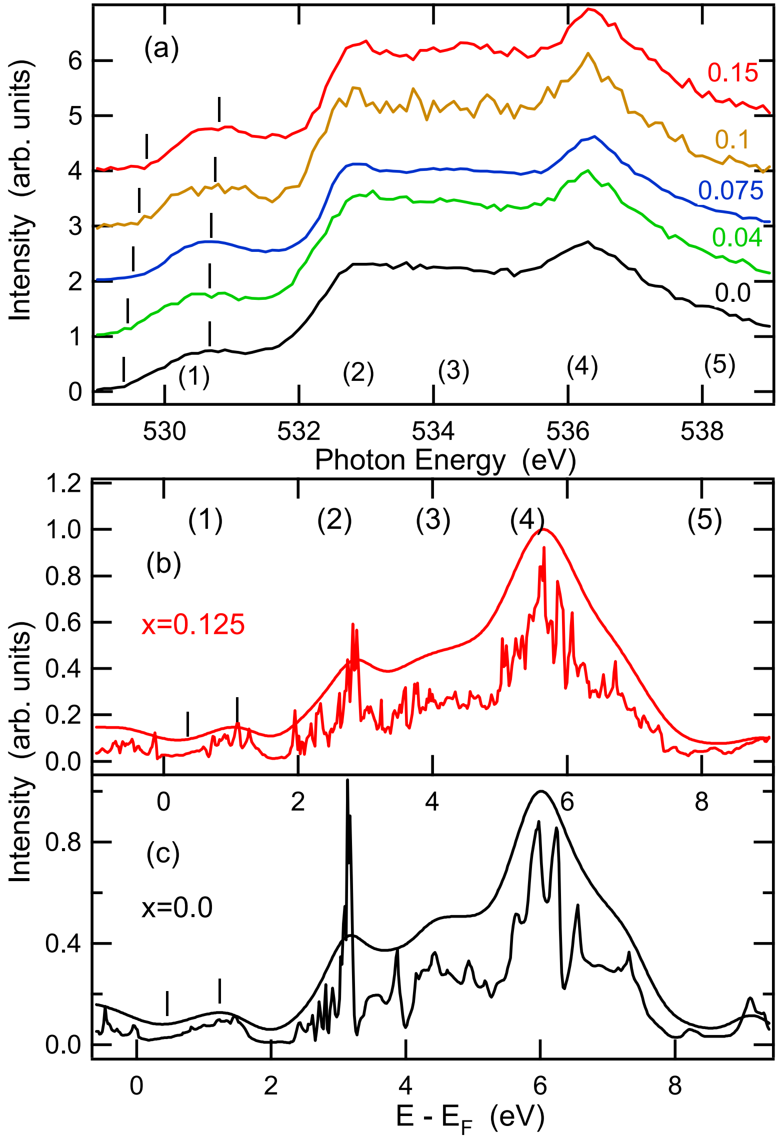
Comparison to LDA P-DOS:

- Good agreement
- core hole effect is small
  ⇒ direct interpretation possible

T. Kroll *et al.*, PRB 2008

Results

X-ray absorption: Oxygen 1s → 2p: doping dependence fluorescence signal



- weak doping dependence

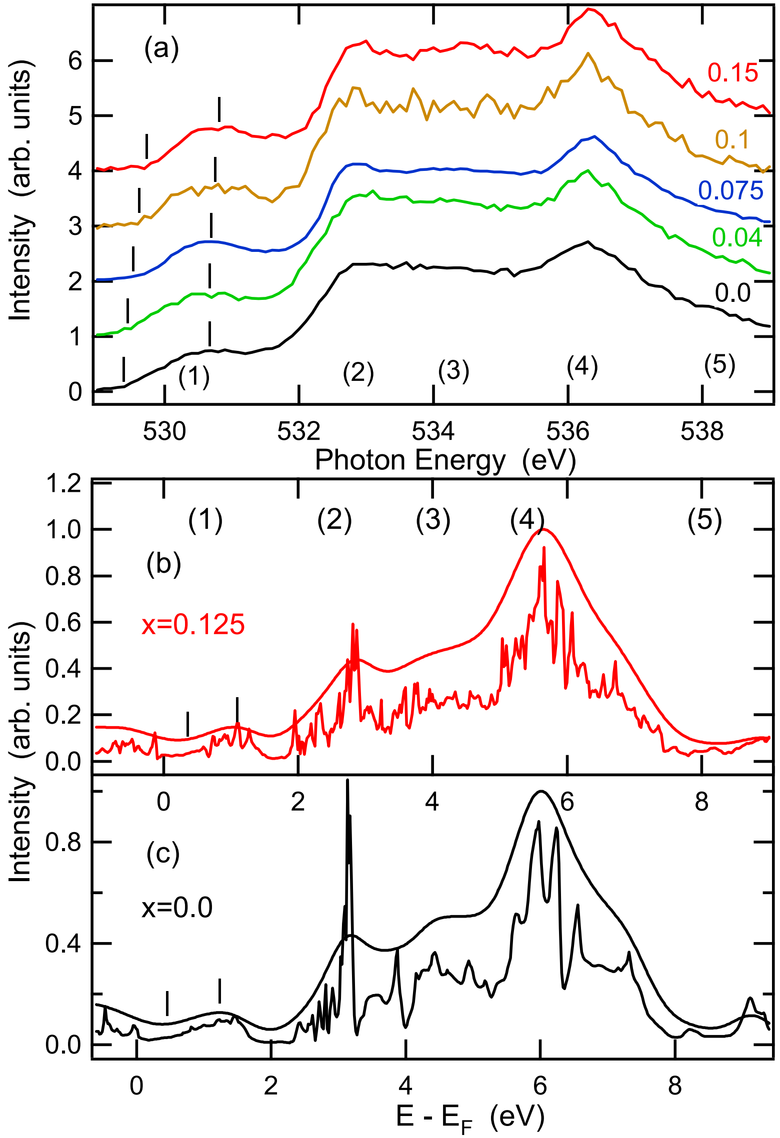
- Shift of Fe peak (1) ≈ 100 meV
  ⇒ change of Madelung potential upon doping

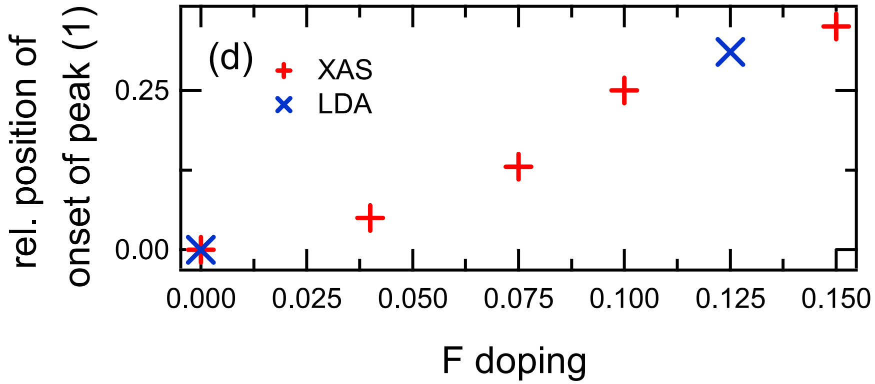
- Shift of onset of peak (1)
  ⇒ shift of chemical potential

- Visible in both experimental and theoretical spectra

Results

X-ray absorption: Oxygen 1s → 2p: doping dependence fluorescence signal

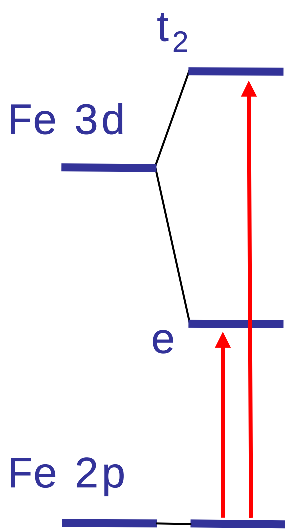


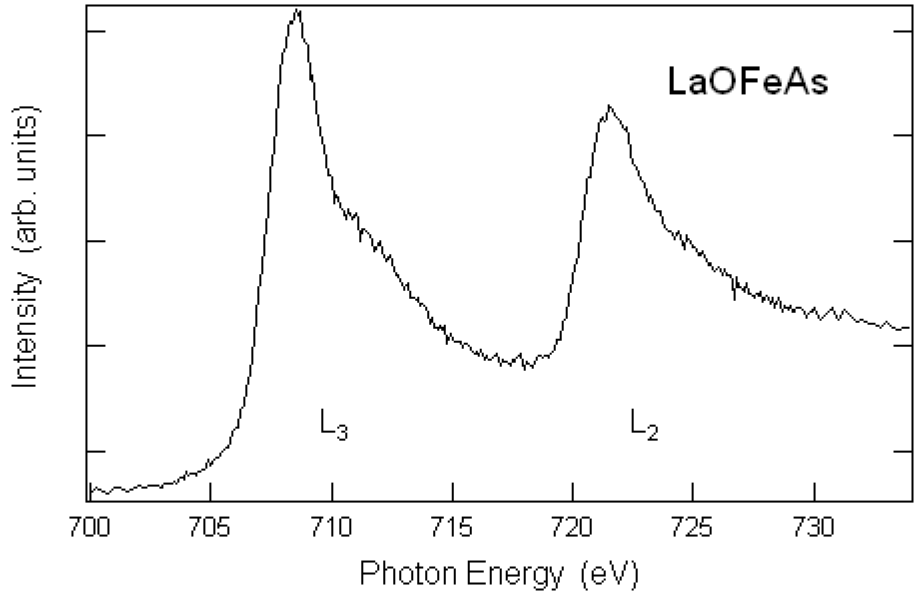


⇒ **O K-edge strongly affected by shift of the chemical potential upon doping**

Results

X-ray absorption: Iron 2p → 3d fluorescence signal



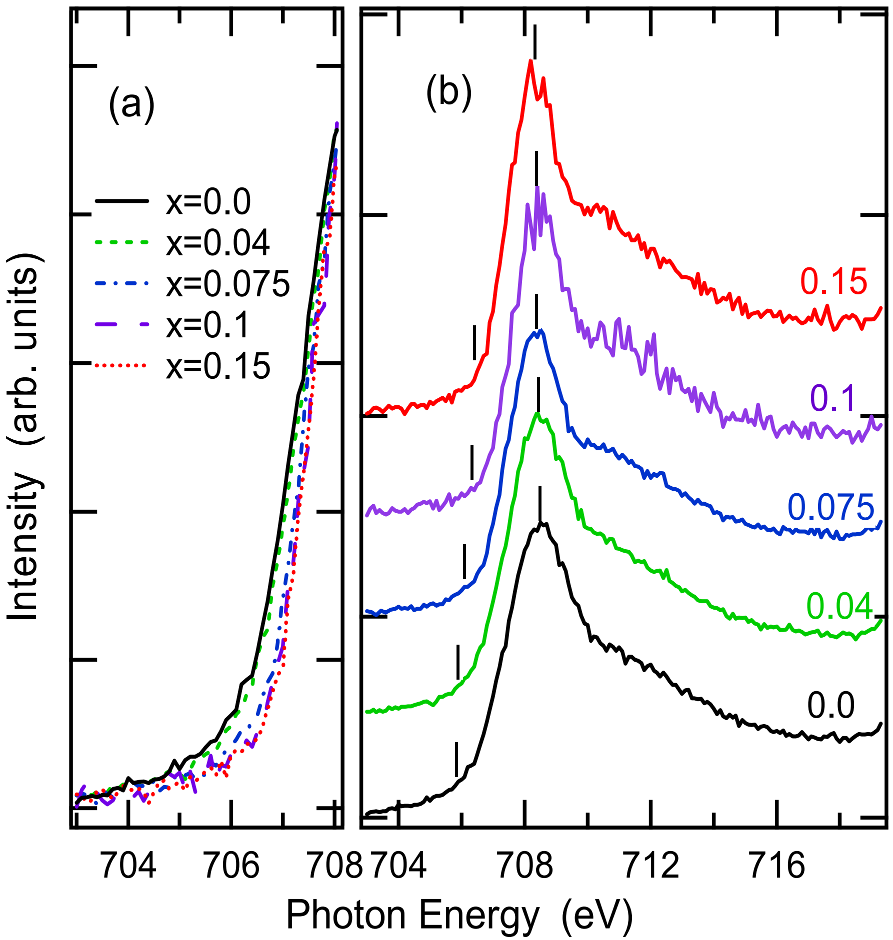


- peaks consists of main peak and high energy shoulder
- no low energy prepeak observable

T. Kroll *et al.*, PRB 2008

Results

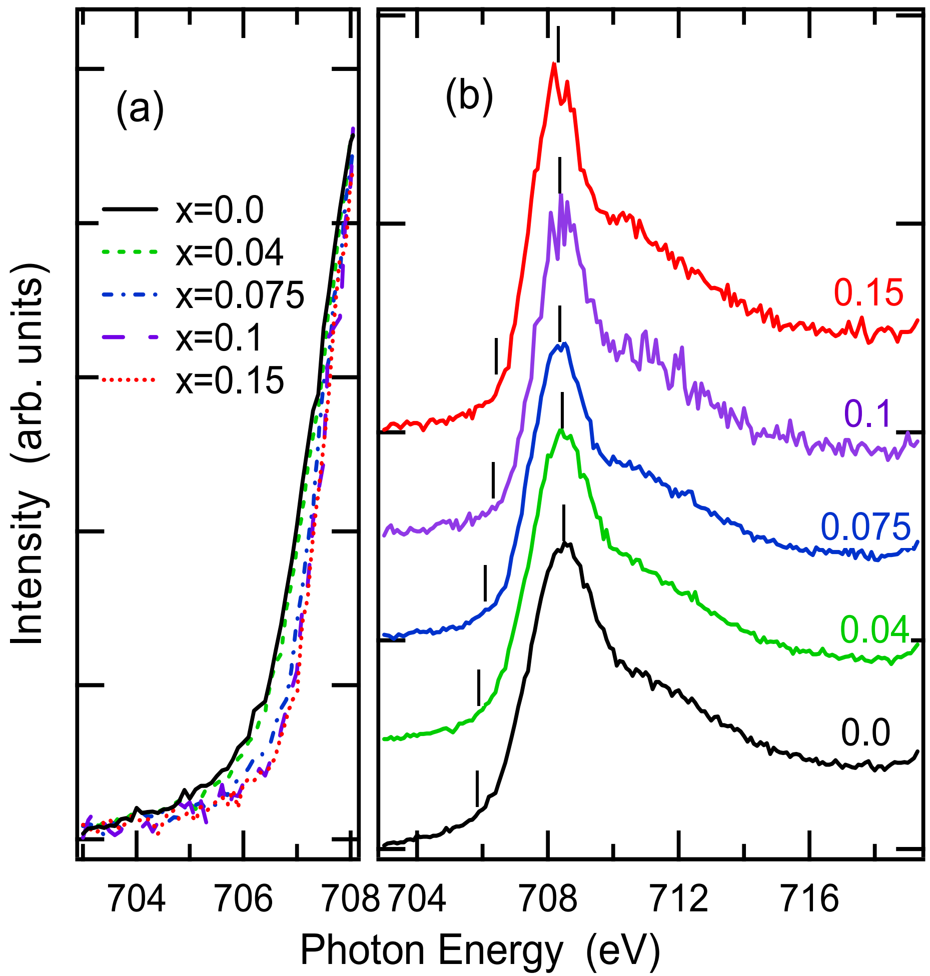
X-ray absorption: Iron 2p → 3d: doping dependence fluorescence signal

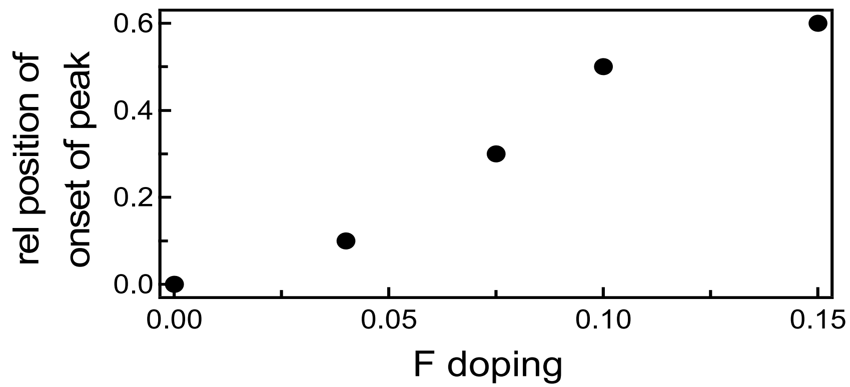


- Slight shift of main peak
- shift of onset of peak
  ⇒ **shift of chemical potential also visible in Fe L-edges**

Results

X-ray absorption: Iron 2p → 3d: doping dependence fluorescence signal





Band effects visible in Fe L-edge

⇒ no strongly correlated material

⇒ moderate/small *U* (*U*<*W*)

Results

X-ray absorption: Iron 2p → 3d
Charge transfer multiplet calculations

Tetrahedral symmetry: T_d

Best fit parameters:

10Dq = 0.2 eV,

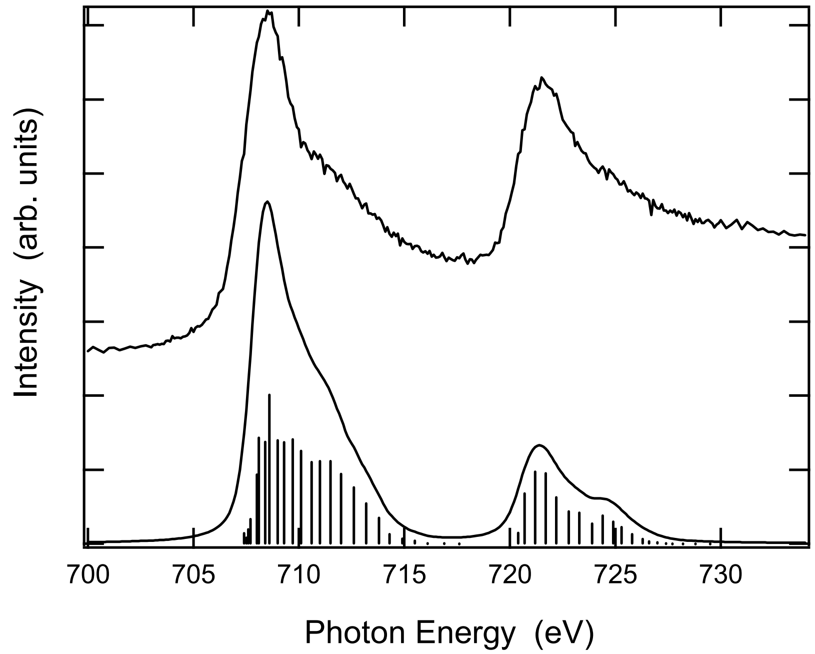
$\Delta = d^7\underline{L}\text{-}d^6 = 1.25$ eV

U = 1.5 eV (multiplet averaged)

$|pd\pi| = 0.27$ eV, $|pd\sigma| = 0.62$ eV

Slater-Condon: 80%

$\Rightarrow J_{e_g} = 0.90$ eV, $J_{t_{2g}} = 0.78$ eV



⇒ Highly covalent system

$\varphi = ad^6 + bd^7\underline{L} + cd^8\underline{L}^2$, $a^2 = 0.56$, $b^2 = 0.39$, $c^2 = 0.05$

⇒ High Spin S=2

T. Kroll *et al.*, PRB 2008

Conclusions XAS:

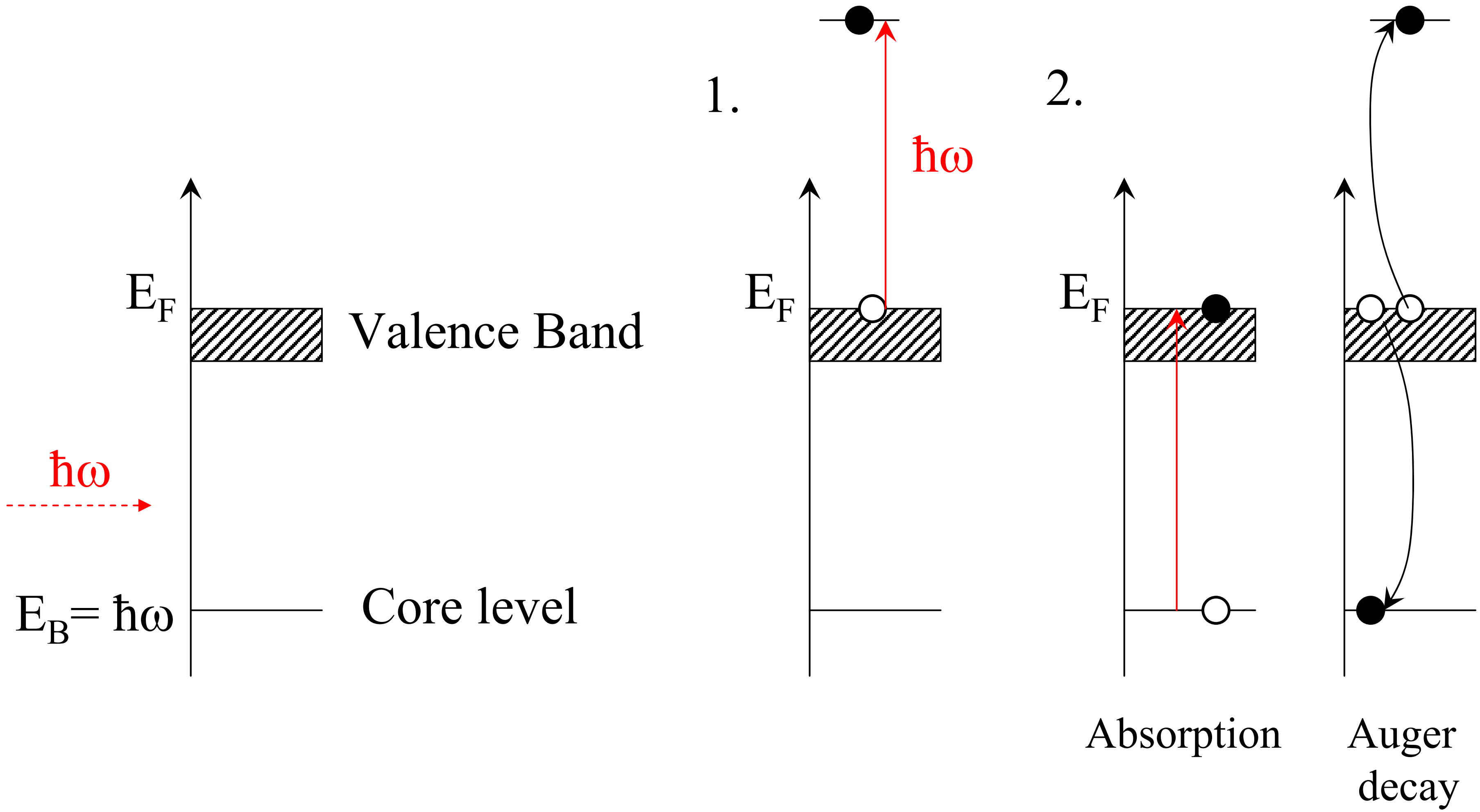
Photoemission:

- Low energy states purely Fe 3*d* states

Absorption:

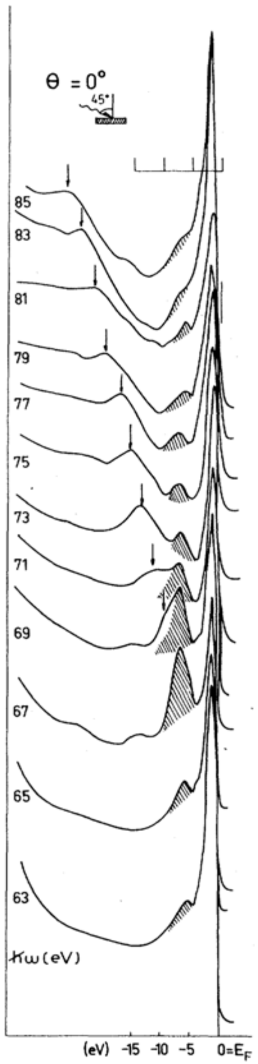
- Shift of chemical potential visible on O K- and Fe L-edges
  - ⇒ band effects important in $LaO_{1-x}F_xFeAs$ absorption edges
  - ⇒ emphasises small/moderate *U*
- Charge transfer multiplet calculations:
  - low Hubbard *U*, $\Delta = d^7\underline{L} - d^6 = 1.25$ eV
  - strongly covalent system
- No significant changes as seen by XAS and PES upon
  - rare earth ion exchange
  - temperature

Basic aspects I



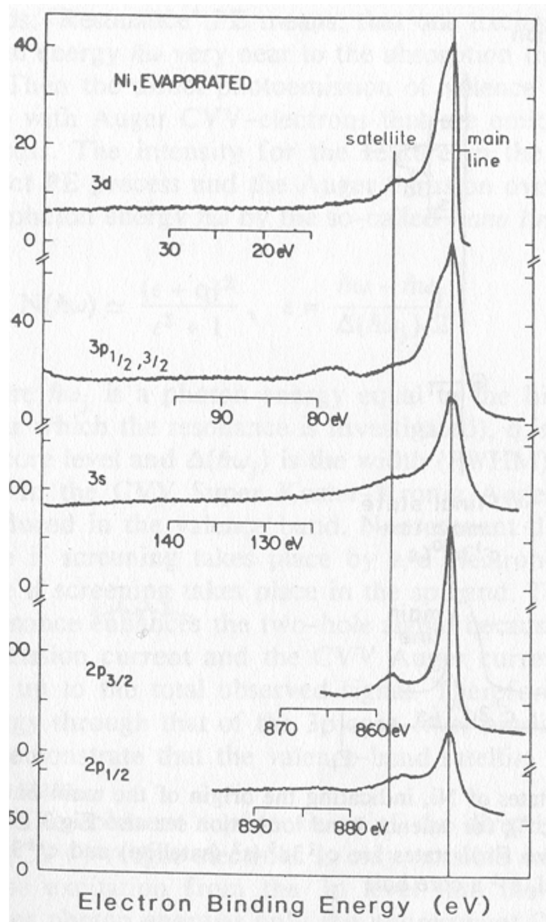
Satellites in Photoemission spectra I

Nickel metal



•Satellite feature due to two-hole (d^8) final state *poorly screened*
•Main valence band in a *well screened* (d^9) state

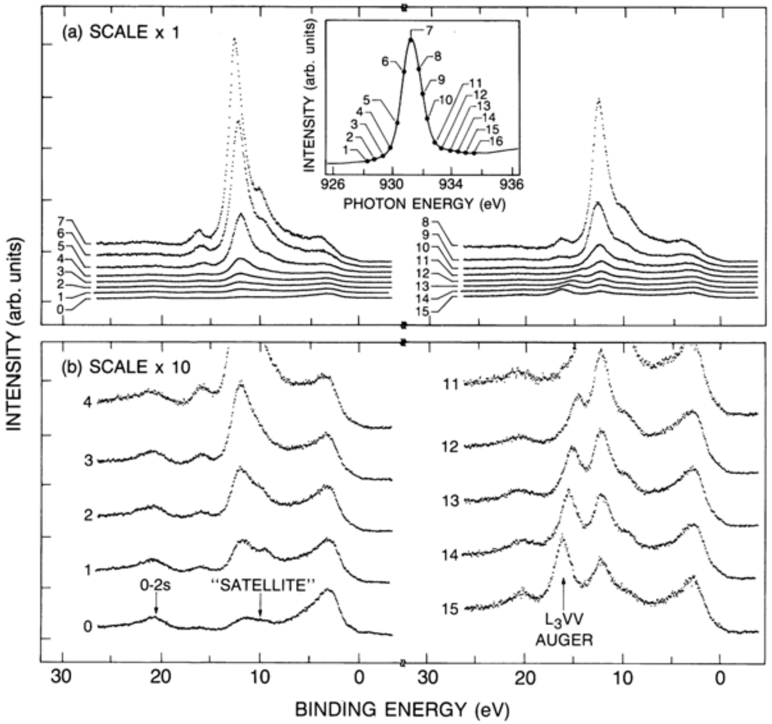
•Satellite observed for all core levels at appr. same energy difference



Guillot et al., Phys. Rev. Lett. 39, 1632 (1977)
S. Hüfner et al., Phys. Lett. 51A, 299 (1975)

Satellites in Photoemission spectra II

CuO



- Satellite: two-hole (d^8) final state, *poorly screened*
- Main valence band: *well screened* (d^9L) state

Tjeng et al., Phys. Rev. Lett. 67, 501 (1991)

$$\Delta E = \sqrt{(U-\Delta)^2 + 4V_{eff}^2}$$ **Two level mixing model**

van der Laan et al., Phys. Rev. B 23, 4369 (1981)

Basic aspects II

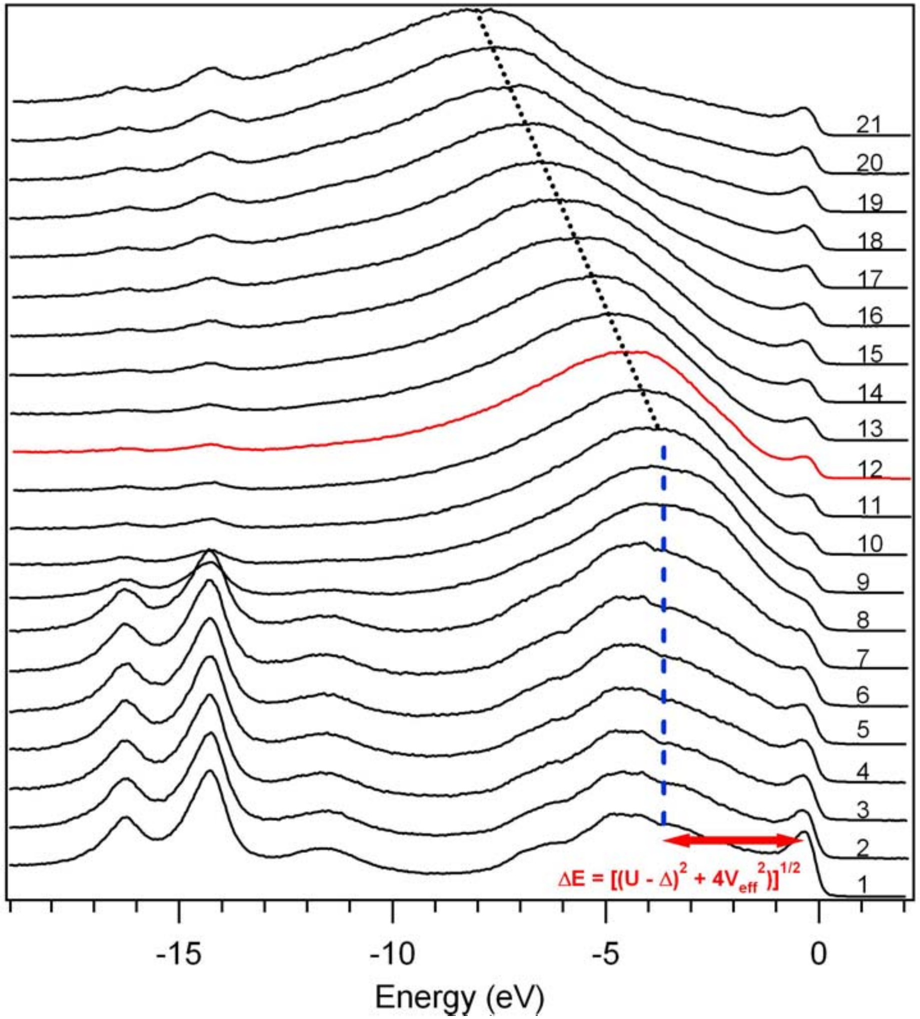
$2p^6 3d^n \rightarrow 2p^6 3d^{n-1} + e^-$ (Normal Photoemission)

$2p^6 3d^n \rightarrow 2p^5 3d^{n+1} \rightarrow 2p^6 3d^{n-1} + e^-$ (Auger decay)

The resonance enhances the satellite !

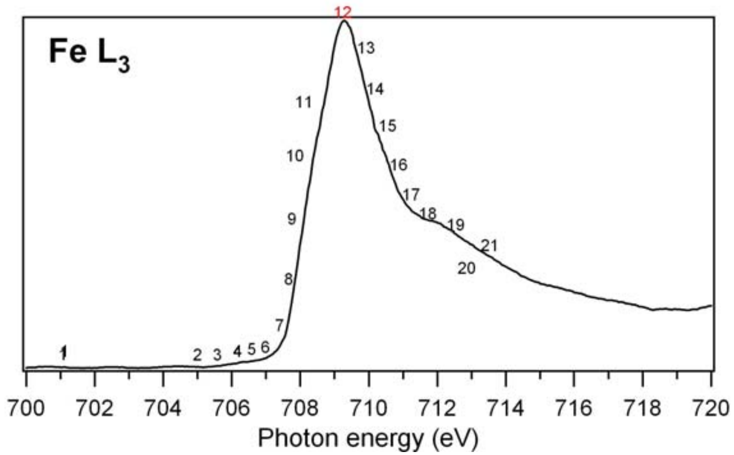
Results

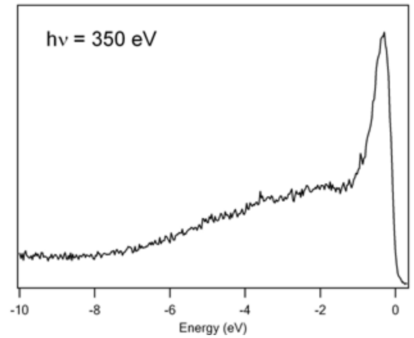
Valence band $BaFe_2As_2$ single crystals



XAS:
U = 1.5 eV
V_{eff} = 1.4 eV

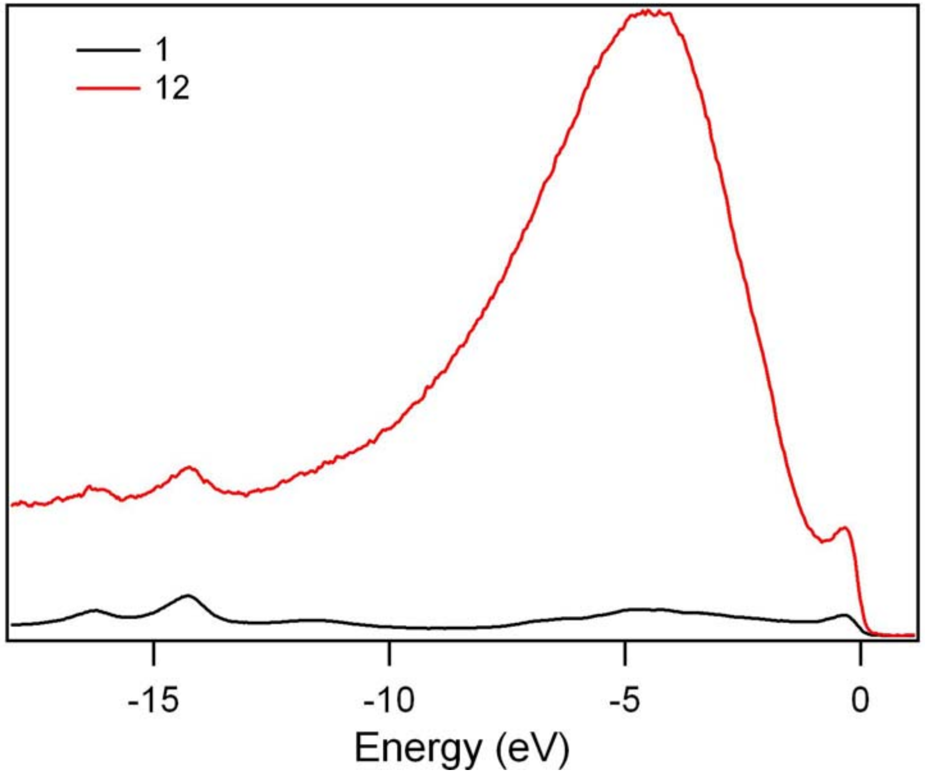
T. Kroll et al., PRB (2008)

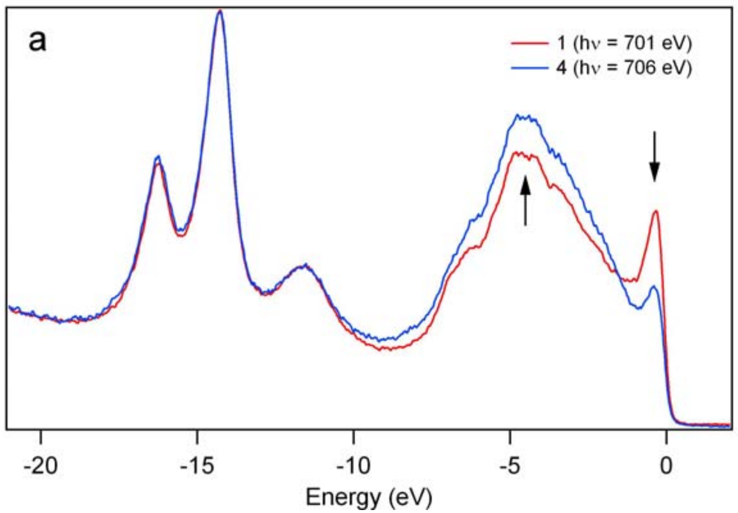




Results

Resonance Profile



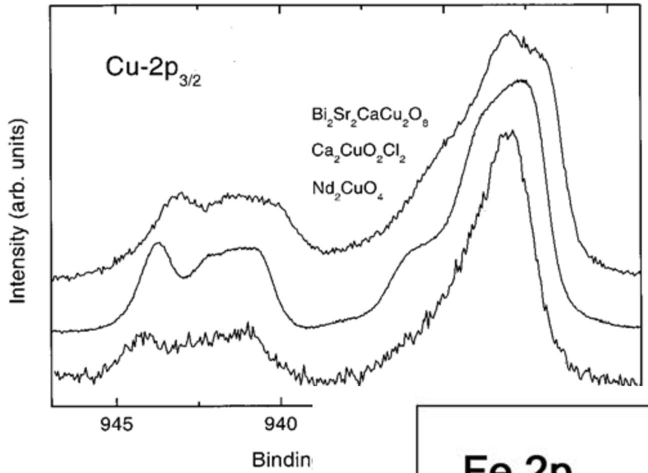


•Resonance/Antiresonant behavior

Results

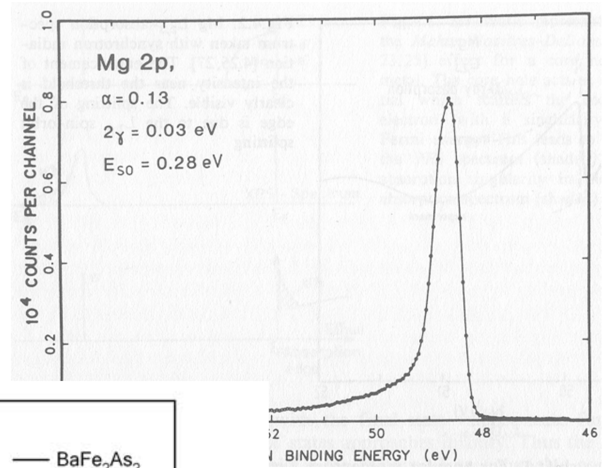
Fe 2p core level

Strong Correlations: Cuprates

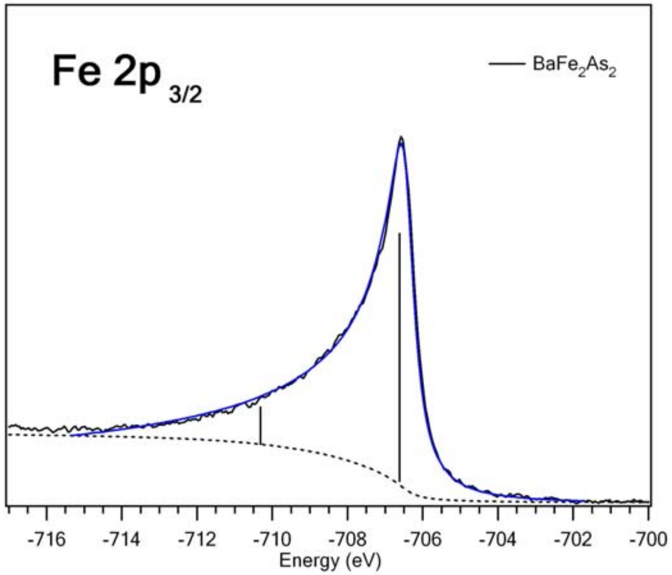


A. Koitzsch et al.,

Weak Correlations: Mg

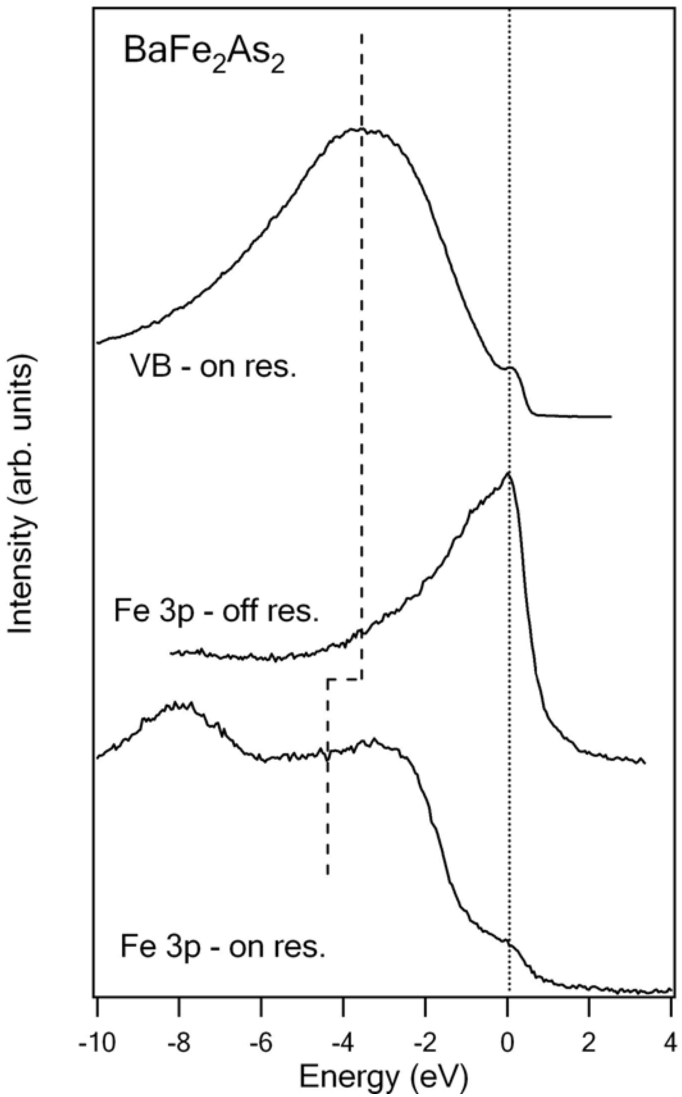


t al., *Photoemission in*
Springer



•Doniach-Sunjic lineshape for simple metals

Fe 3p core level



Strong multiplets spread over large energy range

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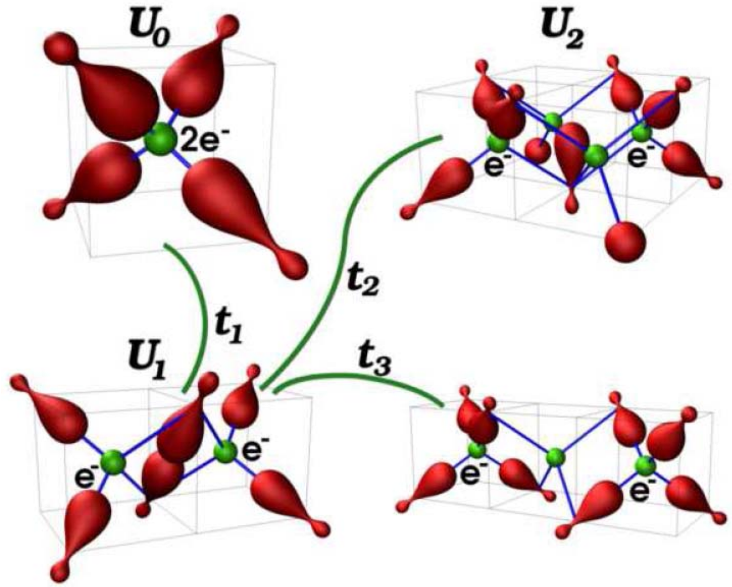
Conclusions Resonant Photoemission

- Observation of the two-hole satellite by resonant photoemission for (Ba,K)Fe_2As_2 single crystals
- Previously obtained parameterset with U = 1.5 eV matches energy position well, U retains a clear physical meaning.
- Consistent description of valence band, Fe 2p and Fe 3p excitations
- Appearance of a conventional metal with hidden correlations

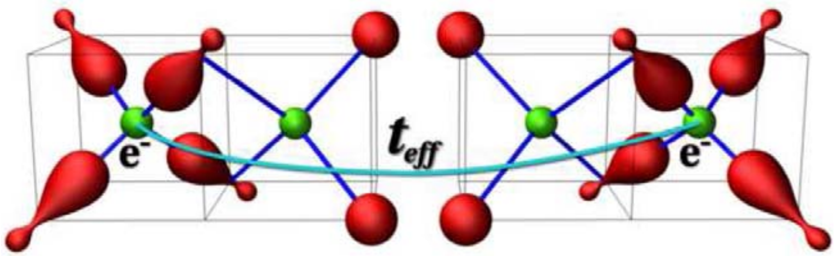
Possible origin of small U:

As highly polarisable:
⇒ Fe surrounded by polarised As
⇒ electronic polarons
⇒ strong screening of Coulomb repulsion

electronic bipolarons:



single electronic polaron:



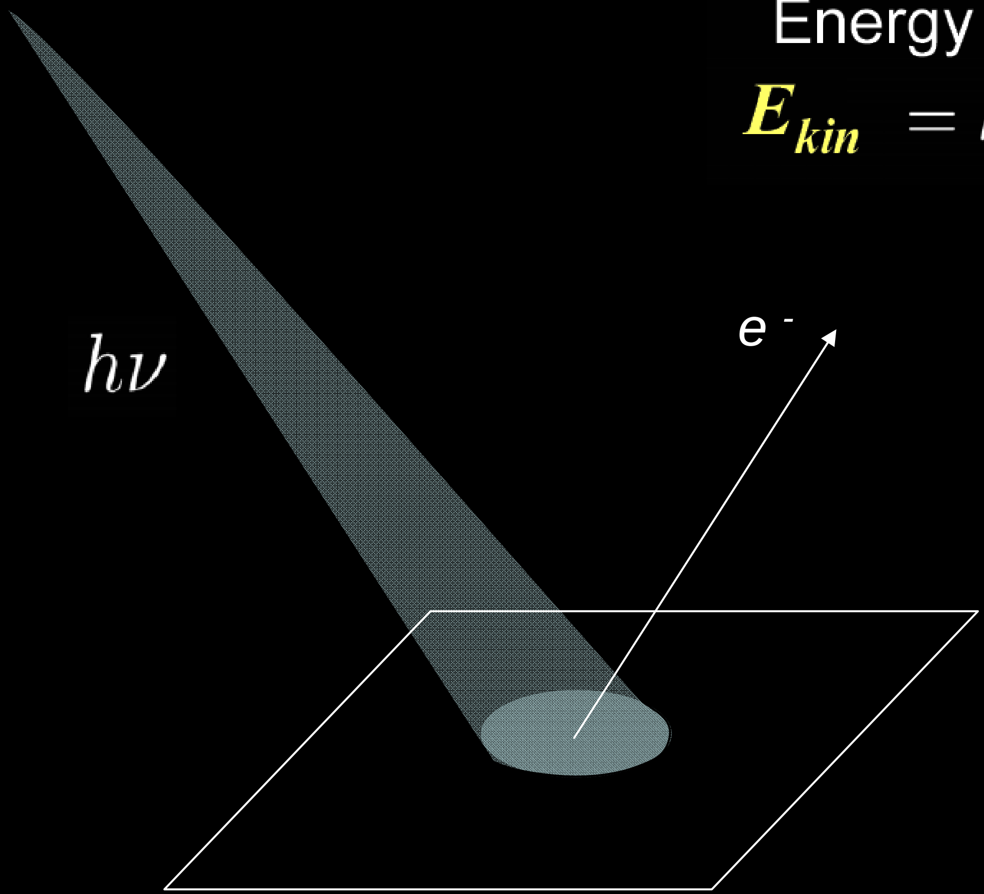
- signifficant screening of U_H
- attractive interaction due to non-2D geometry

Sawatzky et al., arXiv:0808.1390
Berciu et al., arXiv:0811.0214

OUTLINE

- „Local physics“, Hubbard U etc.
- **ARPES, Fermi surface etc.**
- „Pseudogap“, Strange T dependencies
- Normal state resistivity
- Charge inhomogeneity (NQR)

Photoelectric effect

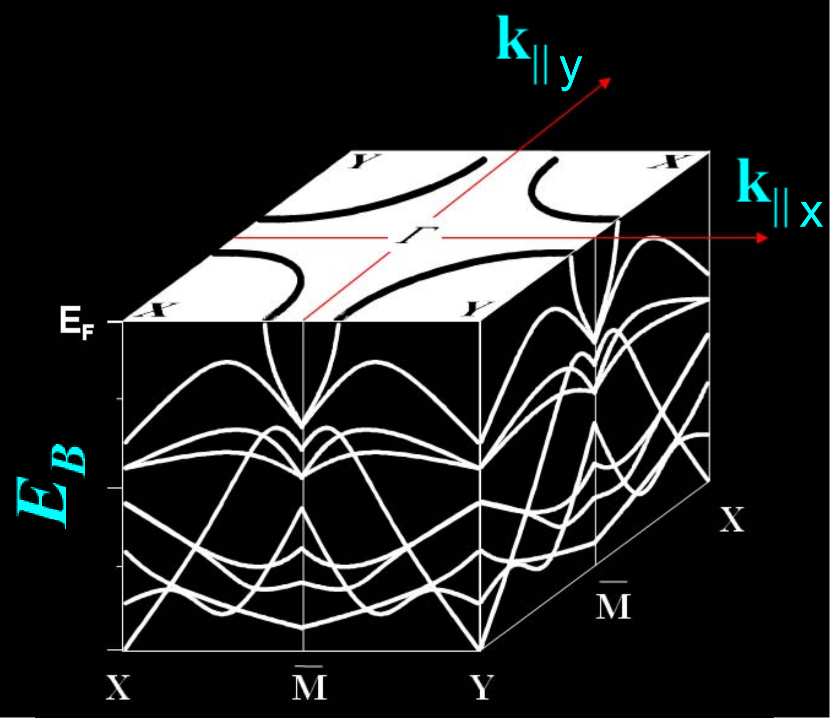


Energy Conservation

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

Momentum Conservation

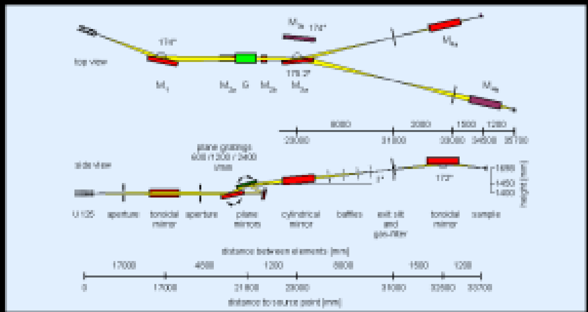
$$\hbar \mathbf{k}_{||} = \hbar \mathbf{K}_{||} = \sqrt{2mE_{kin}} \cdot \sin\vartheta$$



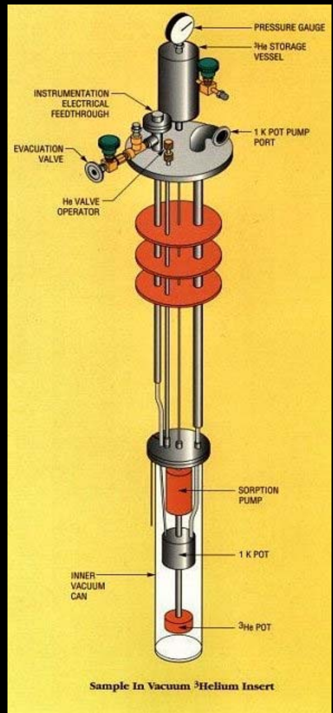
S.V. Borysenko
IFW-Dresden

Low temperature ARPES at BESSY

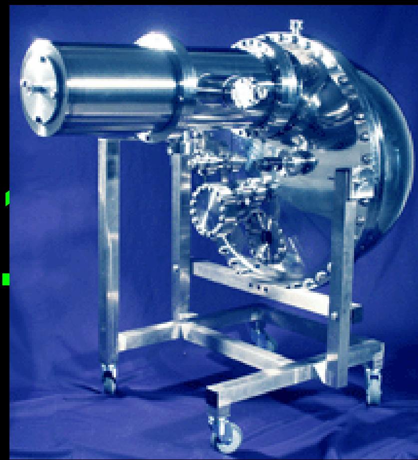
Low-energy PGM beamline



UHV compatible
He3 cryostat



Electron-energy
analyzer

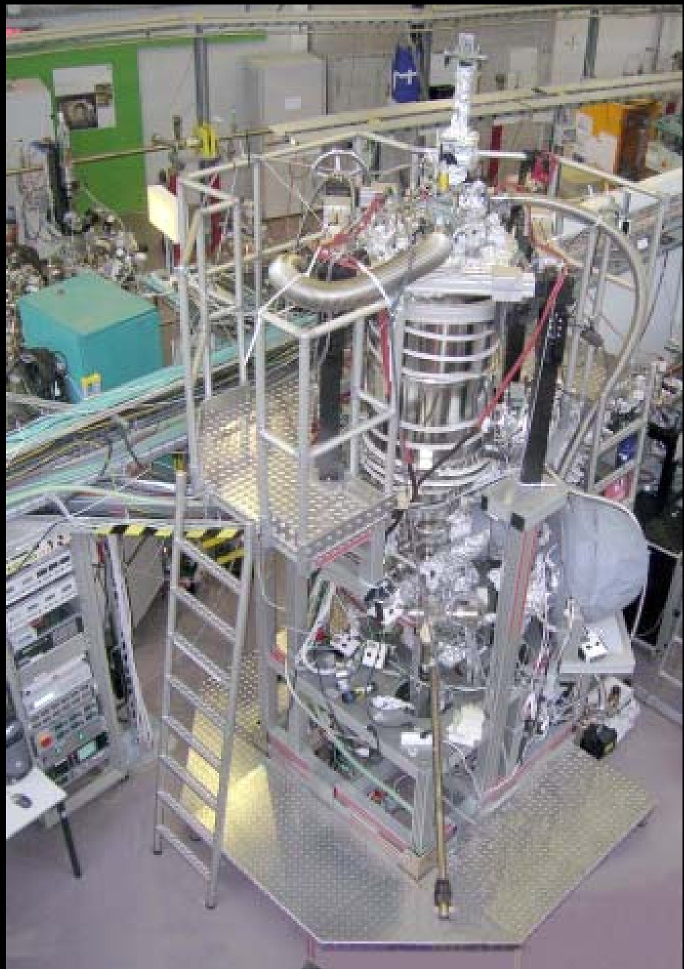


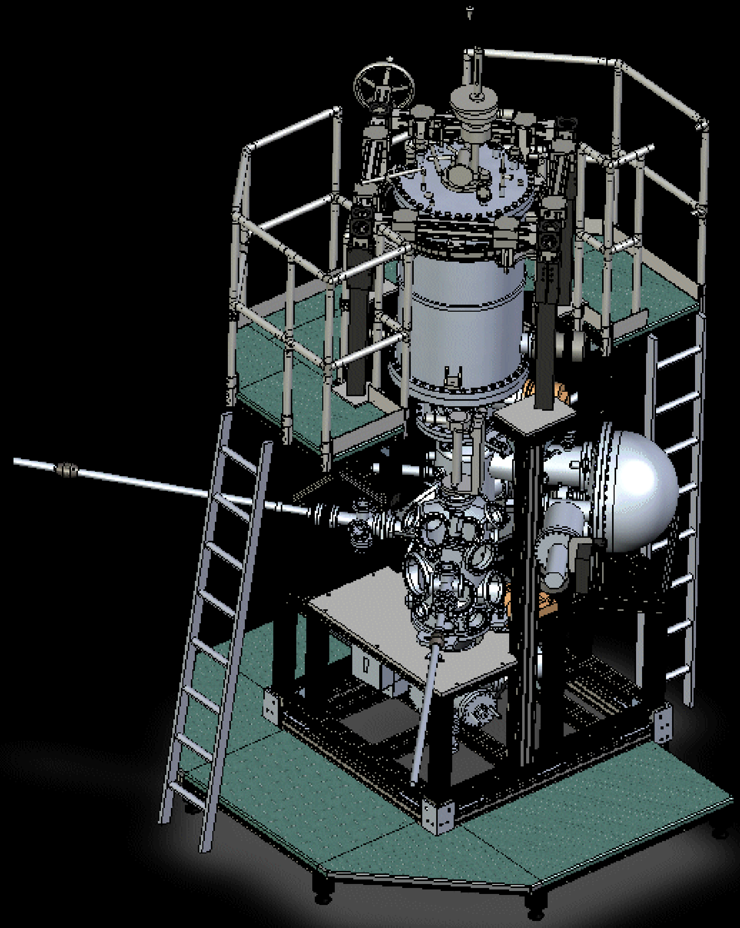
1

=

1 meV 1 K 1 meV

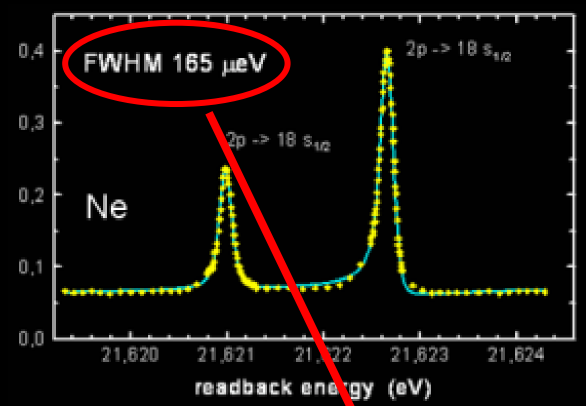
1^3 - ARPES facility

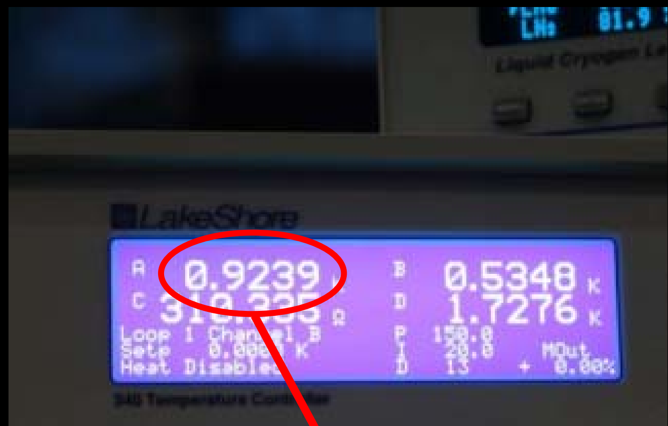


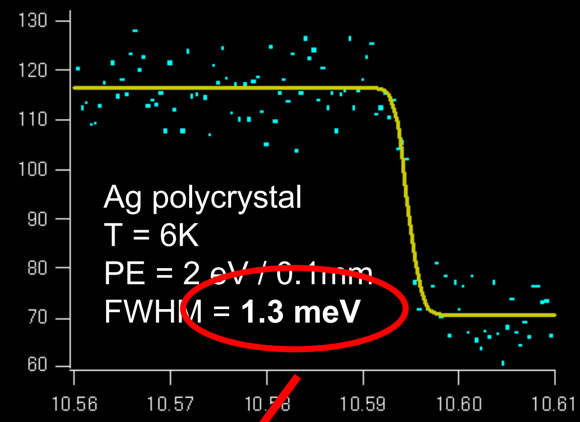


The goal is nearly achieved !

Expected: **1 meV** **1 K** **1 meV**



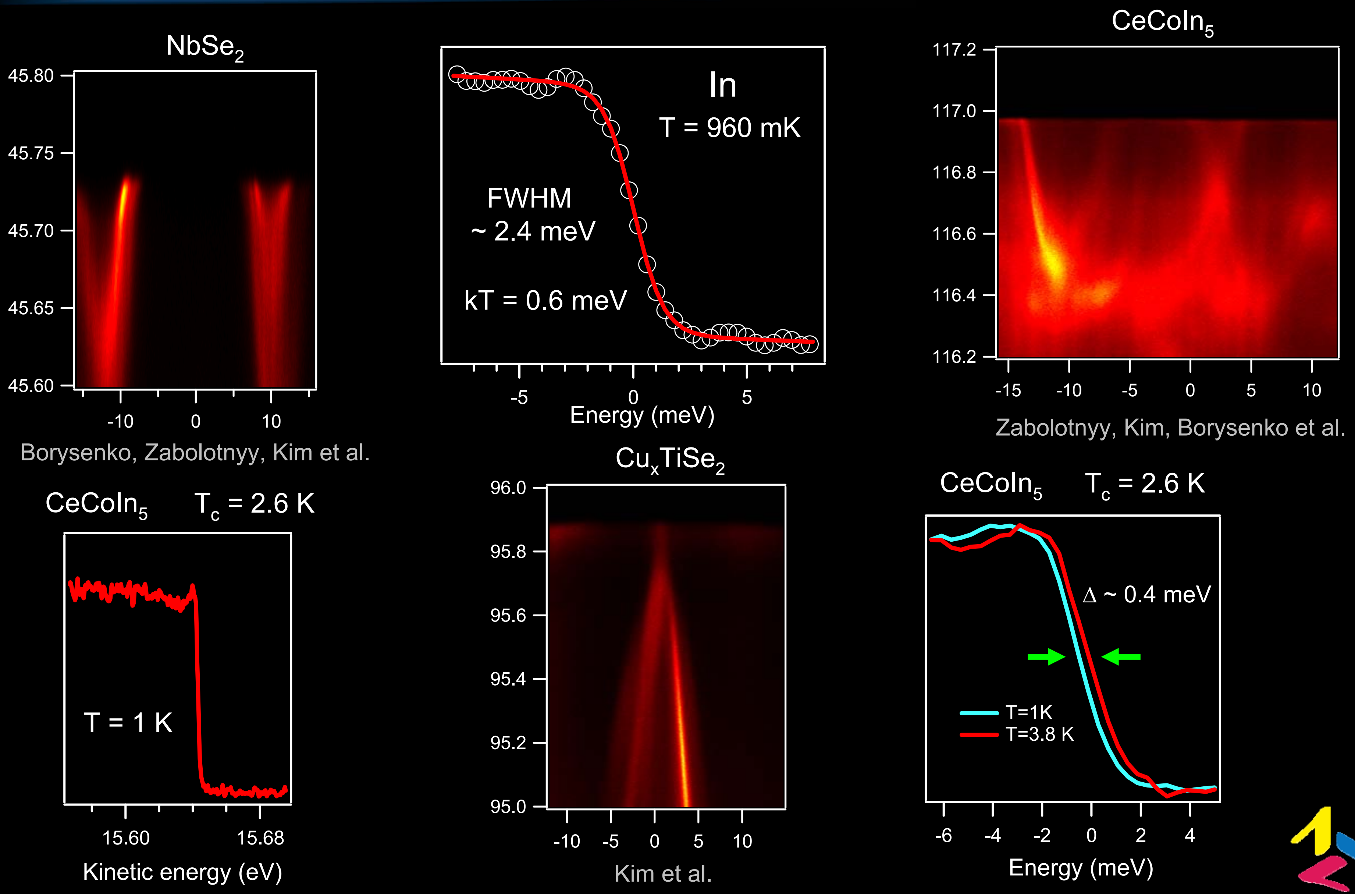


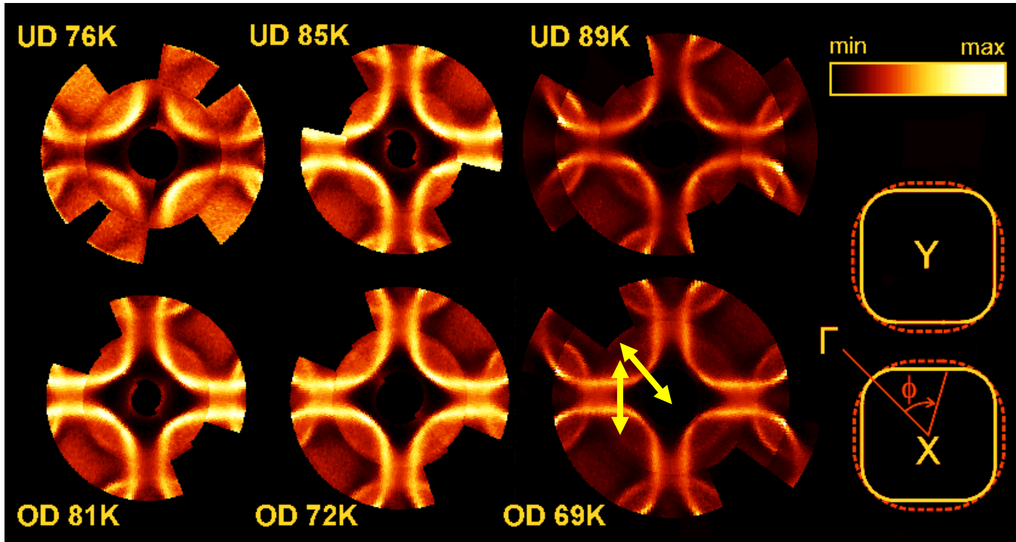


Follath et al.

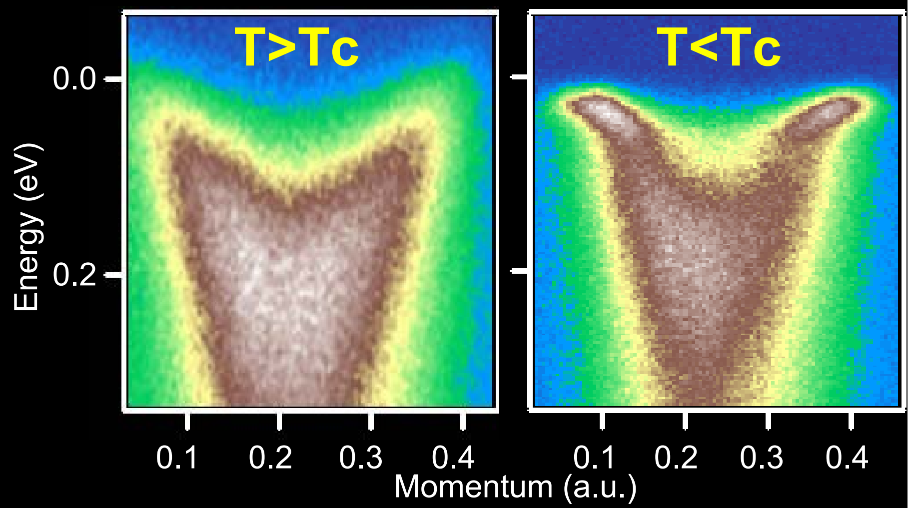
Achieved: **0.165 meV** **0.92 K** **1.3 meV**

ARPES below 1K



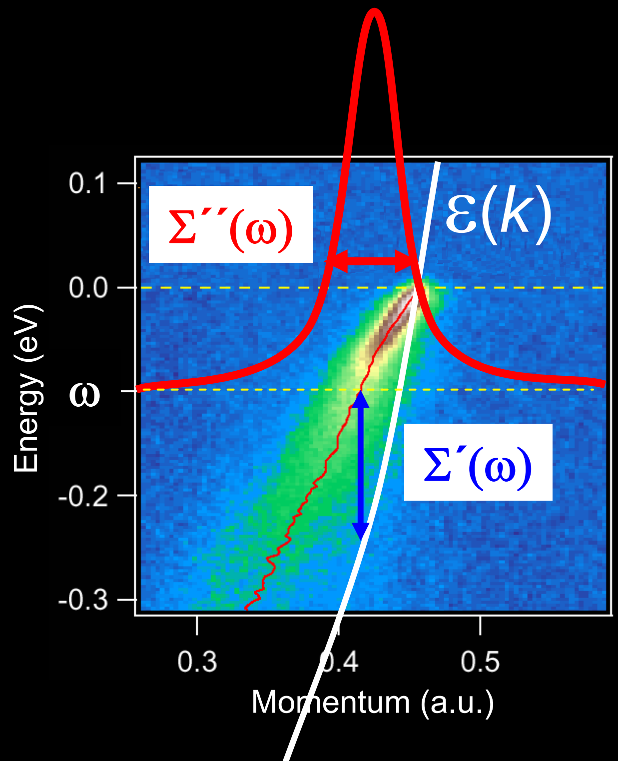


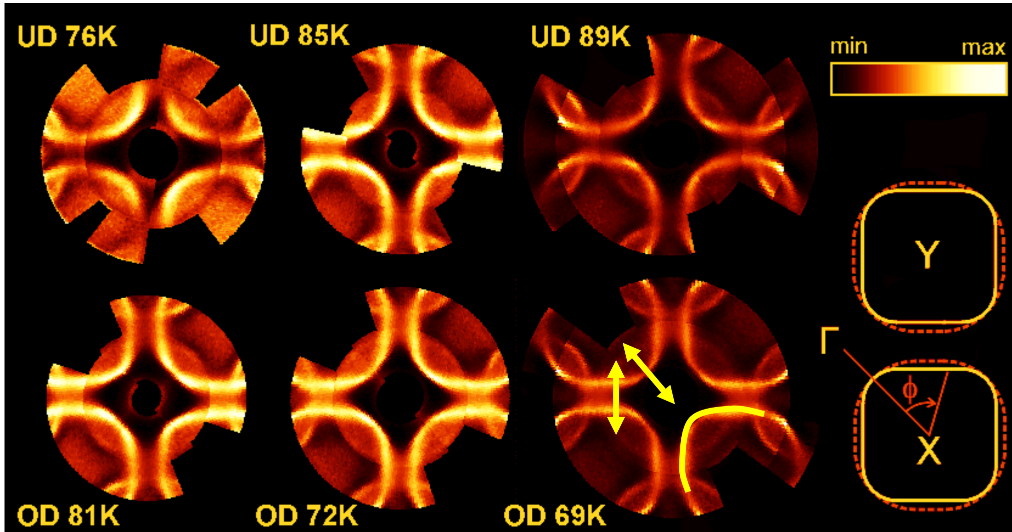
Kordyuk et al. PRB 02



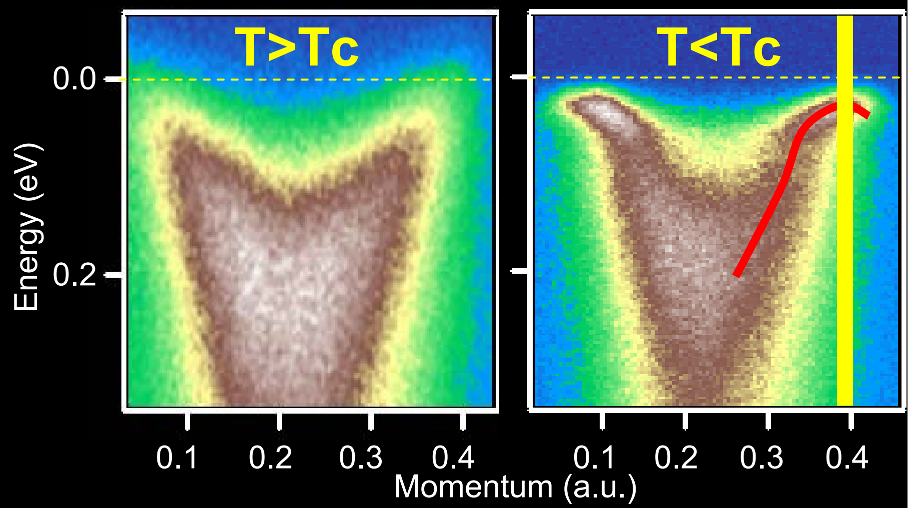
Borysenko et al. PRL 03

BSCCO



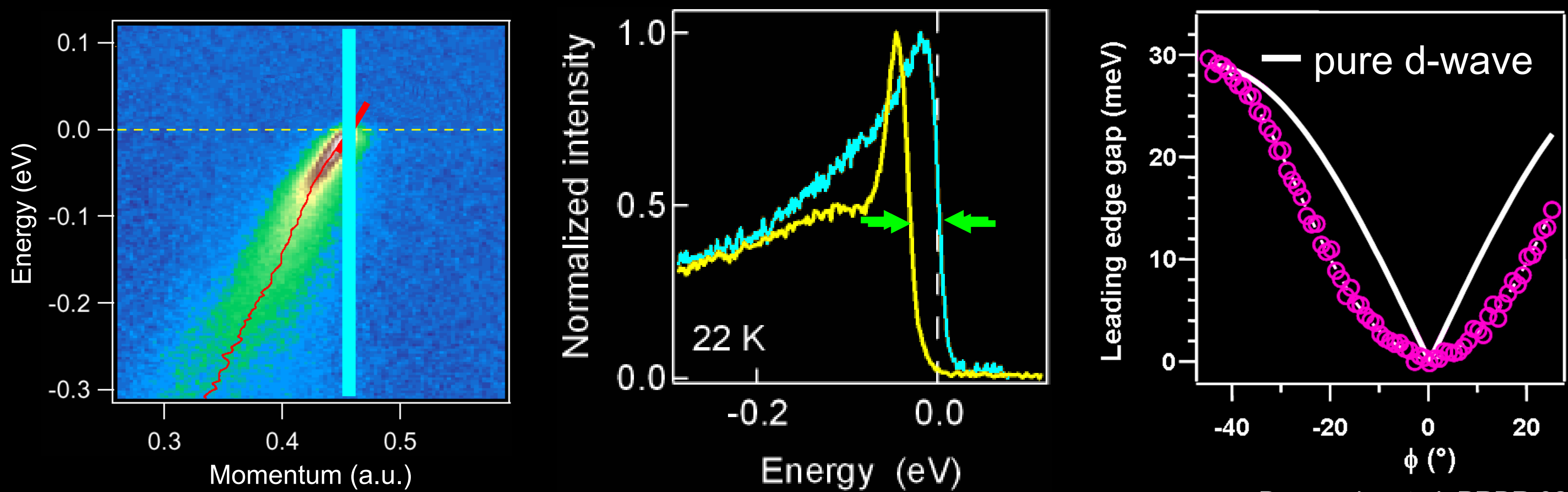


Kordyuk, SVB et al. PRB 02

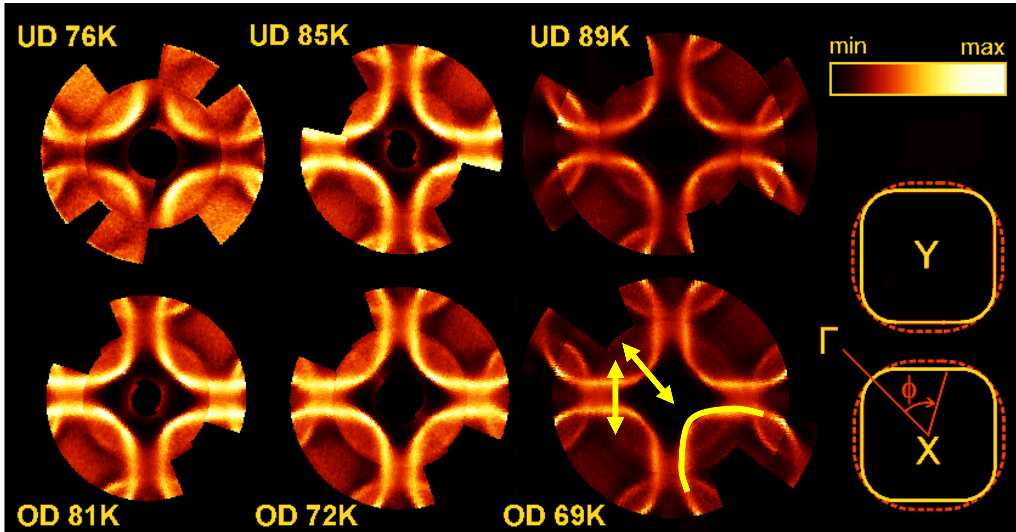


Borysenko et al. PRL 03

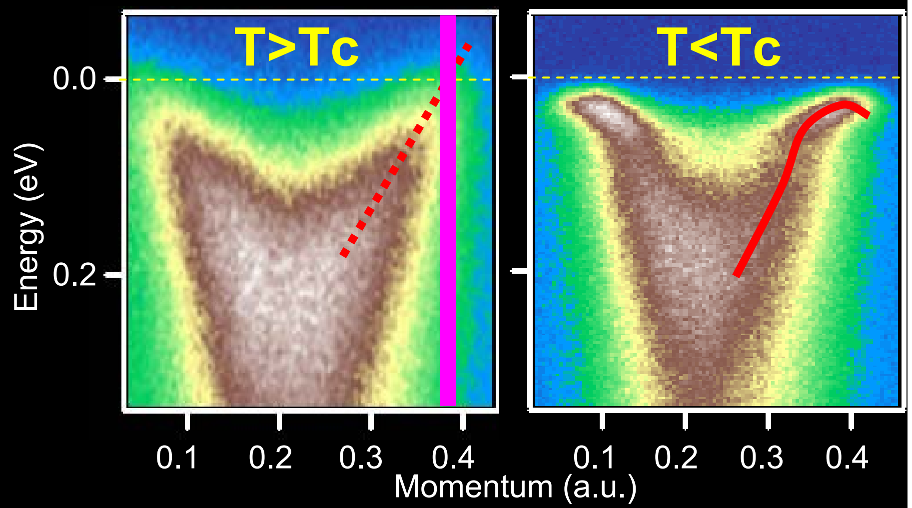
BSCCO



Borysenko et al. PRBR 02

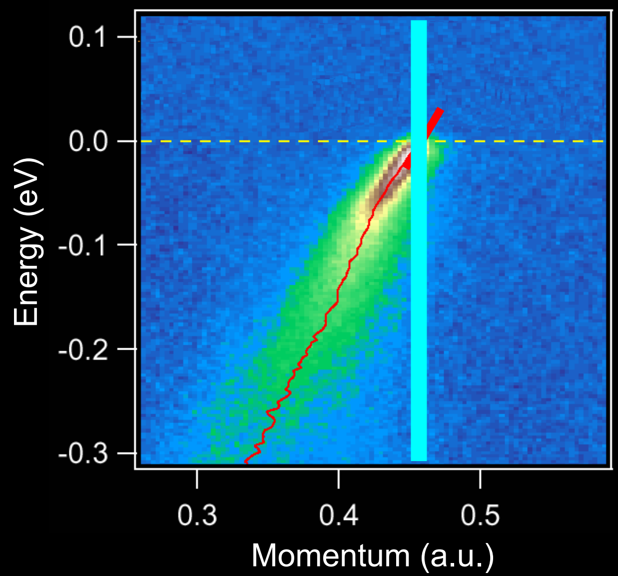


Kordyuk, SVB et al. PRB 02

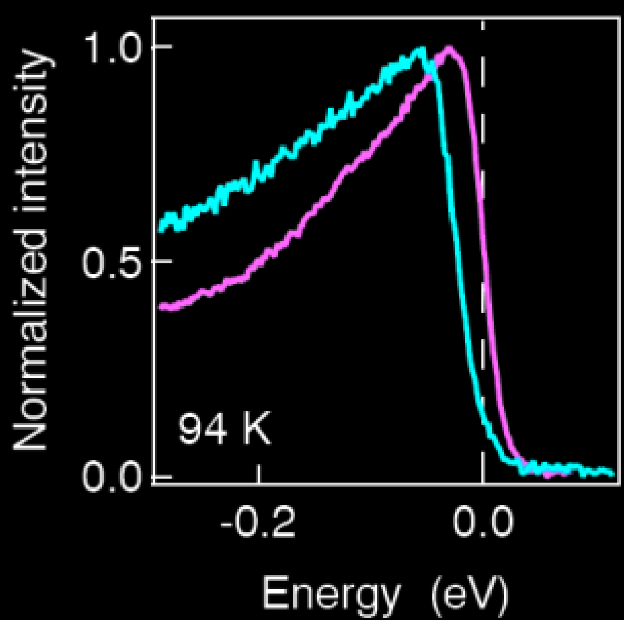


Borysenko et al. PRL 03

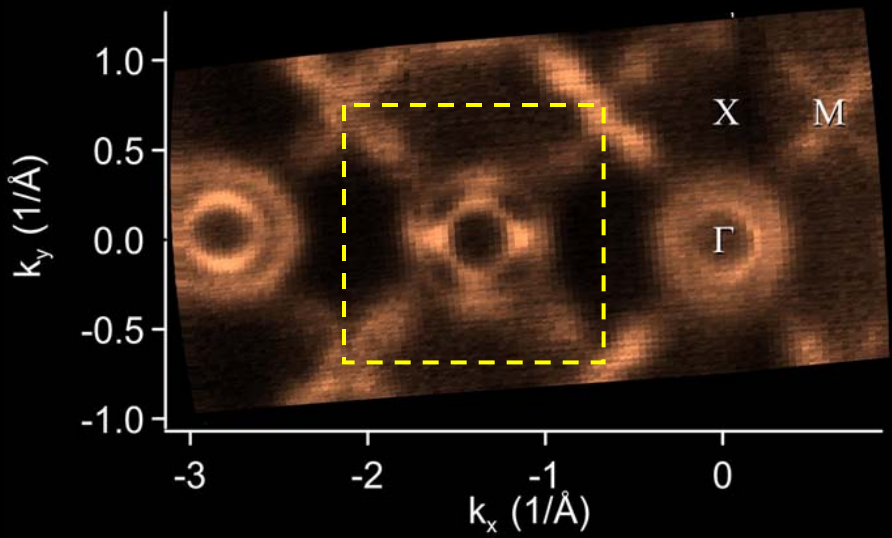
BSCCO

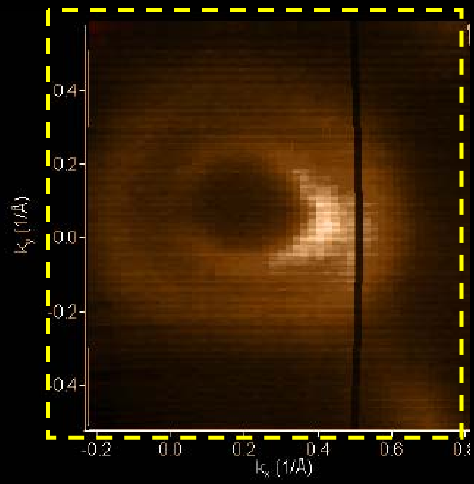


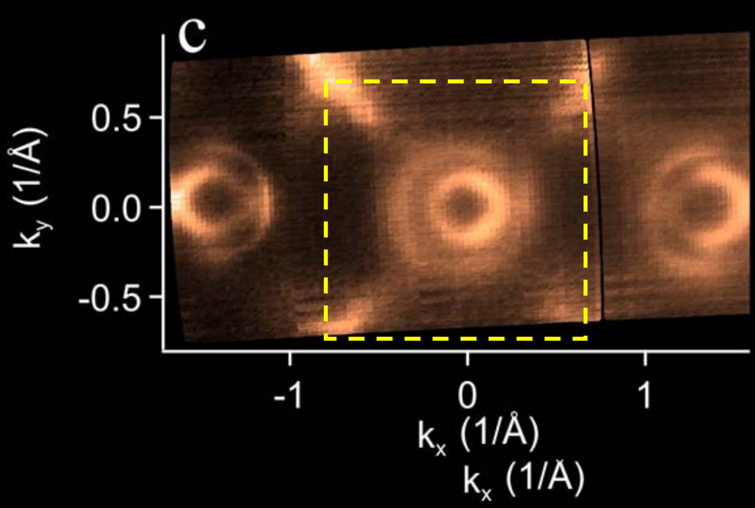
„Pseudo“ gap

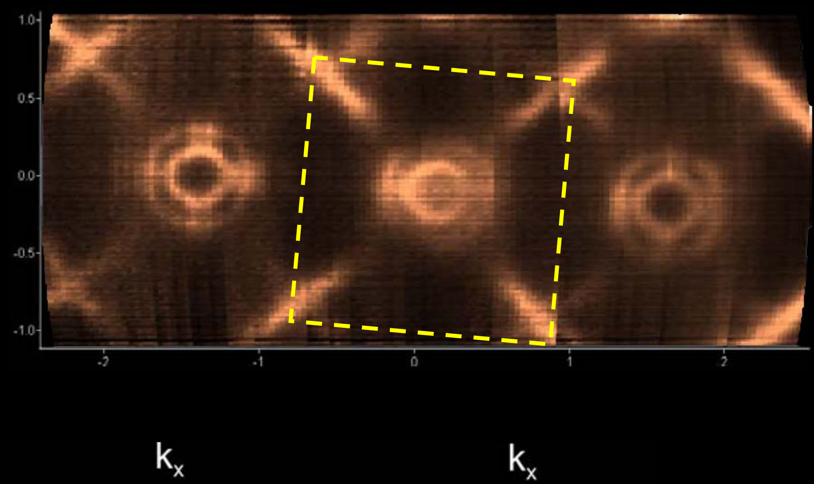


Fermi surface of BKFA (our experiment)





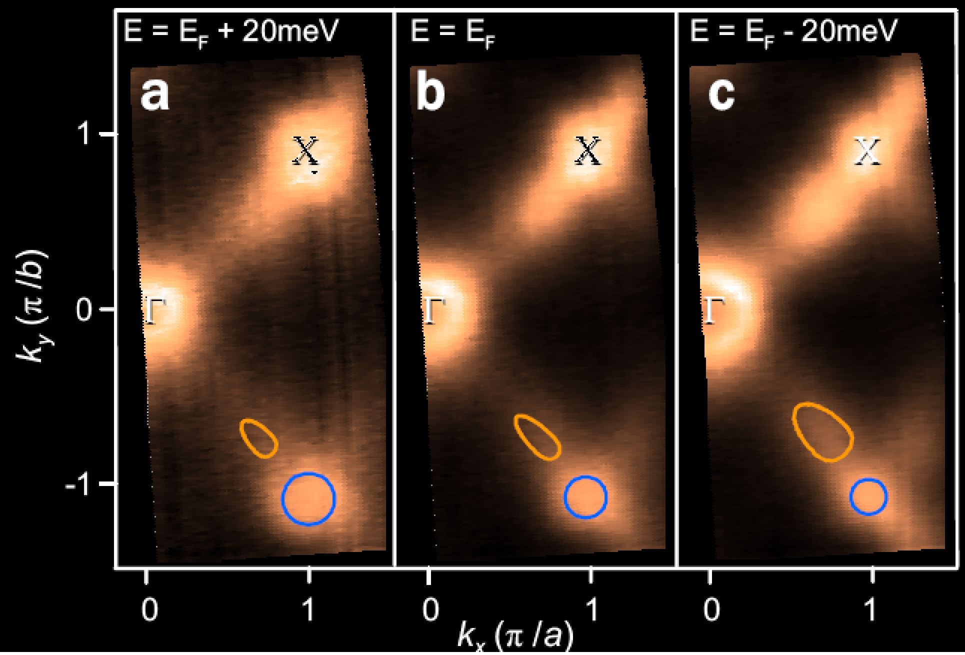


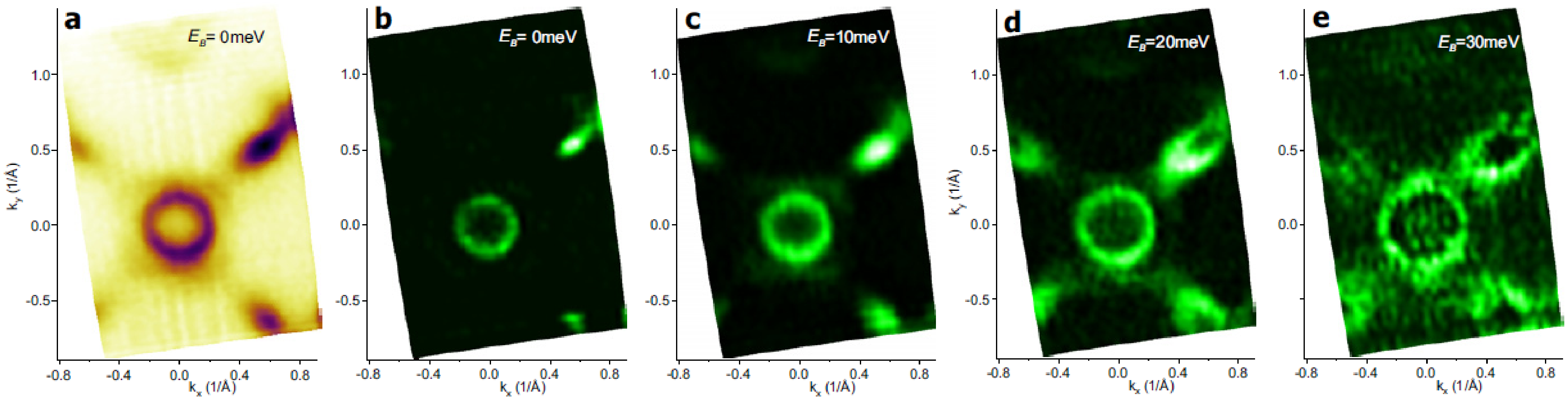


Zabolotnyy et al. Nature 09

Fermi surface of BKFA (our experiment)

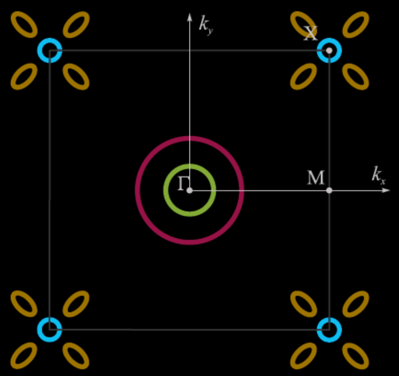
150 K

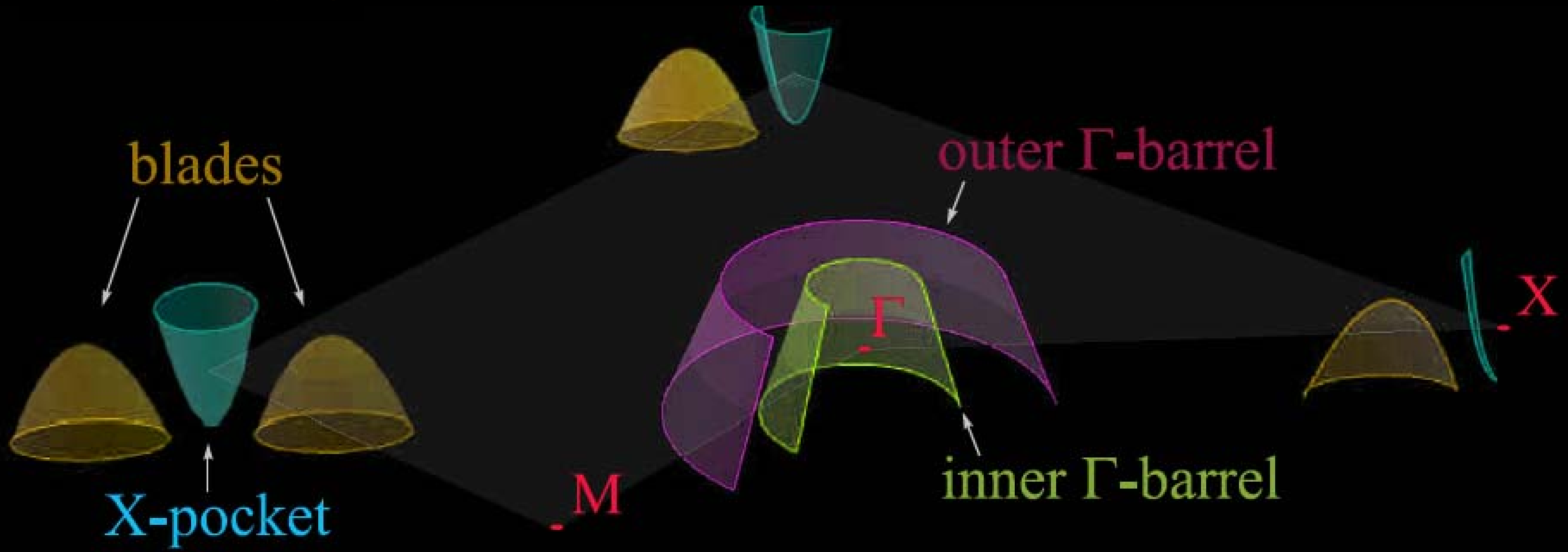




Fermi surface topology

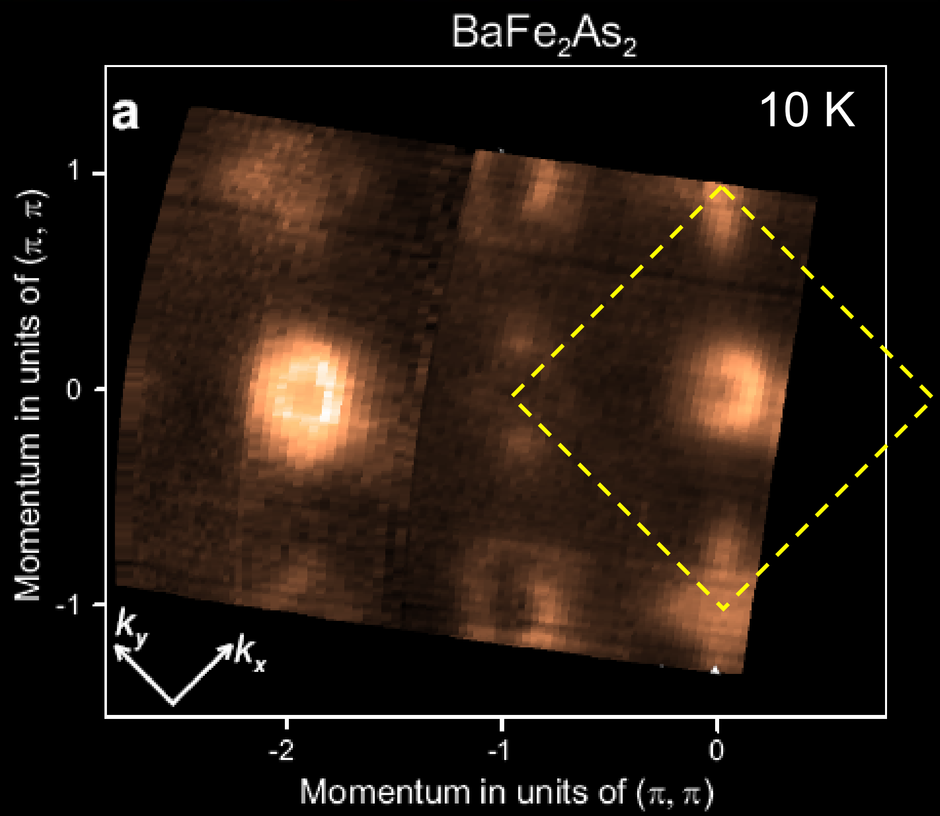
$Ba_{1-x}K_xFe_2As_2$

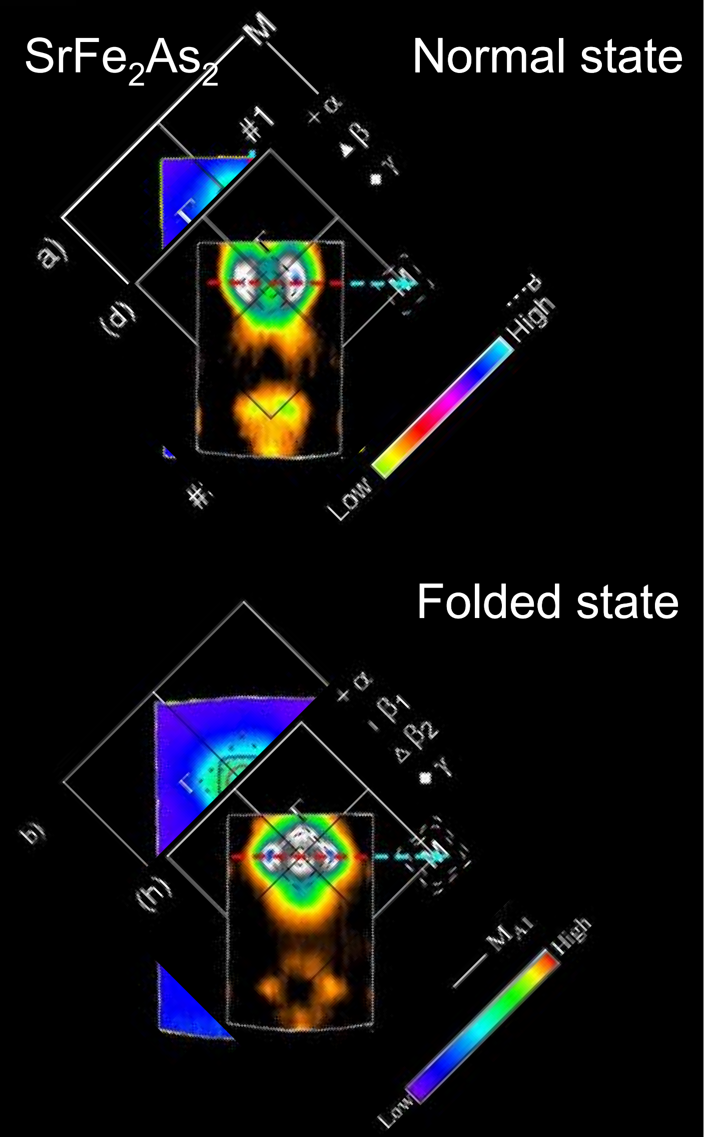




Evtushinsky *NJP* 2009

Fermi surface of parent compounds

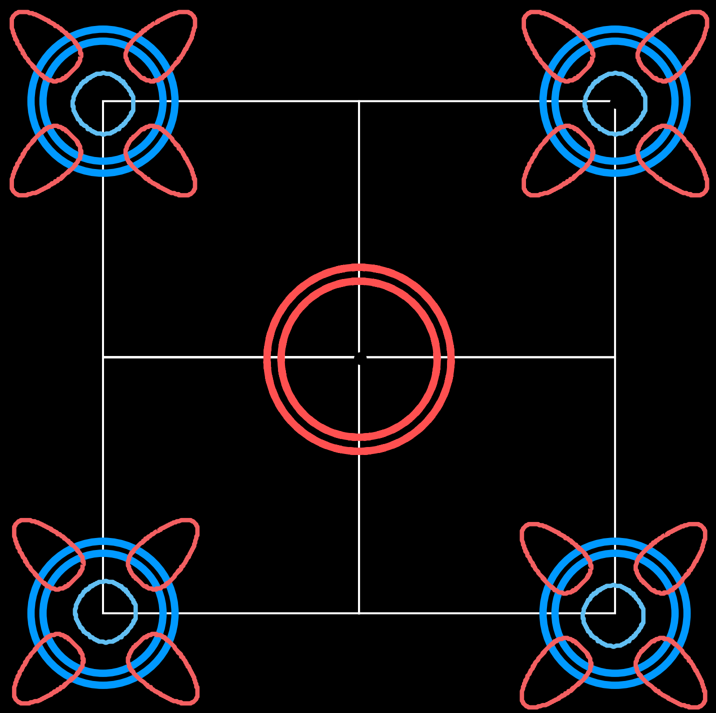


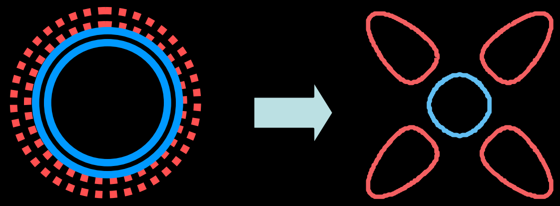


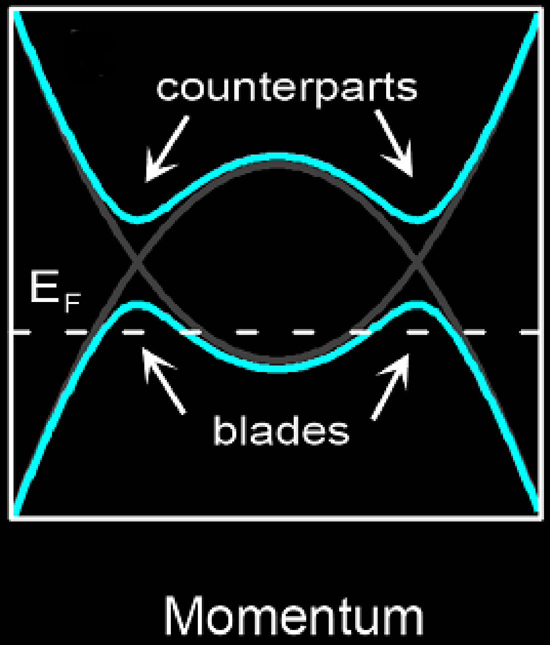
Zabolotnyy et al. Nature 09

L. X. Yang et al., arXiv:0806.2627 / Y. Zhang et al., arXiv:0808.2738

(π, π) reconstruction







Zabolotnyy et al. Nature 09

Fermi surface topology

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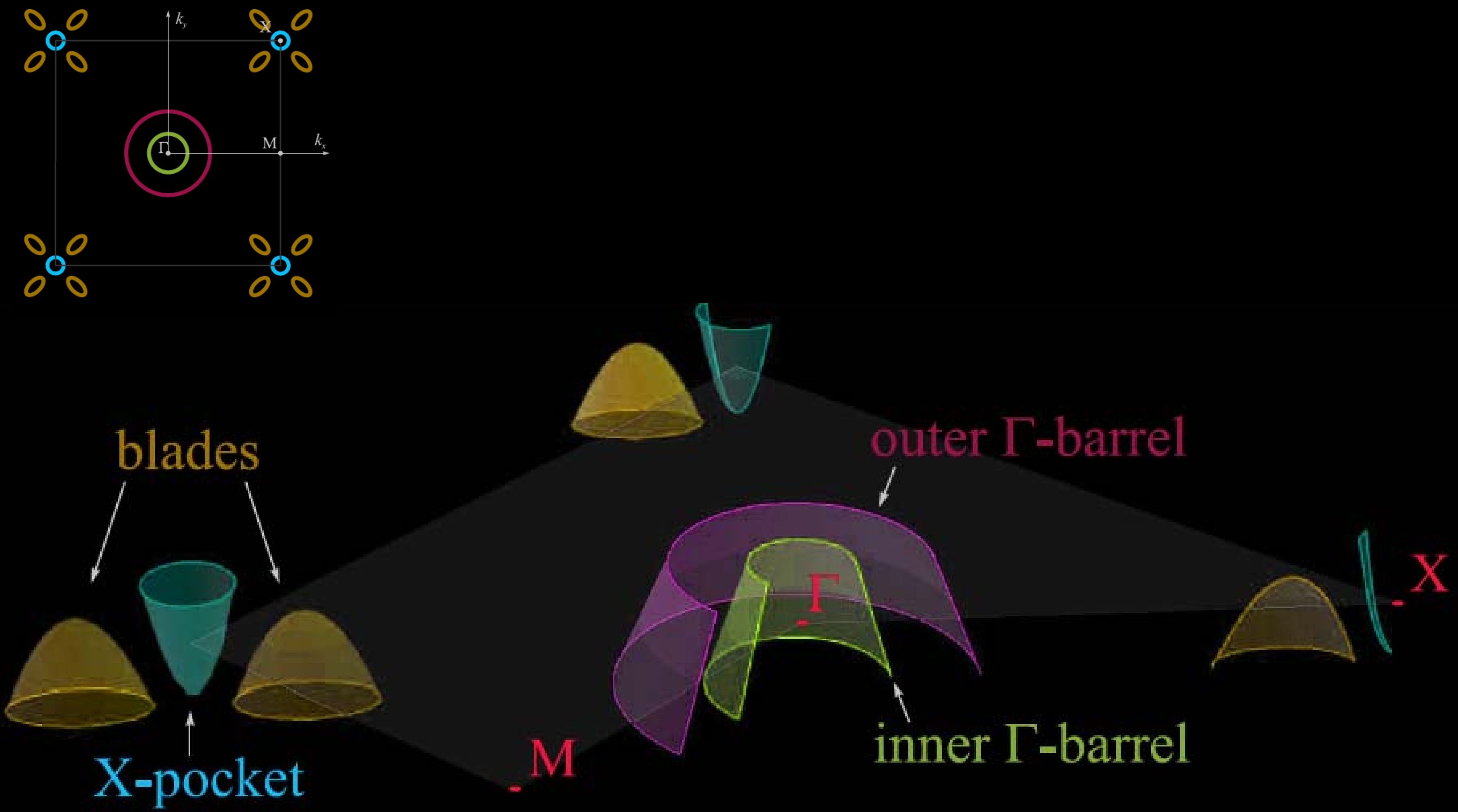
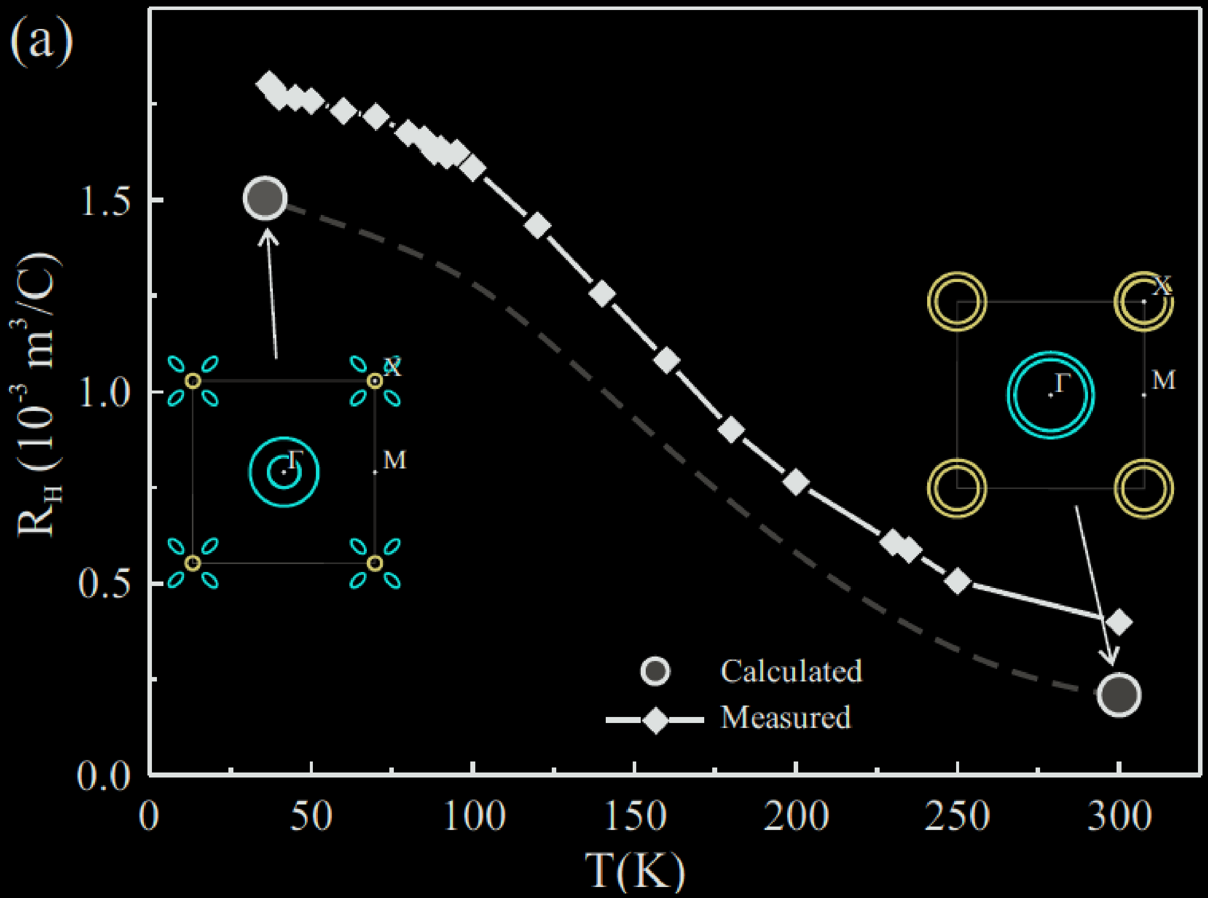


Evtushinsky *NJP* 2009

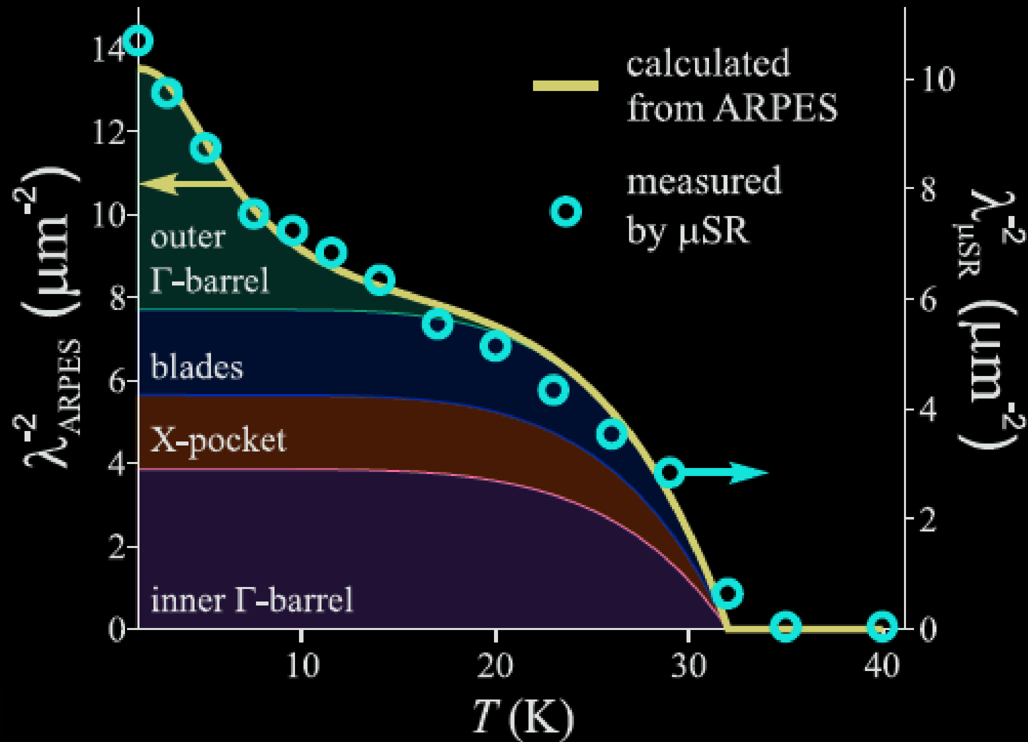
Hall coefficient from ARPES: $Ba_{1-x}K_xFe_2As_2$

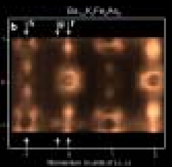


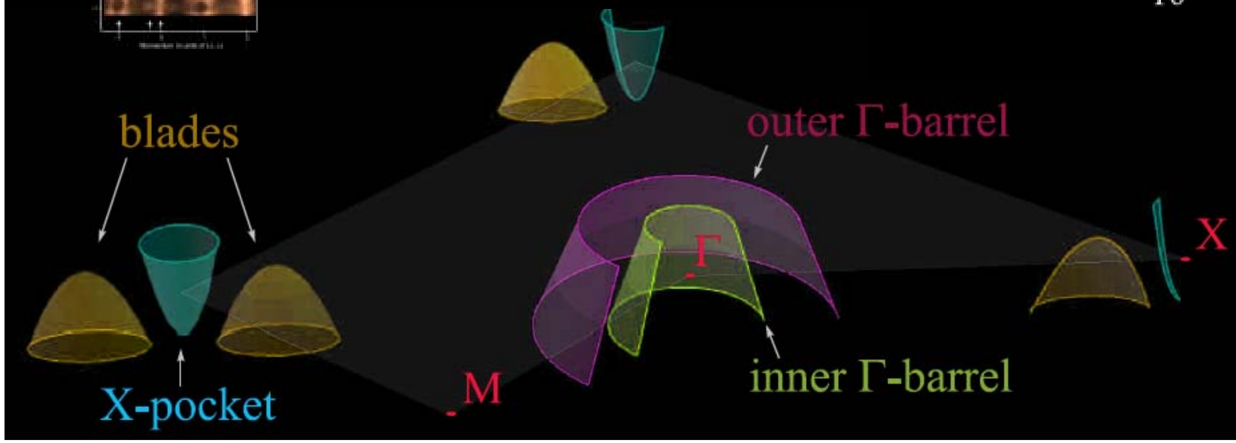
Evtushinsky et al.

Agreement with μSR data

ARPES → **μSR**





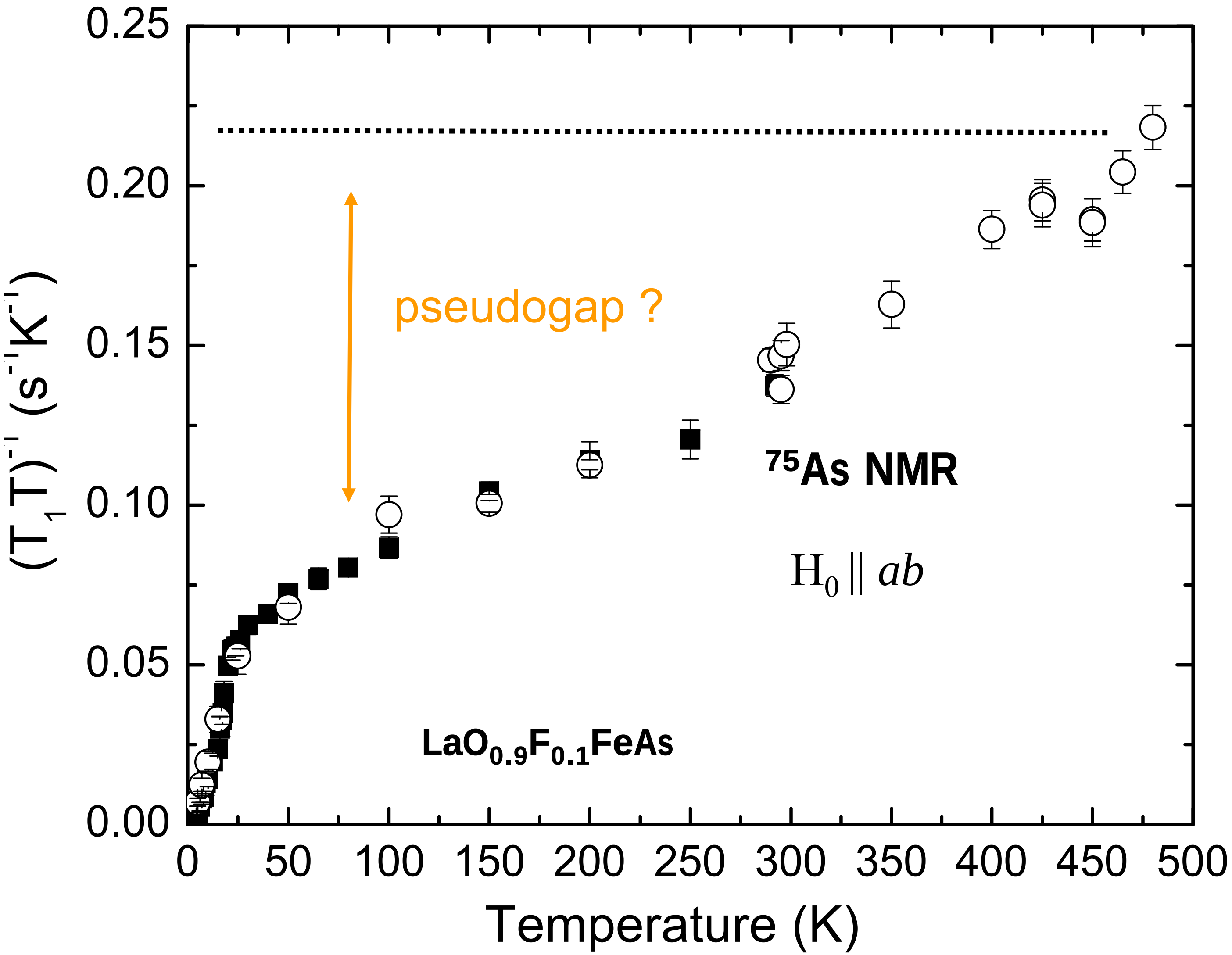


Evtushinsky et al. NJP 09

OUTLINE

- „Local physics“, Hubbard U etc.
- ARPES, Fermi surface etc.
- **„Pseudogap“, Strange T dependencies**
- Normal state resistivity
- Charge inhomogeneity (NQR)

Spin lattice relaxation rate, T_1^{-1}, normal state

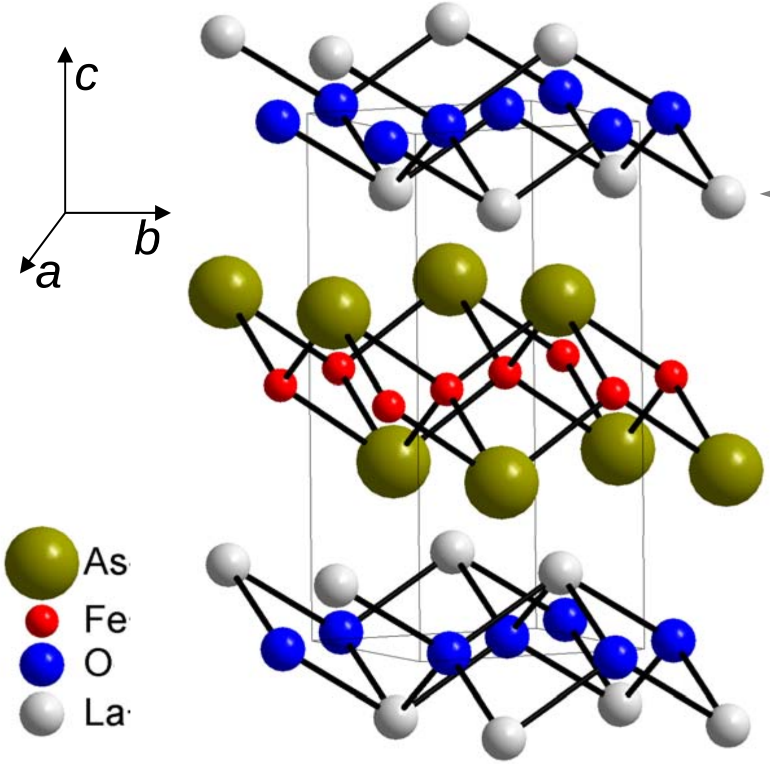


H.-J. Grafe et al., PRL 101, 047003 (2008)
H.-J. Grafe et al., New J. Phys. 2009

NMR on $LaO_{1-x}F_xFeAs$

NMR/NQR

local probe

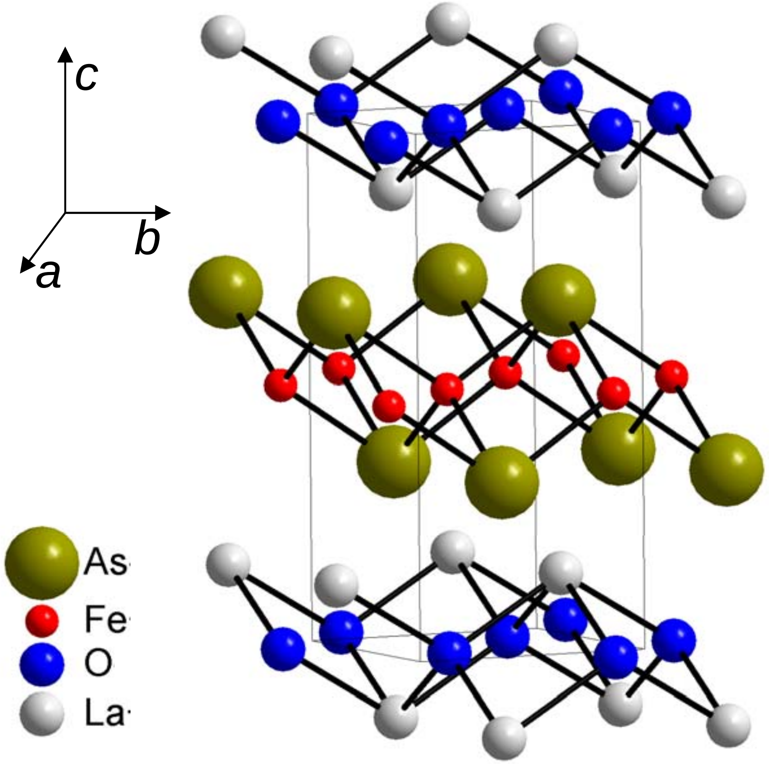


^{139}La: I=7/2, Q≠0,
outside the FeAs plane

^{57}Fe: I=1/2, Q=0

^{75}As: I=3/2, Q≠0,
inside the FeAs plane

Nuclear Magnetic and Quadrupole Resonance



$$\mathcal{H} = \gamma\hbar H_0(1 + K)\hat{I}_z$$

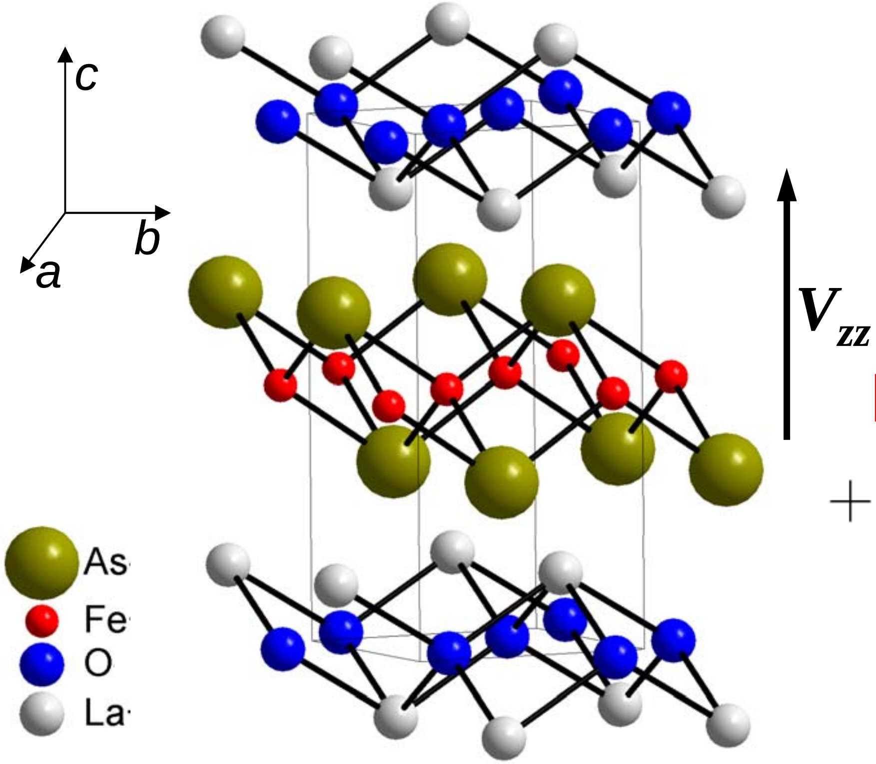
local susceptibility:

$K = K_s + K_{orb}$

$K_s = A_{hf} \cdot \chi_s(q=0, \omega=0)$

Nuclear Magnetic and Quadrupole Resonance

$$\mathcal{H} = \gamma\hbar H_0(1 + K)\hat{I}_z$$



local susceptibility:

$$K = K_s + K_{orb}$$

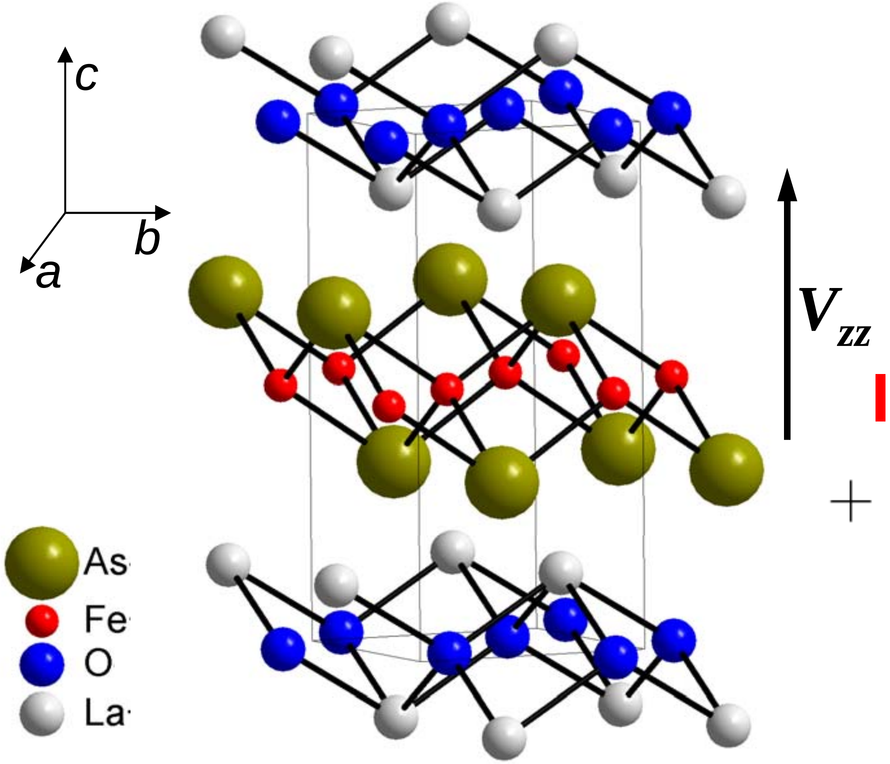
$$K_s = A_{hf} \cdot \chi_s(q=0, \omega=0)$$

local charge environment:

$$+ \frac{h\nu_Q}{6}[(3\hat{I}_{z'}^2 - \hat{I}^2) + \eta(\hat{I}_{x'}^2 - \hat{I}_{y'}^2)]$$

$$\nu_Q = \frac{3eQV_{zz}}{2I(2I-1)h}\sqrt{1 + \eta^2/3}$$

Nuclear Magnetic and Quadrupole Resonance



$$\mathcal{H} = \gamma\hbar H_0(1+K)\hat{I}_z$$

local susceptibility:

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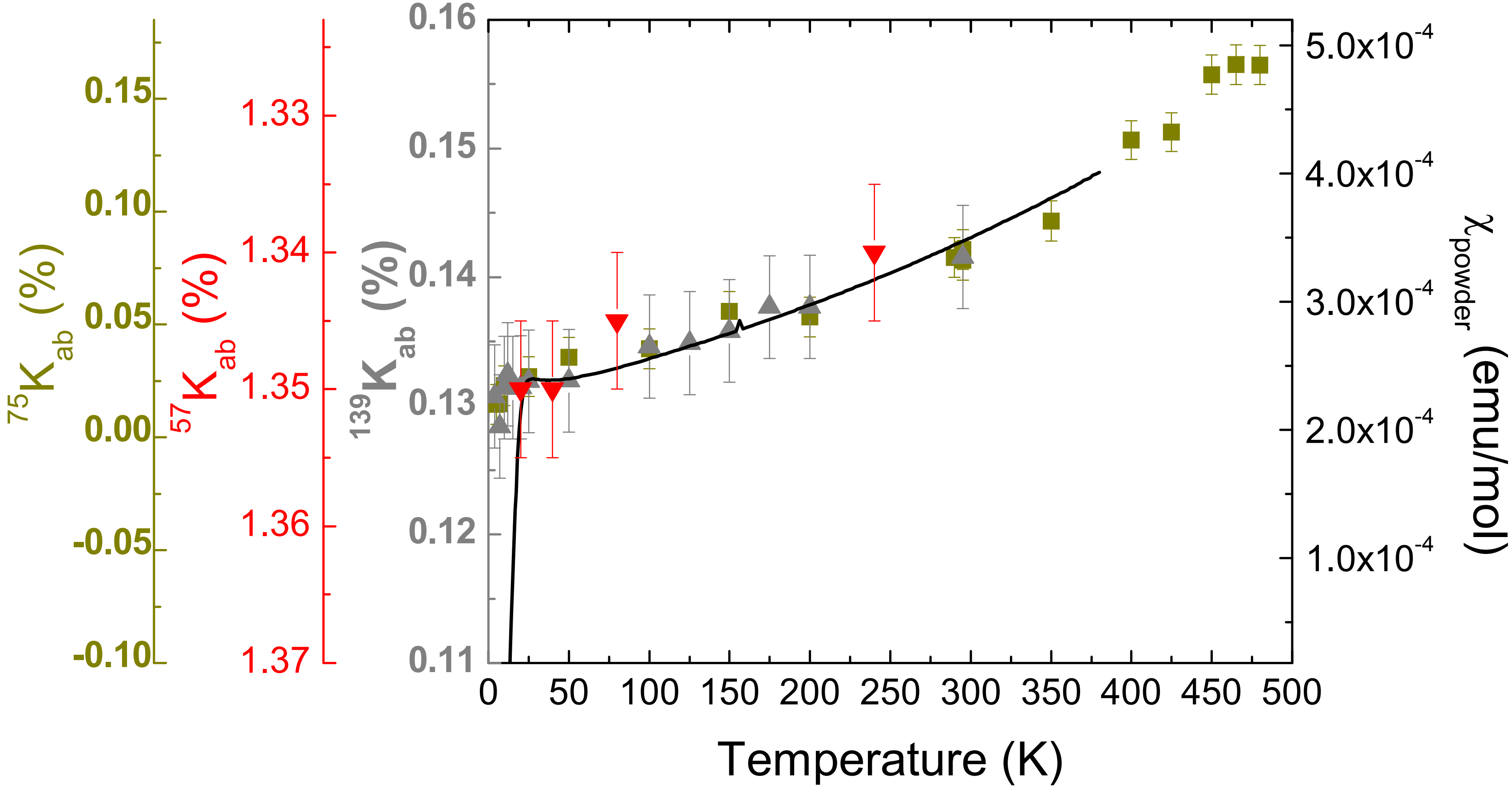
$$\nu_Q = \frac{3eQV_{zz}}{2I(2I-1)h}\sqrt{1+\eta^2/3}$$

local *dynamic* susceptibility:

$$(T_1T)^{-1} \sim A_{hf}(q)^2 \cdot \chi''(q, \omega)$$

$$\omega \sim 10\text{-}100 \text{ MHz}$$

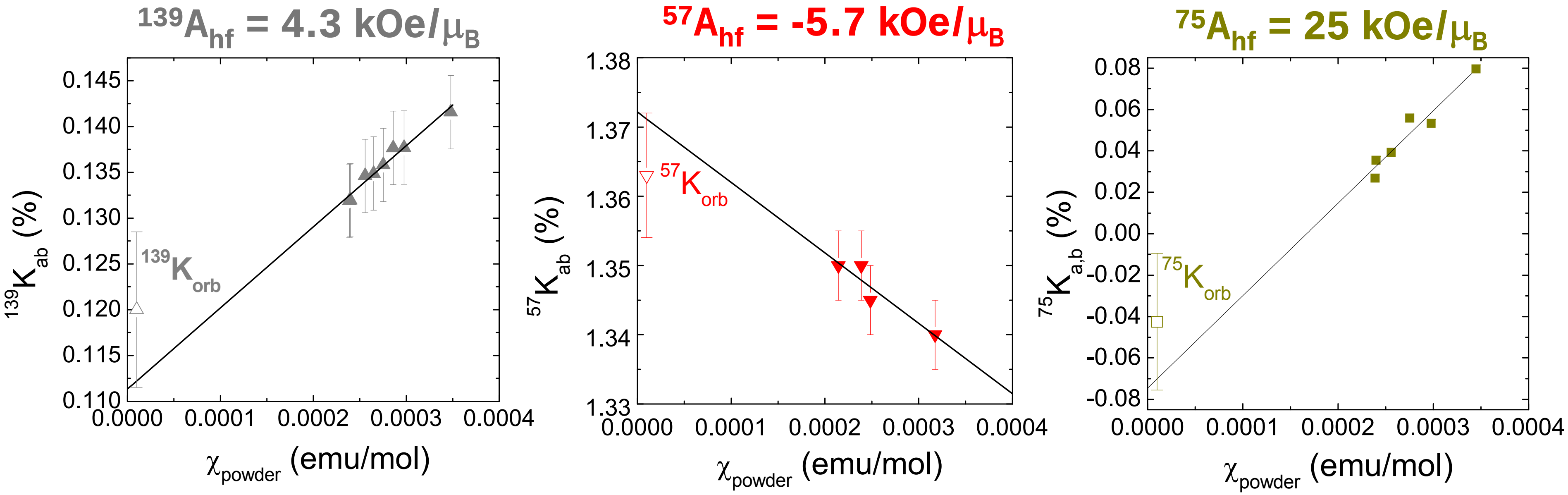
Knight shift for H_0 || *a*,*b*: $LaO_{0.9}F_{0.1}FeAs$



$K=K_s+K_{orb}$

$K_s=A_{hf}\cdot\chi_s(q=0,\omega=0)$

Hyperfine couplings for ^{139}La, ^{57}Fe and ^{75}As in $LaO_{0.9}F_{0.1}FeAs$



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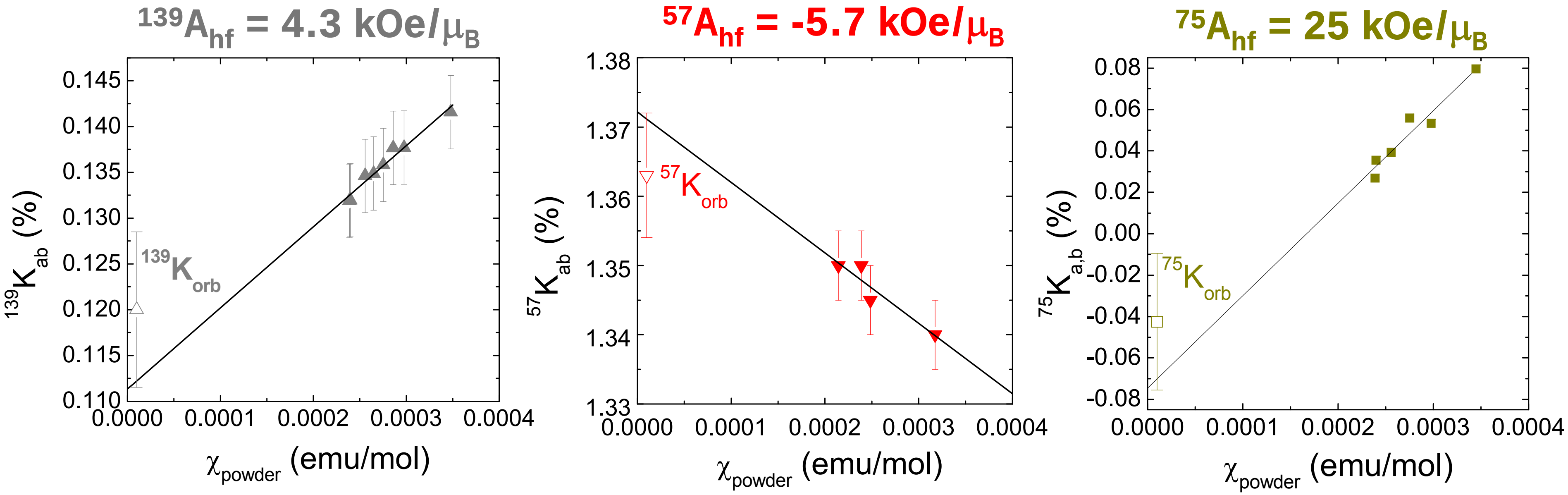


$H_{int}(La) = {}^{139}A_{hf} \cdot \mu(Fe)$

undoped LaOFeAs:

$H_{int,x=0}(La) = 2.5$kOe

Nakai, JPSJ 77, 073701 (2008)

⇒ ordered Fe moment of ~0.58 μ_B

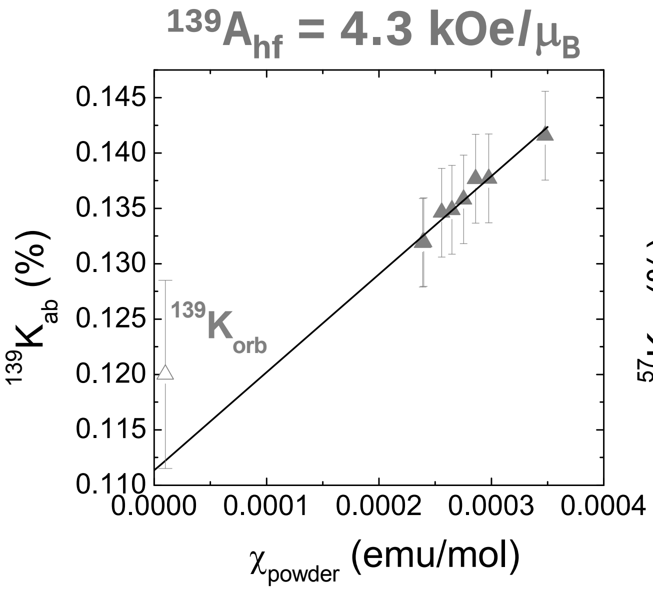
Neutron scattering: ~0.36 μ_B

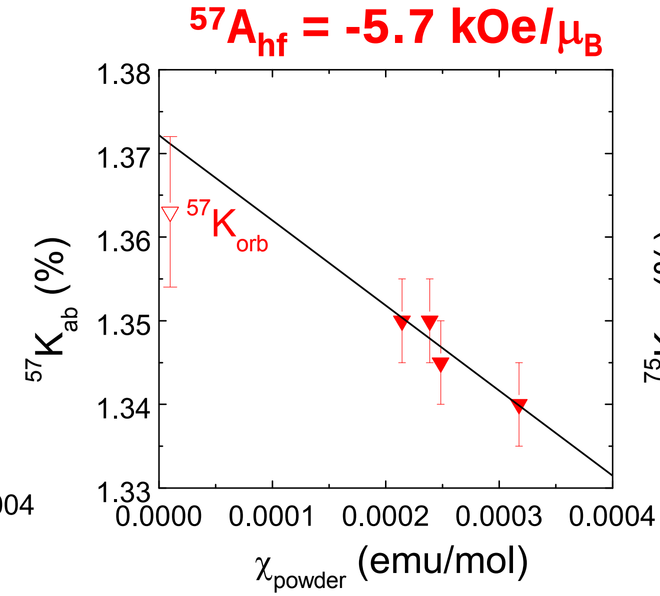
de la Cruz et al., Nature 453, 899 (2008)

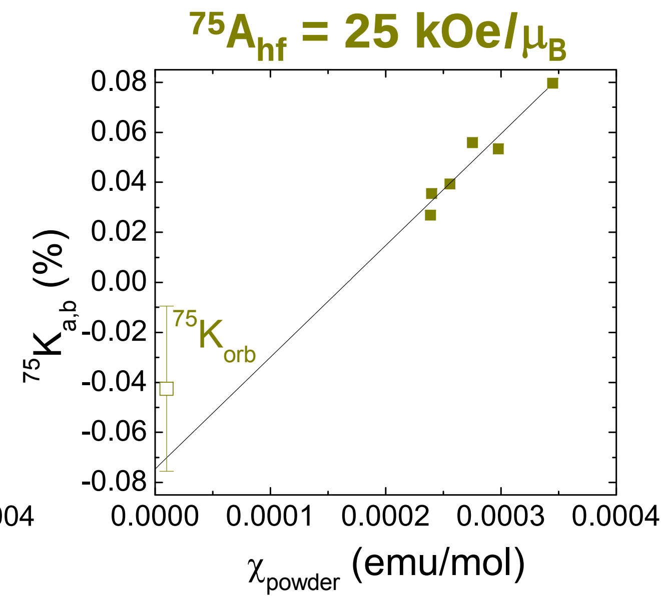
Mößbauer spectroscopy: ~0.3 μ_B

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

Hyperfine couplings for ^{139}La, ^{57}Fe and ^{75}As in $LaO_{0.9}F_{0.1}FeAs$







$H_{int}(La) = {}^{139}A_{hf} \cdot \mu(Fe)$

undoped LaOFeAs:

$H_{int,x=0}(La)$ = 2.5kOe

Nakai, JPSJ 77, 073701 (2008)

$\Rightarrow$ **ordered Fe moment of ~0.58 μ_B**

Neutron scattering: ~0.36 μ_B

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

Mößbauer spectroscopy: ~0.3 μ_B

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

^{57}Fe: negative hyperfine coupling:

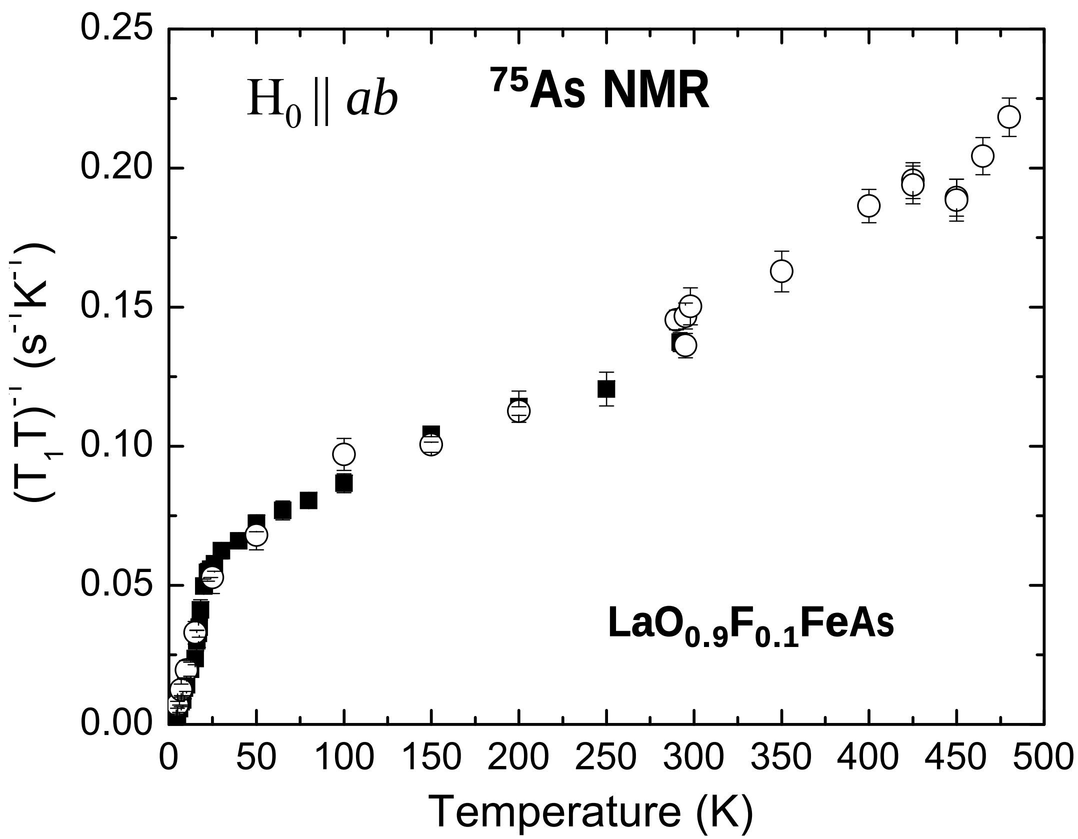
$$^{57}A_{hf} = A_{cp} + A_{4s}$$

If A_{cp} (core polarization) is large and negative and A_{4s} large and positive, then $^{57}A_{hf}$ can be small and negative.

Spin lattice relaxation rate, T_1^{-1}, normal state

$$\frac{1}{T_1} = \frac{2\gamma_n^2 k_B T}{(\gamma_e \hbar)^2} \lim_{\omega \to 0} \sum_{q} A_q A_{-q} \frac{\chi''_\perp(q,\omega_0)}{\omega_0}$$

measure of the dynamic spin susceptibility



- $(T_1T)^{-1}$ is not constant in the normal state, no simple Fermi liquid behavior
- Pseudo gap like decrease of $(T_1T)^{-1}$ in the normal state, but no “peak“ up to 500 K

H.-J. Grafe et al., PRL 101, 047003 (2008)

Spin lattice relaxation rate, T_1^{-1}, normal state

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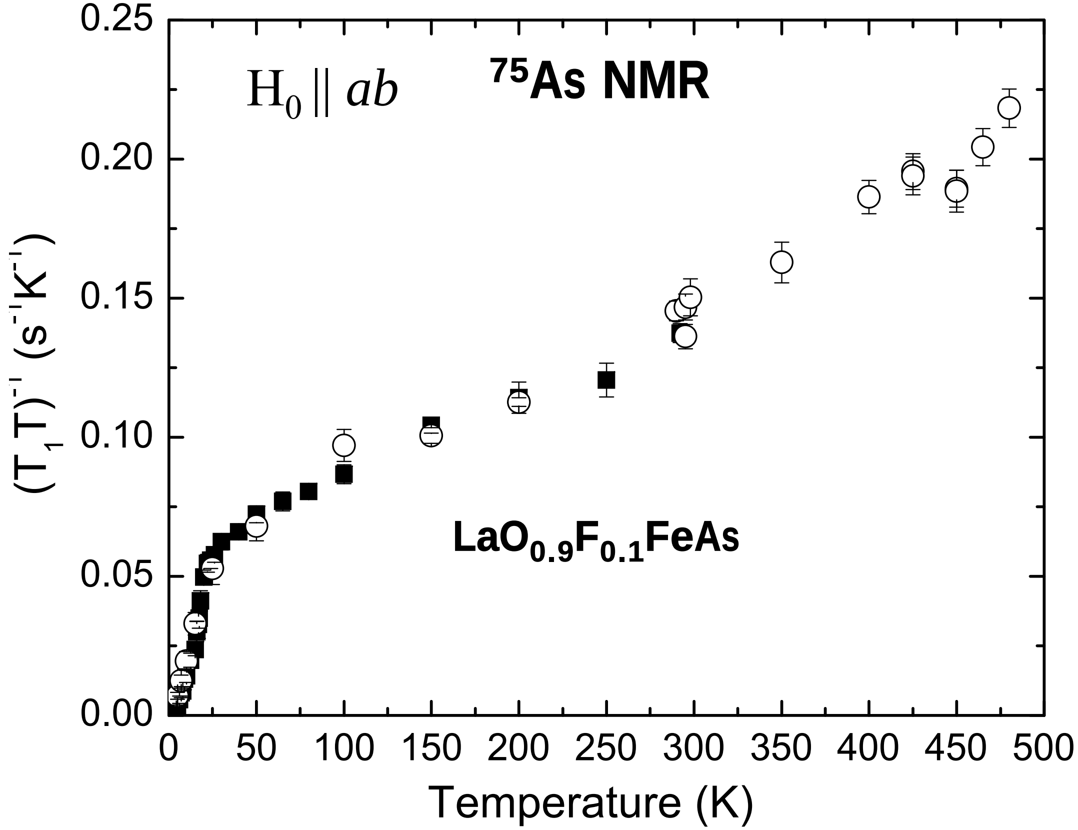
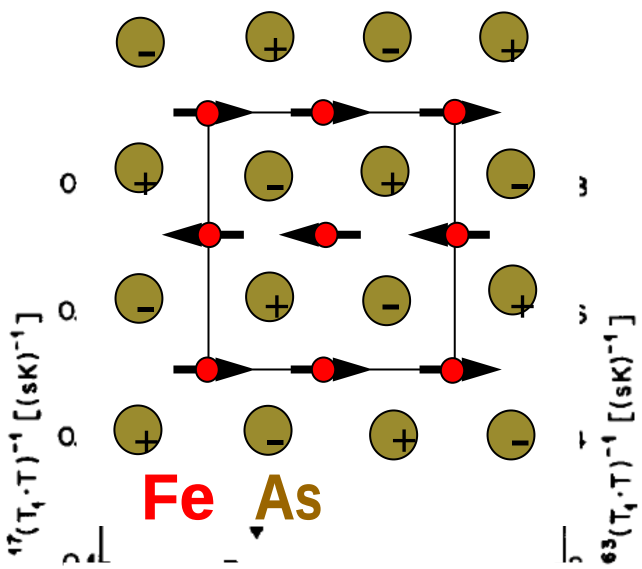
→ measure of the dynamic spin susceptibility

→ *q*-dependent form factor (hyperfine coupling of the nucleus)





Fe maximal at q=(π,π)

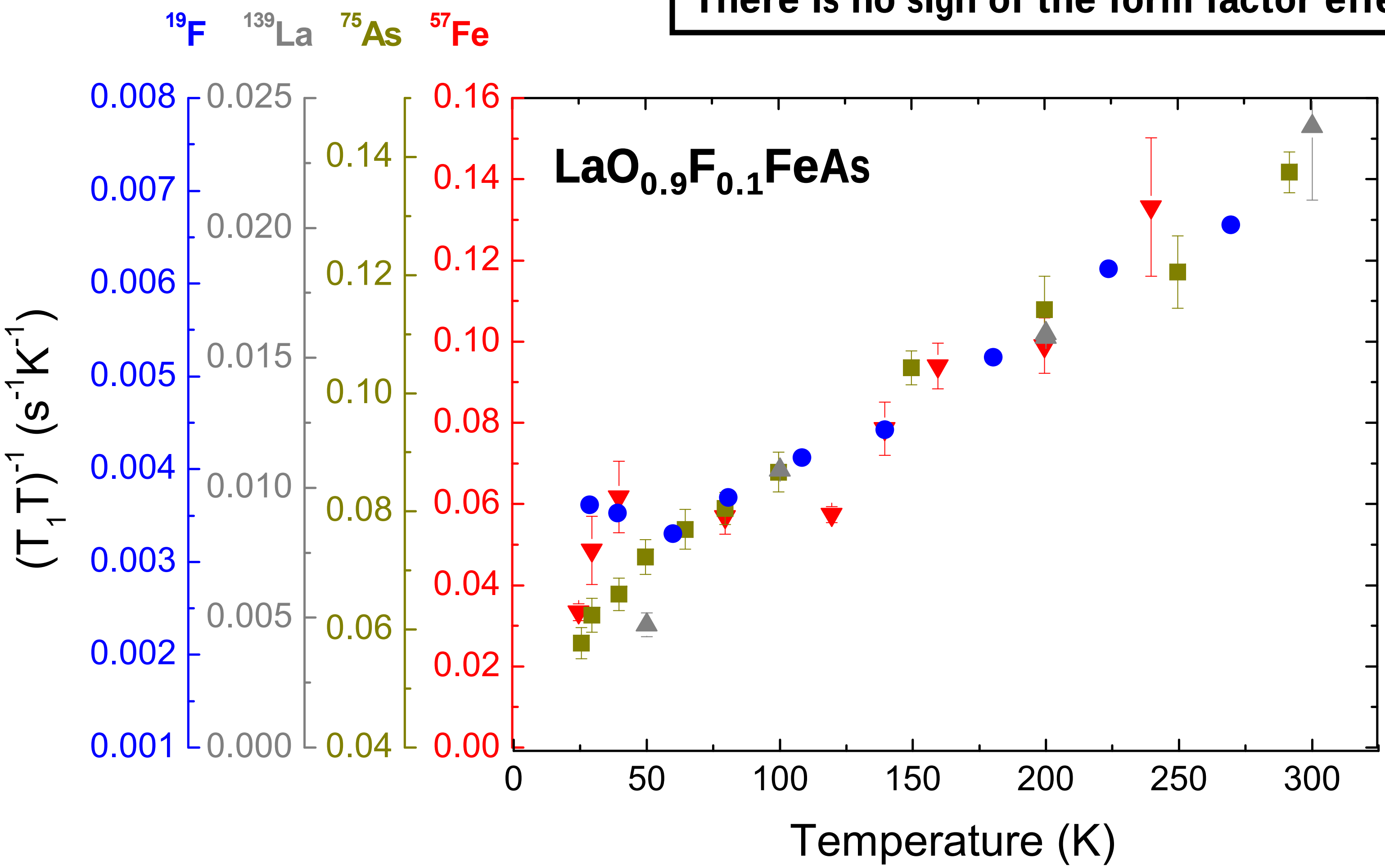
As maximal at q=(0,0)

Mangelschots, Physica C 1993

Comparison of ^{57}Fe, ^{75}As, ^{139}La and ^{19}F T_1^{-1}, normal state

$$\frac{1}{T_1} = \frac{2\gamma_n^2 k_B T}{(\gamma_e \hbar)^2} \lim_{\omega \to 0} \sum_{\boldsymbol{q}} A_{\boldsymbol{q}} A_{-\boldsymbol{q}} \frac{\chi''_\perp(\boldsymbol{q}, \omega_0)}{\omega_0}$$

There is no sign of the form factor effect.



^{19}F data from Ahilan *et al.*
Phys. Rev. B **78**, 100501(R) (2008)

Comparison of ^{57}Fe, ^{75}As, ^{139}La and ^{19}F T_1^{-1}, normal state

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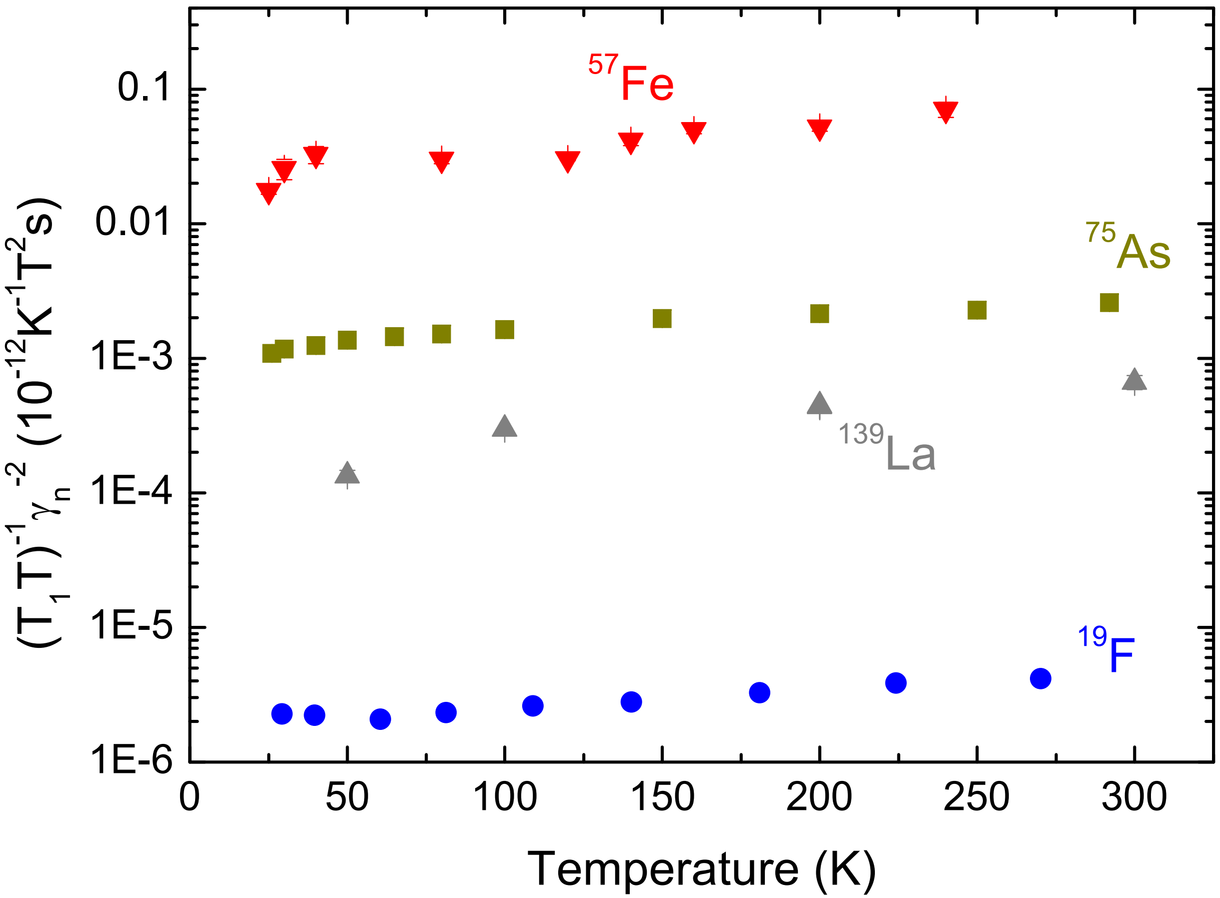
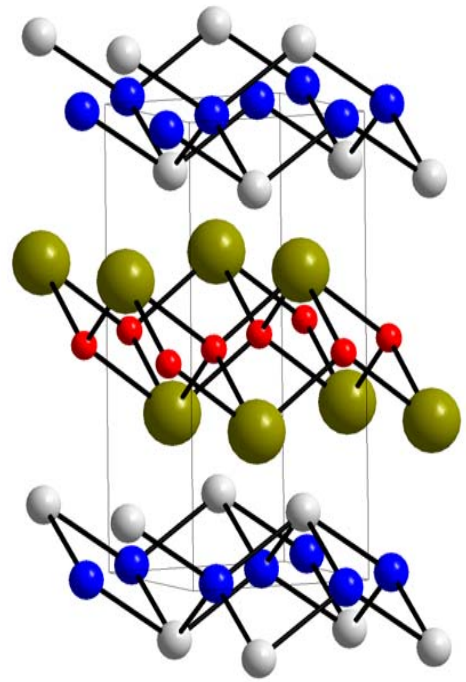
$LaO_{0.9}F_{0.1}FeAs$





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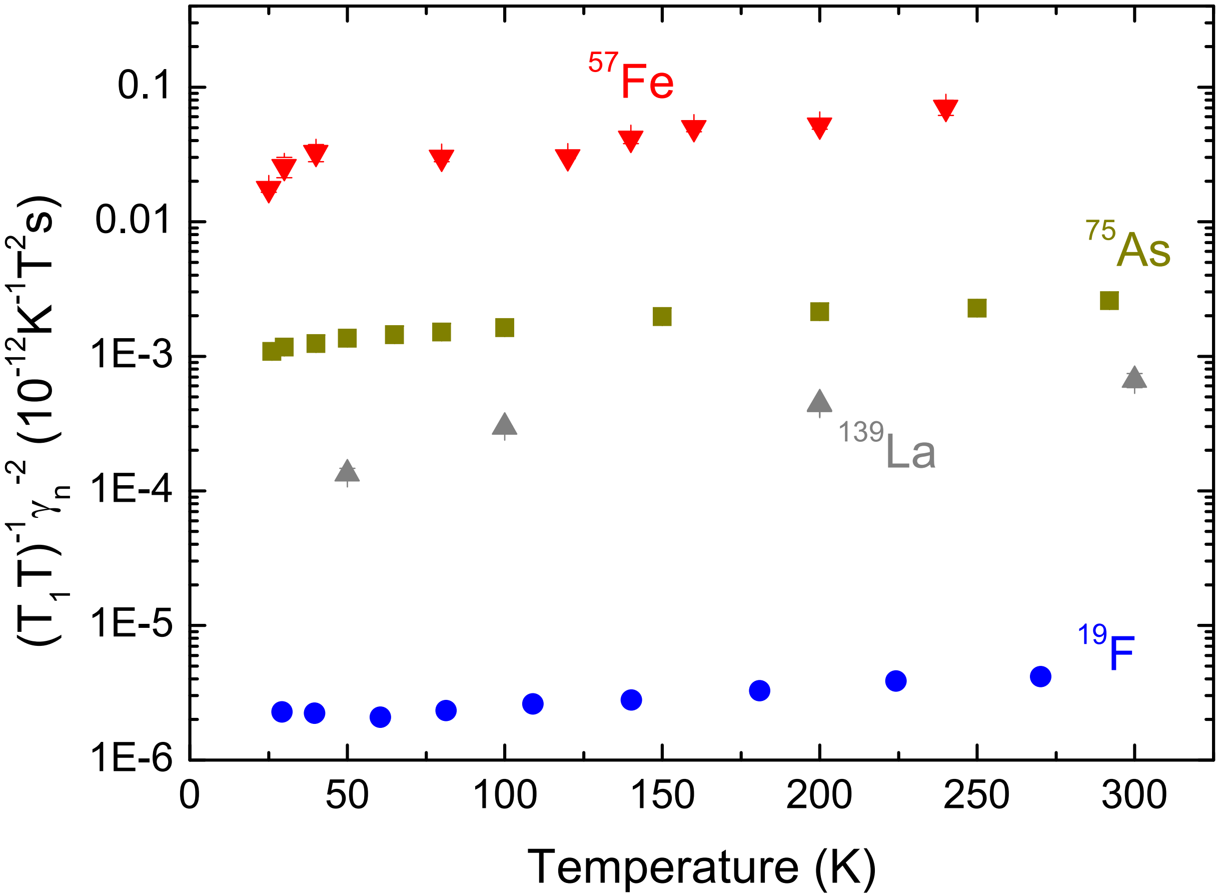
$LaO_{0.9}F_{0.1}FeAs$

$$\frac{^{57}A_{hf}(q=0)^2}{^{75}A_{hf}(q=0)^2} = \frac{-5.7^2\ (\mathrm{kOe}/\mu_B)^2}{25^2\ (\mathrm{kOe}/\mu_B)^2} = 0.05$$



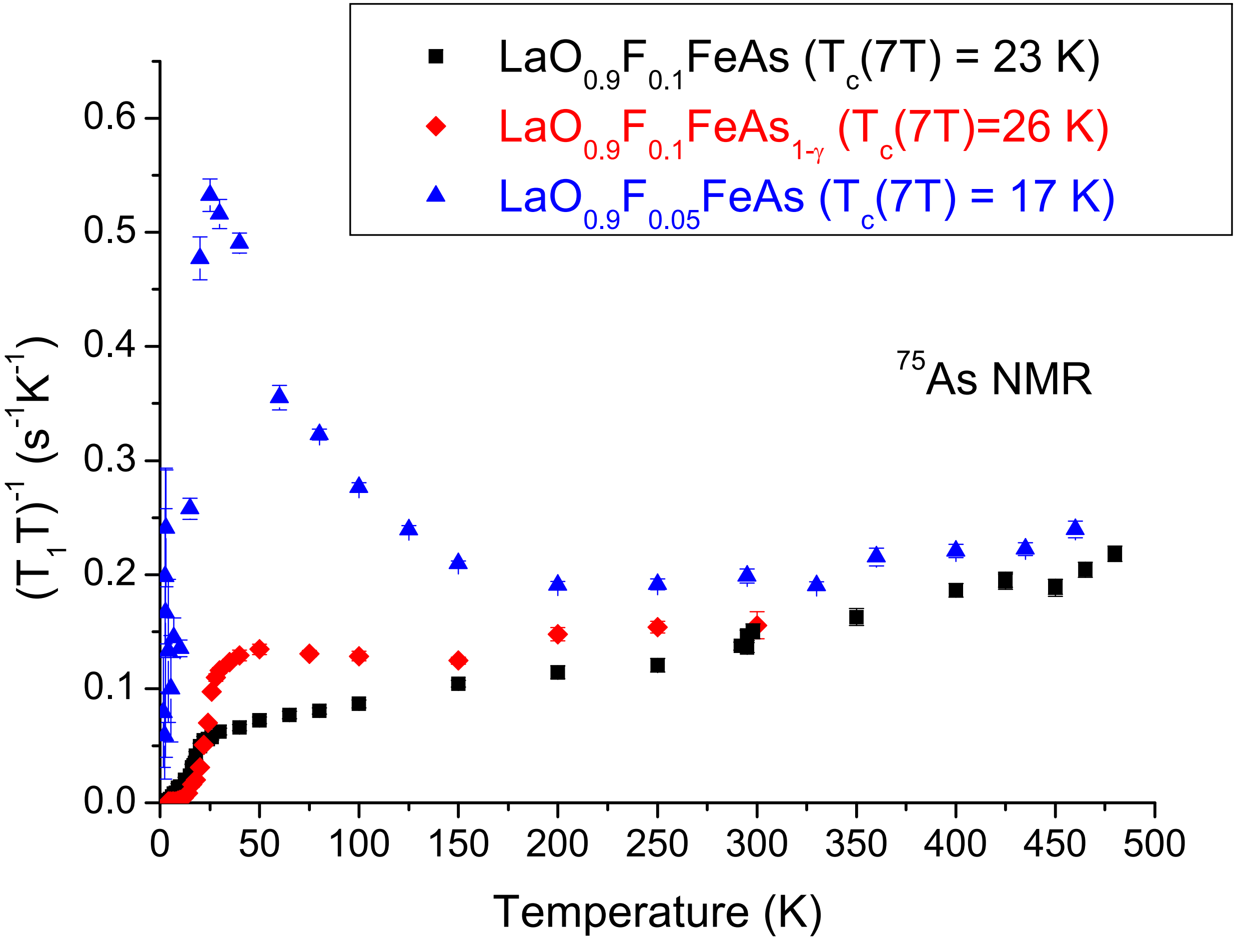
$$\frac{^{75}(T_1 T \gamma_n^2)}{^{57}(T_1 T \gamma_n^2)} = 20\text{-}30$$

Either strong q dependence or quasi particle scattering.

In case of quasi part. scatt. $^{57}A_{cp}$ adds as the sum of the squares, rather than a direct sum.

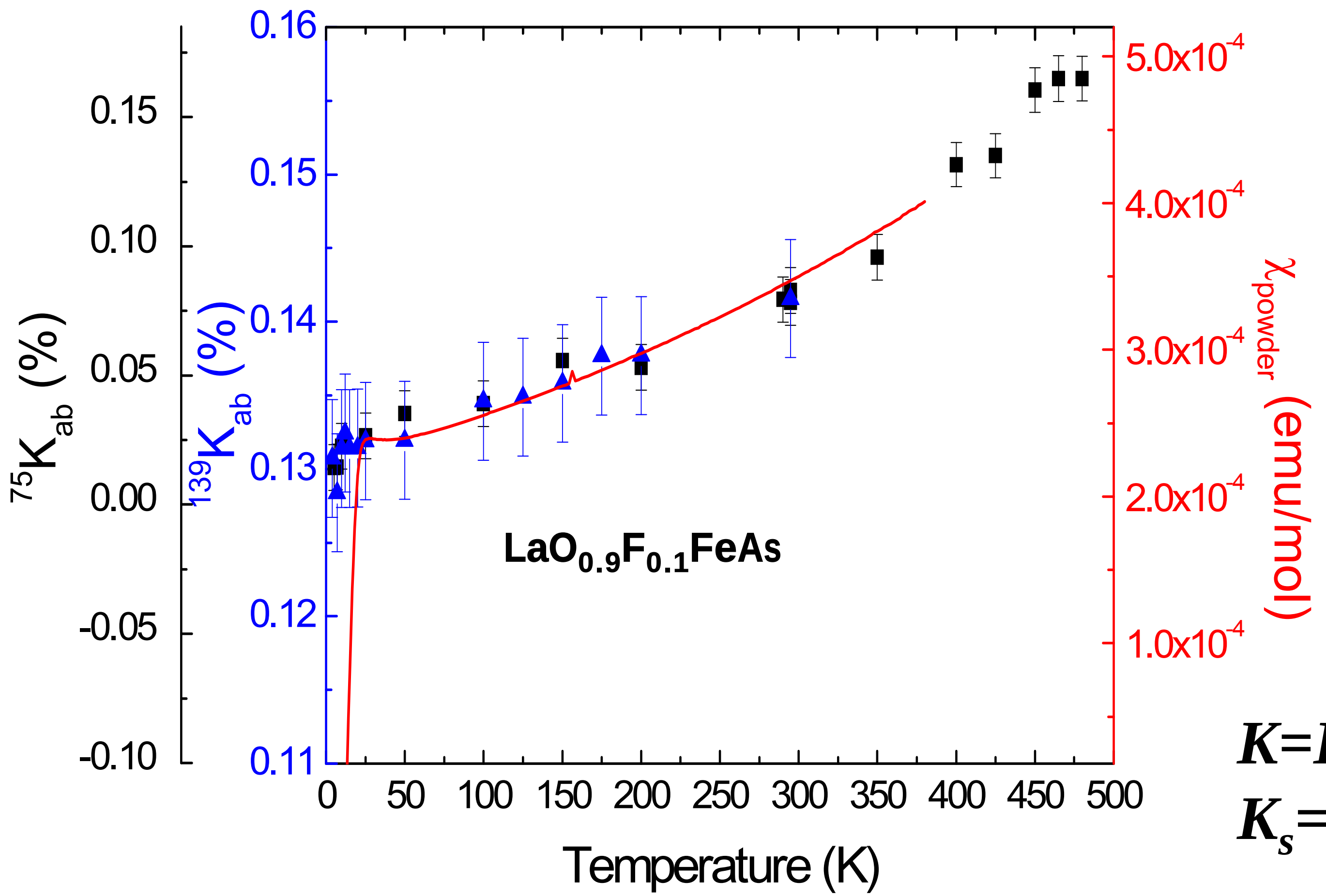
^{19}F data from Ahilan *et al.*
Phys. Rev. B **78**, 100501(R) (2008)

Spin lattice relaxation rate, T_1^{-1}, normal state



- $(T_1T)^{-1}$ is not constant in the normal state, no simple Fermi liquid behavior
- Pseudo gap like decrease of $(T_1T)^{-1}$ in the normal state, but no pseudo gap peak up to 500 K
- Spin fluctuations in the underdoped region

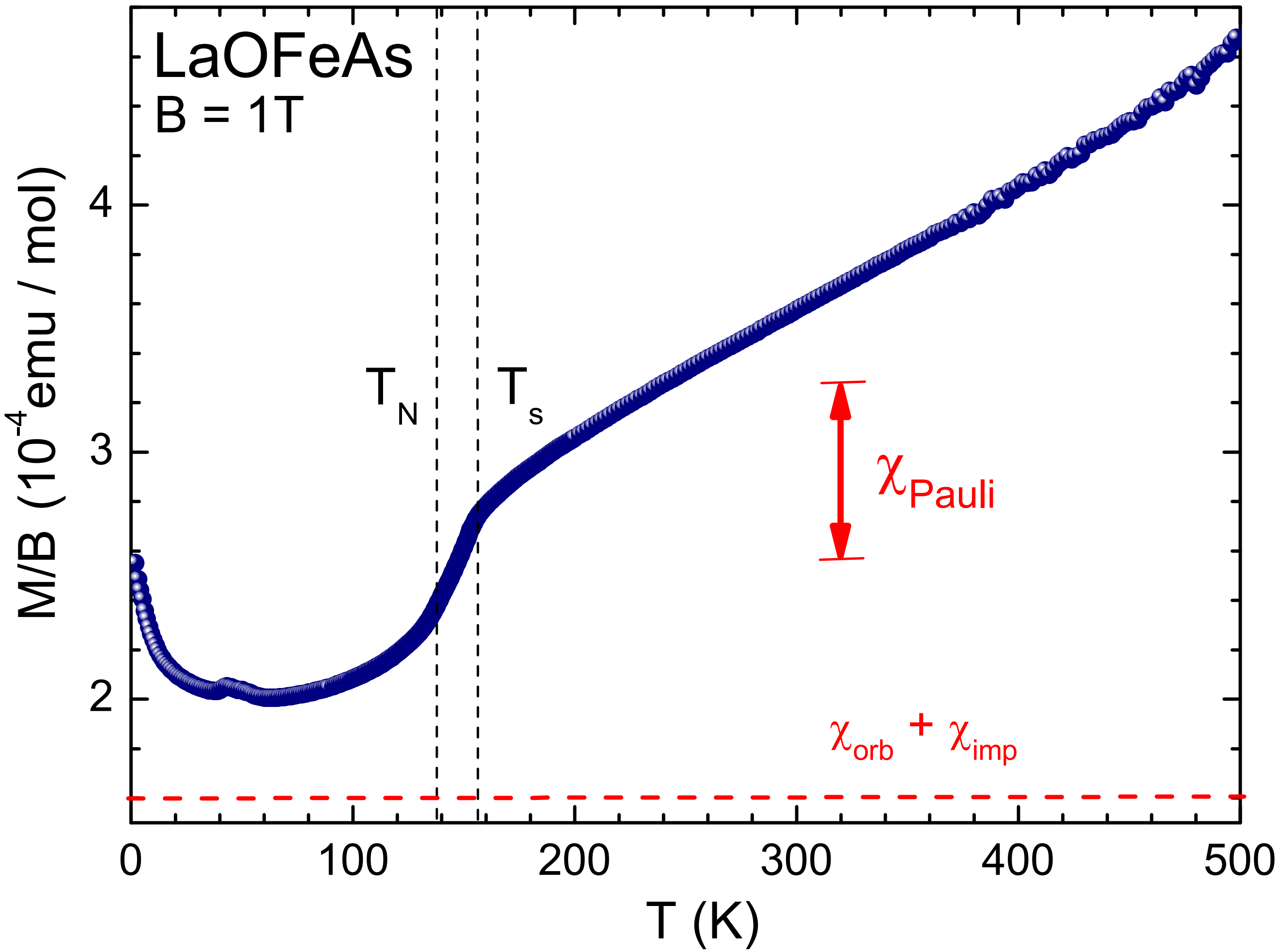
NMR on La($O_{1-x}F_x$)FeAs: Knight shift



$$K = K_s + K_{orb}$$
$$K_s = A \cdot \chi_s(q=0, \omega=0)$$

- **Pseudo gap like decrease of Knight shift, but no “peak“ up to 500 K**
- **Macroscopic susceptibility is not affected by impurities**

Magnetic Susceptibility of LaOFeAs



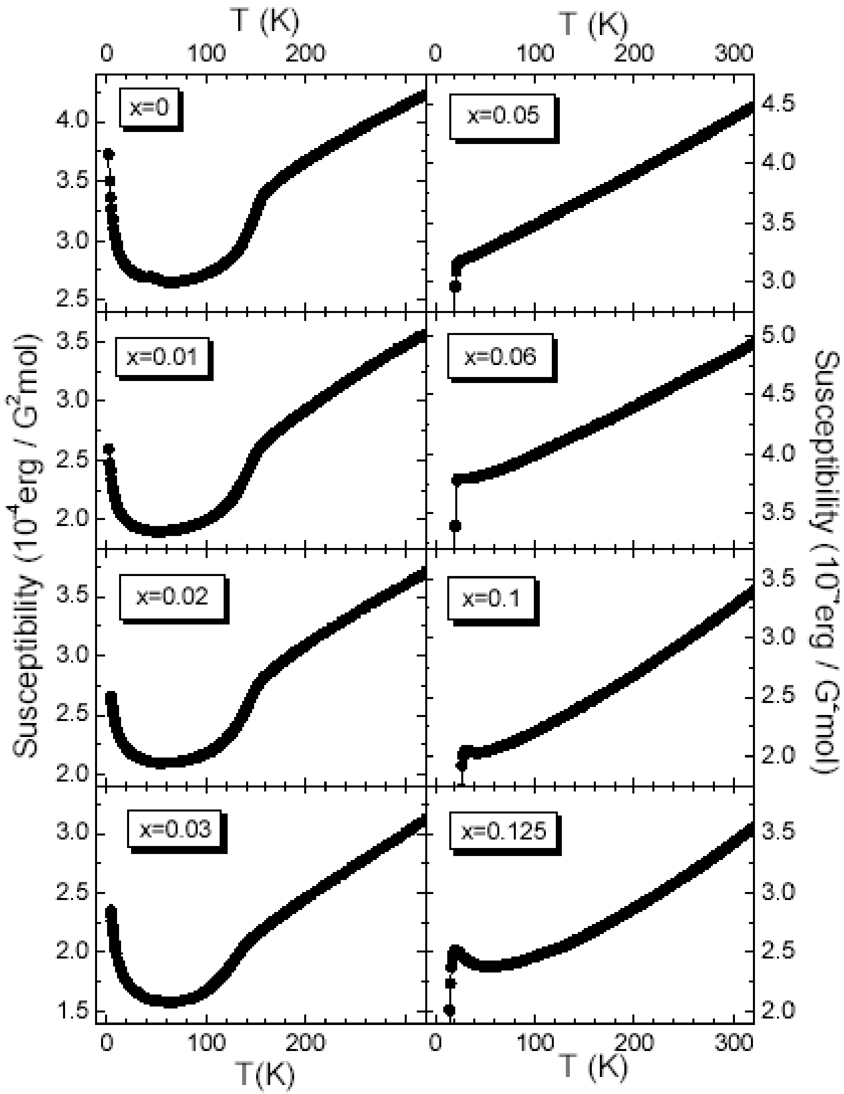
- 'Poor' metal
- No Curie-Weiss behavior
- No simple Pauli behavior

$$\chi_P = \frac{3\mu_B^2}{\pi^2 k_B^2}\gamma$$

R. Klingeler et al., archiv:0808.07080

χ_{orb}: T. Imai et al., archiv 0810.0305

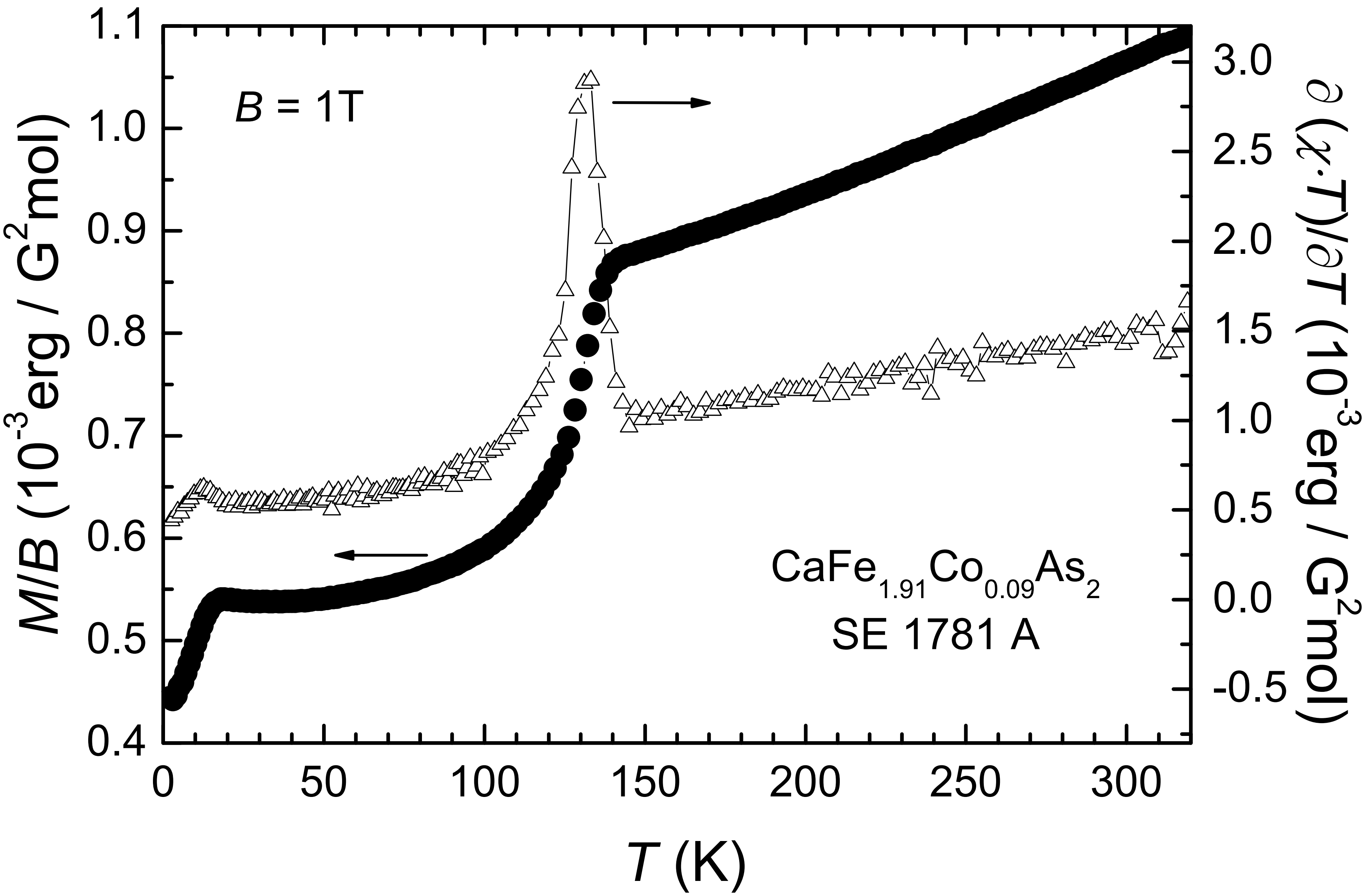
Magnetic Susceptibility of $La(O_{1-x}F_x)FeAs$



Normal State χ

- χ increases with T (up to 500K)
- absolute values of χ “small”
- similar T dependence for all doping concentrations
- similar absolute values of χ for all doping concentrations

R. Klingeler et al., arXiv: 0808.0708


B = 1T
CaFe1.91Co0.09As2
SE 1781 A
M/B (10-3erg / G2mol)
∂(χ·T)/∂T (10-3erg / G2mol)
T (K)
0
50
100
150
200
250
300
0.4
0.5
0.6
0.7
0.8
0.9
1.0
1.1
-0.5
0.0
0.5
1.0
1.5
2.0
2.5
3.0

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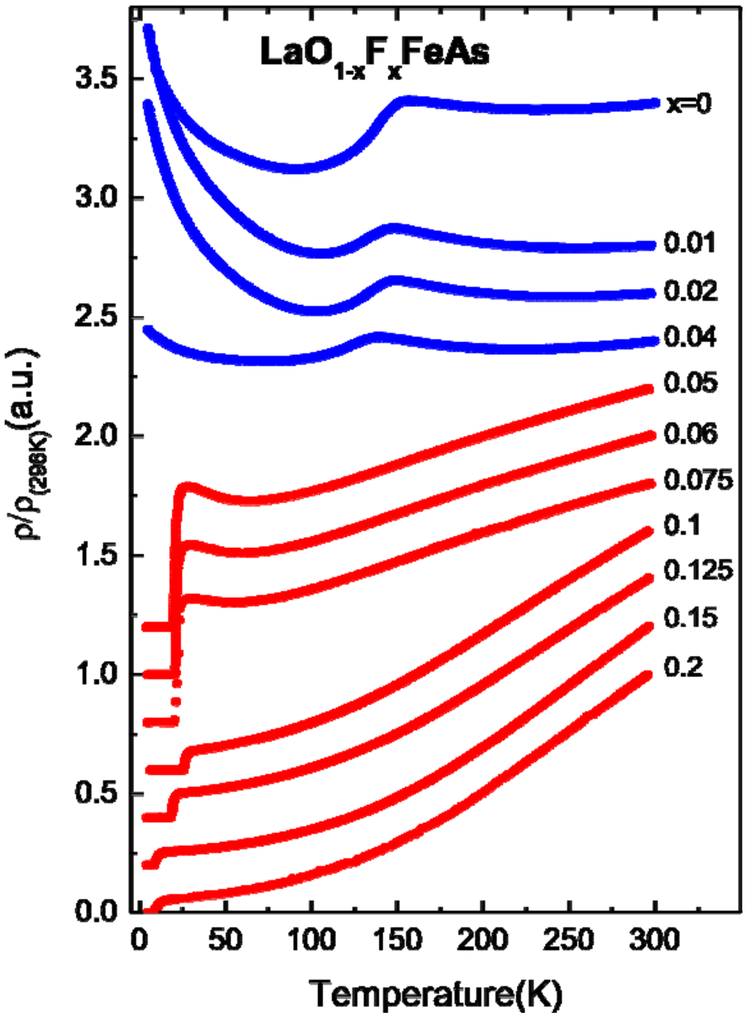
Electronic Properties of Pnictide Superconductors

OUTLINE

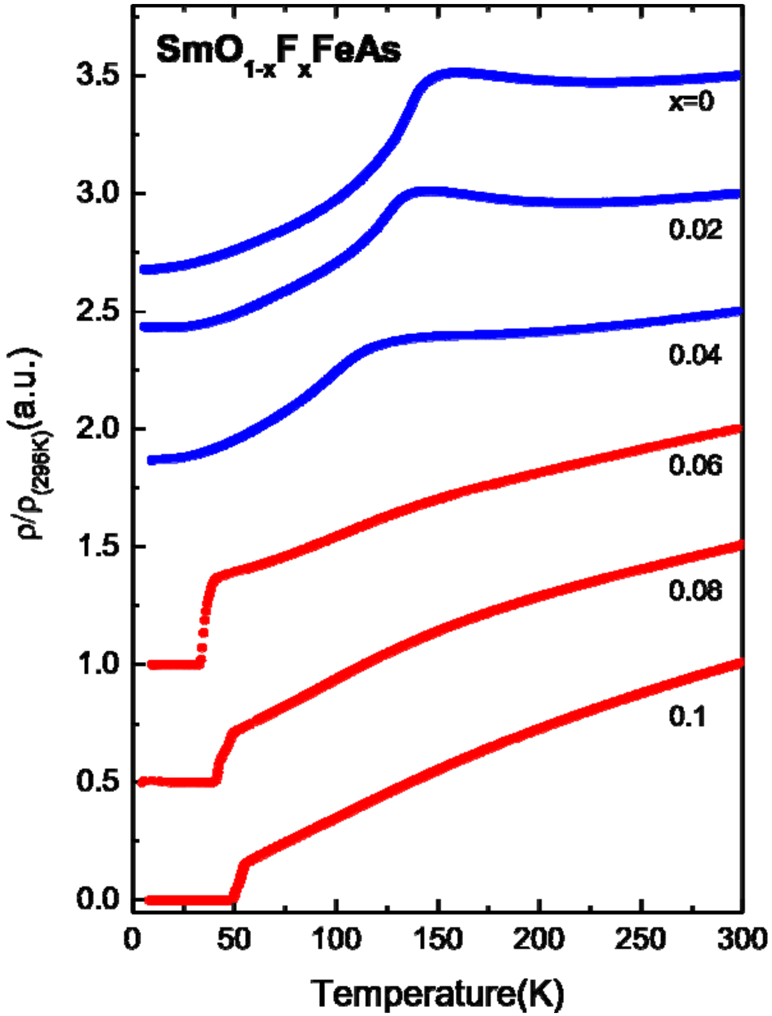
- „Local physics“, Hubbard U etc.
- ARPES, Fermi surface etc.
- „Pseudogap“, Strange T dependencies
- **Normal state resistivity**
- Charge inhomogeneity (NQR)

$(RE)O_{1-x}F_xFeAs$ – Normal State Resistivity

$LaO_{1-x}F_xFeAs$ – lowest T_c



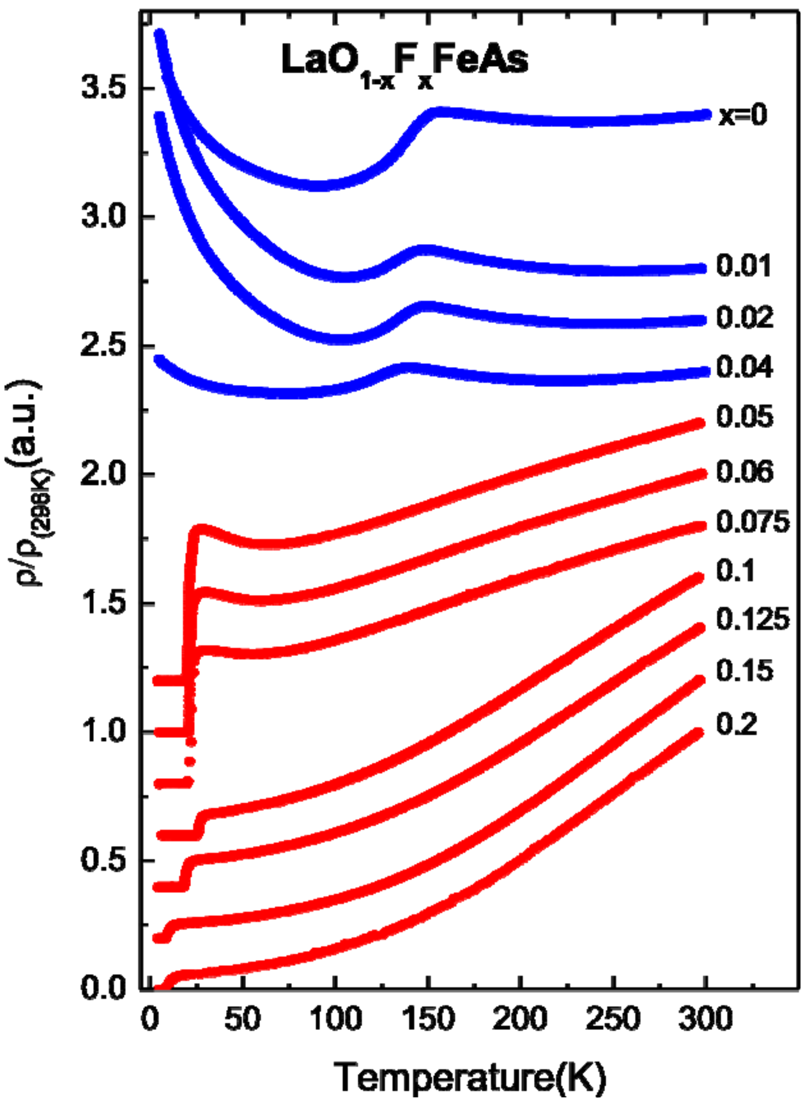
$SmO_{1-x}F_xFeAs$ – highest T_c



What are the electronic properties in the normal state?

C. Hess et al., EPL (2009)

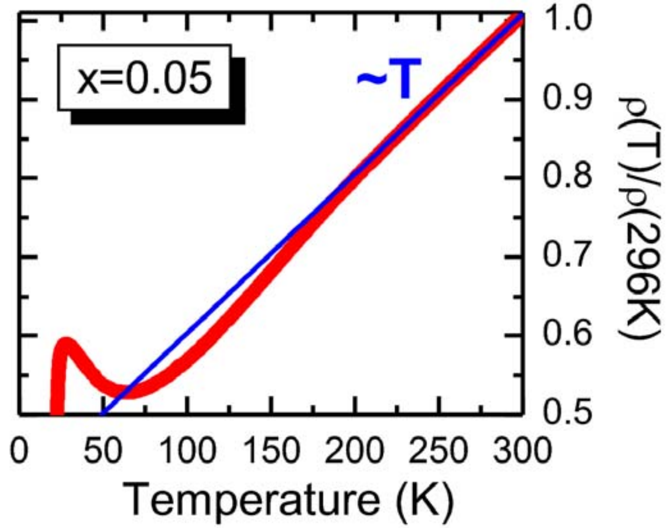
$LaO_{1-x}F_xFeAs$ - Normal State Resistivity



C. Hess et al., EPL (2009)

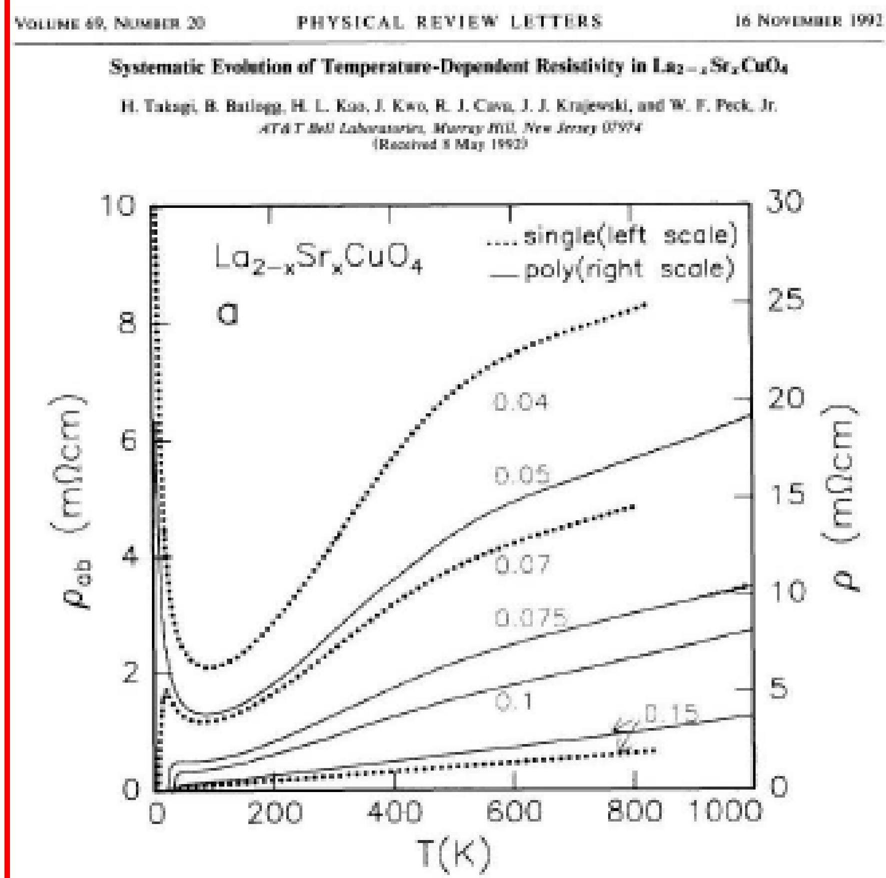
Superconducting
„underdoped"

- High T_c (>20K)
- No structural transition
- No SDW (μSR)
- Low-T upturn
- Linear at high T
- Inflection point at ~150K!



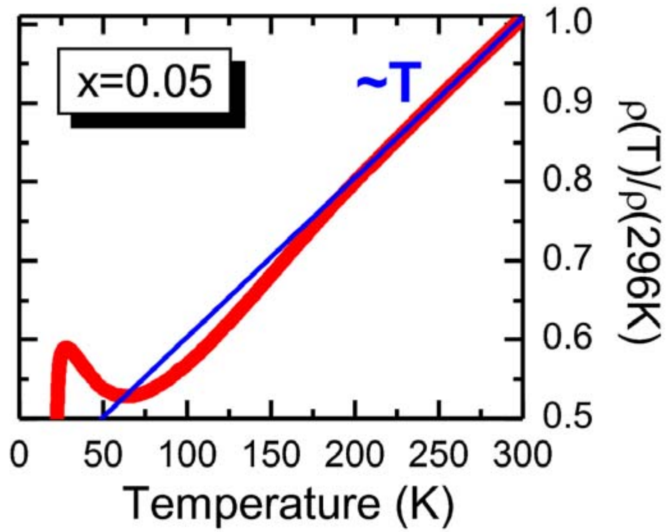
$LaO_{1-x}F_xFeAs$ - Normal State Resistivity

Looks like underdoped Cuprates!



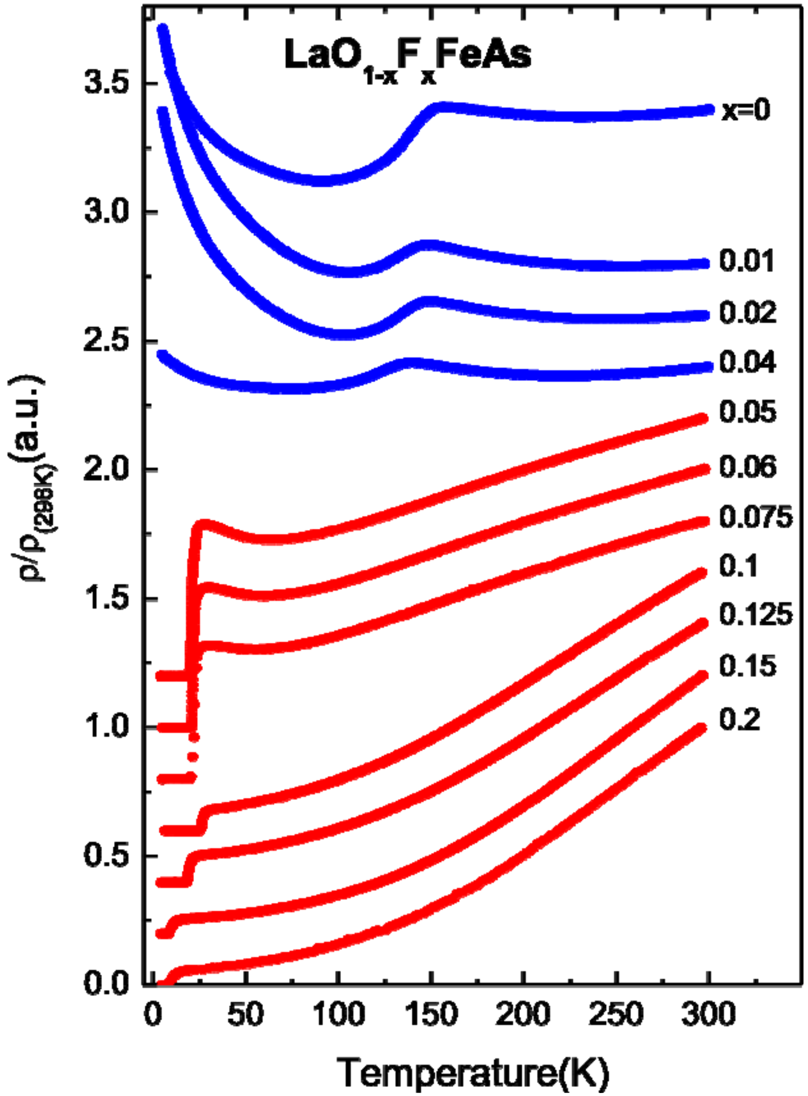
Superconducting
„underdoped“

- High T_c (>20K)
- No structural transition
- No SDW (μSR)
- Low-T upturn
- Linear at high T
- Inflection point at ~150K!



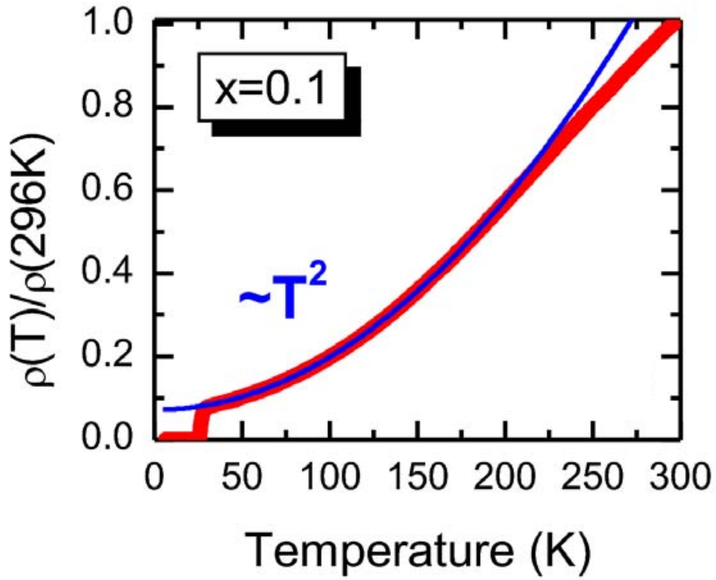
C. Hess et al., EPL (2009)

$LaO_{1-x}F_xFeAs$ - Normal State Resistivity



Superconducting
„overdoped“

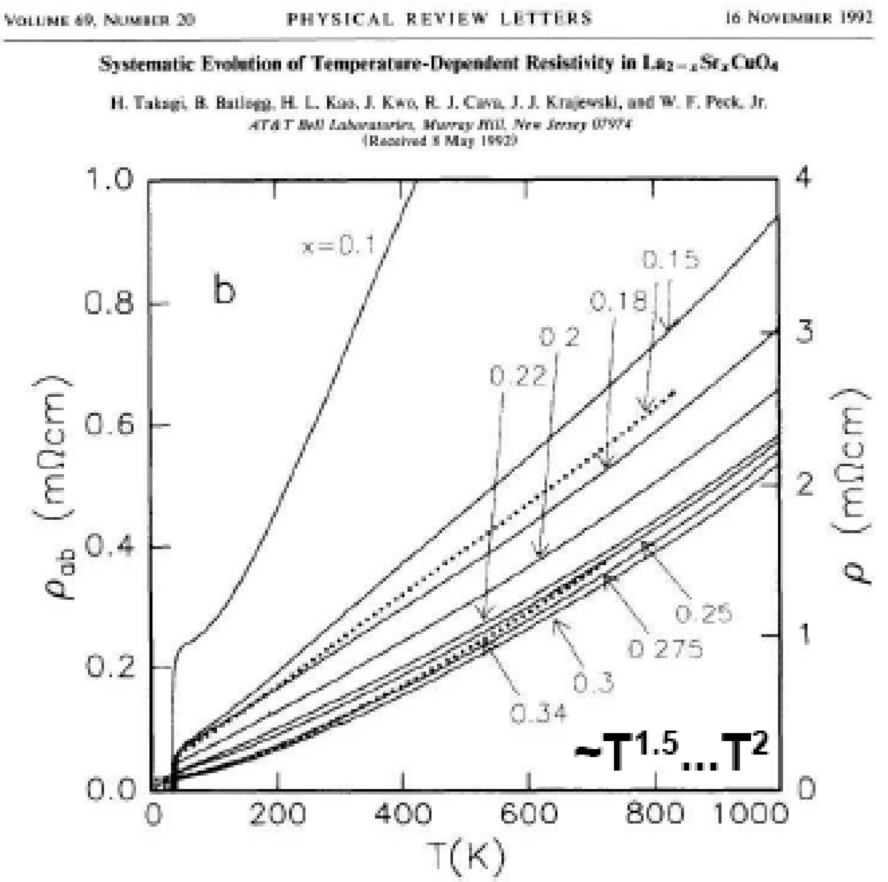
- Highest T_c (26.8K) at x=0.1
- No Low-T upturn
- Inflection point vanishes
- Linear at high T
- ~T^2 at low T



C. Hess et al., EPL (2009)

$LaO_{1-x}F_xFeAs$ - Normal State Resistivity

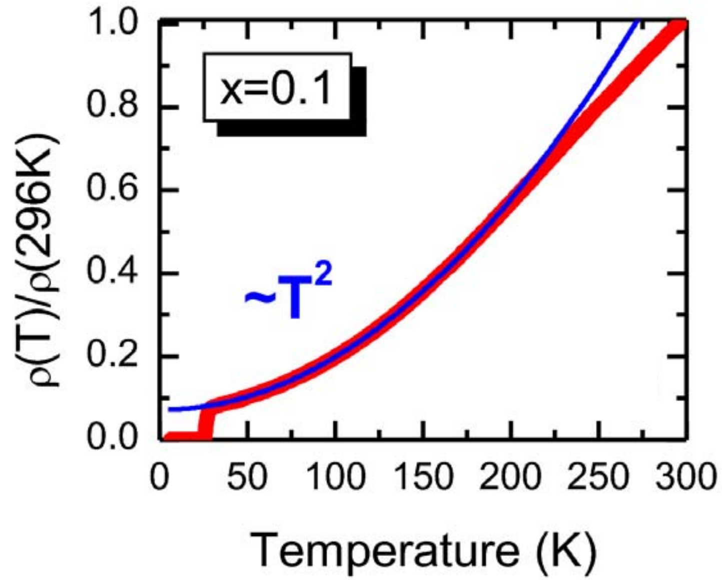
Similar to overdoped Cuprates!



Superconducting

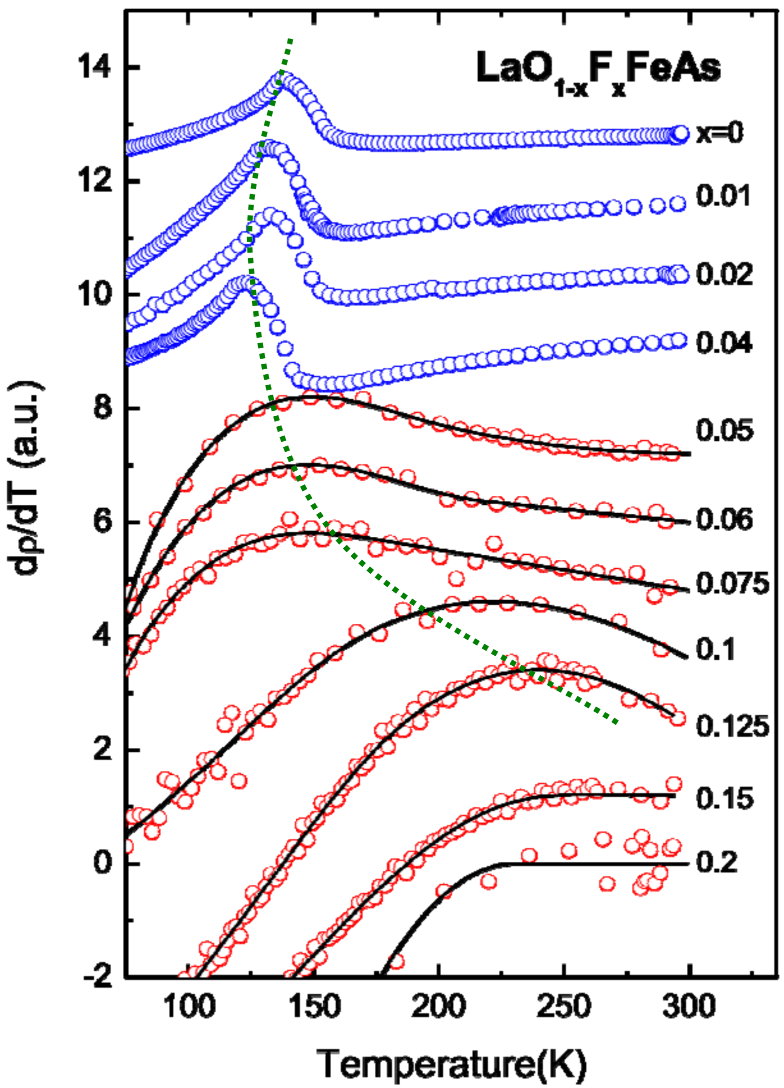
„overdoped“

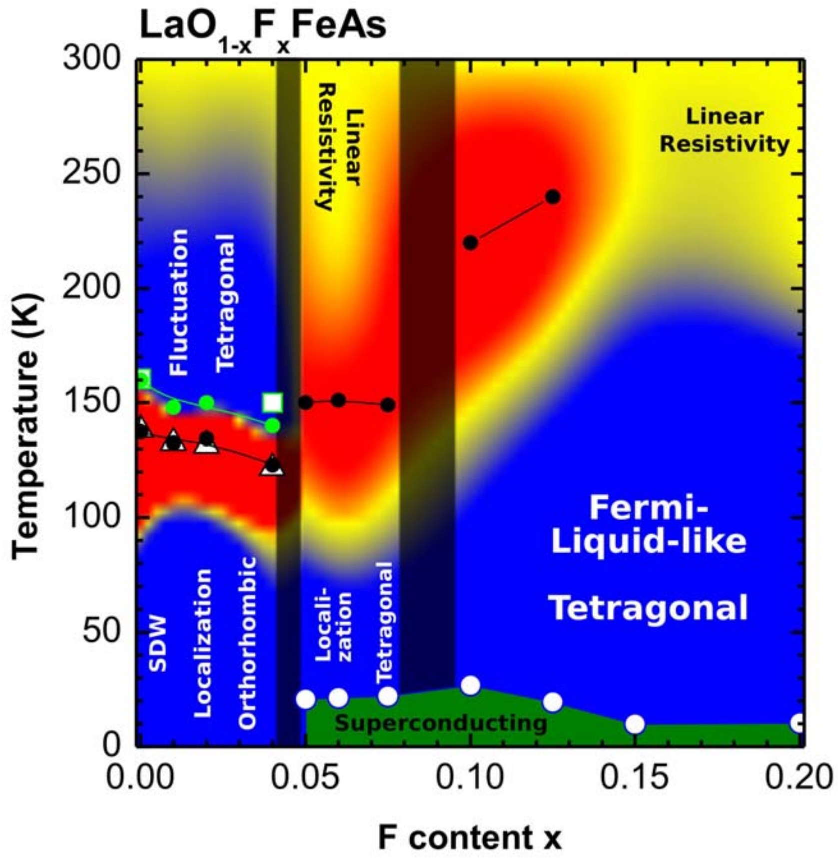
- Highest T_c (26.8K) at x=0.1
- No Low-T upturn
- Inflection point vanishes
- Linear at high T
- $\sim T^2$ at low T



C. Hess et al., EPL (2009)

$LaO_{1-x}F_xFeAs$ – Construct phase diagram…





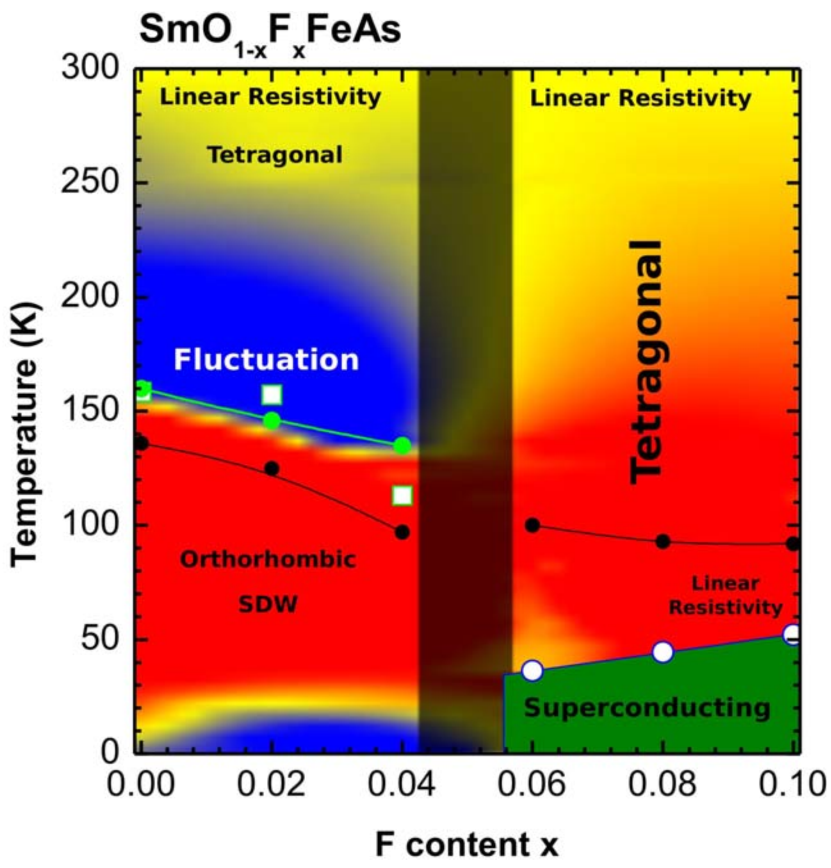
Colors:

$d\Delta/dT \approx 0$ → *yellow*

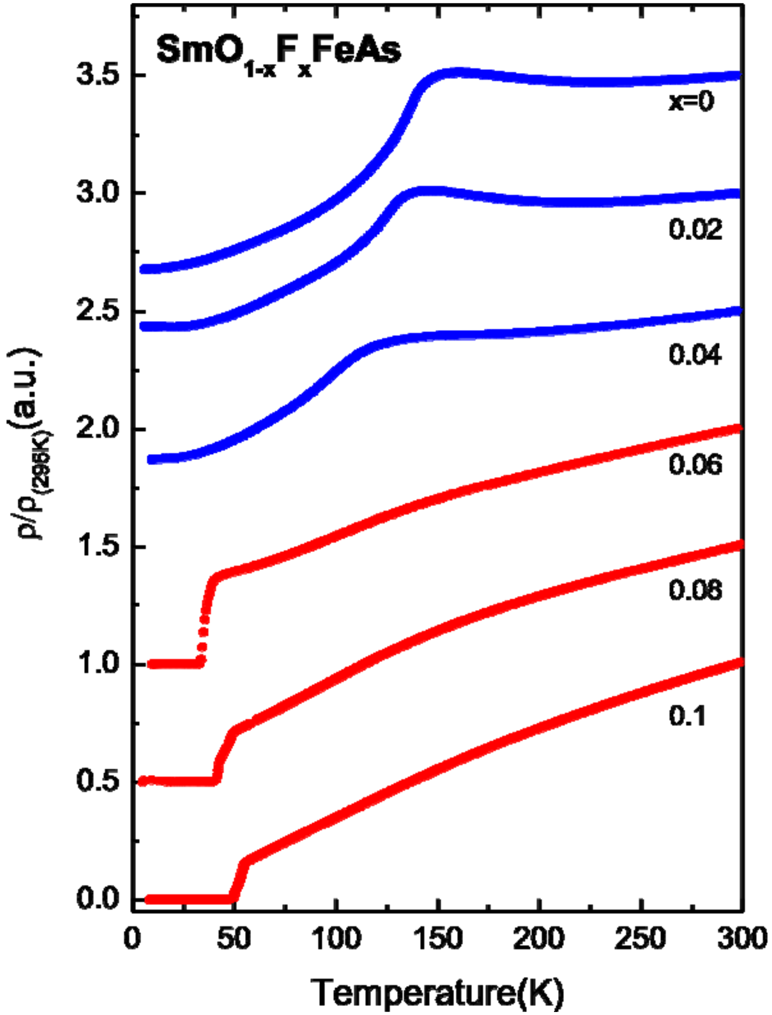
$d\Delta/dT > 0$ → *red*

$d\Delta/dT < 0$ → *blue*

$SmO_{1-x}F_xFeAs$ - Phase diagram



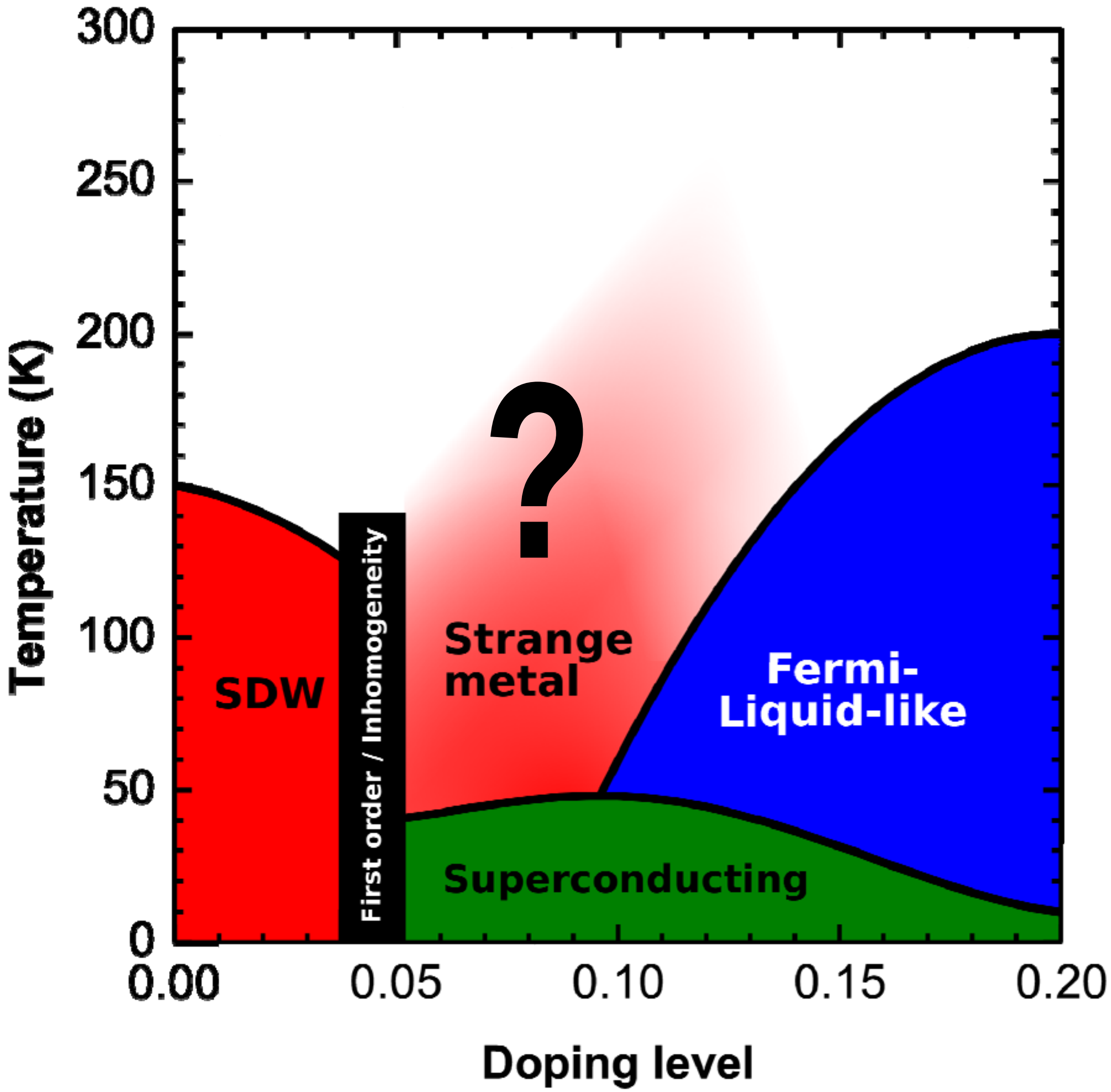
$SmO_{1-x}F_xFeAs$ – highest T_c



- Anomaly at ~ 150 K even stronger
- Higher T_c
- No Fermi-liquid region

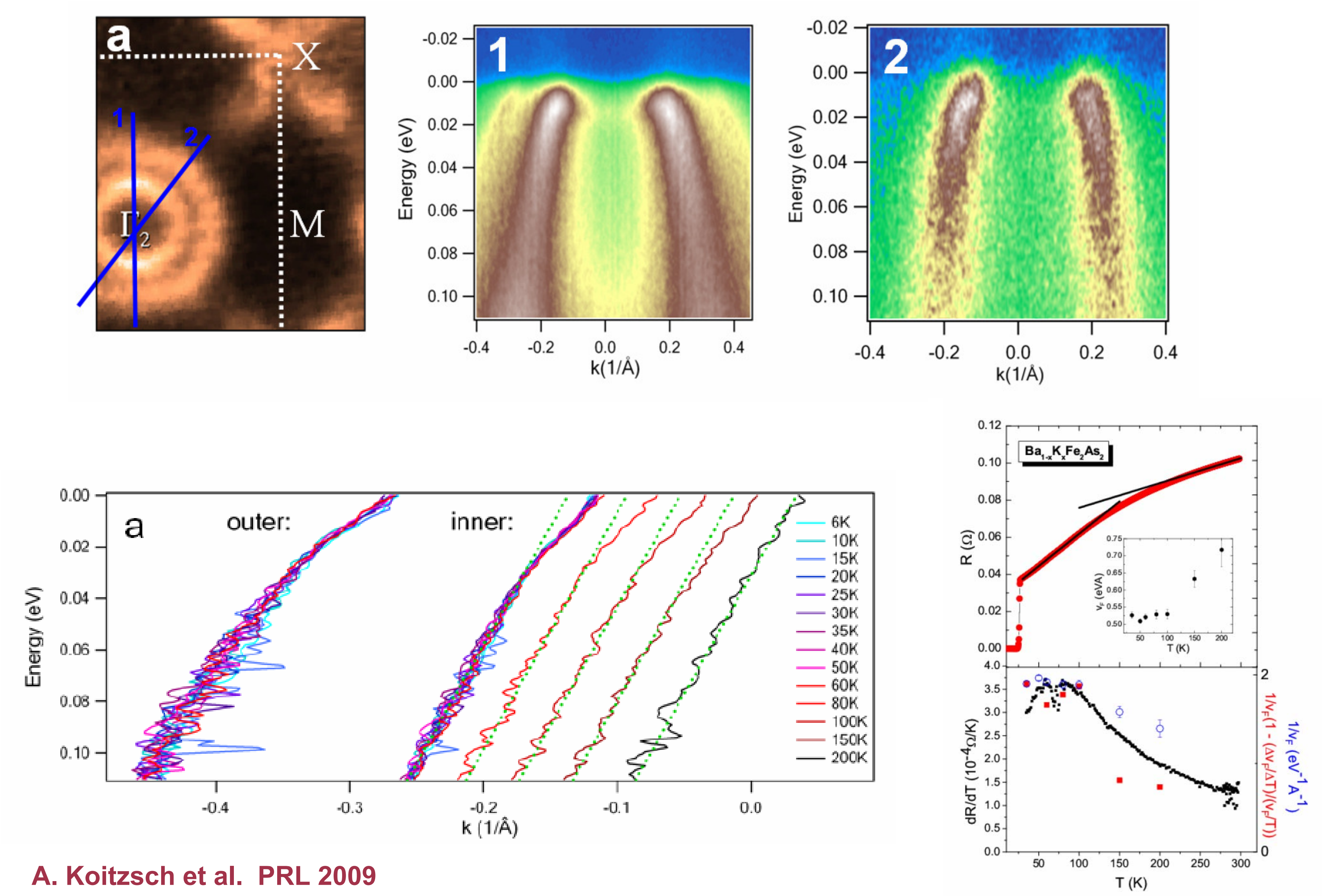
C. Hess et al., EPL (2009)

Proposed generic phase diagram



C. Hess et al., EPL (2009)

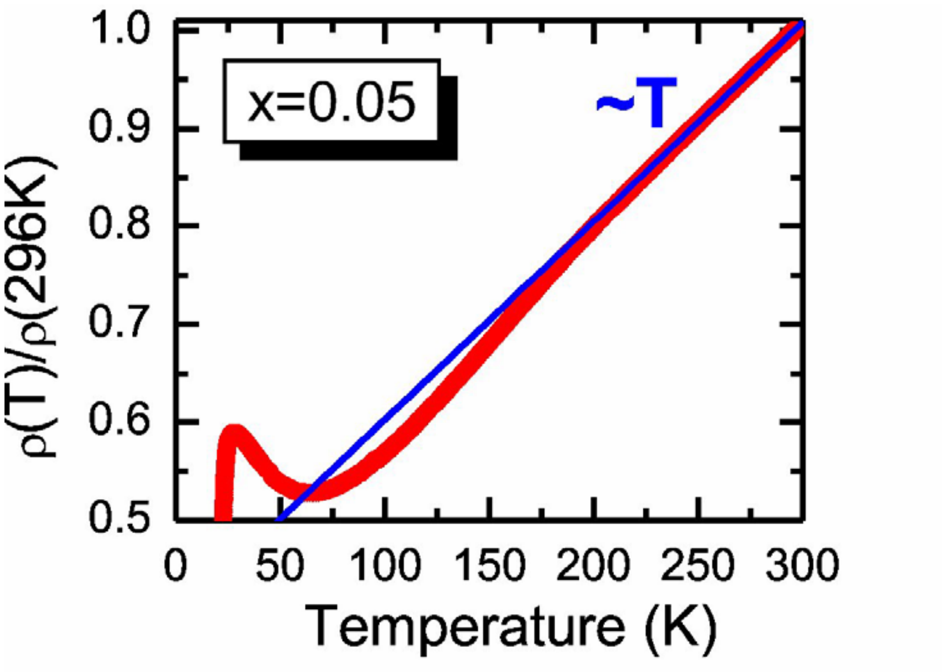
"Kinks" in the dispersion of $Ba_{1-x}K_xFe_2As_2$

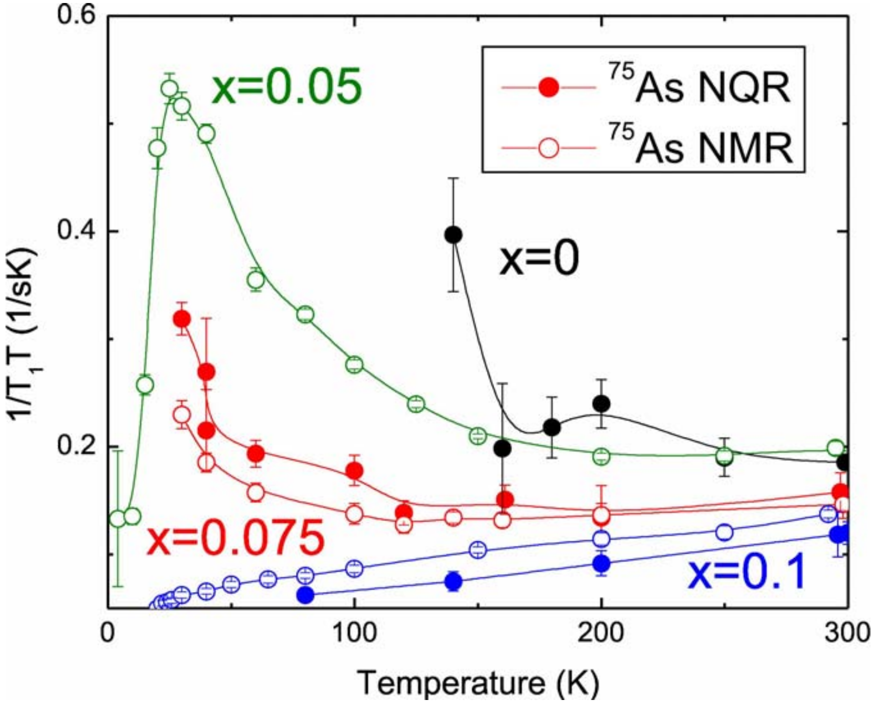


A. Koitzsch et al. PRL 2009

Magnetic fluctuations couple to electronic transport

$LaO_{1-x}F_xFeAs$

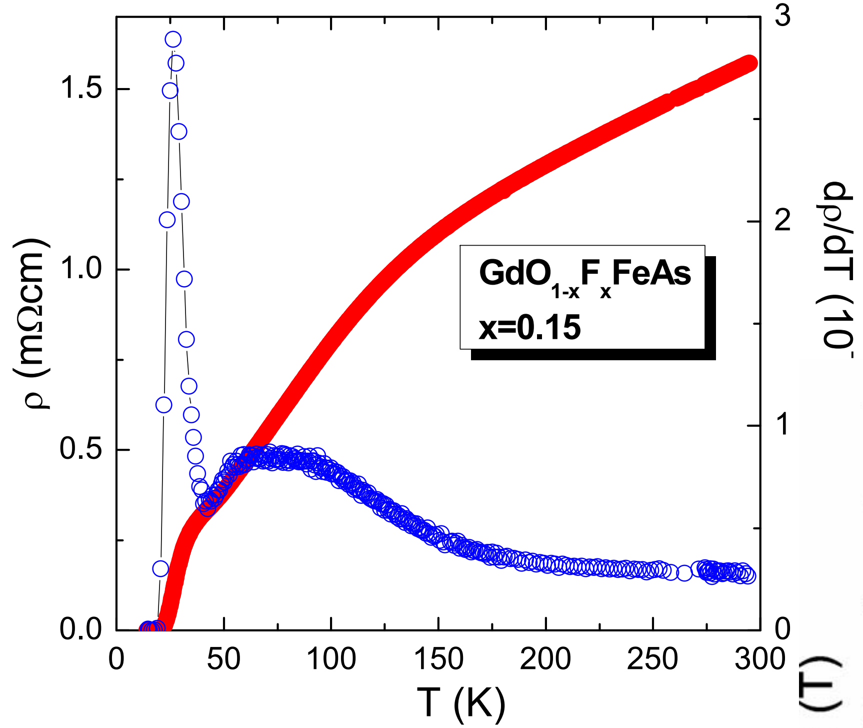


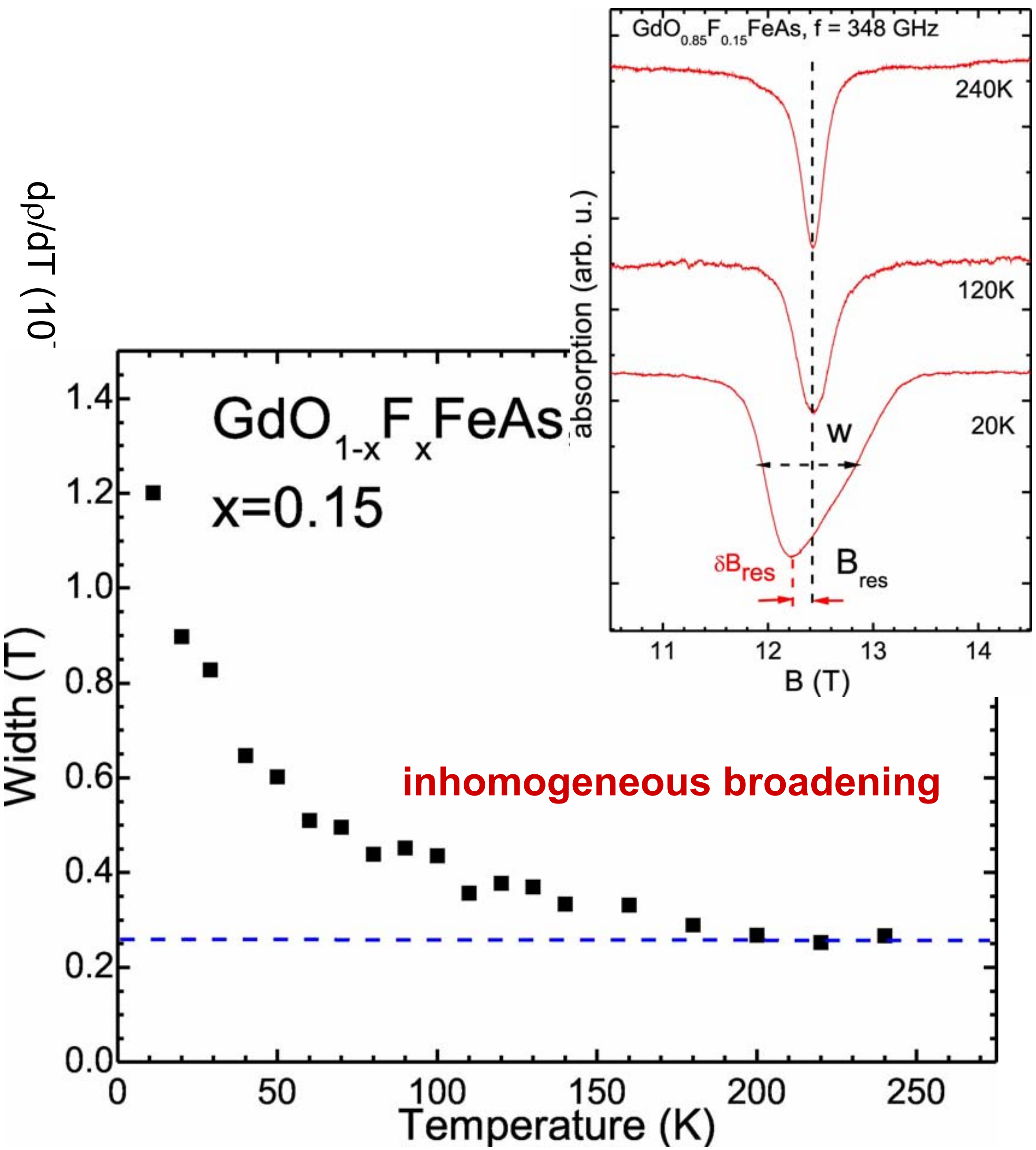


Anomaly of ρ

Slowing down of spin fluctuations

Further evidence: ρ and ESR on $GdO_{1-x}F_xFeAs$





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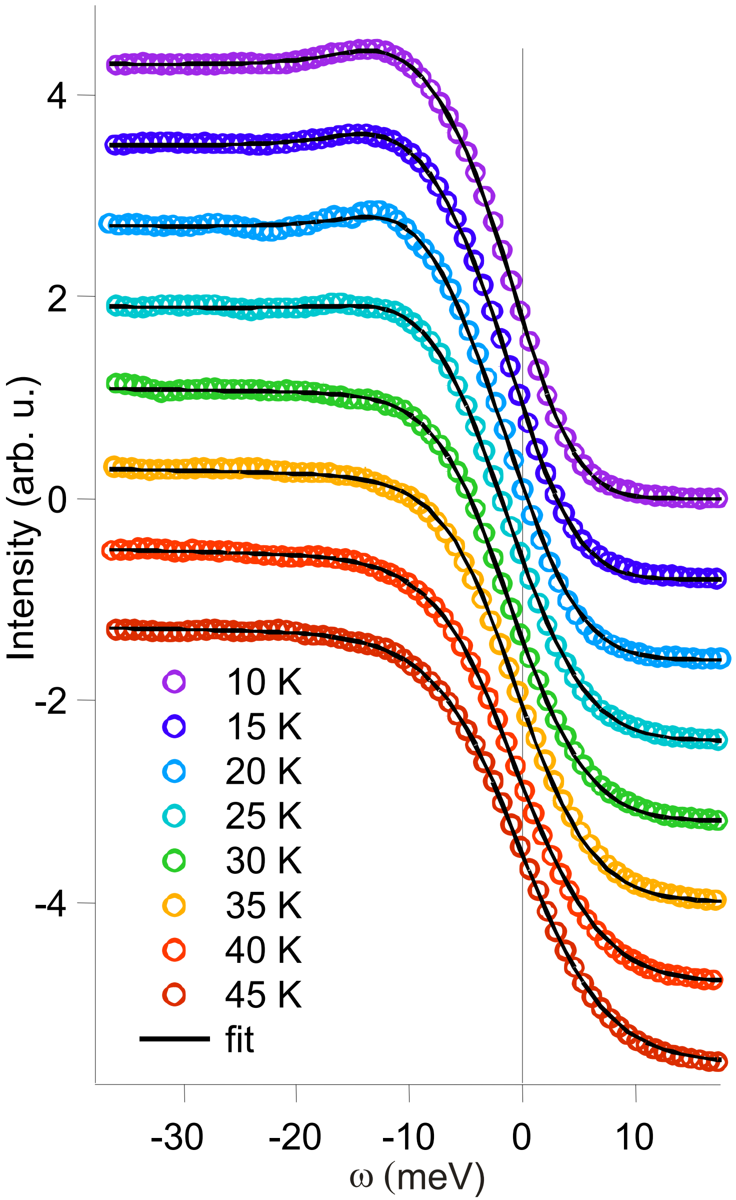
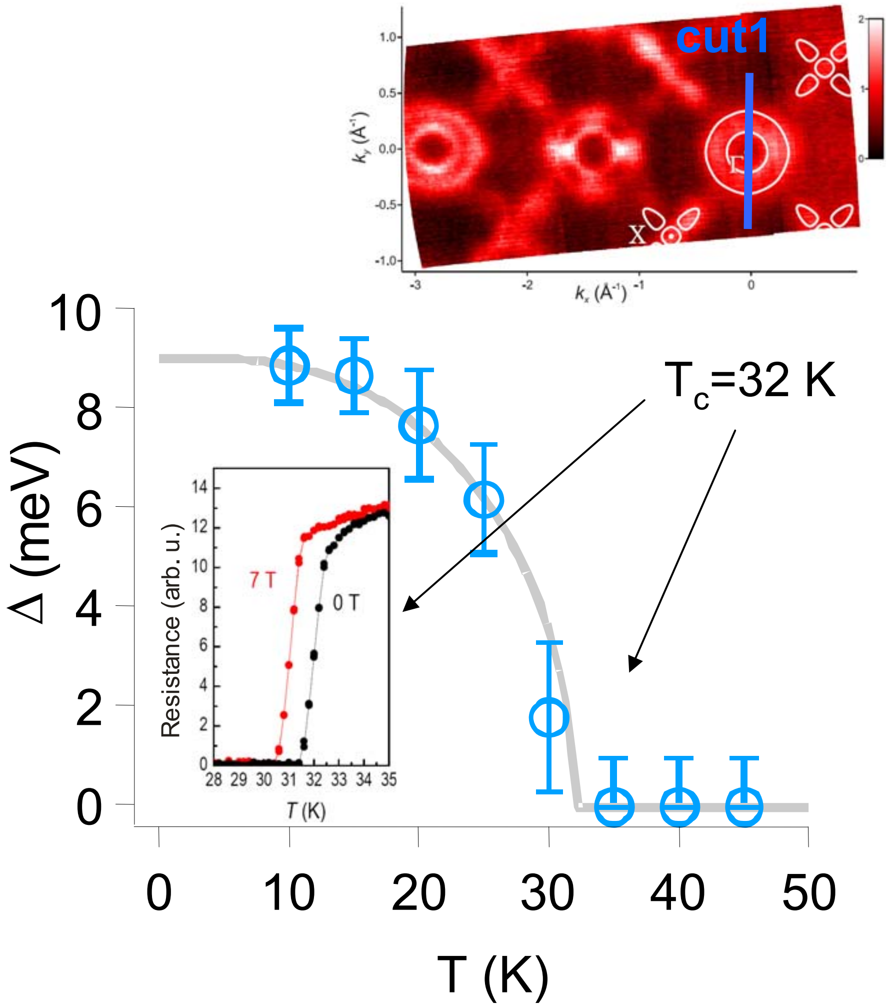
OUTLINE

- „Local physics“, Hubbard U etc.
- ARPES, Fermi surface etc.
- „Pseudogap“, Strange T dependencies
- Normal state resistivity
- **Charge inhomogeneity (NQR)**

Gap on the inner Γ-barrel, ΓM

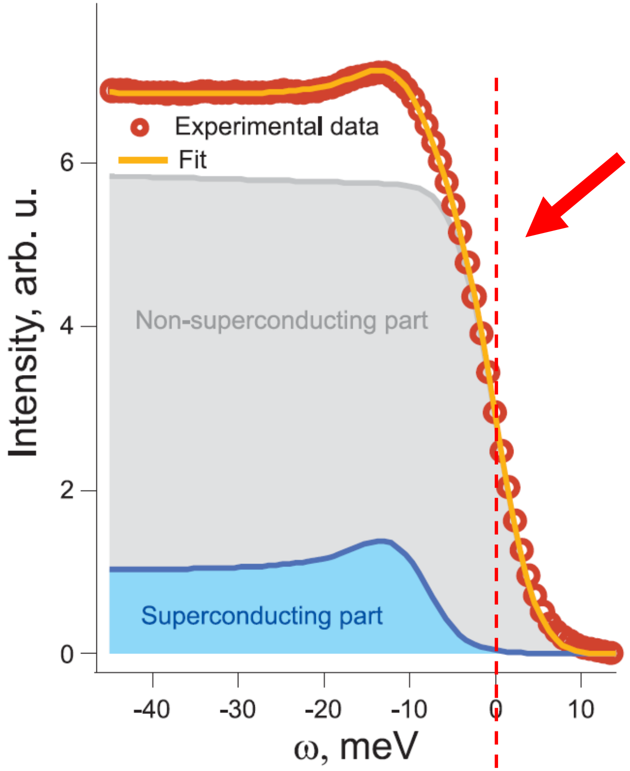


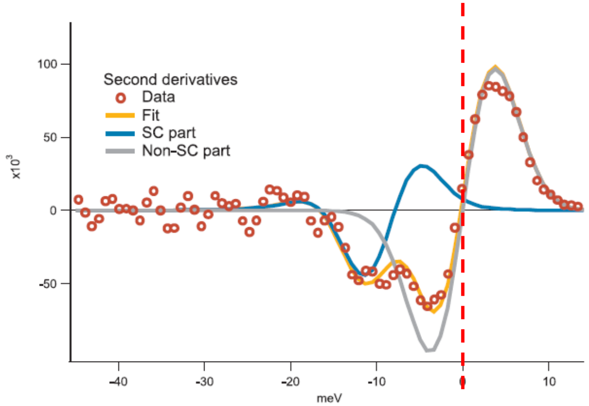


$$9.1 \pm 0.7\,\mathrm{meV}$$

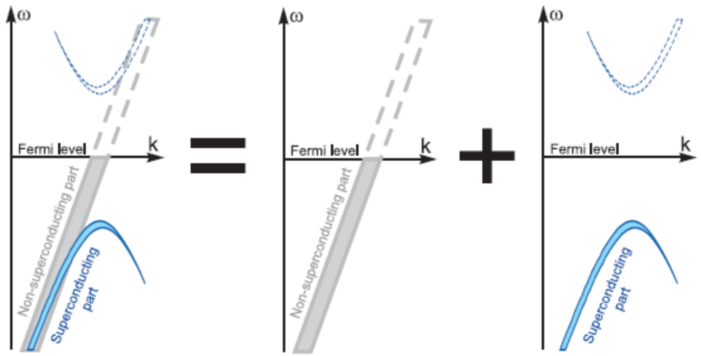
D.V. Evtushinsky et al., PRB 2009

Non-superconducting fraction below T_c

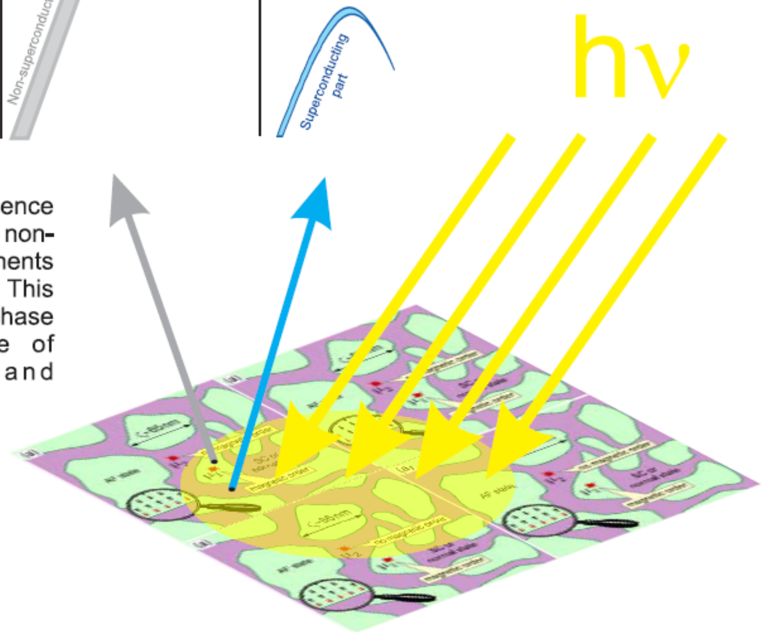




D.V. Evtushinsky et al., PRB 2009



Sketch, illustrating presence of superconducting and non-superconducting components in the same spectrum. This observation supports phase separated coexistence of superconductivity and magnetism.



Only 23±3% of the spectra refer to the superconducting part

μSR: 29% non-magnetic

J. T. Park et. al., PRL 2009

T. Goko et. al., arXiv:0808.1425 (2008)

Non-superconducting fraction below Tc

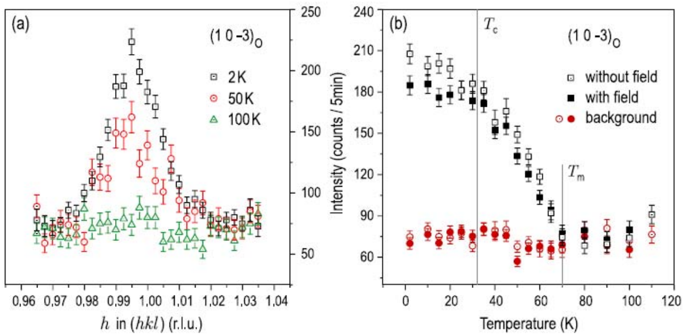
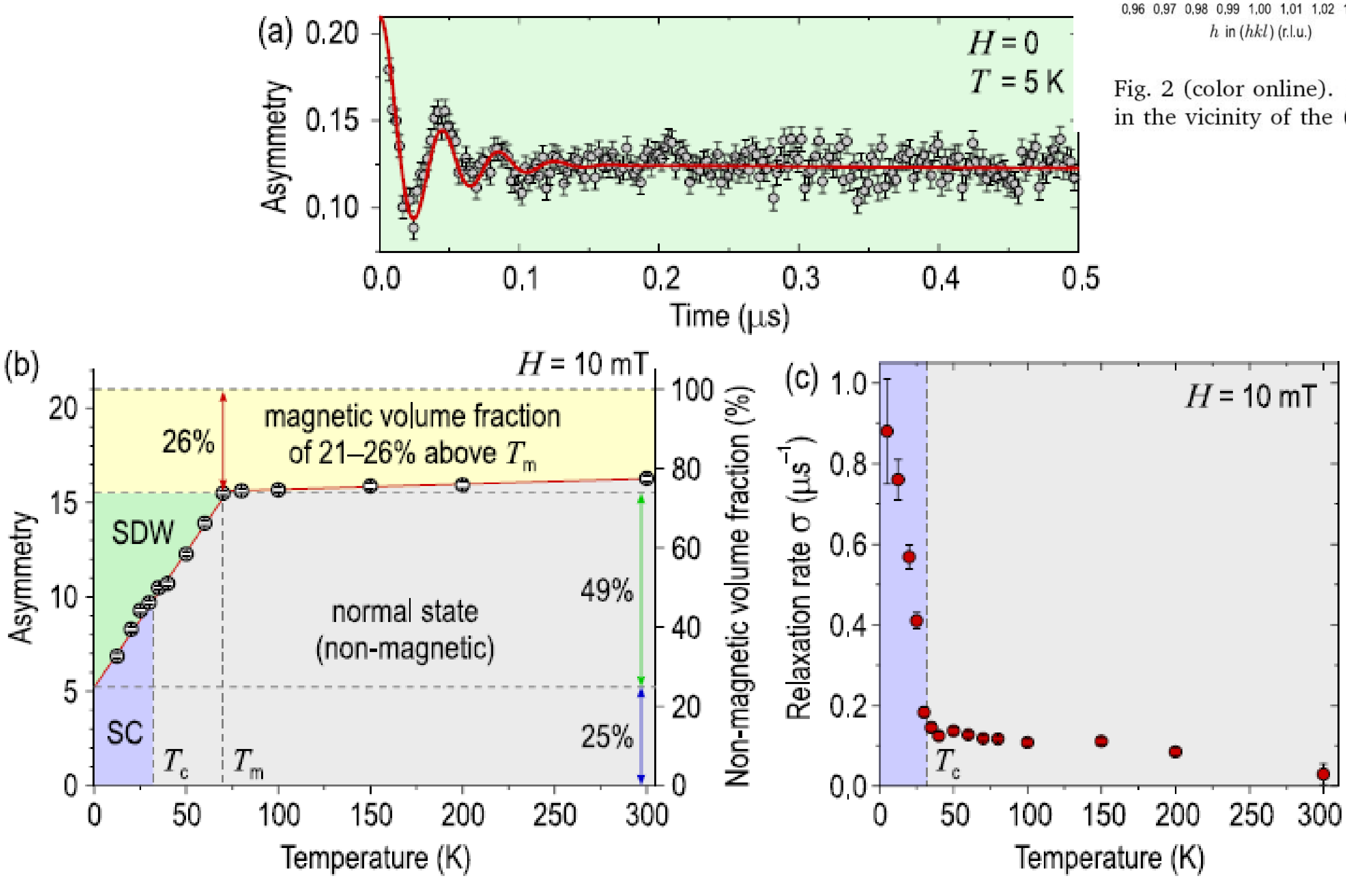
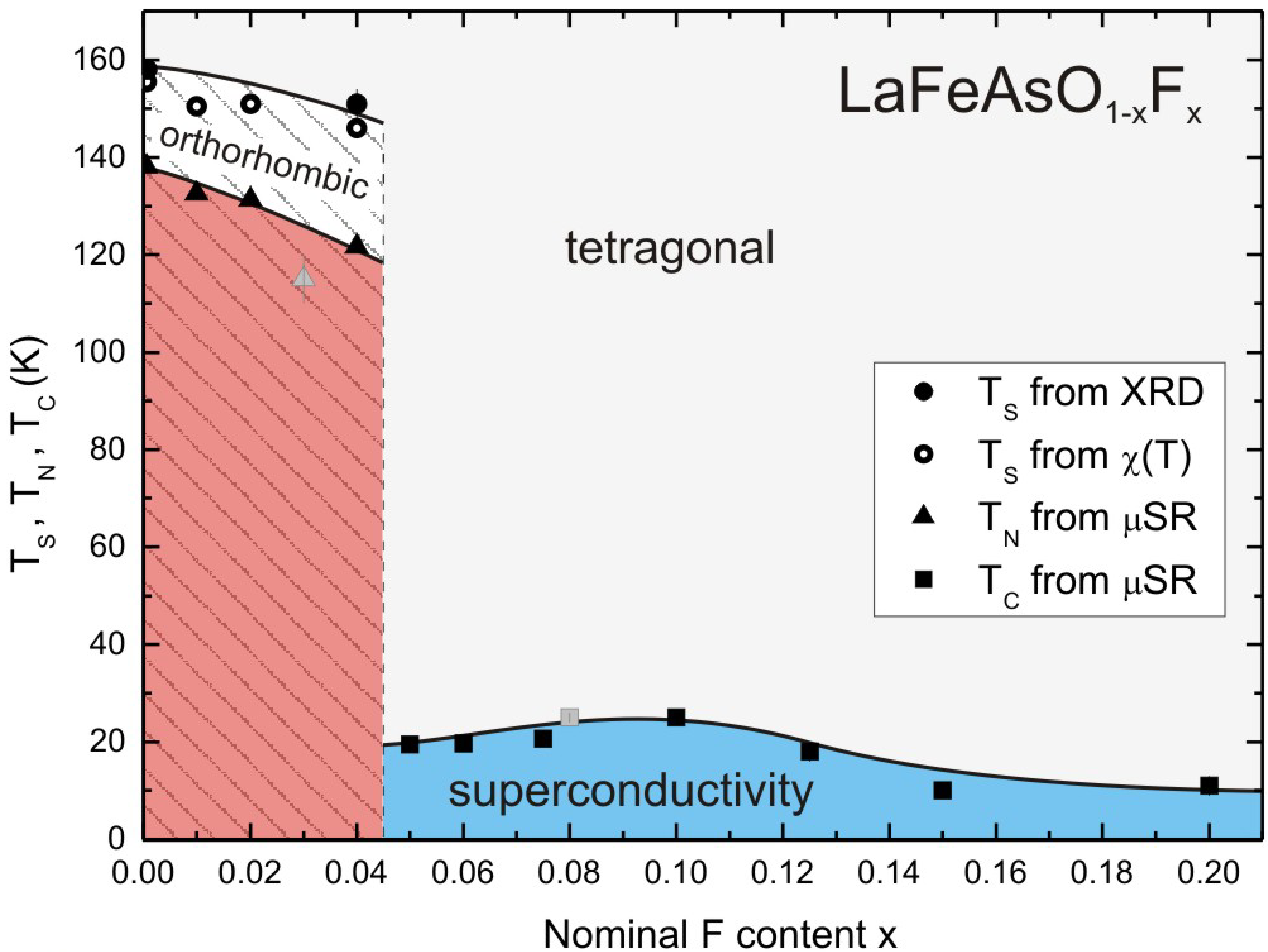


Fig. 2 (color online). Elastic neutron scattering data measured in the vicinity of the $(1\,0\,{-3})_O$ magnetic Bragg peak (O stands



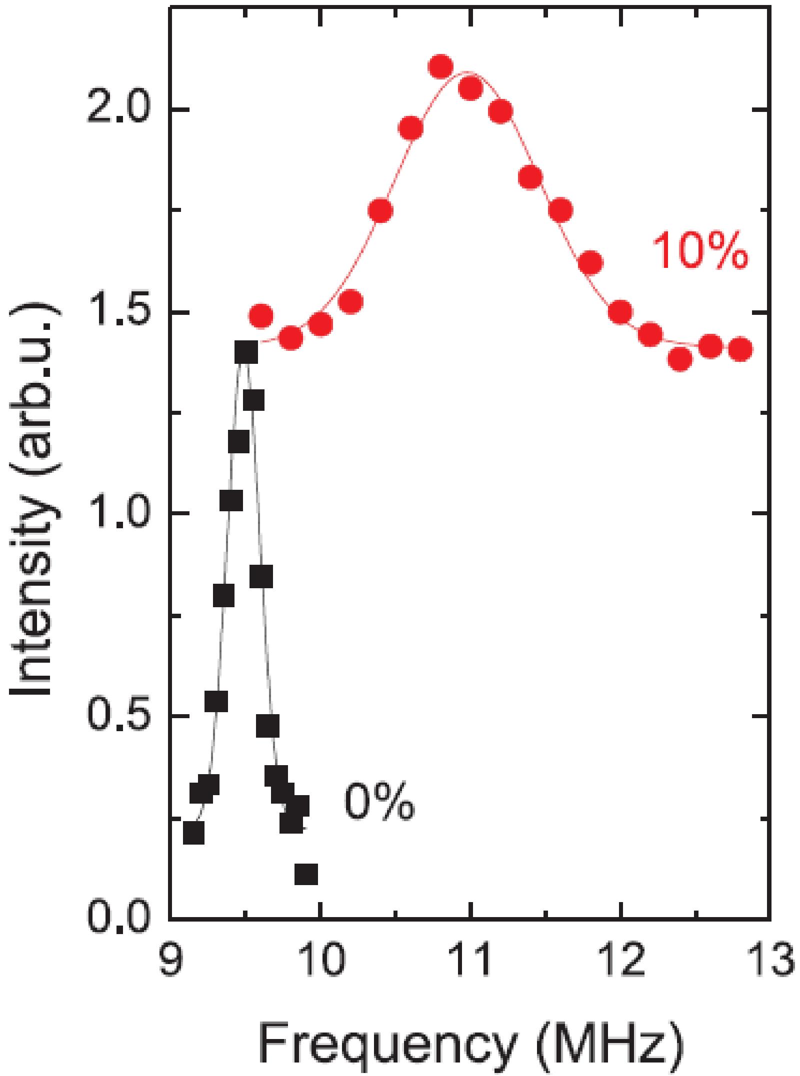
J. T. Park et. al., arXiv:0811.2224 (2008)

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



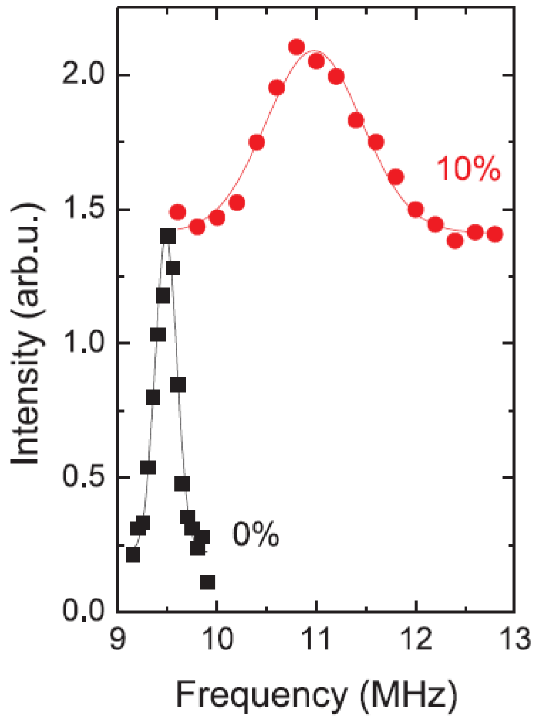
H. Luetkens et al., Nature Materials 2009

NQR of $La(O_{1-x}F_x)FeAs$: Electrical field gradient at the As nucleus → Charge distribution in the FeAs layers

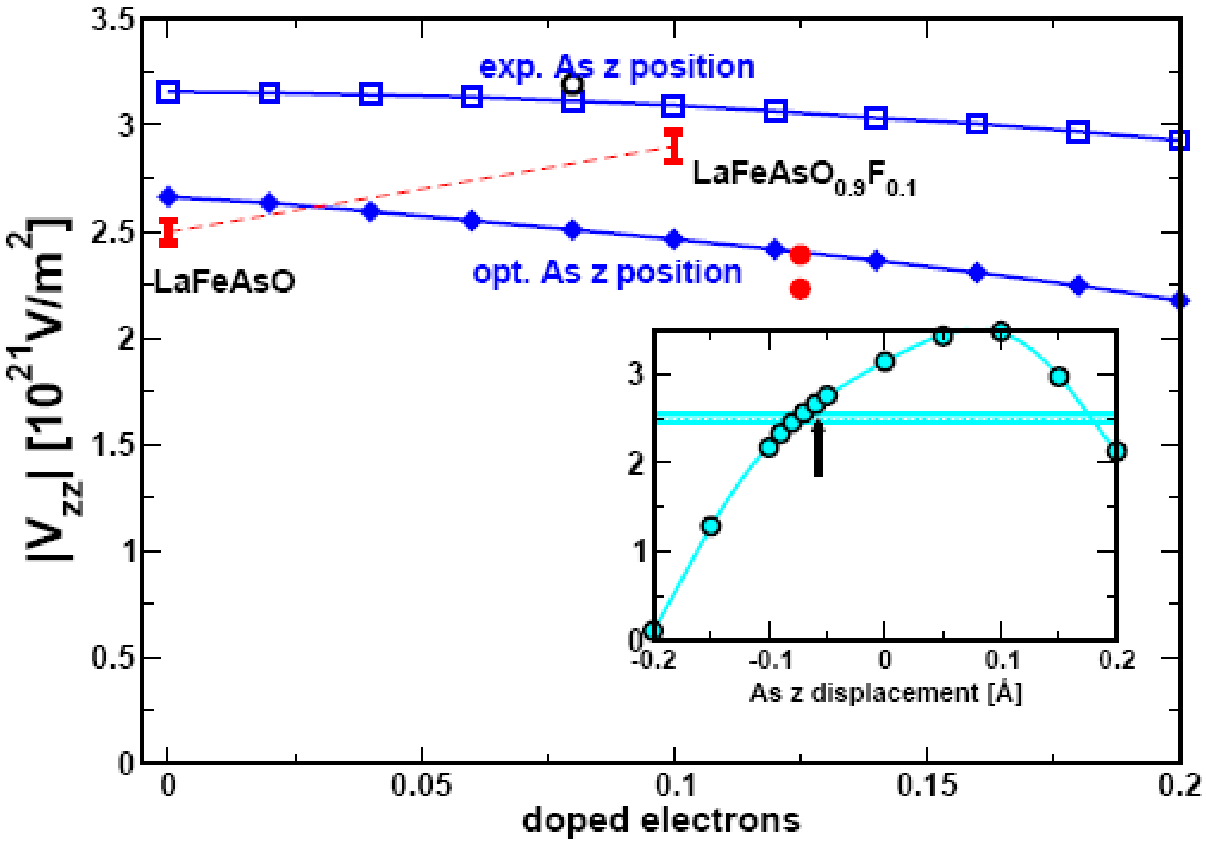


Grafe et al., New J. Phys. 2009

NQR of La($O_{1-x}F_x$)FeAs : Electrical field gradient at the As nucleus → Charge distribution in the FeAs layers

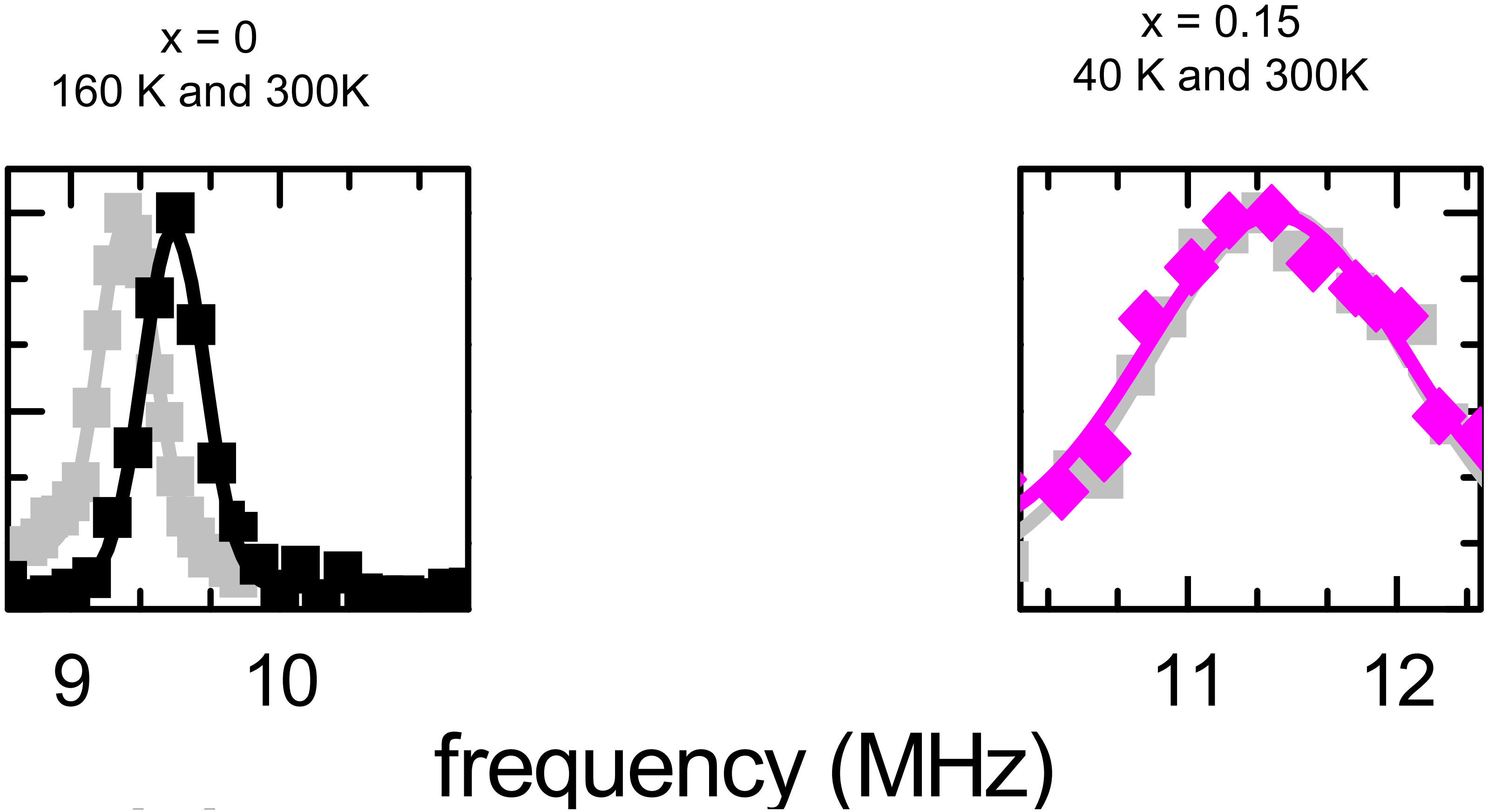


Bandstructure calculations

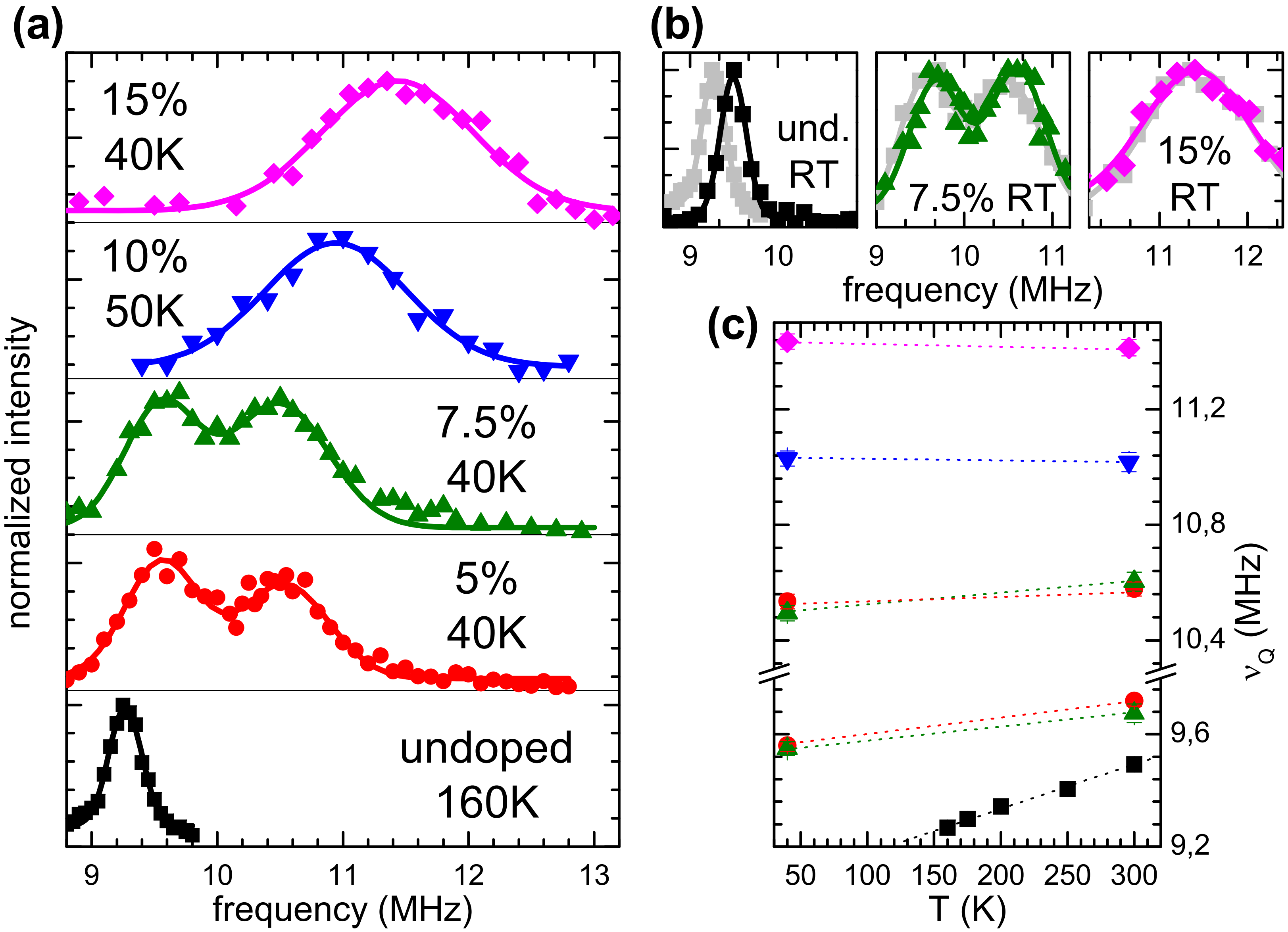


Grafe et al., New J. Phys. 2009

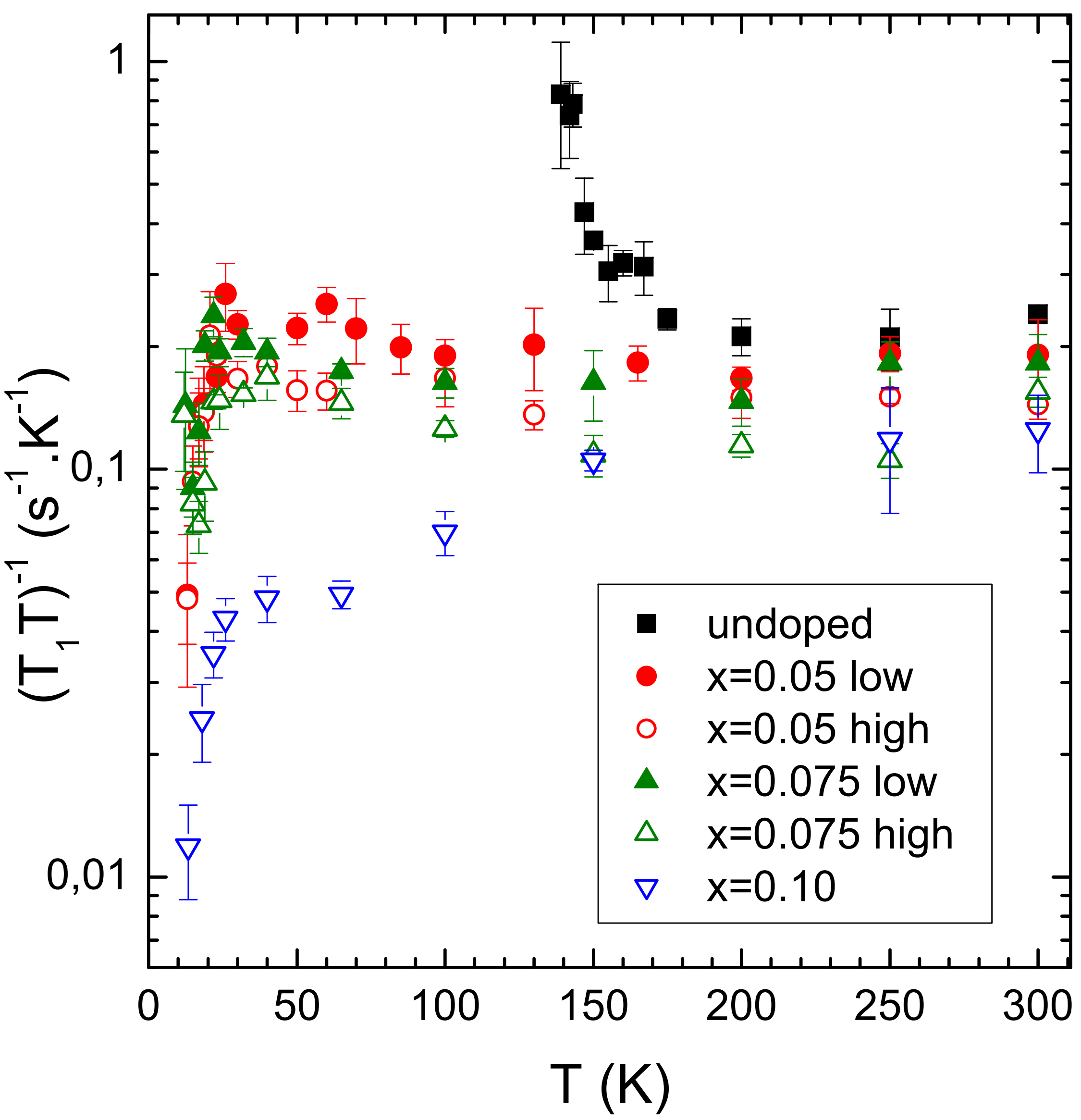
NQR of La($O_{1-x}F_x$)FeAs : T dependence



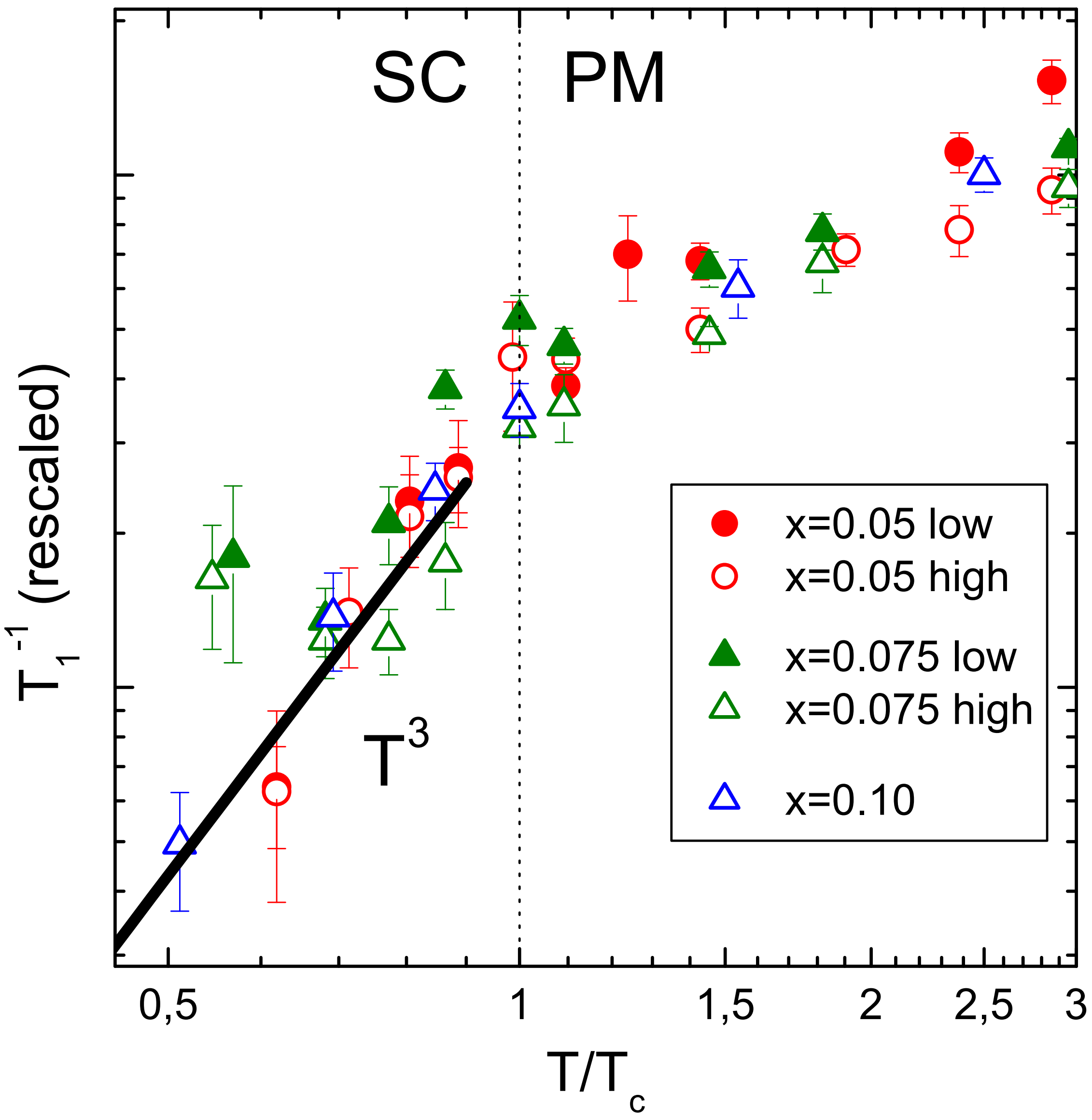
NQR of $La(O_{1-x}F_x)FeAs$: Spatial variation of the doping



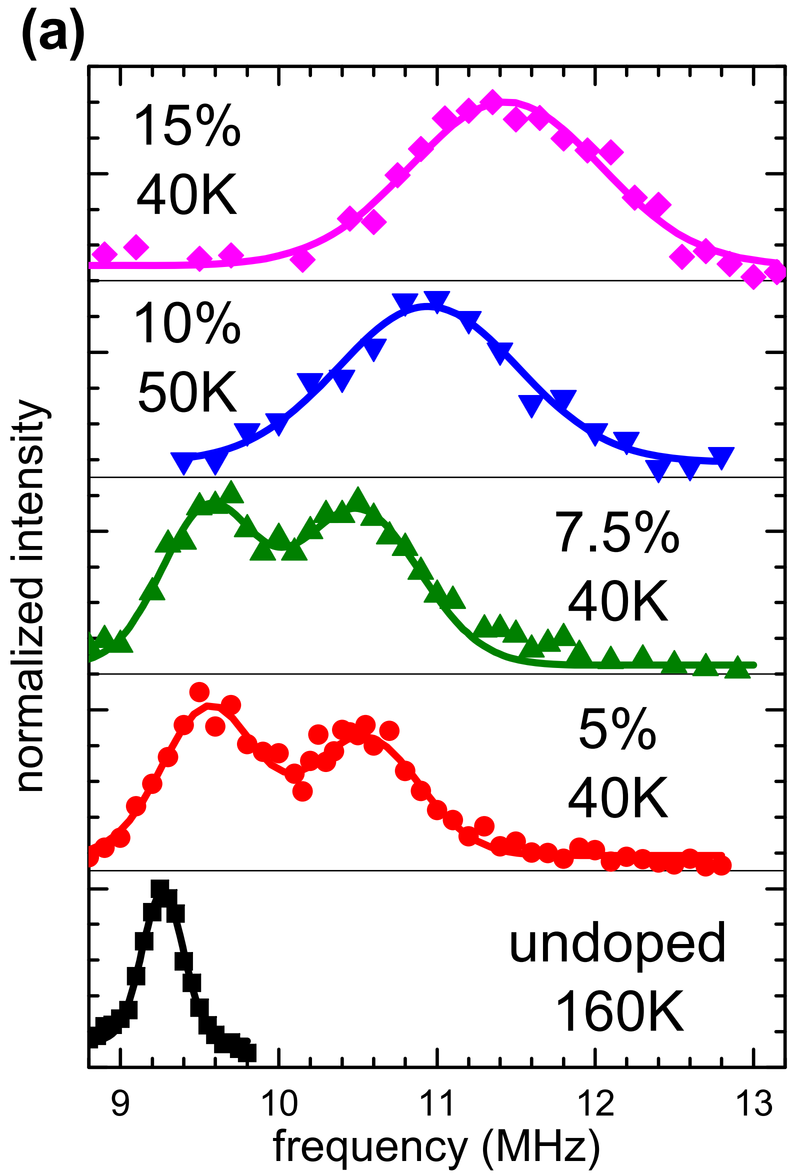
NQR of $La(O_{1-x}F_x)FeAs$: Spatial variation of the doping



NQR of $La(O_{1-x}F_x)FeAs$: Spatial variation of the doping



Spatial variation of the doping on the atomic or nm scale

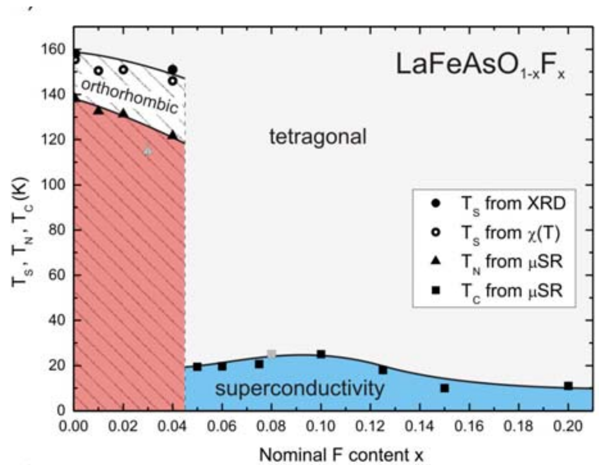


Underdoped pnictides:
Local charge distribution varies
(~undoped and ~optimally doped)

2 well defined frequencies
Not disorder
Not distribution of F atoms

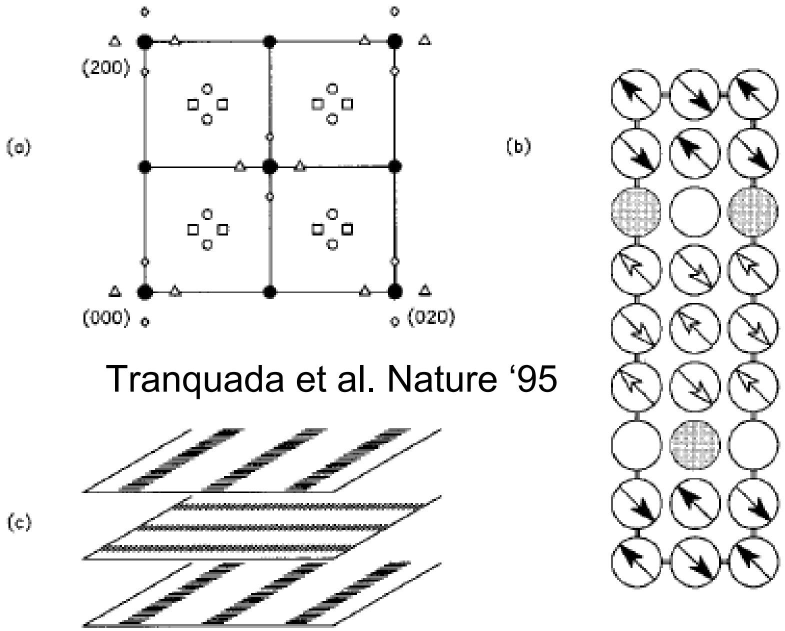
No traces of magnetism in μSR
„undoped" regions too small?

2 peaks with similar behavior at T_c
ordered structure (e.g. „stripes etc.")
regions too small (< ξ)

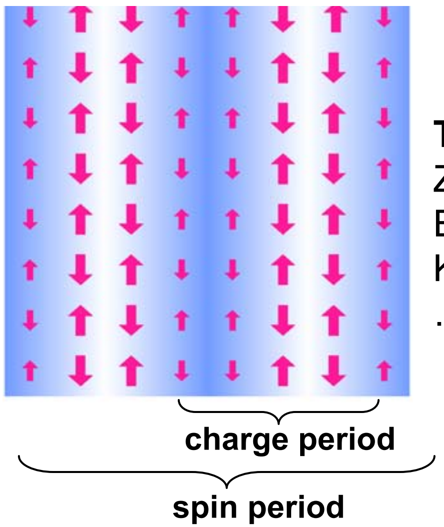


Stripes in Cuprate Superconductors

Static Stripes in $(La,Nd)_{7/8}Sr_{1/8}CuO_4$

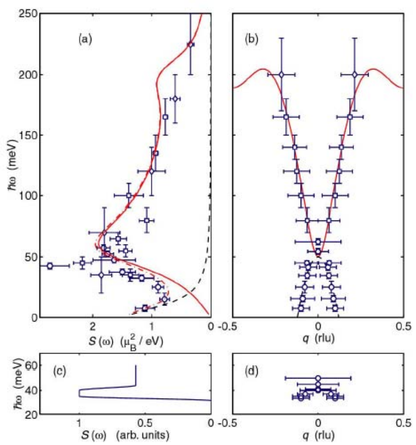


Tranquada et al. Nature '95

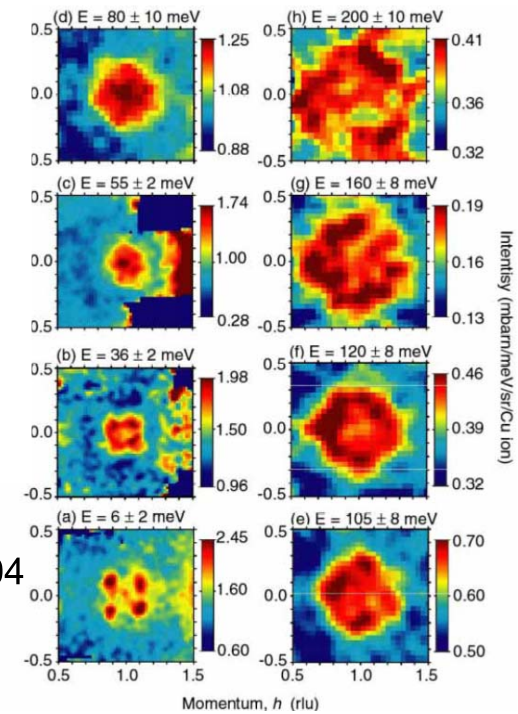


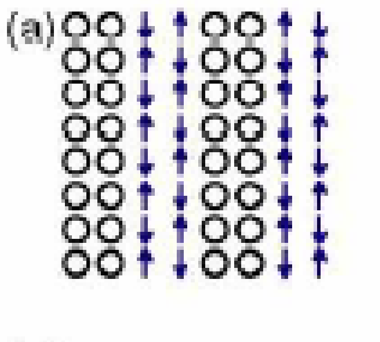
Theory
Zaanen et al. '89
Emery et al.
Kivelson et al.
…

Stripes and/or neutron resonance



Tranquada et al. Nature '04

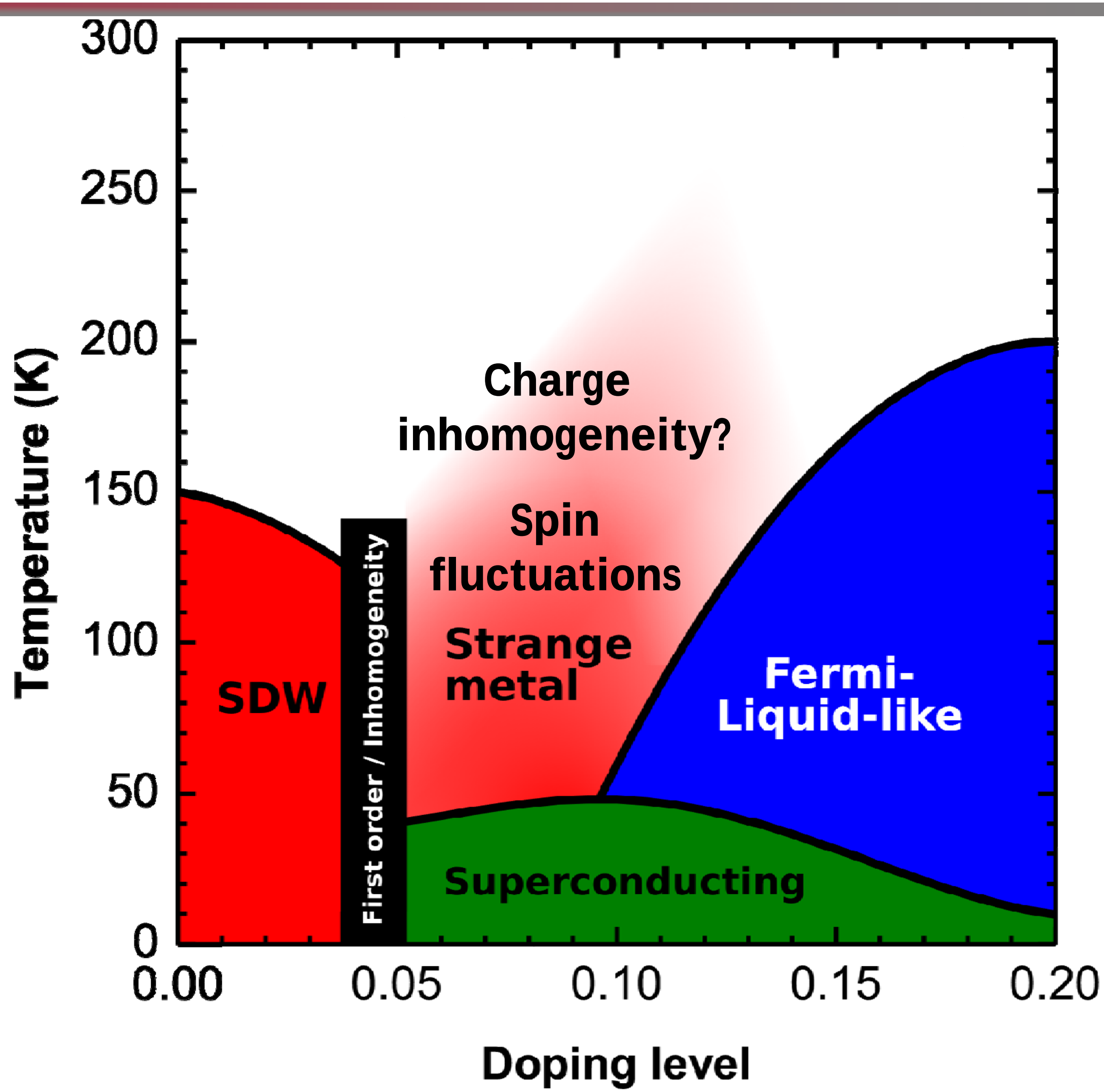


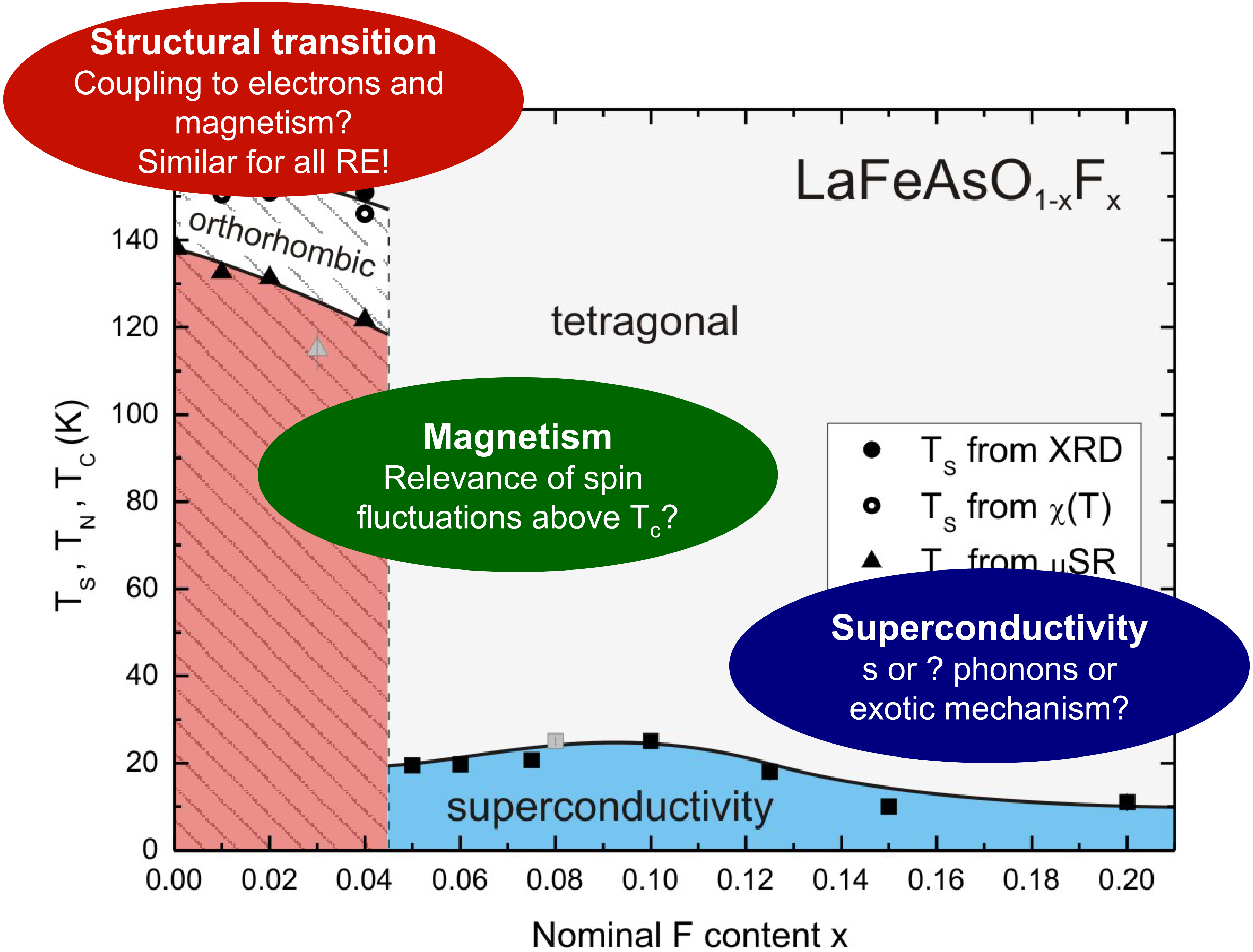


Theory and further experiments:
Hayden et al.
Keimer et al.
Vojta et al
Uhrig et al.
...

Direct obervation of charge stripes:
Abbamonte et al. Nature Physics '05

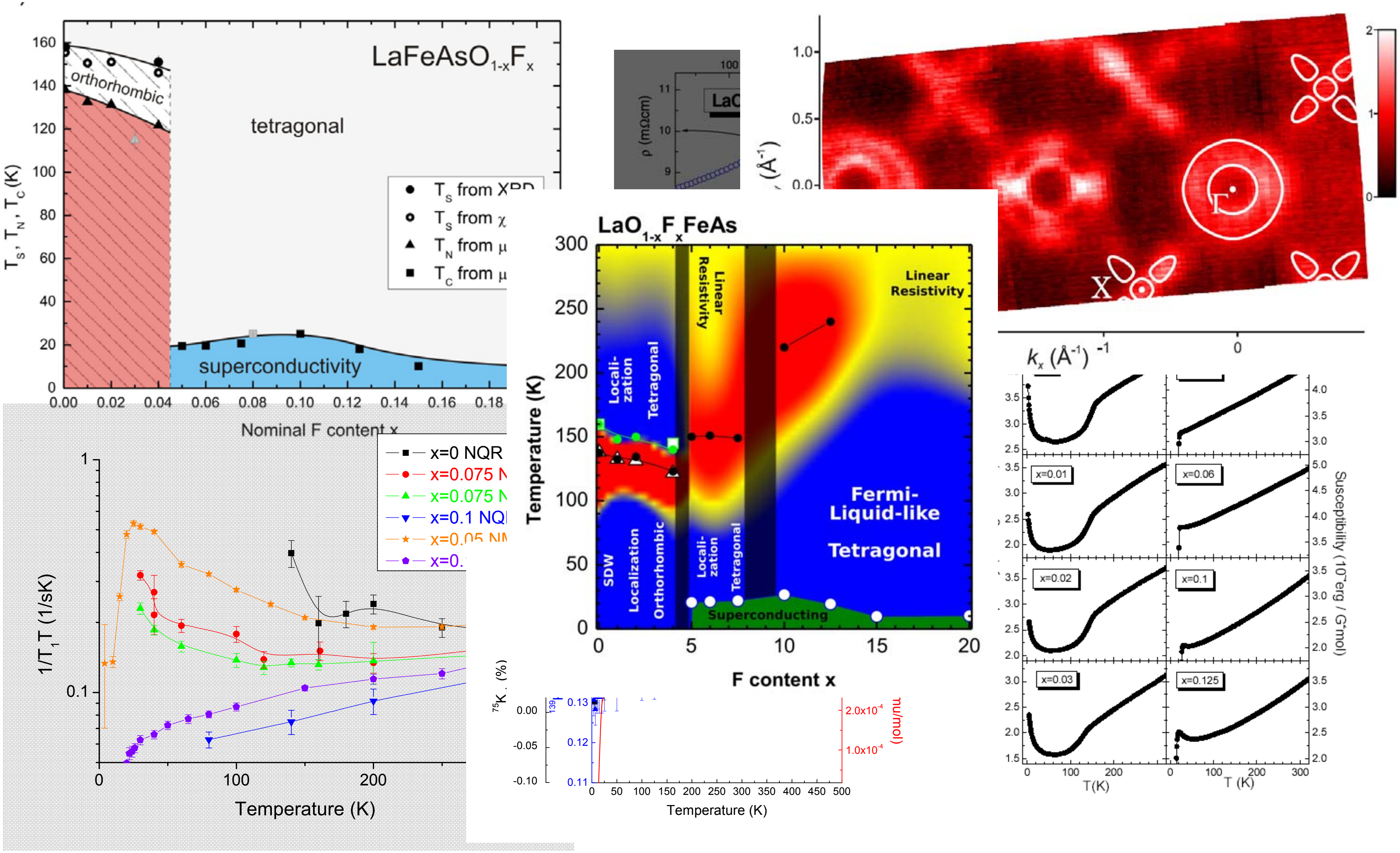
Proposed generic phase diagram





Structural transition
Coupling to electrons and magnetism?
Similar for all RE!
LaFeAsO1-xFx
orthorhombic
tetragonal
Magnetism
Relevance of spin fluctuations above Tc?
Ts from XRD
Ts from χ(T)
Superconductivity
s or ? phonons or exotic mechanism?
superconductivity
Ts, TN, TC (K)
Nominal F content x
0.00
0.02
0.04
0.06
0.08
0.10
0.12
0.14
0.16
0.18
0.20
0
20
40
60
80
100
120
140

Thank you for your attention

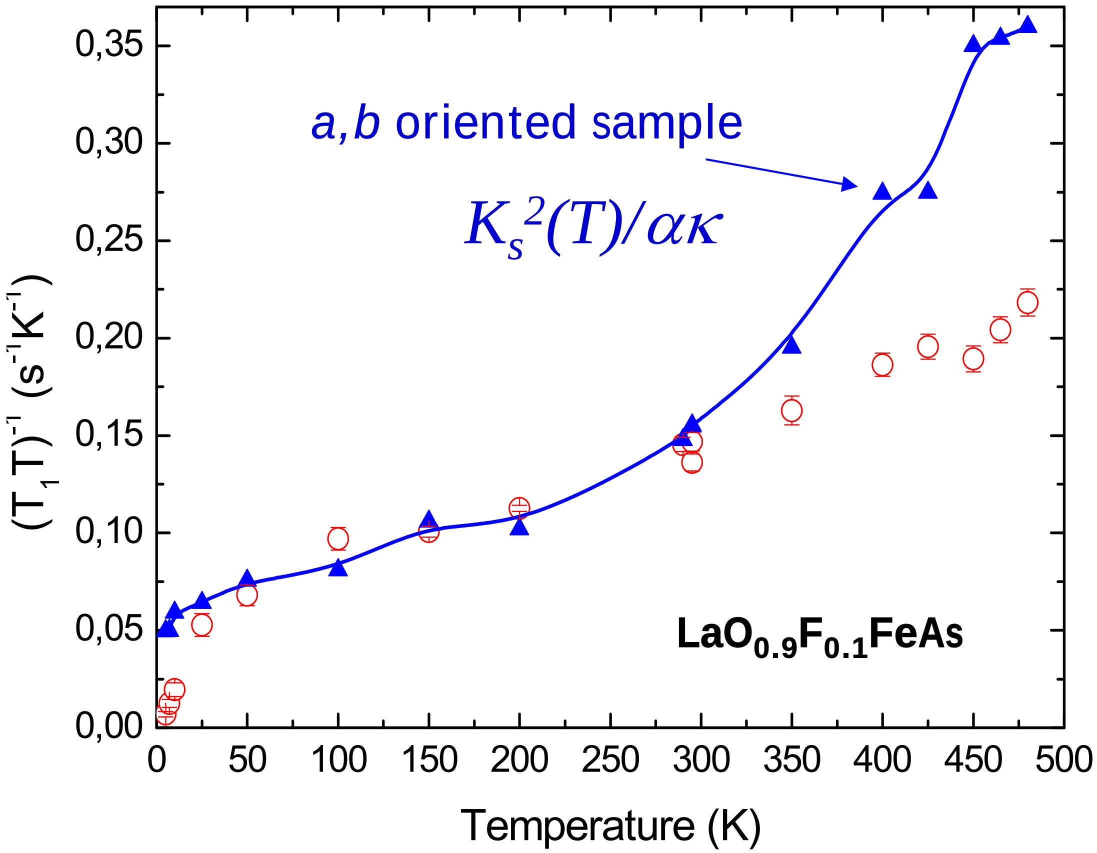


Knight shift and T_1^{-1}: Korringa relation

$$(T_1 T)^{-1} \cdot K_s^2 = \alpha\kappa$$

$$\kappa = \hbar\gamma_e^2/4\pi\, k_B^{75}\gamma^2$$

$$\alpha = 1.8$$



H.-J. Grafe et al., PRL 101, 047003 (2008)