Mini workshop on iron-based superconductors (Minipgm)

Kavli Insitute for Theoretical Physics, Santa Barbara,10 Jan. 2011

NMR investigation on iron-based superconductors

Interplay between magnetism and superconductivity

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JST – TRIP

Collaborators

NMR

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Sample: $BaFe_2(As_{1-x}P_x)_2$

Kyoto Univ.


S. Kasahara


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Sample: $LaFeAs(O_{1-x}F_x)$

Tokyo Inst. of Technology


Y. Kamihara


H. Hosono

Contents

1. Introduction to iron-based superconductors & NMR

2. NMR results in 122 superconductorBa$Fe_2(As_{1-x}P_x)_2$

  - ● P-concentration dependence of magnetic fluctuations
  - ● Comparison with K- & Co-doped $BaFe_2As_2$
  - ● Suppression of internal field at low P concentrations

3.Comparison with other iron-based families

4.Summary

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1. Introduction to iron-based superconductors & NMR

2. NMR results in 122 superconductor$BaFe_2(As_{1-x}P_x)_2$

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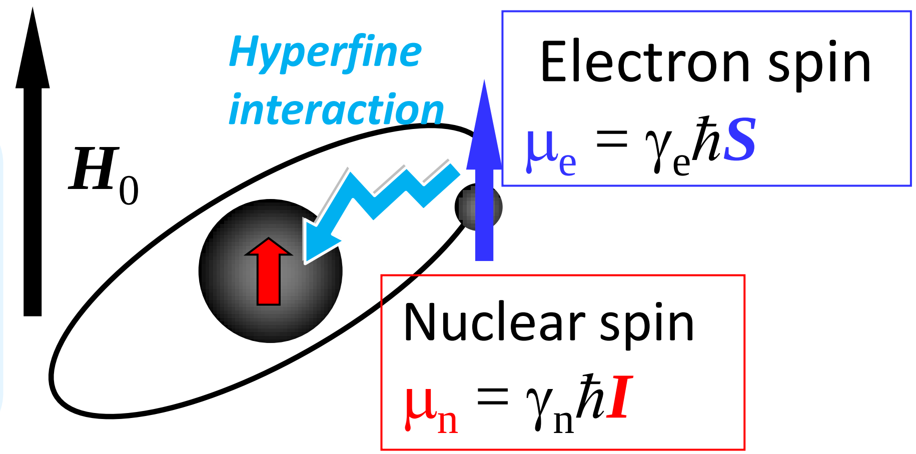
3. Comparison with other iron-based families

4. Summary

Hyperfine Interaction between Nuclear and Electronic Spins

Nuclear spins (***I***) are coupled with electronic spins (***S***) polarized by magnetic field (***H*~0~**).



Hamiltonian of the nuclear spins

$$\mathrm{H_Z} = -\gamma_n \hbar \, \boldsymbol{I} \, \boldsymbol{H}_0 + \mathbf{A} \, \boldsymbol{I} \, \boldsymbol{S} = -\gamma_n \hbar \, \boldsymbol{I} \, \boldsymbol{H}_{\mathrm{Loc}}$$

A: *Hyperfine coupling tensor*

Local field at the nuclear site

$$\boldsymbol{H}_{\mathrm{Loc}} = \boldsymbol{H}_0 - \frac{\mathbf{A}}{\gamma_n \hbar} \boldsymbol{S} = \boldsymbol{H}_0 - \frac{\mathbf{A}}{\gamma_n \hbar} \{ \underbrace{\langle \boldsymbol{S} \rangle}_{\text{Av. static}} + \underbrace{\delta \boldsymbol{S}}_{\text{dynamics}} \}$$

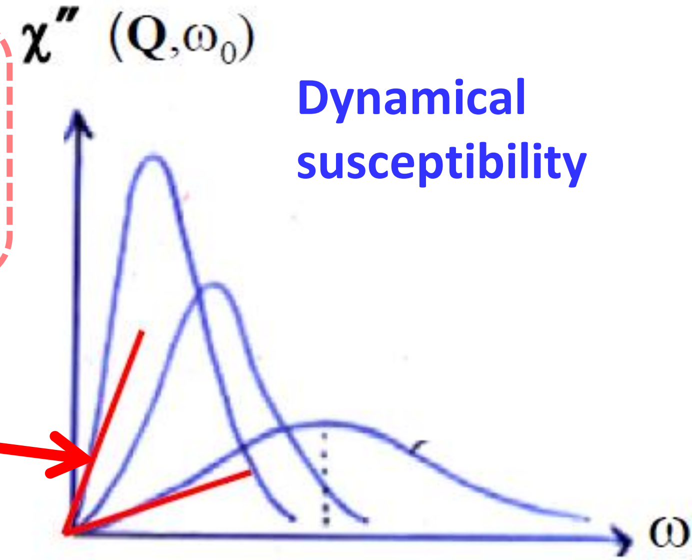
Knight Shift (proportional to spin susceptibility $\chi(q = 0)$)

$$\mathbf{K} = \frac{\mathbf{H}_0 - \langle \mathbf{H}_{\mathrm{Loc}} \rangle}{\mathbf{H}_0} = \frac{\mathrm{A}}{\gamma_n \hbar} \cdot \frac{\langle \mathbf{S} \rangle}{\mathbf{H}_0} = \frac{\mathrm{A}}{N_A \gamma_e \gamma_n \hbar^2} \chi(q = 0)$$

Nuclear spin-lattice relaxation rate: $1/T_1$

Dynamical component of hyperfine interaction

$$H = -\gamma_n \hbar \vec{I} \cdot \underline{\delta \vec{S}} = -\gamma \hbar \left\{ I_z \delta S_z + \frac{1}{2}\left(I_+ \delta S_- + I_- \delta S_+ \right) \right\}$$



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

$$= \frac{4\pi}{\hbar} \frac{(\gamma_n \hbar A)^2}{N^2} \underline{N^2(E_F)} k_B T$$

Korringa law : $T_1 T$ = const.
(Characteristics of Metal)

***q*-sum information on spin fluctuations with very low energy (~mK order)**

⇔Neutron experiments

Magnetic fluctuations

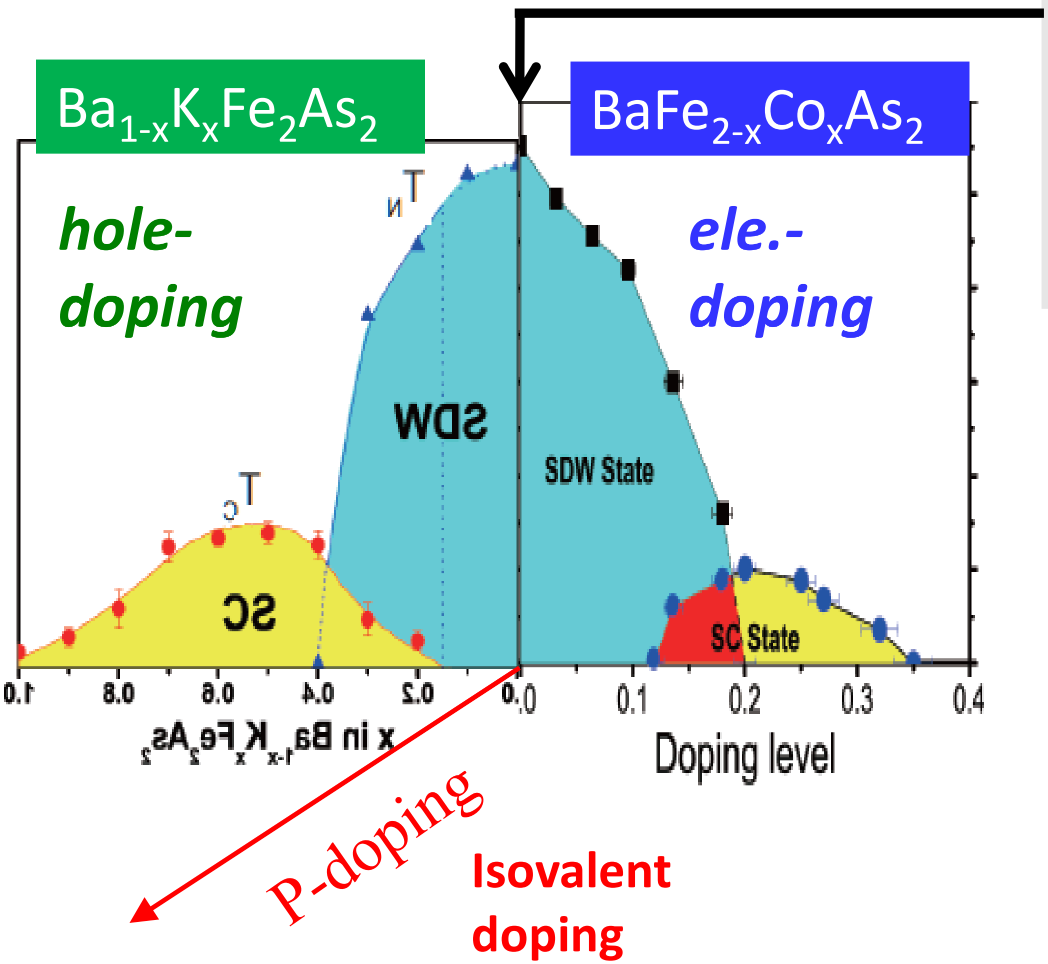
$$\frac{1}{T_1} = \frac{T}{(T - T_M)^n}$$

- 2D FM n=3/2, AFM n=1
- 3D FM n= 1, AFM n=1/2

Moriya *et al.*

$1/T_1$ = const. for a paramagnetic state of local moment systems

Superconductivity in $BaFe_2As_2$ (122) system

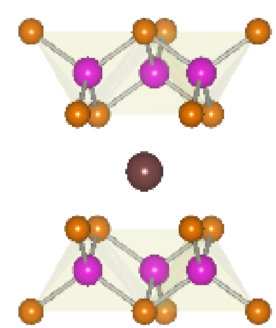


$BaFe_2As_2$:
Magnetic and Structural ordering at ~135 K
Bad metal

⇔Cuprates (Mott insulator)

Isovalent P substitution induces superconductivity.

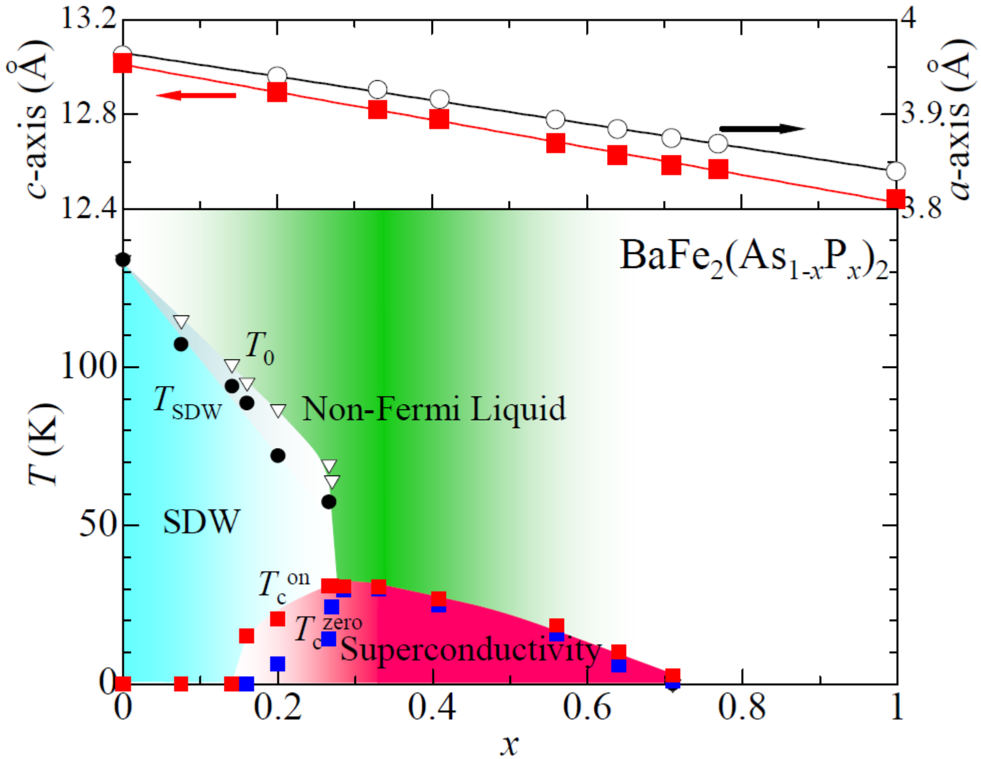
S. Jiang *et al.* J. Phys: Cond.Matt. 21 382203 (2009)

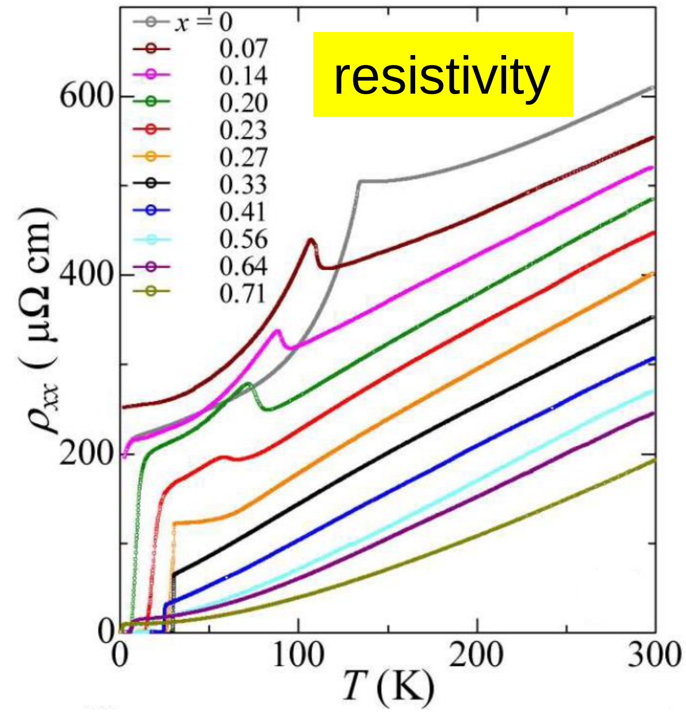


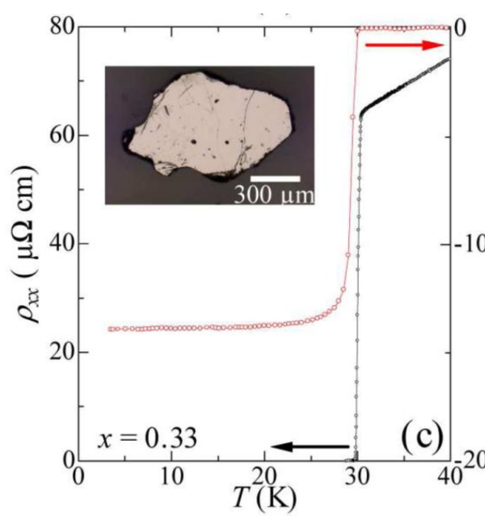
H.Chen *et al.* EPL**85**, 17006 (2009)
X.F.Wang *et al.* arXiv. 0811.2920

Isovalent P doped superconductor $BaFe_2(As_{1-x}P_x)_2$

Kasahara *et al*., Phys. Rev. B **81** (2010) 184519
Jiang *et al.* J. Phys: Cond. Mat. 21 382203 (09)







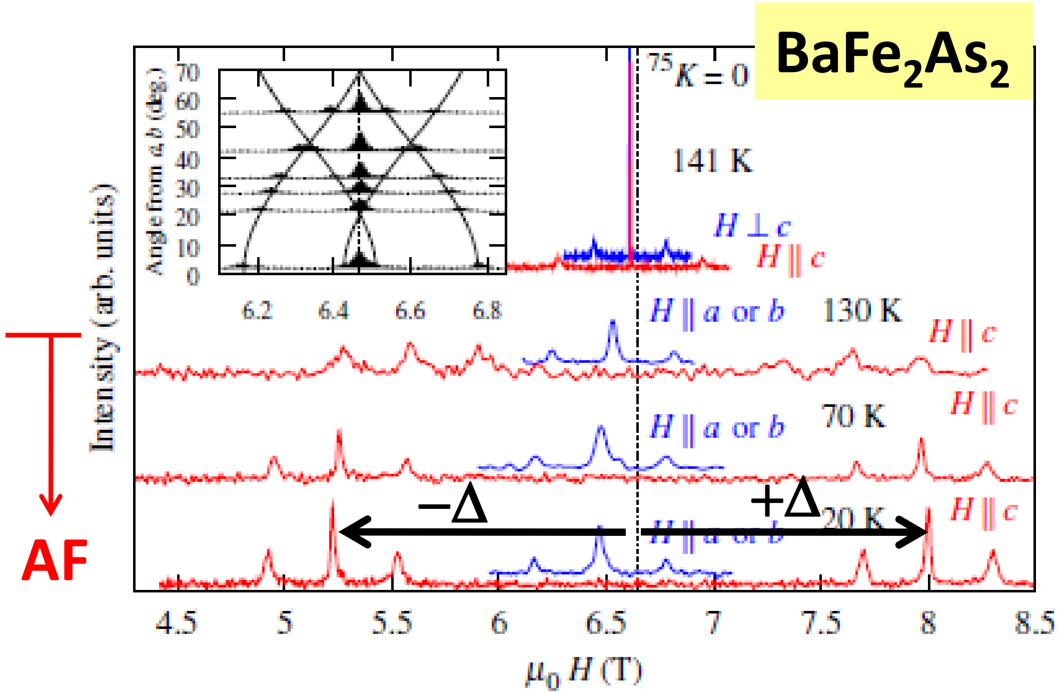
Quite sharp SC transition

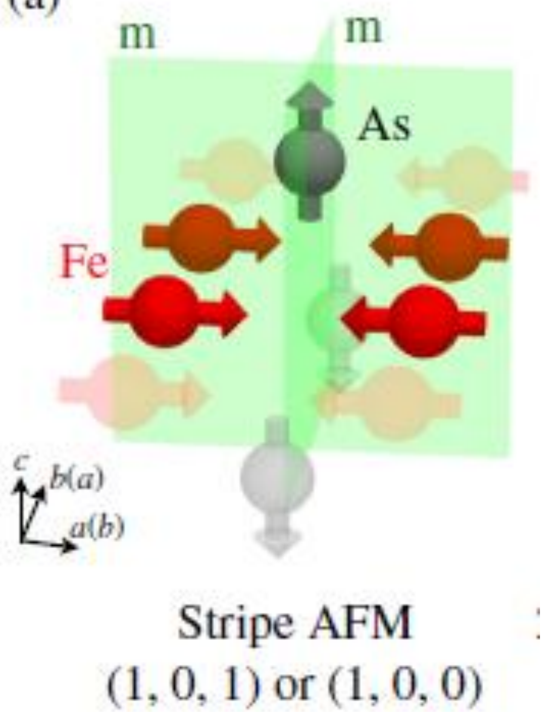
- Superconductivity with T_c =30 K is realized by isovalent P doping.
- High-quality single crystal

  dHvA signal observed above x ~0.4.

Form Factor at As (P) site

K. Kitagawa *et al*., JPSJ **78** (2009) 063706.





$T < T_{SDW}$: Internal field (Δ) at the As site

H_{appl} || c-axis: $$H_{res} = H_{Appl} \pm \Delta$$

H_{appl} || a or b-axis: $$H_{res} = \sqrt{H_{Appl}^{\ 2} + \Delta^2}$$

NMR spectra indicate that internal field Δ is parallel to the *c*-axis.

Hyperfine Fields at As (P) site

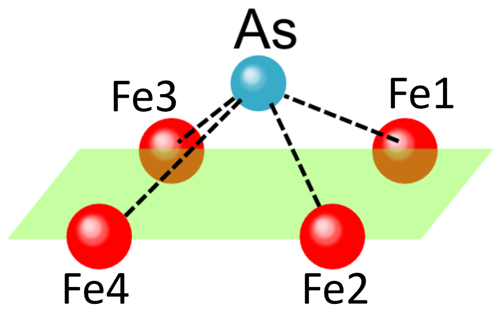
Hyperfine field determined by neighboring Fe spins

$$H^{\mathrm{As}} = \sum_{i=1}^{4} A_i S_i^{\mathrm{Fe}} = \tilde{A} S_1^{\mathrm{Fe}}$$

H^{As} : HF at the ^{75}As site

S^{Fe} : Spin at the Fe site

$\tilde{A}$: HF coupling tensor



K. Kitagawa *et al.*, JPSJ **78** (2009) 063706.

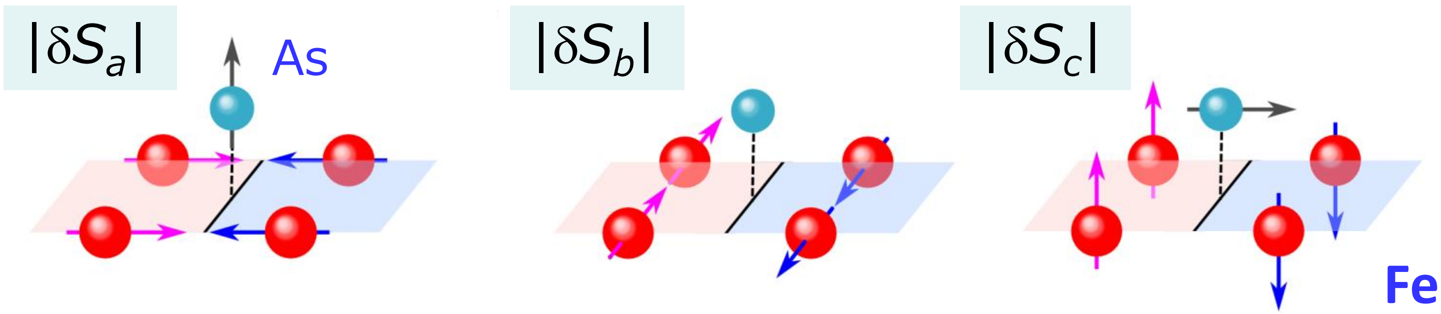
$$\tilde{\mathbf{A}} = \begin{pmatrix} A_{ab} & C & S_1 \\ C & A_{ab} & S_2 \\ S_1 & S_2 & A_c \end{pmatrix}$$

A_i : diagonal terms

$S_{1[2]}$: off-diagonal terms related with(π, 0)[(0,

C : off-diagonal terms related with (π, π) SF

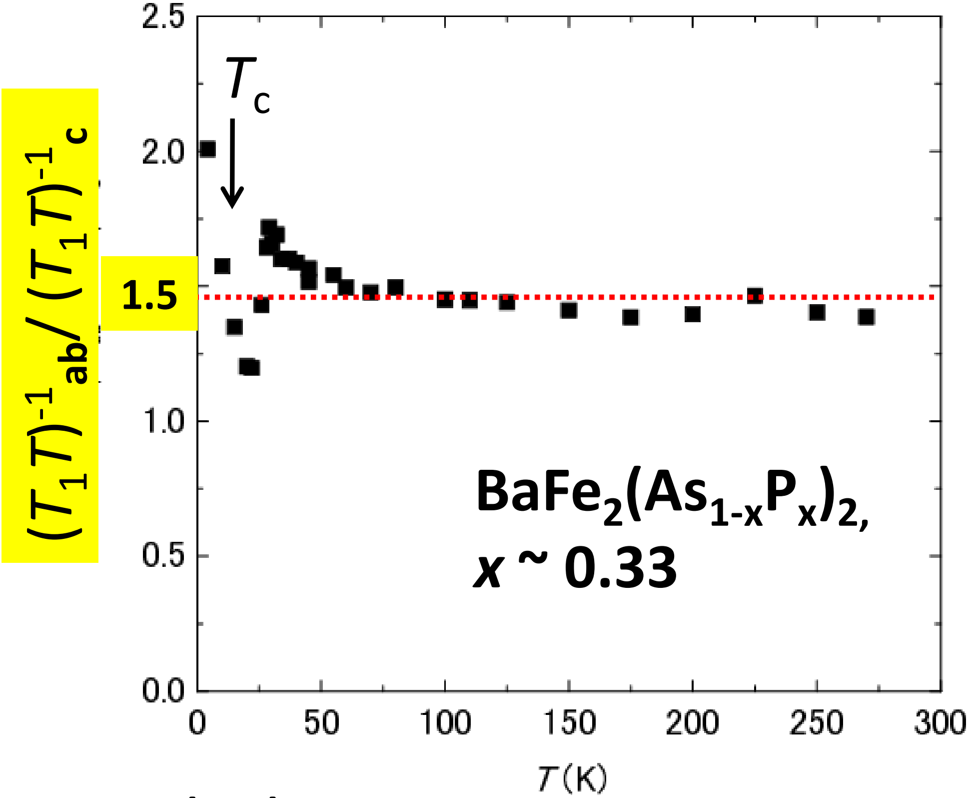
Hyperfine fields due to the stripe spin correlations



$$\begin{pmatrix} |H_a^{\mathrm{As}}| \\ |H_b^{\mathrm{As}}| \\ |H_c^{\mathrm{As}}| \end{pmatrix} \propto \begin{pmatrix} 0 & 0 & S_1 \\ 0 & 0 & 0 \\ S_1 & 0 & 0 \end{pmatrix} \begin{pmatrix} |\delta S_a^{\mathrm{Fe}}| \\ |\delta S_b^{\mathrm{Fe}}| \\ |\delta S_c^{\mathrm{Fe}}| \end{pmatrix} = S_1 \begin{pmatrix} |\delta S_c^{\mathrm{Fe}}| \\ 0 \\ |\delta S_a^{\mathrm{Fe}}| \end{pmatrix}$$

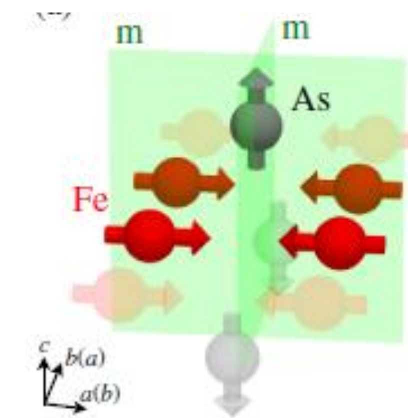
Fe spin in the *ab*-plane creates hyperfine fields along *c*-axis at As & P sites.

Stripe AF spin fluctuations in $BaFe_2(As_{1-x}P_x)_2$ (x ~0.33)



Anisotropy in $(T_1T)^{-1}$ can provide information on ***q*-vector of spin fluctuations.**

$$\delta \mathbf{H}^{As} = 4S \begin{pmatrix} \delta S_z \\ 0 \\ \delta S_x \end{pmatrix}$$



Stripe AFM
(1, 0, 1) or (1, 0, 0)

Stripe (π,0) AFM

$(T_1T)^{-1}_{H//ab} \propto |\delta H_{ab}|^2 + |\delta H_c|^2 \propto 1/2|\delta S_z|^2 + |\delta S_x|^2$

$(T_1T)^{-1}_{H//c} \propto |\delta H_a|^2 + |\delta H_b|^2 = 2|\delta H_{ab}|^2 \propto |\delta S_z|^2$

$\delta S_x^{Fe} \rightarrow \delta H_c$ @As

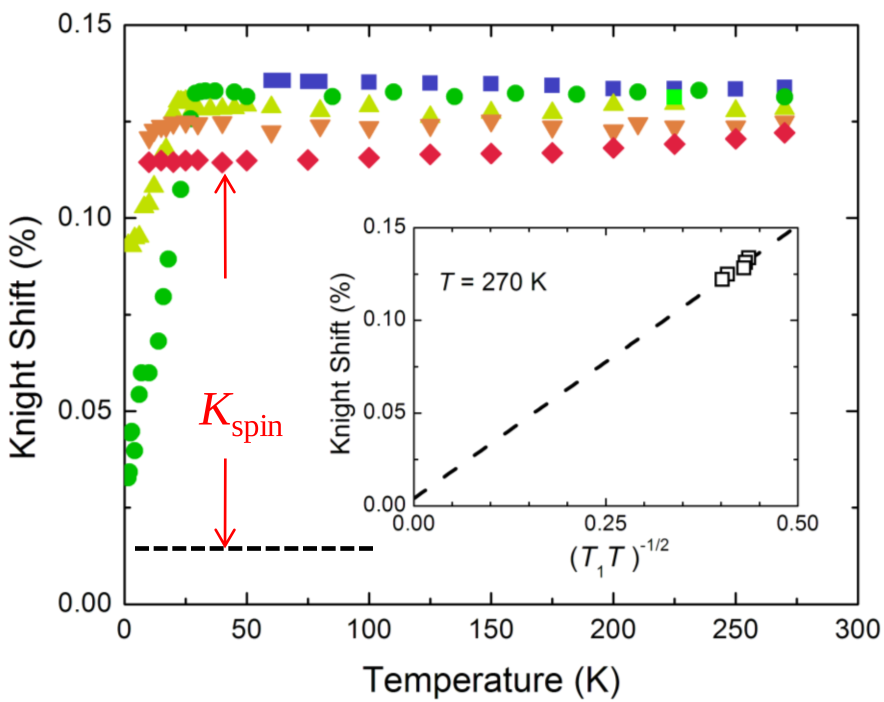
$\delta S_z^{Fe} \rightarrow \delta H_a$ @As

Isotropic spin component $|\delta S_x| = |\delta S_y| = |\delta S_z|$: $\mathbf{(T_1T)^{-1}_{H//ab} / (T_1T)^{-1}_{H//c} = 1.5}$

Contents

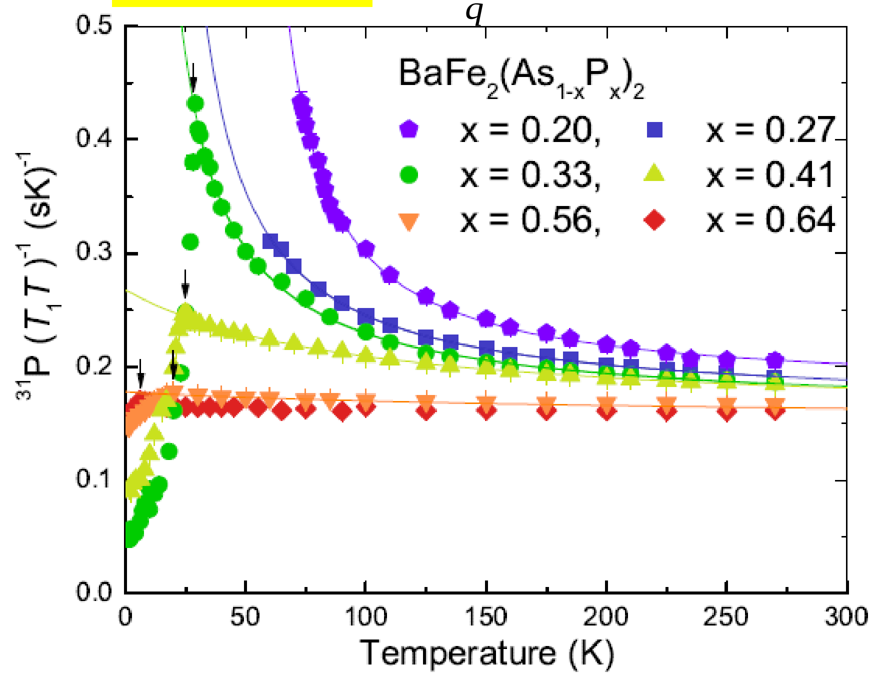
Overview of NMR results in $BaFe_2(As_{1-x}P_x)_2$ (0.2 <= x <= 0.64)

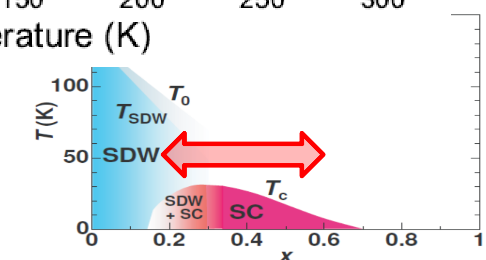
^{31}P Knight shift $\chi(q=0)$



$K_{spin} \propto \chi_{spin} = \mu_B^2 N(E_F)$

^{31}P $(T_1T)^{-1}$ $\sum_q \chi(q, \omega \sim 0)$

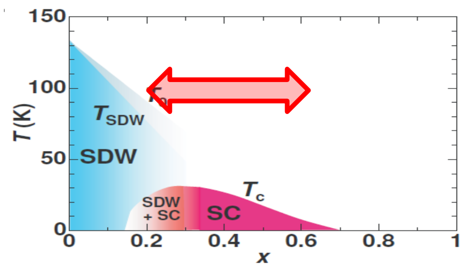


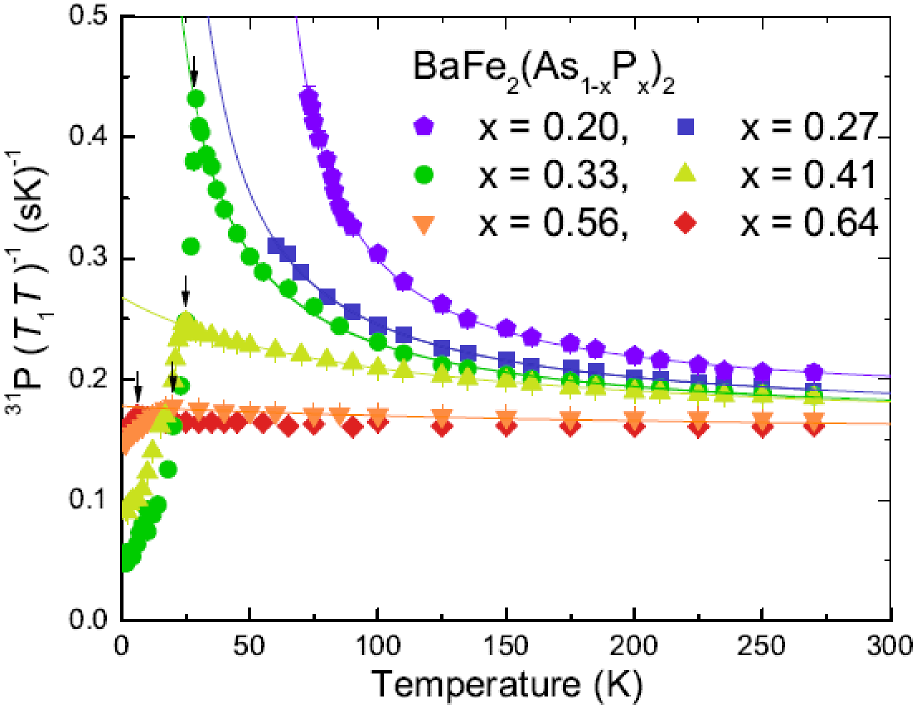


- Knight shift is temperature independent.
- Knight shift is nearly unchanged between x=0.20 and 0.56.
- Significant AFM fluctuations at the optimal P-concentration (x=0.33, T_c=30K).
- The AFM fluctuations are suppressed by P-substitution, and $(T_1T)^{-1}$=const. is observed at x=0.64 (T_c~7 K). *Fermi liquid*

Evolution of AFM fluctuations by P substitution for As

$^{31}P\ (T_1T)^{-1}$



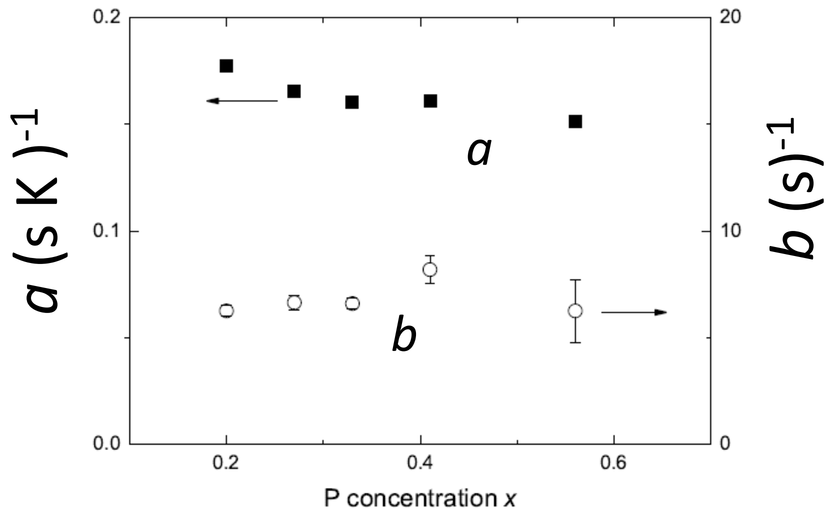


2D AFM
spin fluctuations

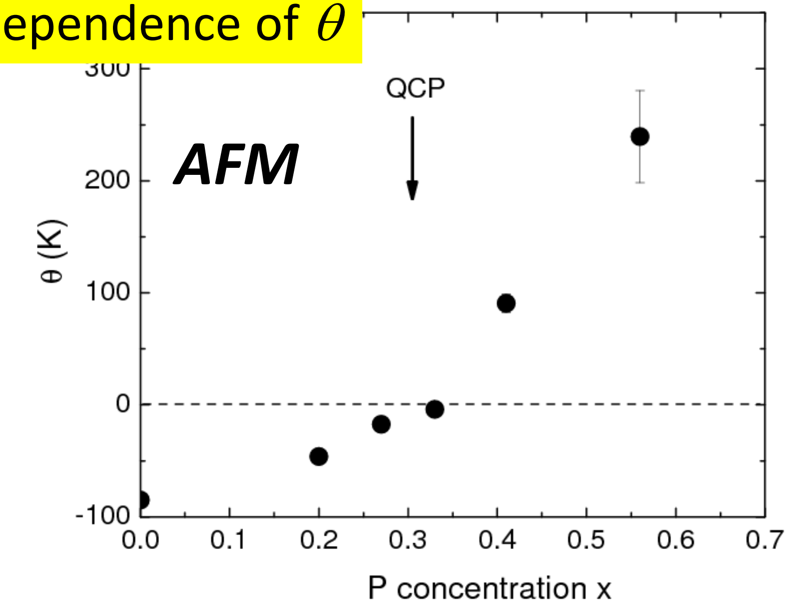
$$\frac{1}{T_1T} = a + \frac{b}{T+\theta}$$

Moriya, Takahashi, Ueda, *JPSJ* **59** (1990) 2905.

P dependence of *a* and *b*

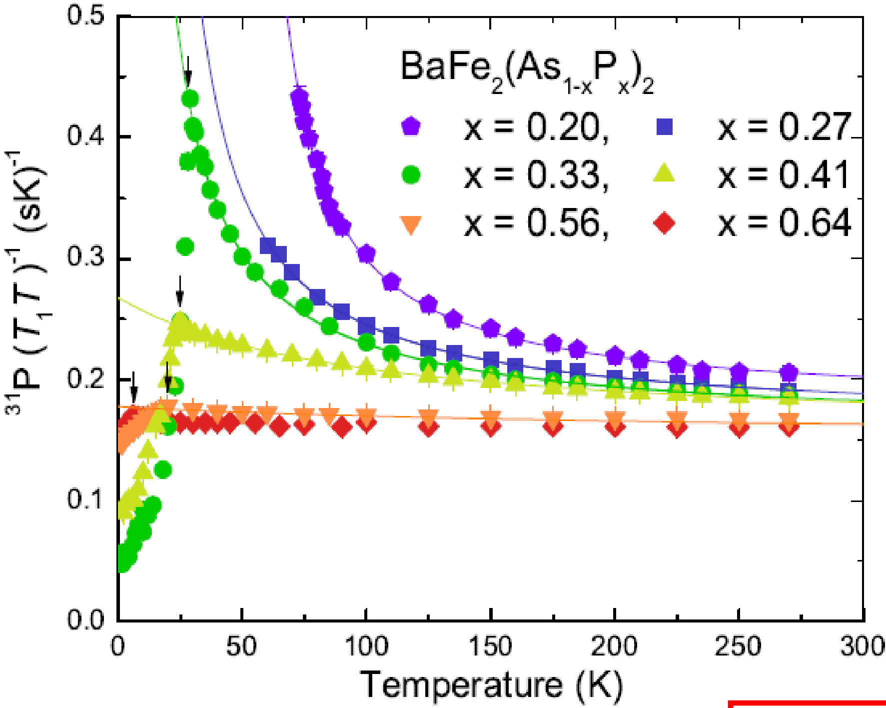


P dependence of θ

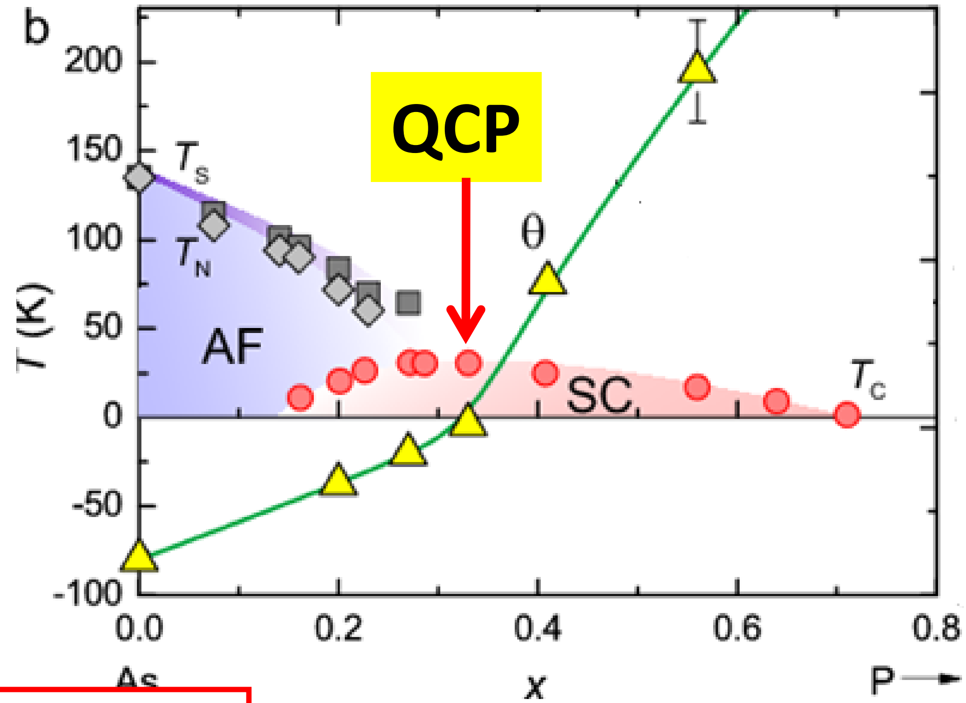


A possible QCP near an optimum concentration (x ~ 0.33)

$^{31}P\ (T_1T)^{-1}$



P dependence of θ and T_c

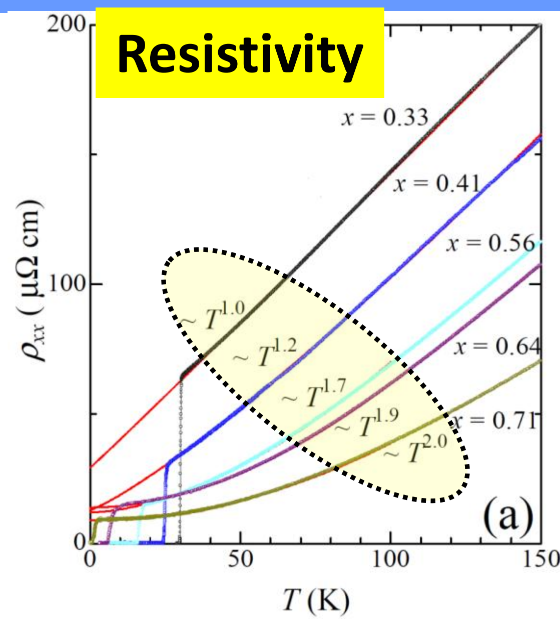


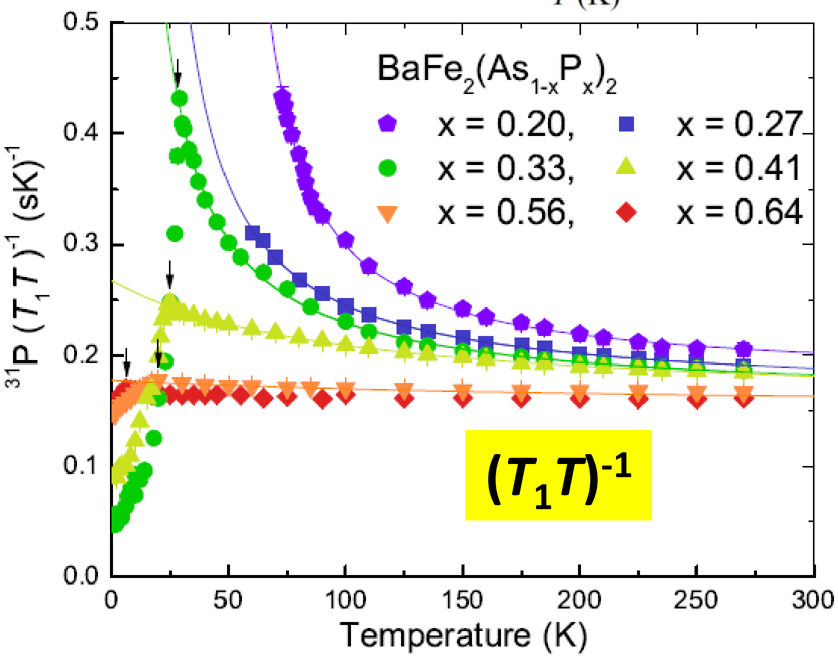
$$\frac{1}{T_1T} = a + \frac{b}{T+\theta}$$

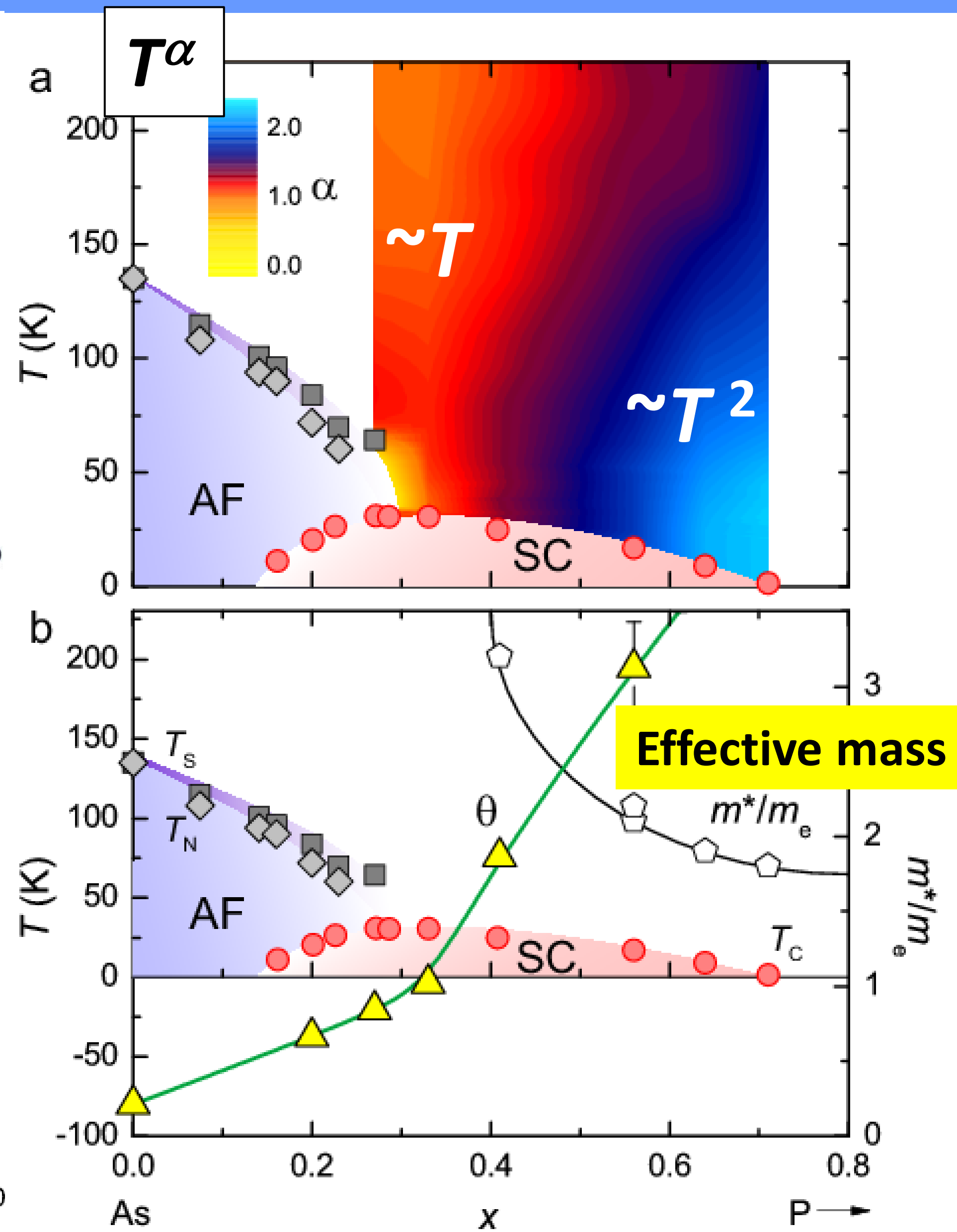
- A QCP inferred from $1/T_1T$ coincides with a T_c maximum in the SC dome of $BaFe_2(As_{1-x}P_x)_2$.

Summary of Experimental Results : ρ , m^* and $(T_1T)^{-1}$

YN *et al.*,
PRL **105**
(2010) 107003.

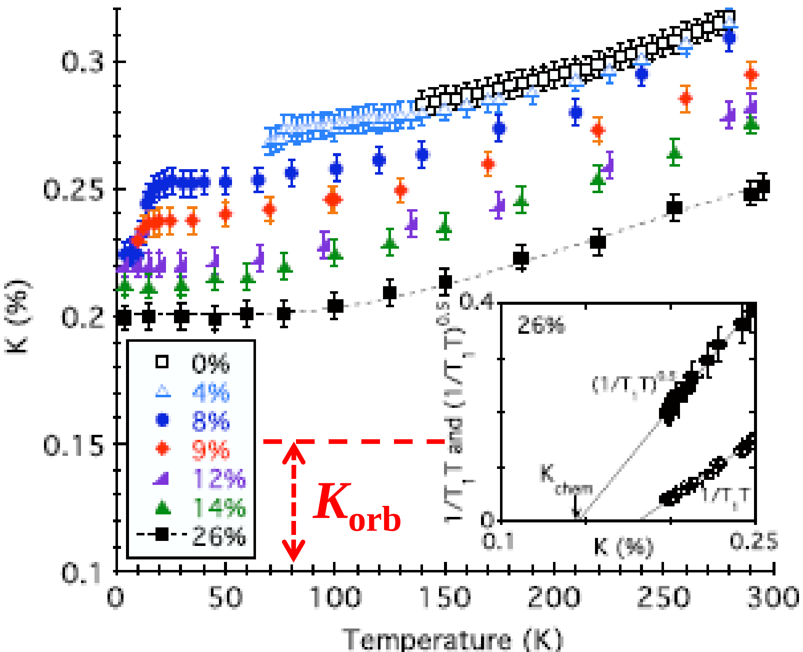




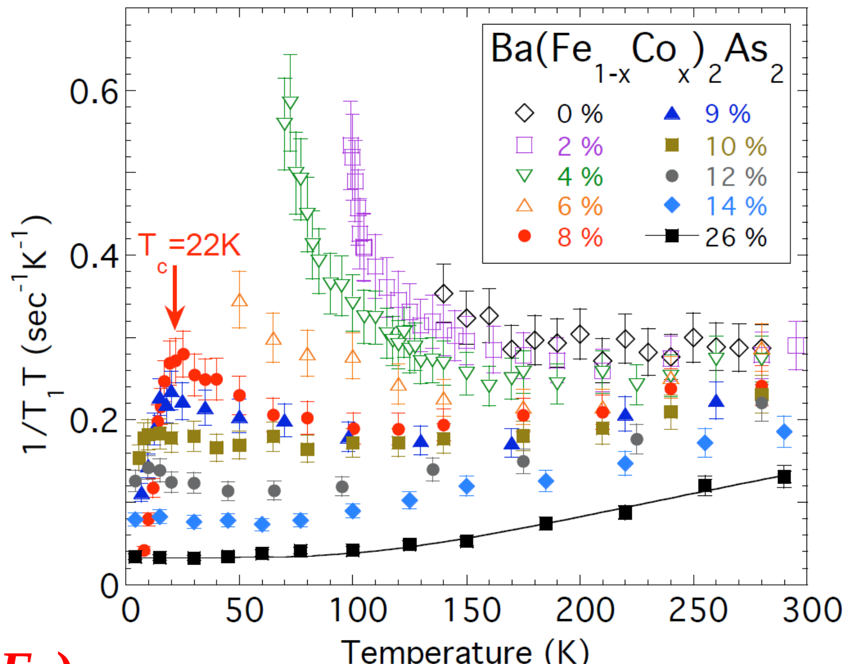


Comparison: $Ba(Fe_{1-x}Co_x)_2As_2$

^{75}As Knight shift

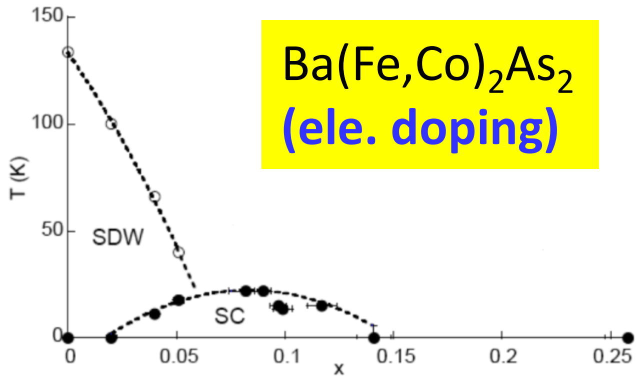


^{75}As $(T_1T)^{-1}$



$$\chi_{spin} = \mu_B^2 N(E_F)$$

Ning *et al.*,
PRL **104** (2010) 037001.

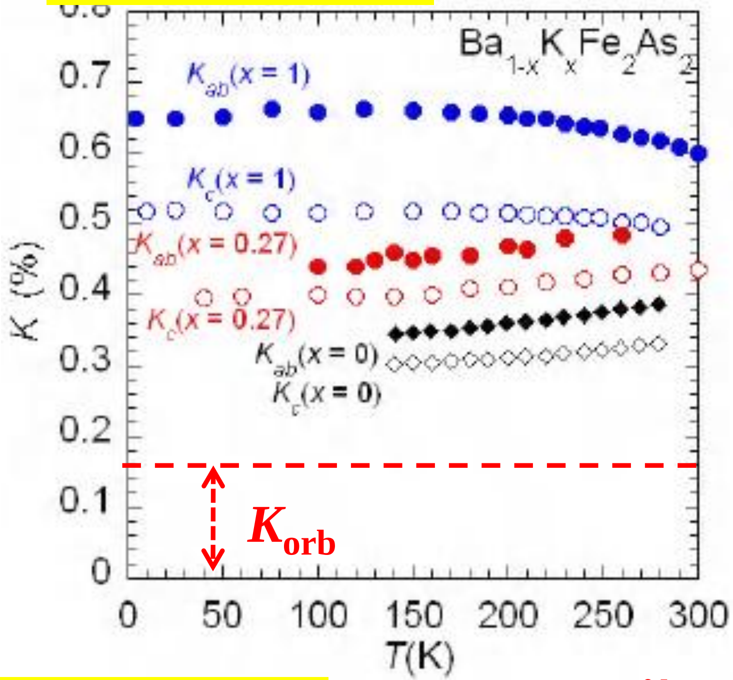


$Ba(Fe,Co)_2As_2$
(ele. doping)

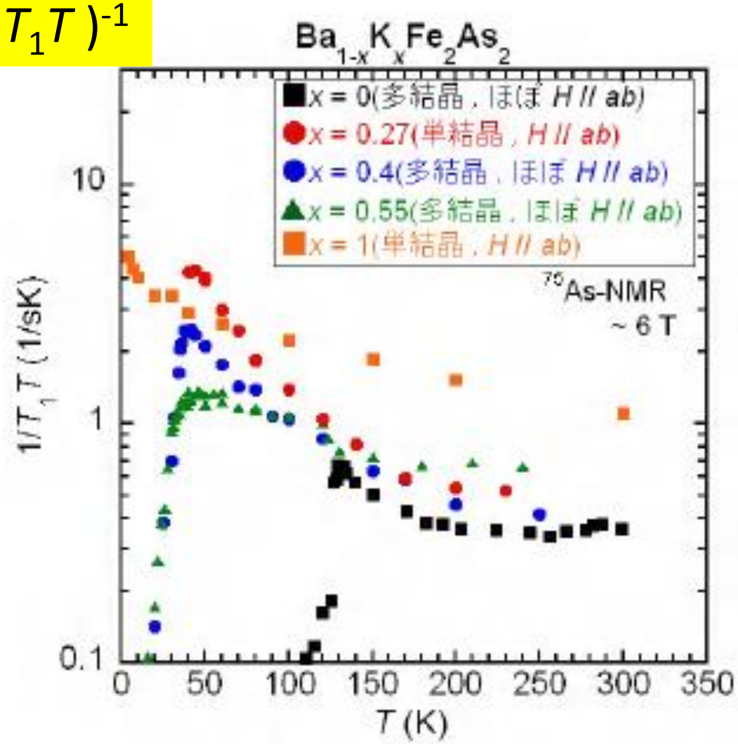
***N*(*E*$_F$) decreases, and**
AF fluctuations are suppressed
by Co(electron) doping.

Comparison: $(Ba,K)Fe_2As_2$

^{75}As Knight shift

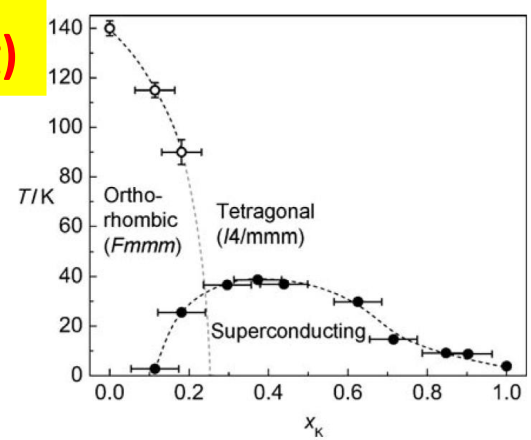


^{75}As $(T_1T)^{-1}$



$(Ba,K)Fe_2As_2$
(hole doping)

$$\chi_{spin} = \mu_B^2 N(E_F)$$



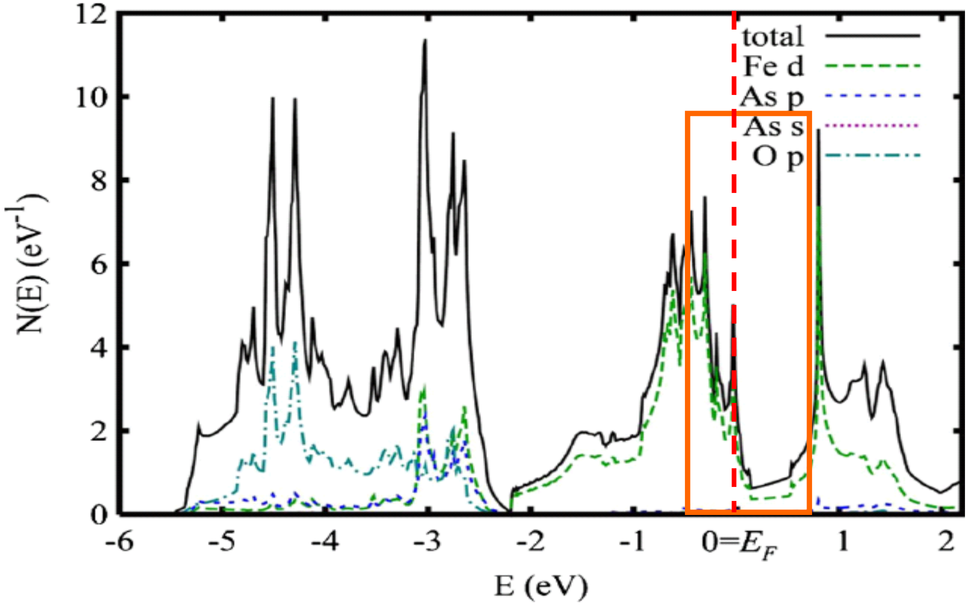
Fukazawa *et al.*, JPSJ **78** (2009) 033704.; *ibid* **78** (2009) 083712.
Yashima *et al.*, *ibid* **78** (2009) 103702.

***N*(*E*$_F$) increases with K(hole) doping**

Strong Energy Dependence of DOS: Possible Origin of χ (q=0,T)

DOS of LaFeAsO

Singh and Du, PRL, **100**, 237003 (2008).

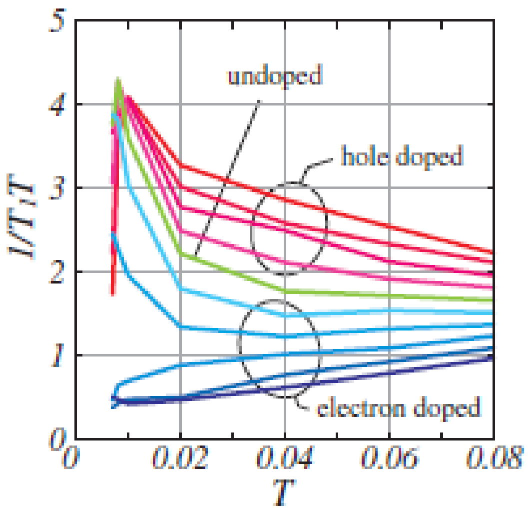


Knight shift & (T_1T)$^{-1}$ data

Electron doping :
DOS decrease

Hole doping :
DOS increase

Isovalent substitution:
DOS *slightly decrease*



Theoretical work considering the band structure effect appears consistent with the data.

H. Ikeda, JPSJ **77**(2008)123707.

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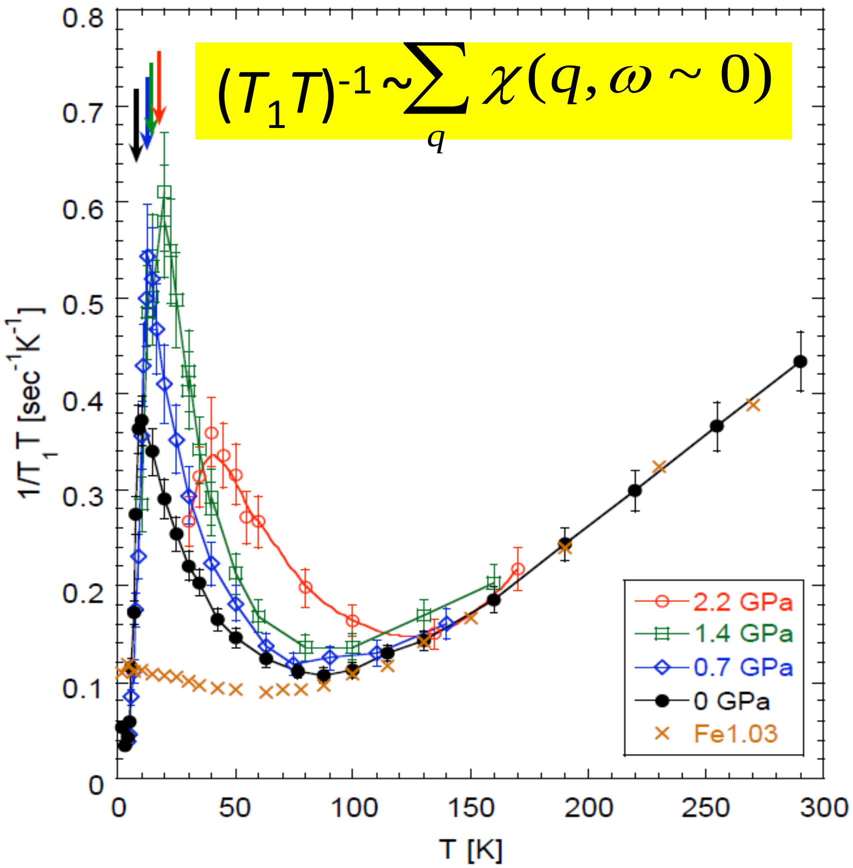
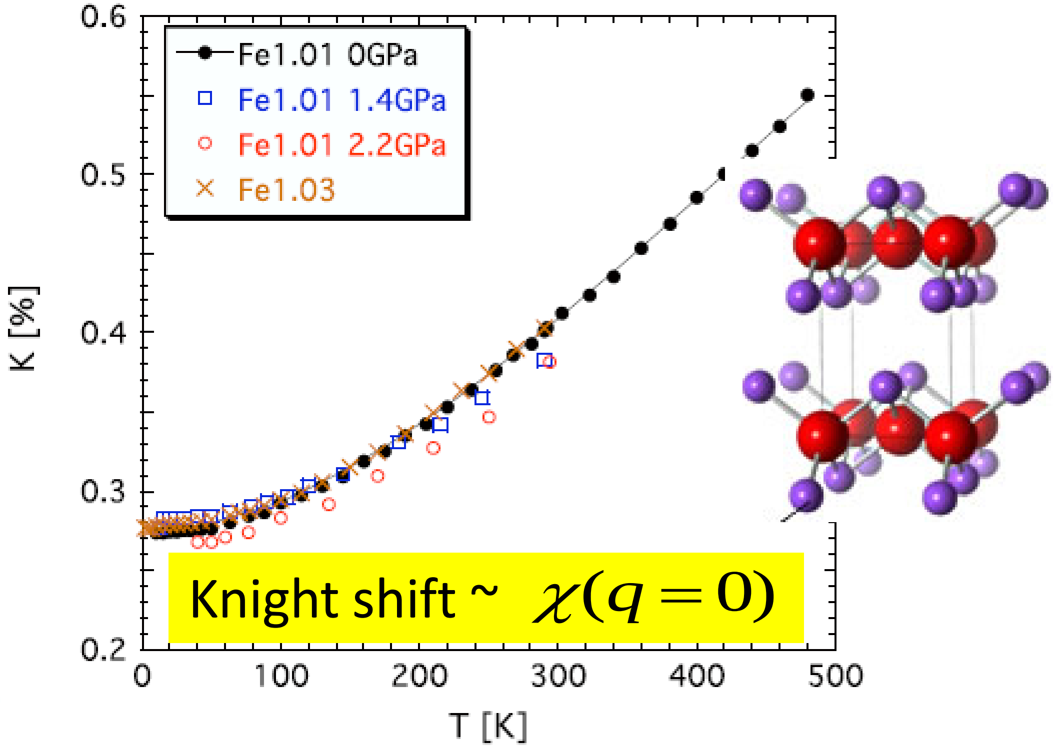
Positive link between AF fluctuations & SC in stoichiometric FeSe



T. Imai *et al.*, PRL **102** (2009) 177005.



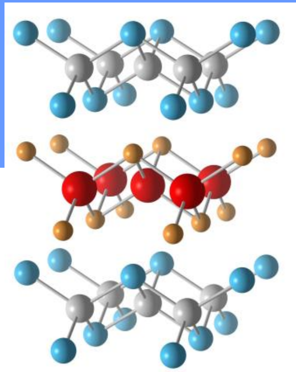
✓At 0 GPa, *AF fluctuations grows prior to superconducting transition.*

✓T_c & AF fluctuations increase under pressure while $\chi(\boldsymbol{q}=0)$ unchanged.

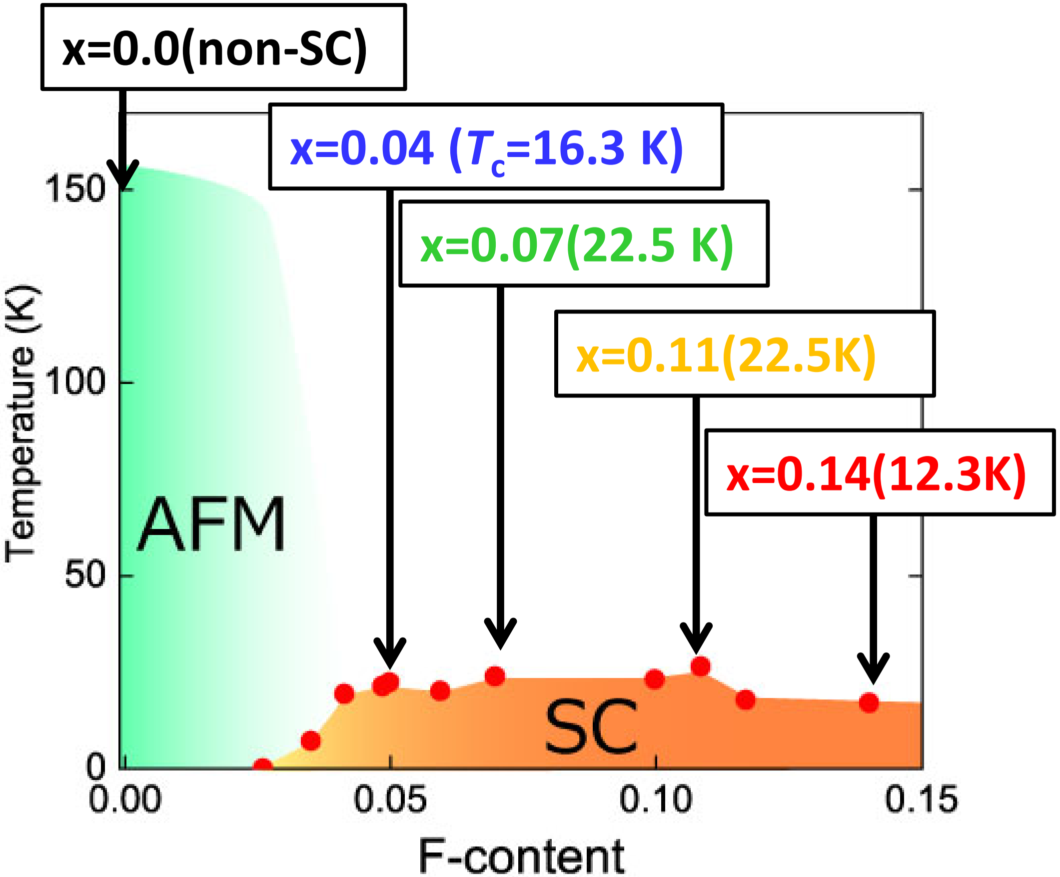
✓Resistivity ρ_{ab} ~ T is observed below 100 K. Non Fermi liquid behavior

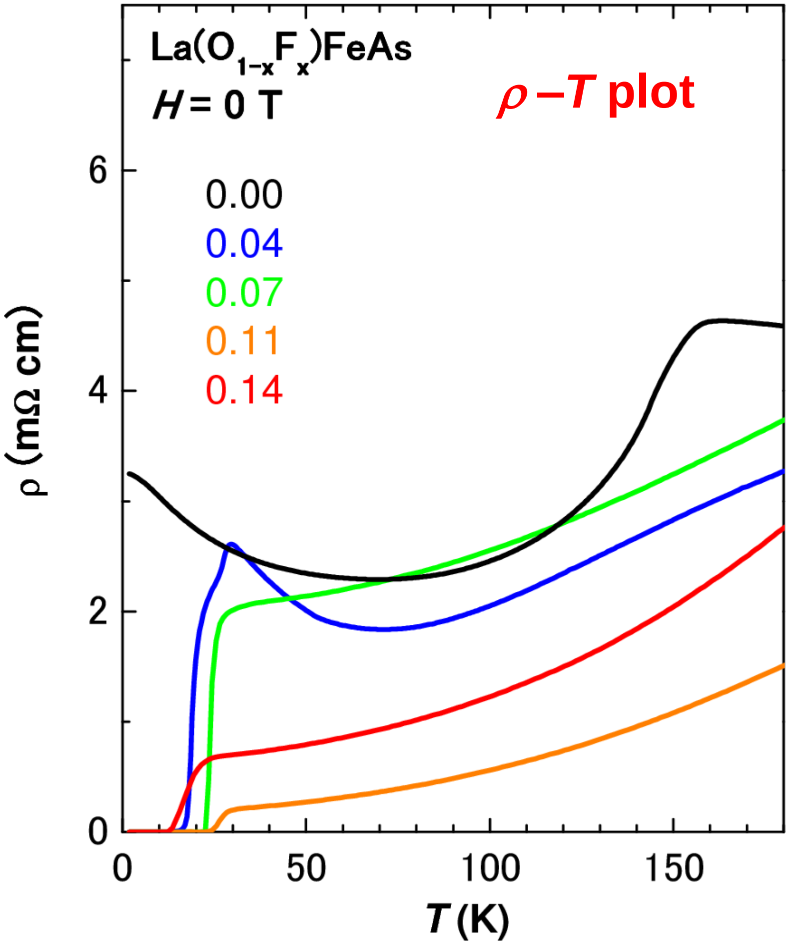
✓Similar to 122 superconductors.

LaFeAs($O_{1-x}F_x$) : Resistivity



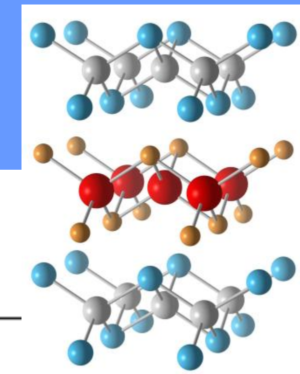
LaFeAs($O_{1-x}F_x$) (x=0.0, 0.04, 0.07, 0.11 and 0.14)



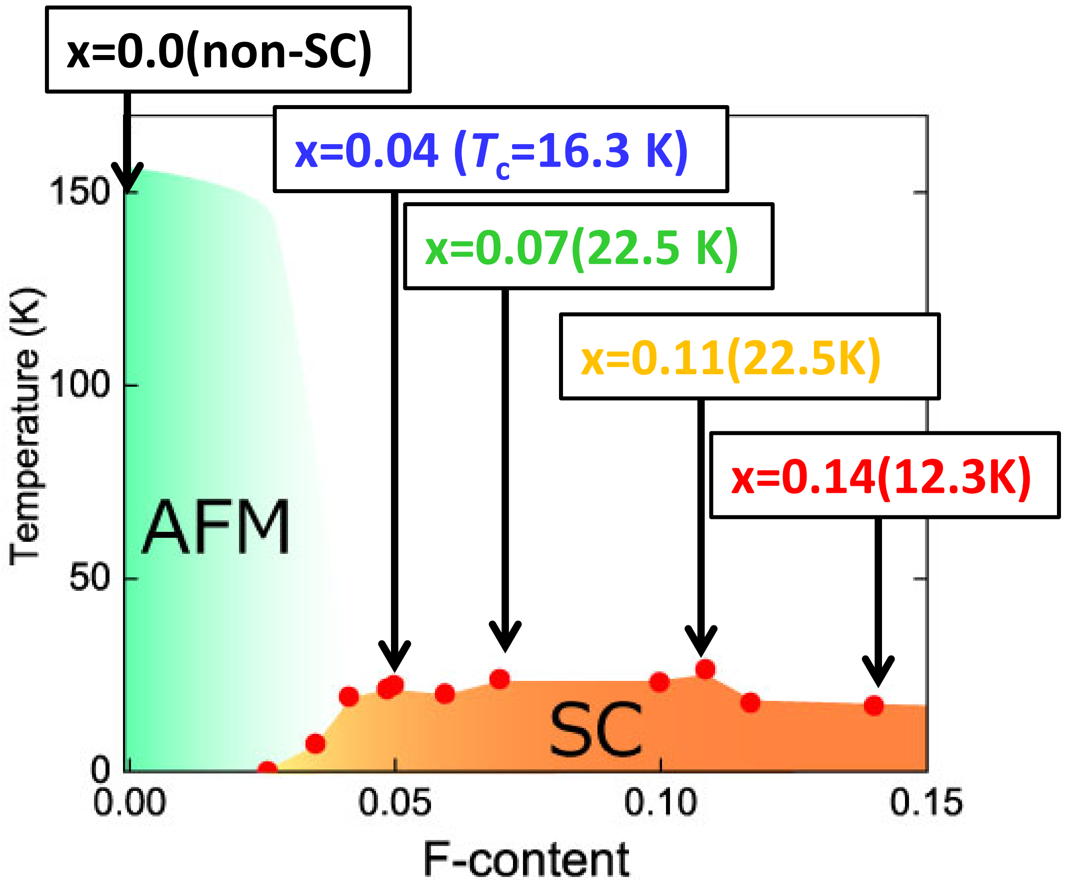


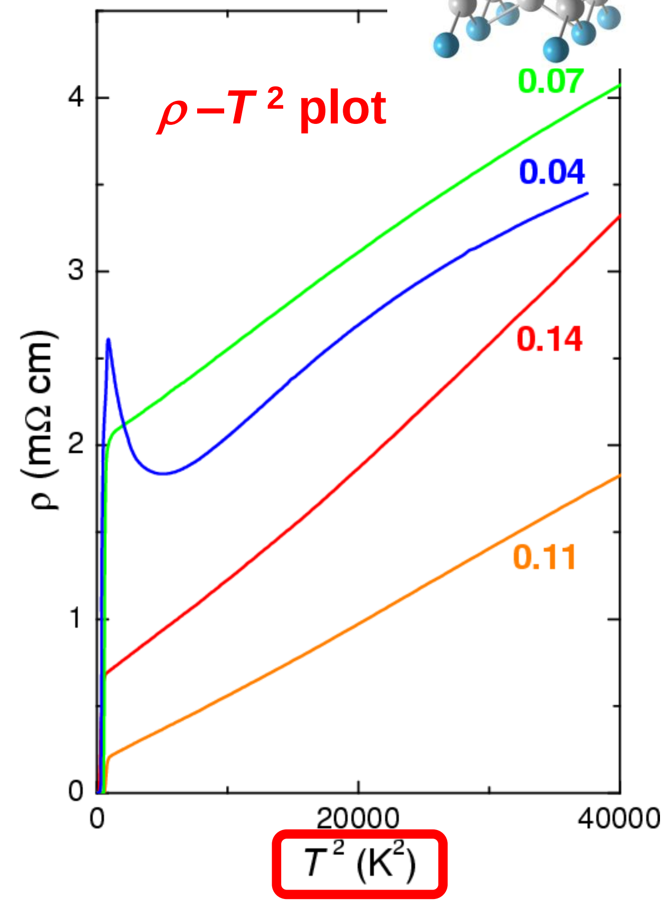
Powdered samples and resistive data are provided by Hosono's group.

LaFeAs($O_{1-x}F_x$) : Resistivity



LaFeAs($O_{1-x}F_x$) (x=0.0, 0.04, 0.07, 0.11 and 0.14)

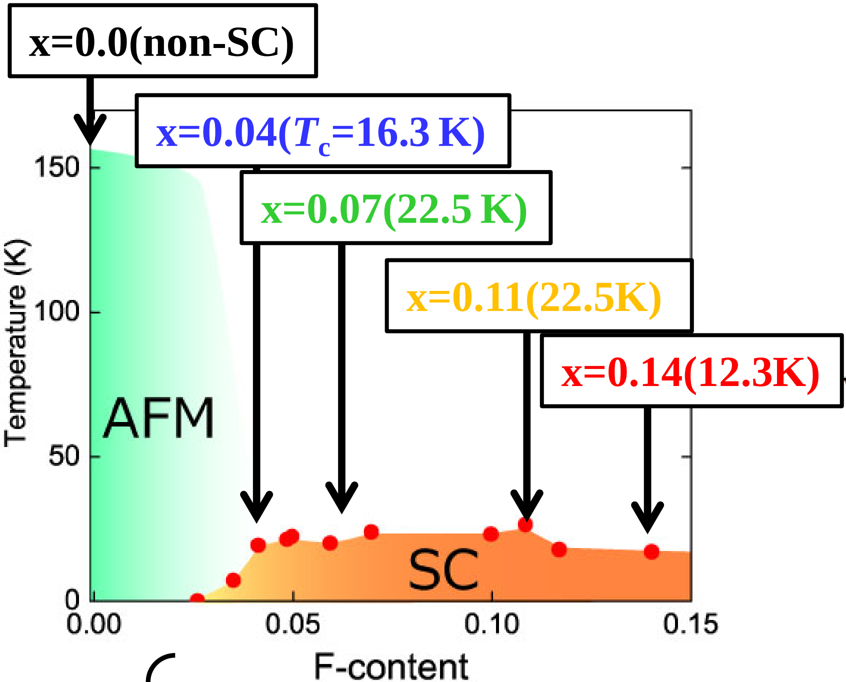




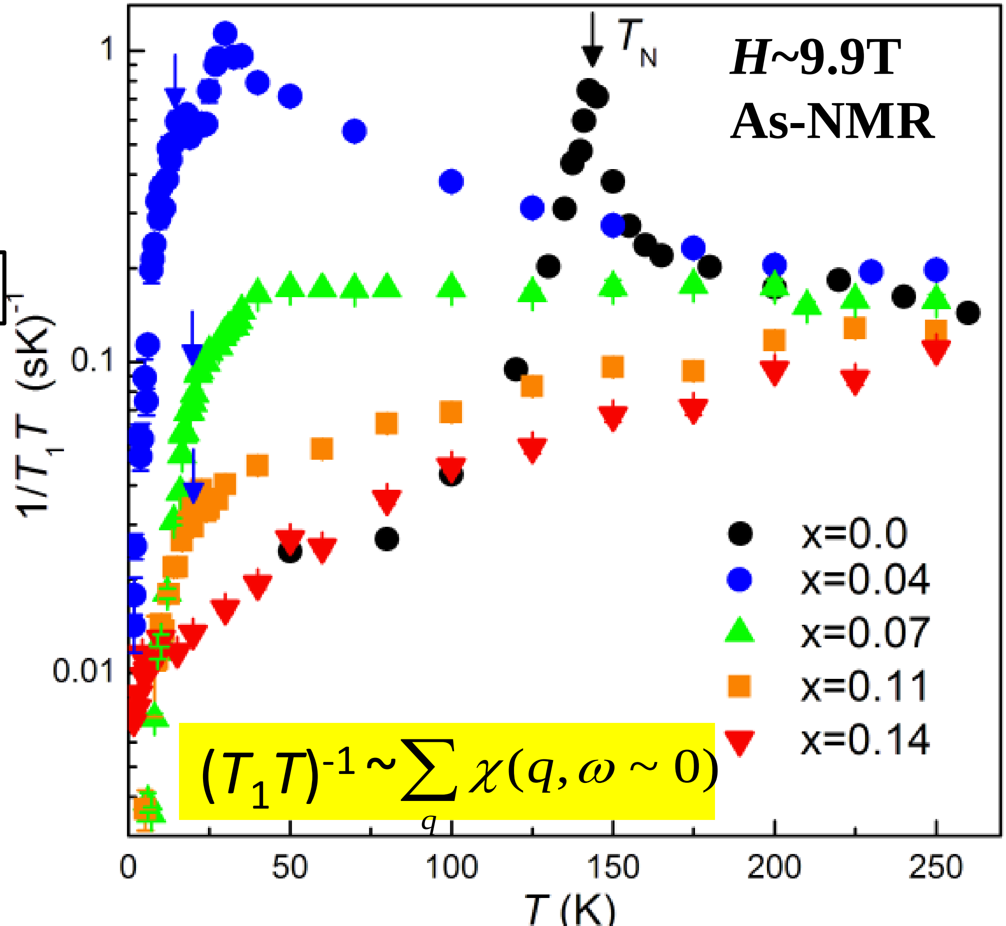
FL behaviors characterized by $\rho \sim T^2$ was observed up to 150K

Evolution of magnetic fluctuations by F-doping in $LaFeAs(O_{1-x}F_x)$

YN *et al.* JPSJ **77**, 073701 (2008).
YN *et al.* New J. Phys. **11**, 045004 (2009).



T_c= 16.3 K (x=0.04), 22.5 K (x=0.07), 22.5 K (x=0.11), 12.3 K (x=0.14)

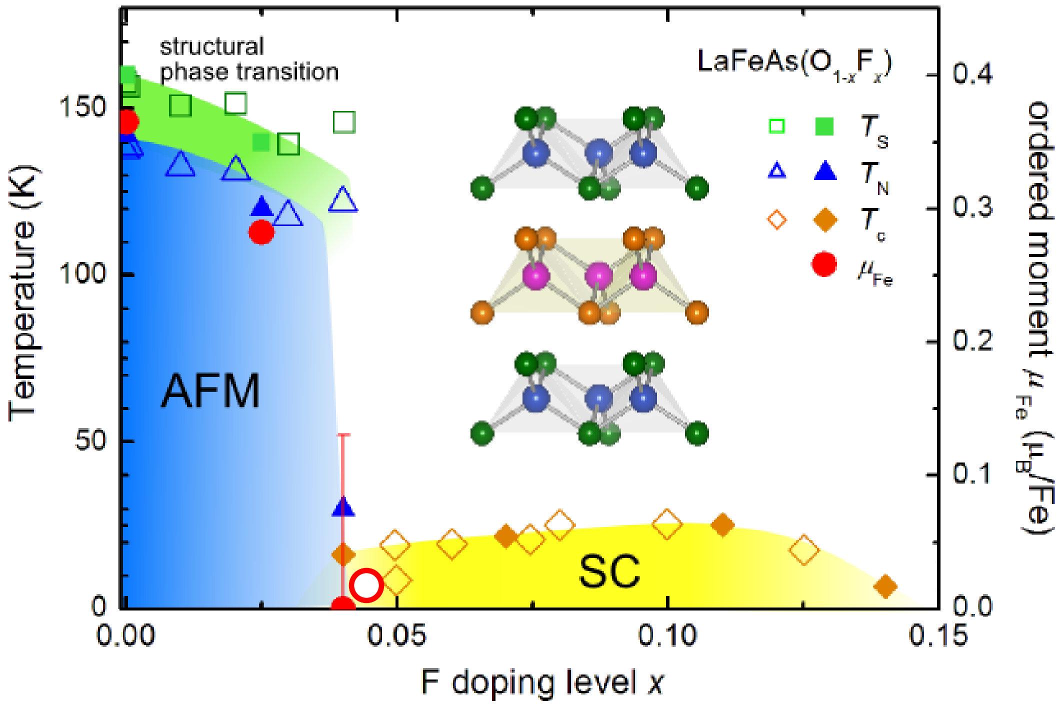


$$(T_1T)^{-1} \sim \sum_q \chi(q, \omega \sim 0)$$

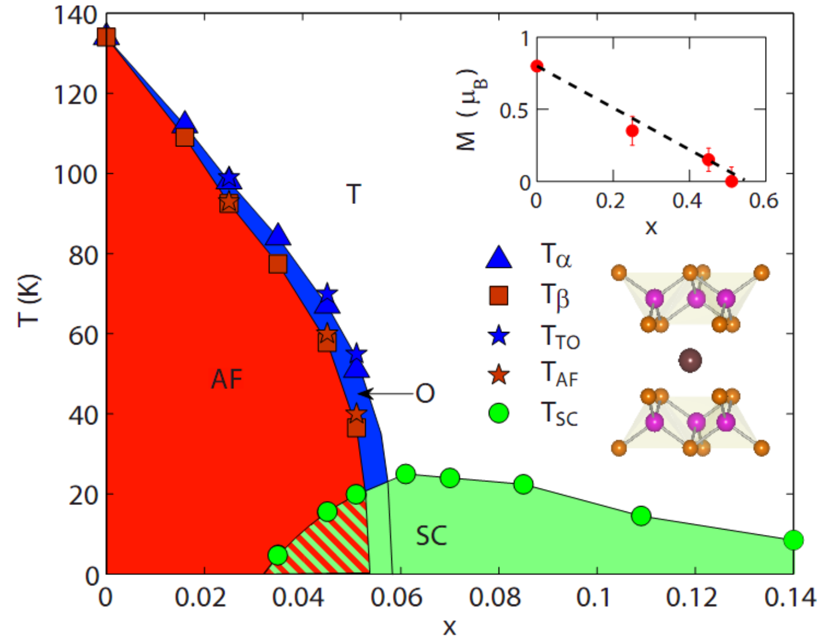
$1/T_1T$ depends strongly on F-doping (2 orders difference!!) ⇔ **T_c changes only by a factor of 2.**

Different Phase diagrams: $LaFeAs(O_{1-x}F_x)$ & Ba-122

$LaFeAs(O_{1-x}F_x)$



$Ba(Fe_{1-x}Co_x)_2As_2$



✓T_N, T_S are sharply suppressed(1[st] order like).

✓Phase separation is suggested.

Luetkens *et al*., Nature Mater. **8**, 305309 (2009).

✓T_N, T_S are gradually suppressed. (2[nd] order like)

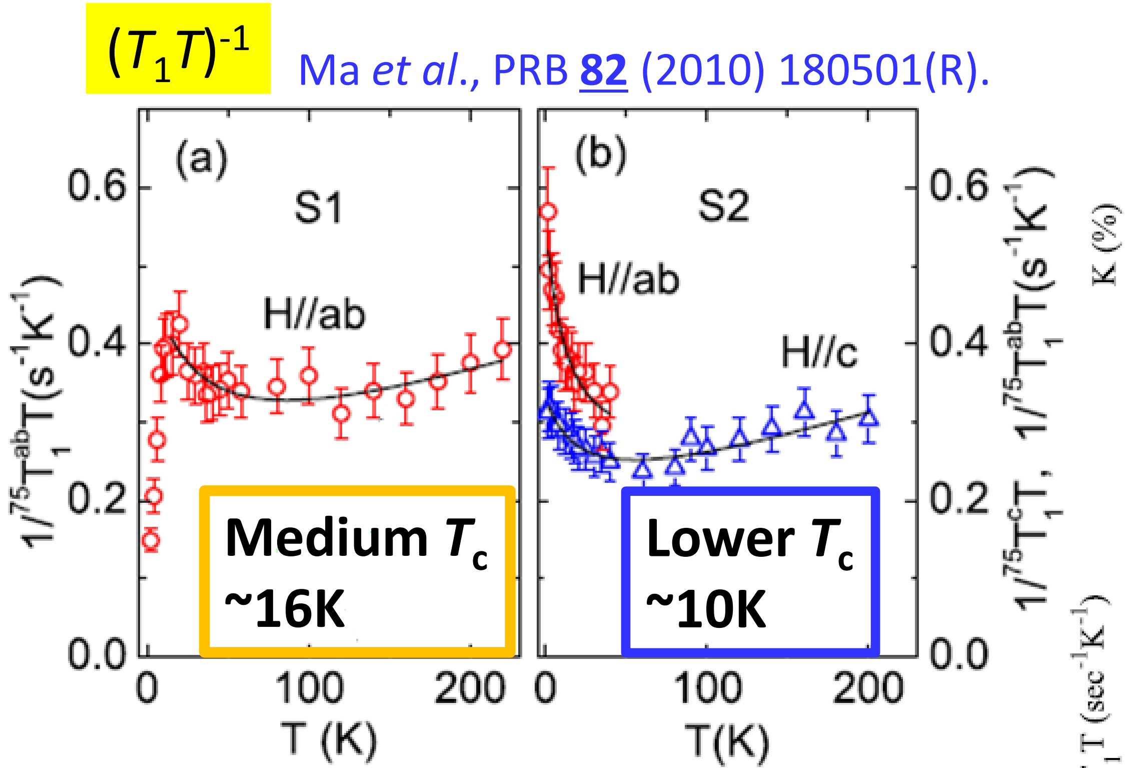
✓Coexistence is suggested.

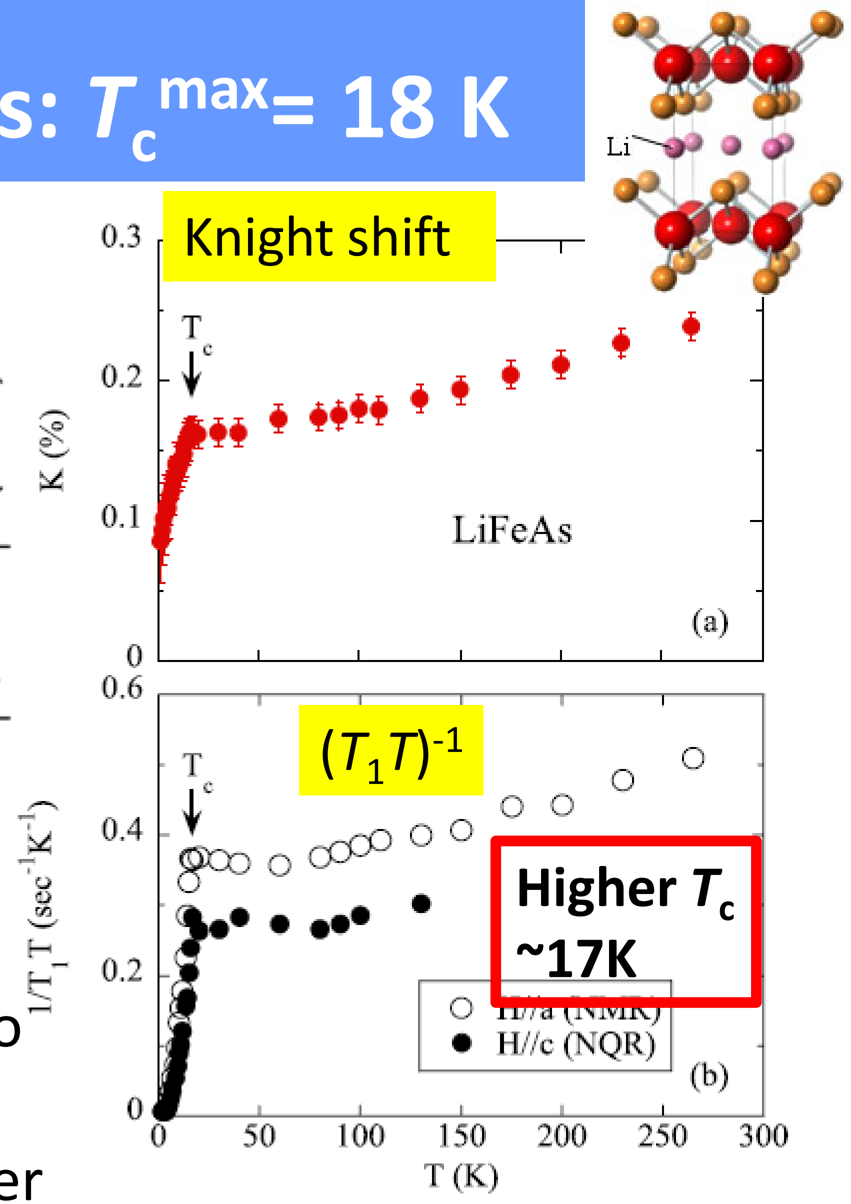
Laplace *et al*., Phys. Rev. B **80**, 140501 (2009).

Relation between antiferromagnetism and superconductivity appears different.

Clean single crystalline samples of 1111 are needed for clarifyng this issue.

111 Superconductor LiFeAs: T_c^{max}= 18 K





✓Strength of spin fluctuations appears to depend on synthesis process.

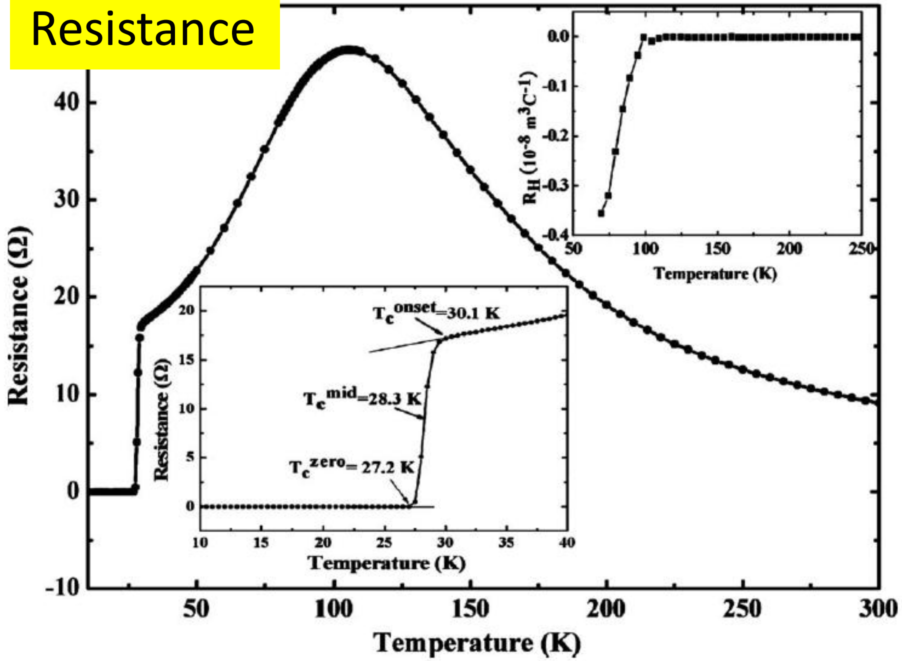
✓Lower T_c samples seem to have stronger AF spin fluctuations.

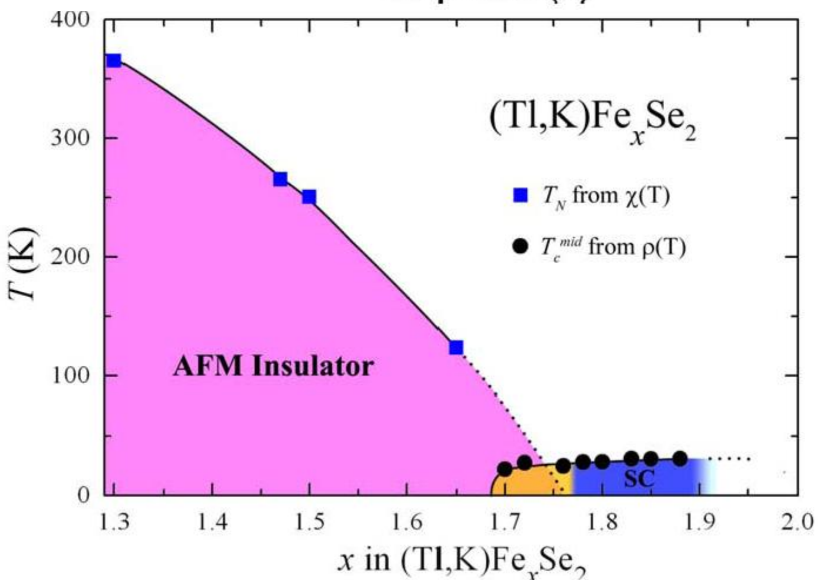
Li *et al.*, JPSJ **79** (2010) 083702.

Systematic investigation on sample characterization is needed.

New high-T_c superconductor $A_yFe_{2-x}Se_2$ T_c up to 40 K (122 structure)

Resistance





J. Guo *et al.*, PRB **82** (2010) 180520(R)

✓Alkali-metal intercalation in between FeSe layers induces a T_c of 30 K in $K_{0.8}Fe_2Se_2$.

M. Fang *et al.*, arXiv:1012.5236.

✓By tuning Fe vacancies, AFM insulators turn into high-T_c superconductors.

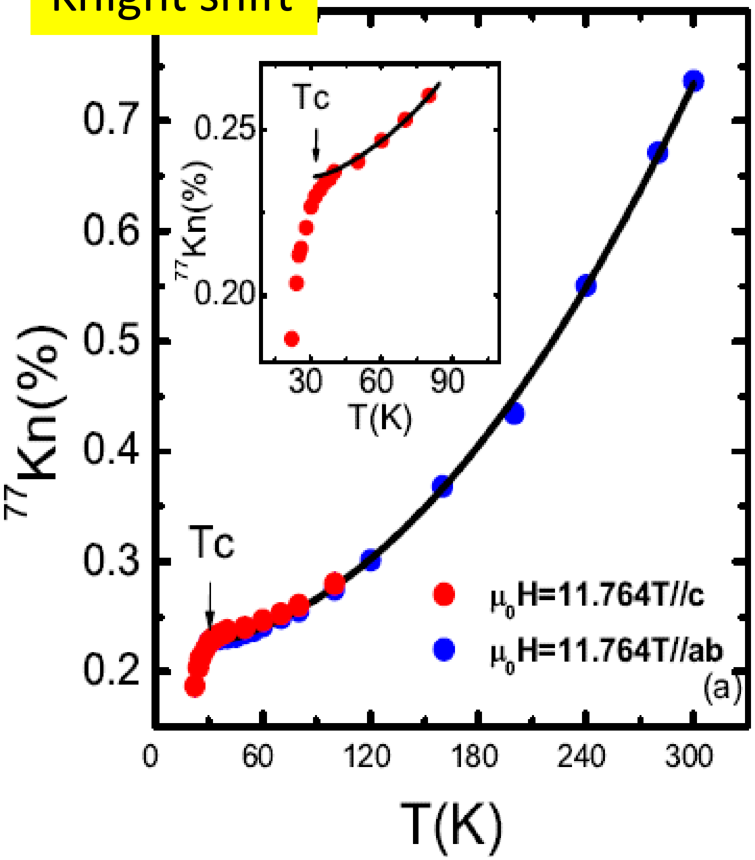
✓Similar to the phase diagram of high-T_c cuprates.

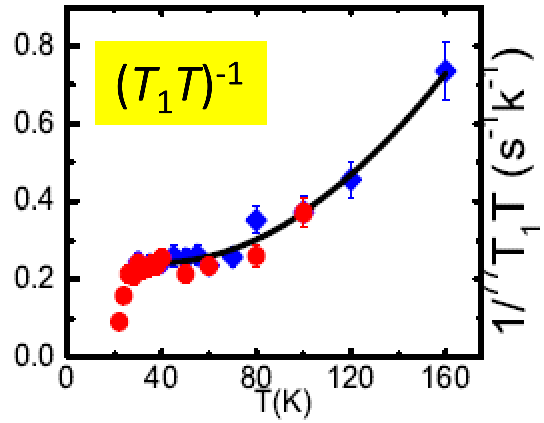
Strong electron correlation plays a role??

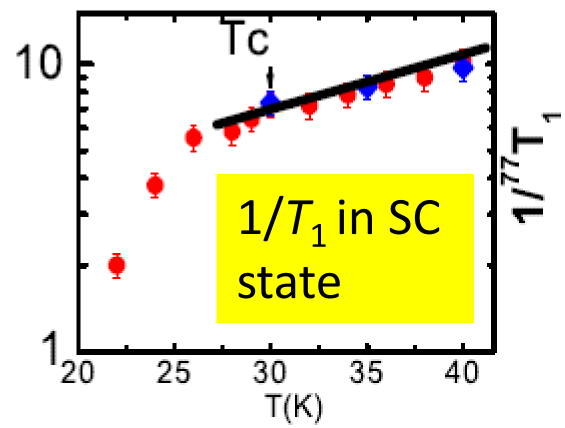
^{77}Se NMR study on $K_{0.8}Fe_{2-x}Se_2$ (T_c = 30 K)

W. Yu *et al.*, arXiv:1101.1071.

Knight shift







✓No enhancement of $(T_1T)^{-1}$ at low T.

✓Korringa law holds (T_1TK^2 = const.)

Fermi liquid

✓No Hebel-Slichter coherence peak?

✓K decreases on cooling.

✓Likely to be spin-singlet.

Issue to be clarified

Absence of spin fluctuations despite its high T_c?

Fe NMR would be very important.

Summary

✓Behavior of spin susceptibility is likely to originate from the DOS at E_F, as inferred from the Knight shift of P-, K-, &Co-doped $BaFe_2As_2$.

✓AFM fluctuations with itinerant 2D nature are largely changed by Co & P substitution, and *a QCP is suggested at optimal concentration for P- & Co-doped $BaFe_2As_2$.*

✓*Similar positive correlation between AFM fluctuations & SC is also observed for stoichiometric FeSe.*

AFM fluctuations likely play a crucial role for superconductivity in the 122 & 11 systems.

However...

Correlation between spin fluctuations & SC is weak in $LaFeAs(O_{1-x}F_x)$.

This may be also the case for newly discovered $K_{1-y}Fe_{2-x}Se_2$.