

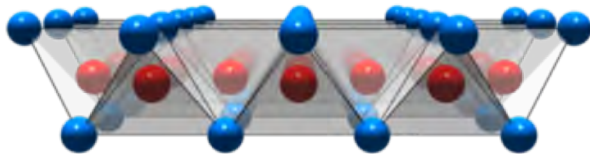
Strain dependent transport and nematicity in Fe based superconductors

Bernd Büchner

IFW Dresden

TU Dresden

GRK 1621



Deutsche
Forschungsgemeinschaft
DFG



Leibniz Institute
for Solid State and
Materials Research
Dresden

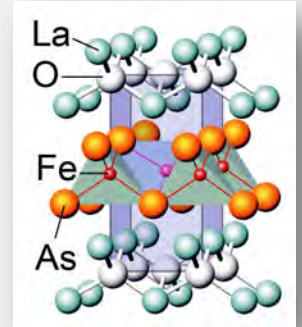


**TECHNISCHE
UNIVERSITÄT
DRESDEN**

OUTLINE

Nematic fluctuations in doped La1111 crystals

- Doped LaOFeAs: an „extraordinary“ Fe based SC
- Magnetic & nematic transitions in LaOFeAs
- Phase diagram of Co-doped LaOFeAs
- Nematic fluctuations in (doped) LaOFeAs



(Development of) methods for strain dependent ...

- Strain dependent NMR on BaFe_2As_2 ; strain up to $(-0.86\%; 0.42\%)$
- Elasto-Seebeck effect on Fe based superconductors
- Elasto-Nernst effect on Fe based superconductors
- ARPES@1³ beamline under strain (ongoing)

Thanks to

Synthesis

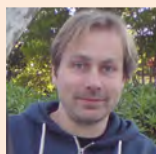


S. Aswartham

S. Wurmehl, **R. Kappenberger**, S. Khim
J. M. Ok, J. S. Kim
S. Ran, L. Bud'ko, P. C. Canfield

IFW Dresden
U Pohang
Ames Lab.

NMR/NQR



H. Grafe



S.H. Baek

G. Lang, P. Lepucki
F. Hammerath, A. Dioguardi
P. Carretta, S. Sanna, G. Prando

IFW Dresden
U. Pavia

Nematic susceptibility



C. Hess

C. Hess, C. Wuttke, **F. Caglieris**, **X. Hong**
F. Wissmann, F. Steckel, s. Sykora

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Thermodynamics Magnetization

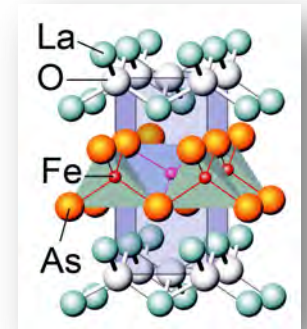
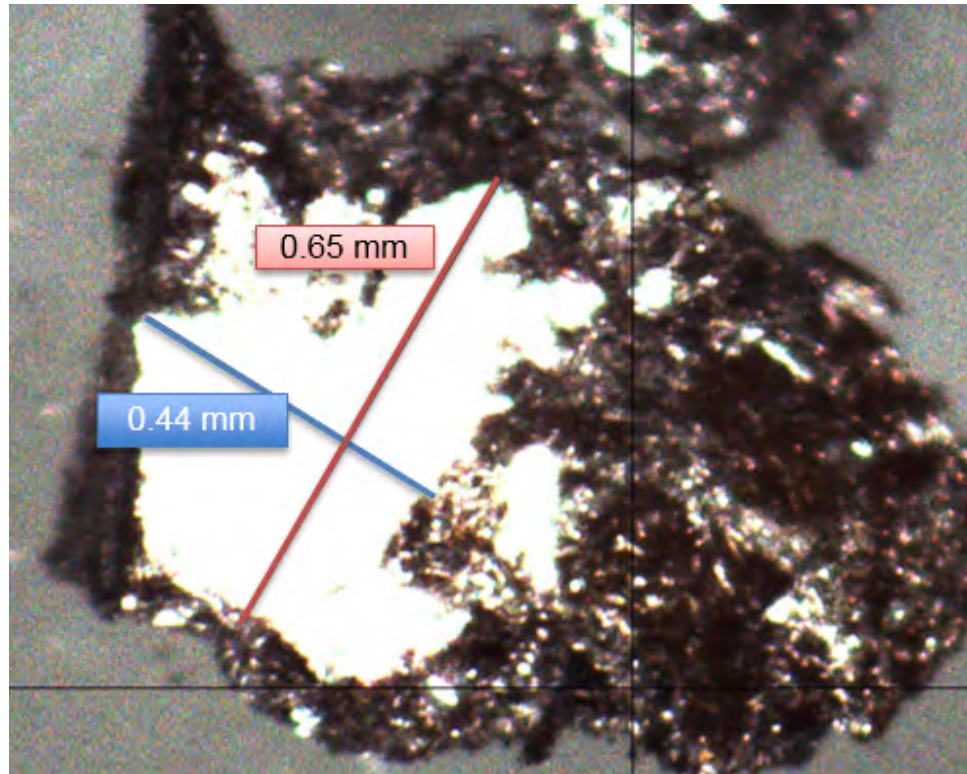


A. Wolter

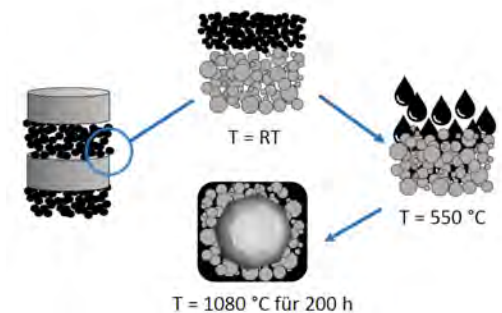
F. Scaravaggi
L. Wang, S. Sauerland, R. Klingeler

IFW Dresden
U Heidelberg

Solid state single crystal growth of LaOFeAs

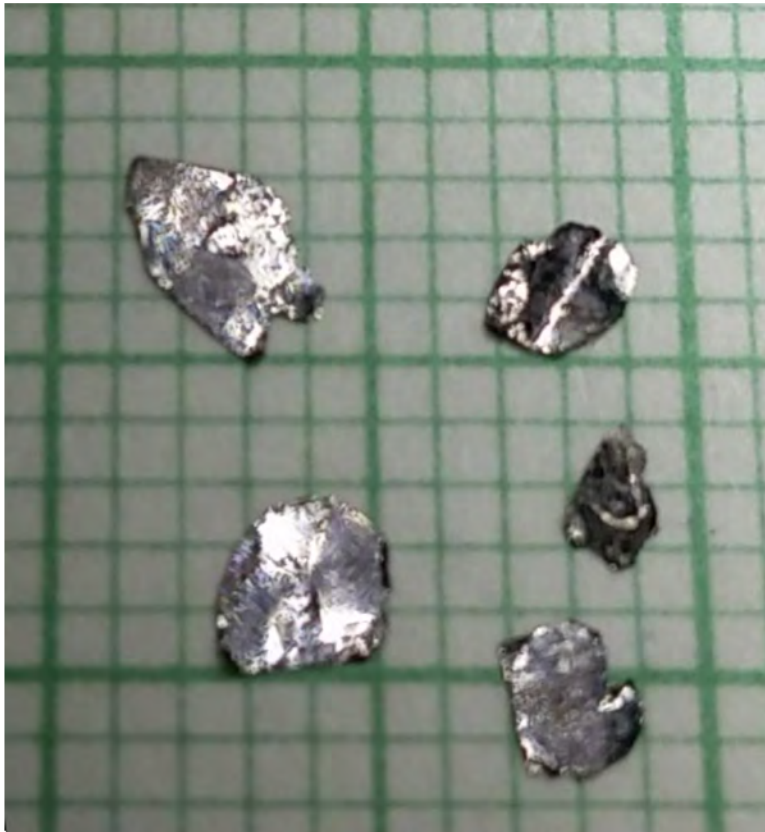


- Subsequent sintering of LaFeAsO polycrystals leads to the formation of crystals
- Optimization of process → large faceted crystals (Solid State Crystal Growth (SSCG))

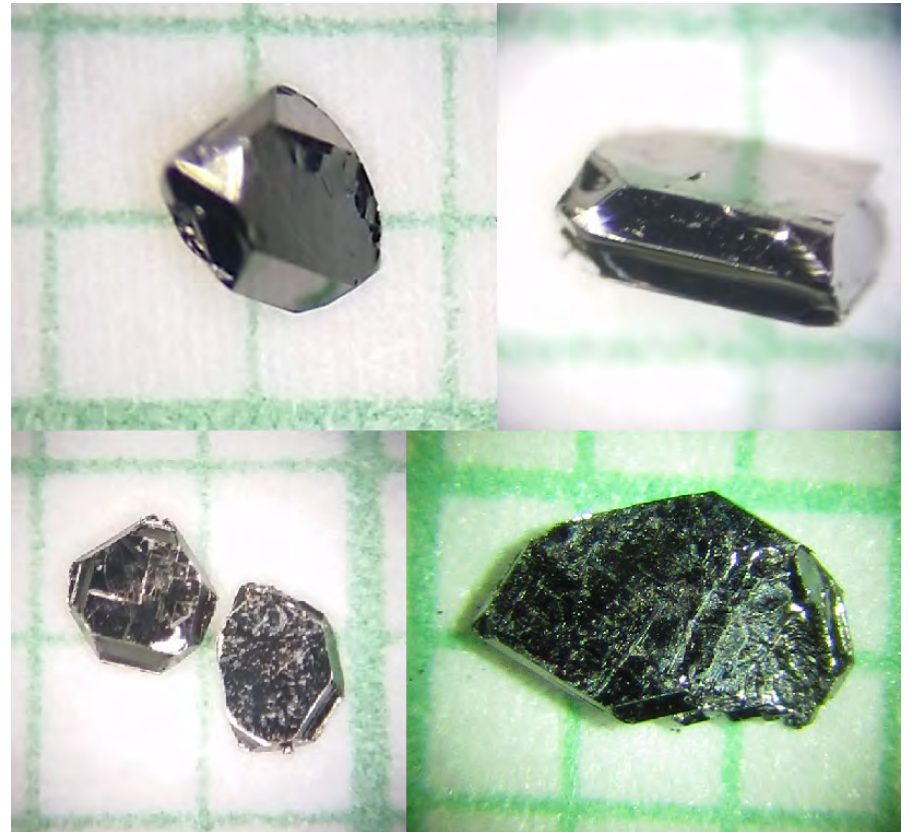


LaOFeAs crystals

24 h @ 1080° C:

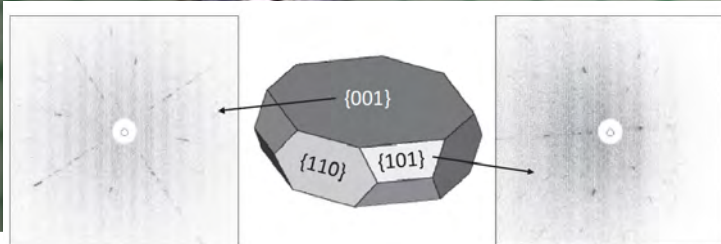
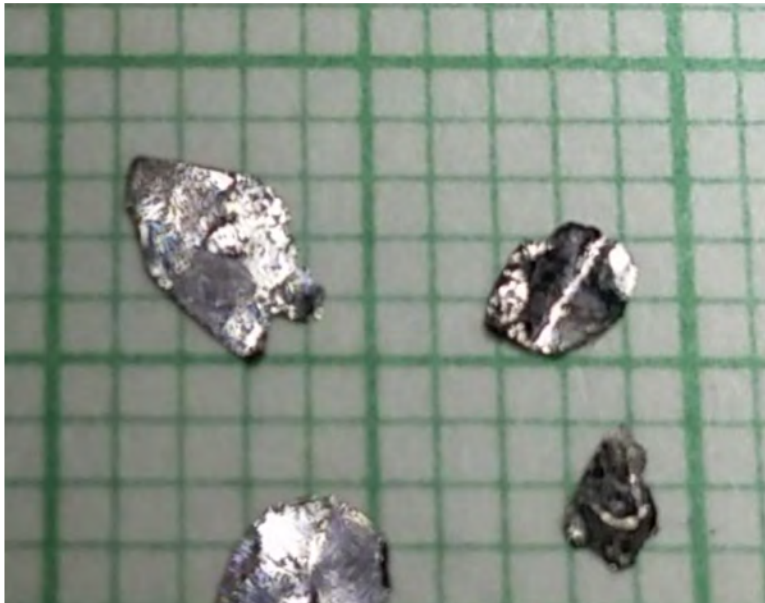


200 h @ 1080° C:

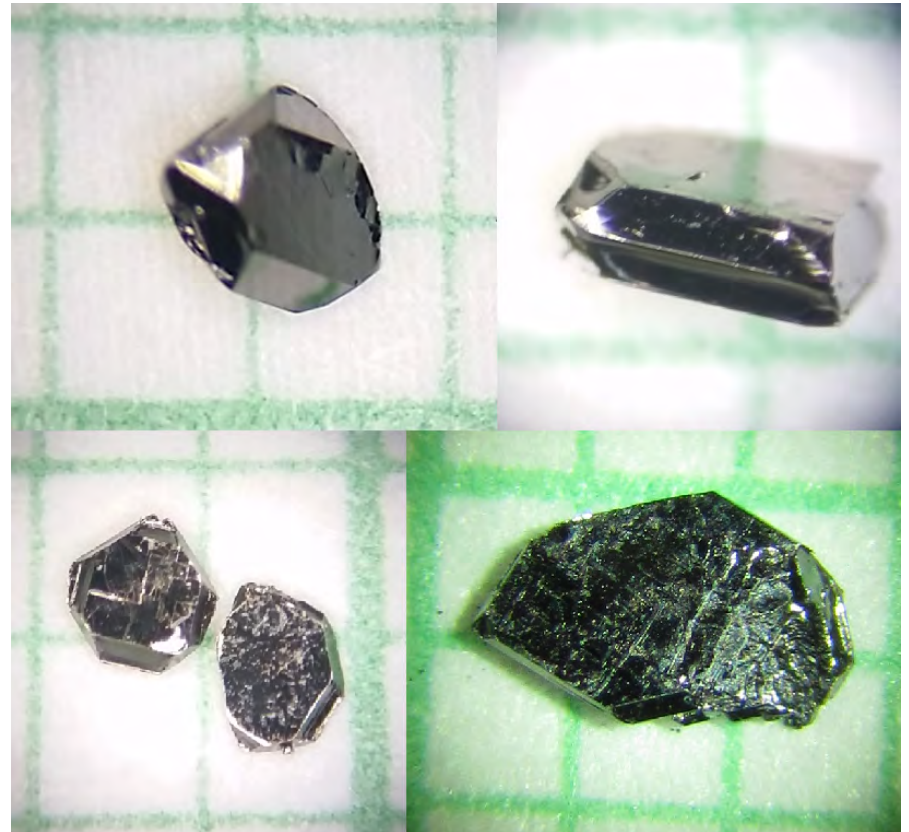


LaOFeAs crystals

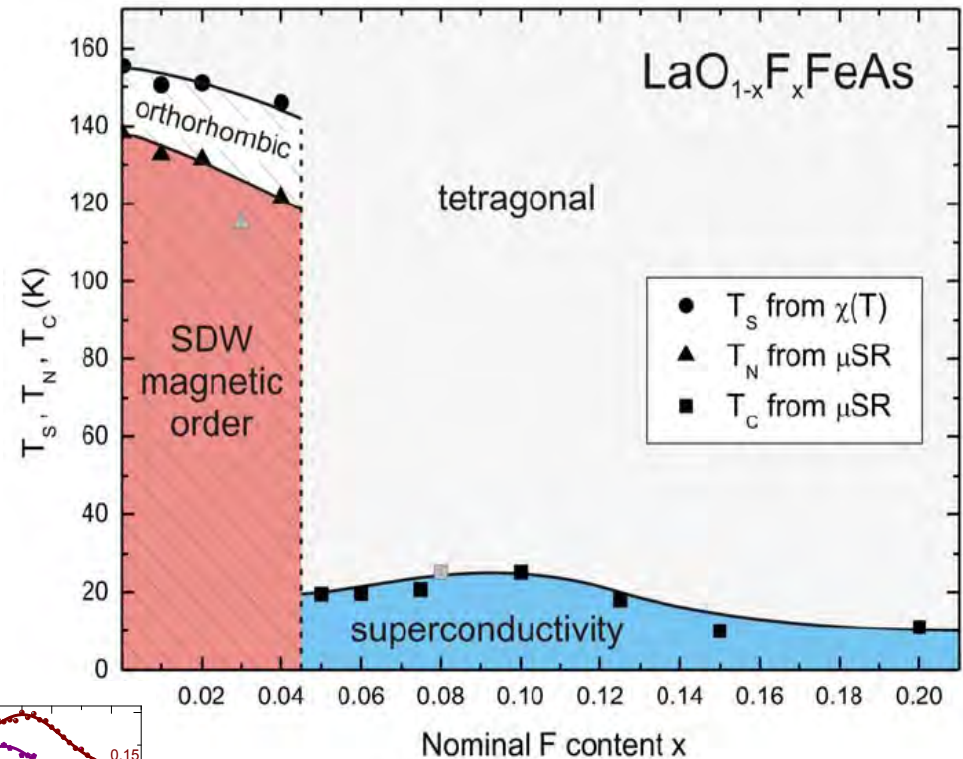
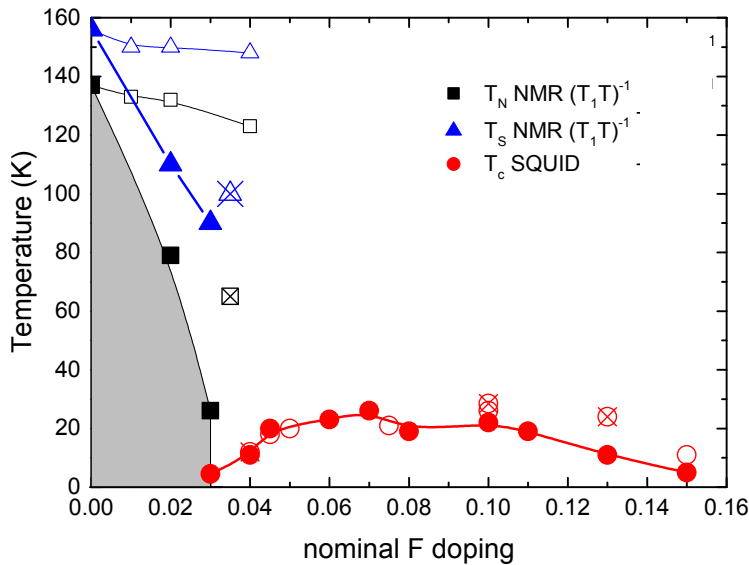
24 h @ 1080° C:



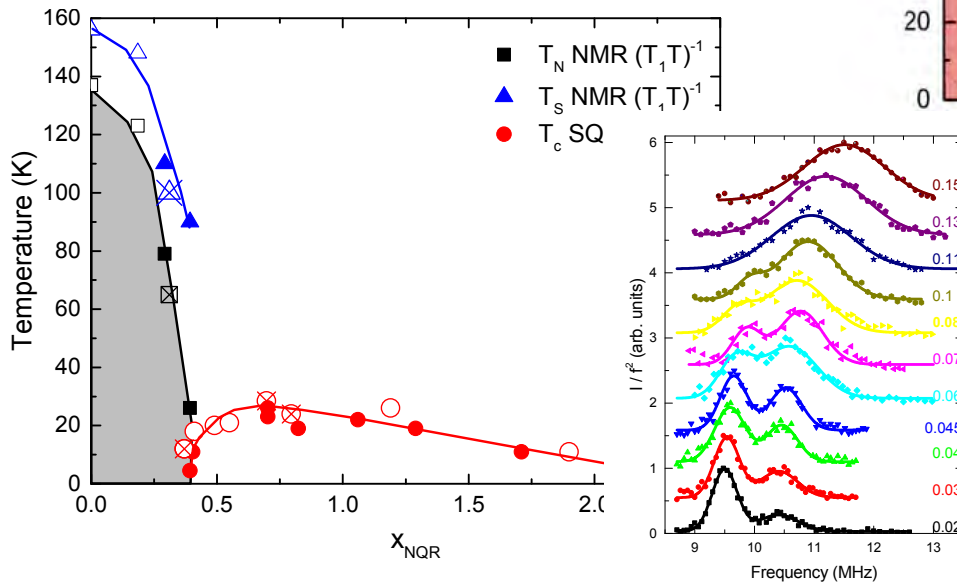
200 h @ 1080° C:



Phase diagram of F doped La 1111: Revisited

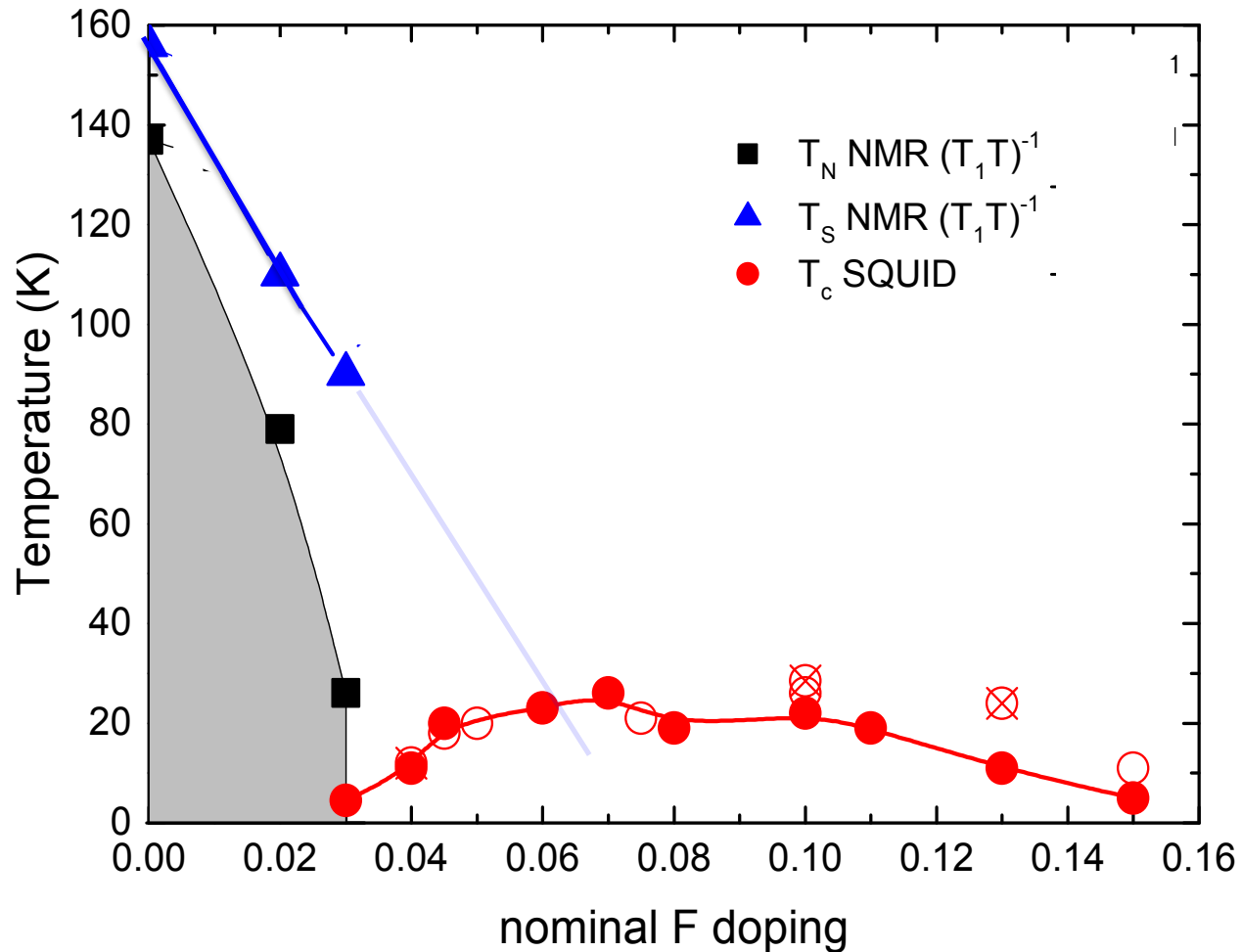


H. Luetkens, BB et al., Nat. Mat. (2009)



- Rapid suppression of T_N
 - Clear separation between T_S and T_N
 - No coexistence of SC and AFM for La1111
- non-magnetic underdoped phase

Revised phase diagram of F doped La 1111

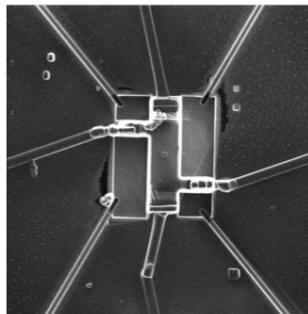
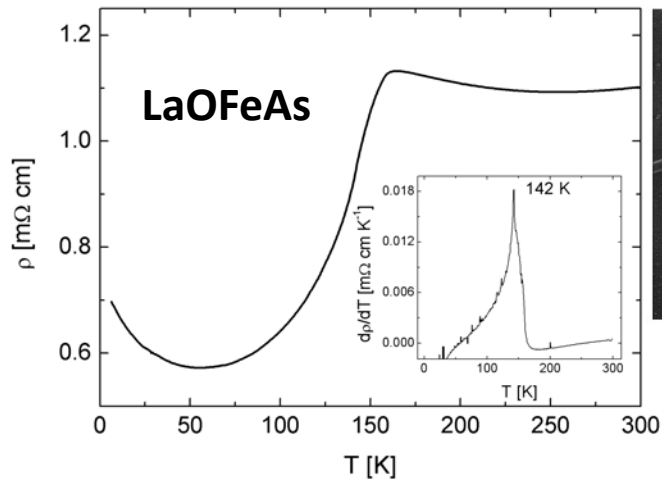


- Rapid suppression of T_N
 - Clear separation between T_S and T_N
 - No coexistence of SC and AFM for La₁₁₁₁
- non-magnetic underdoped phase

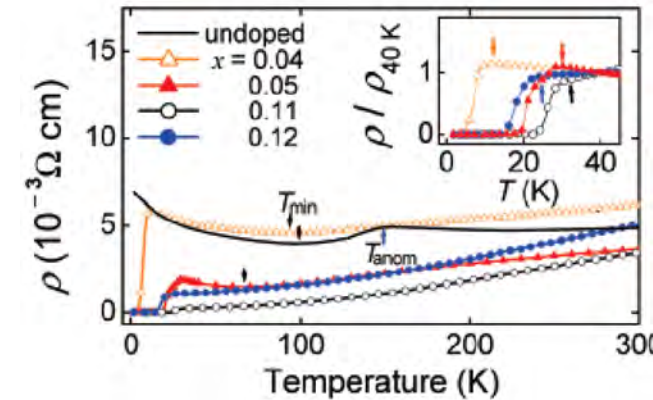
Fe based SC: good and/or bad metals?

Most Fe based superconductors are “good metals”

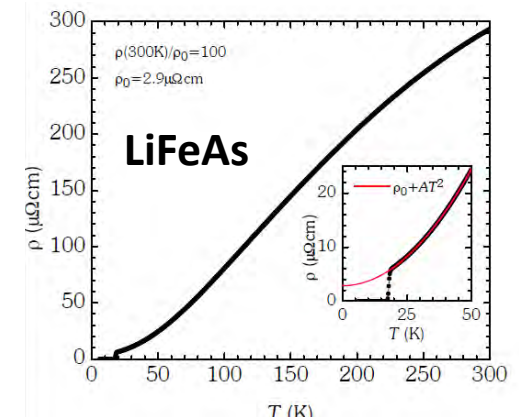
Exception: 1111 (in particular doped LaOFeAs)



F. Caglieris, M. Fujioka et al.

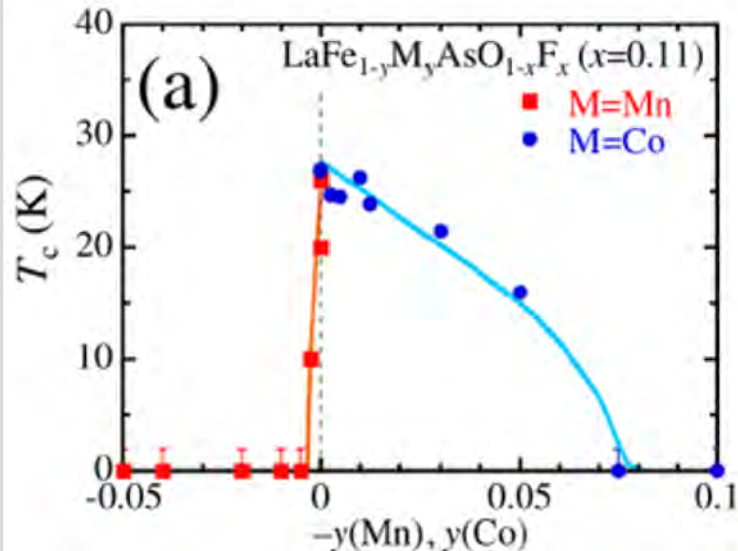


Y. Kamihara et al., J. Am. Chem. Soc. 2008



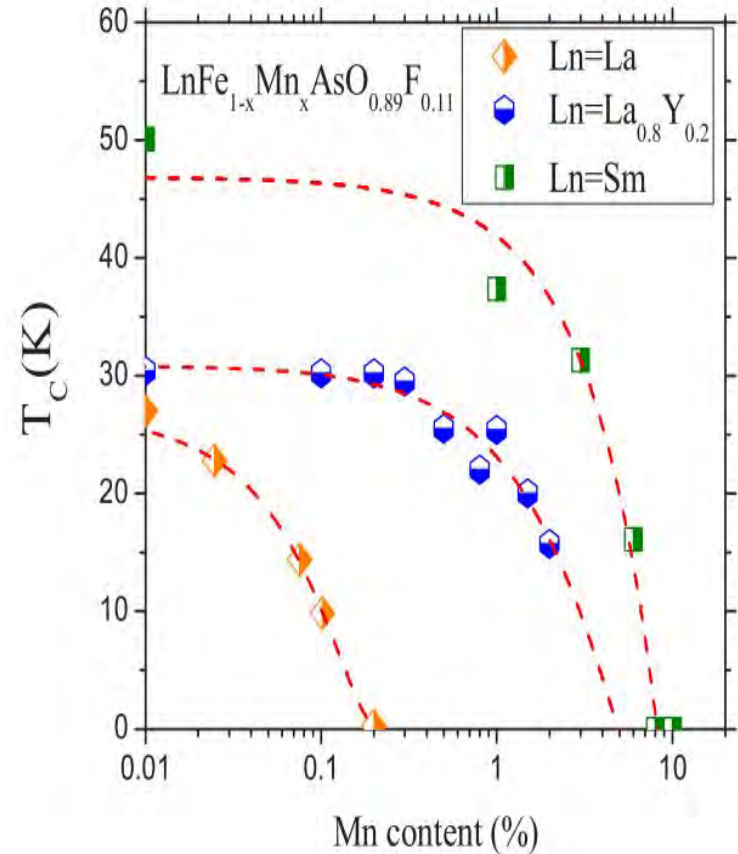
O. Heyer, C. Hess, BB et al., PRB 2011

Poisoning effect of Mn doping in La 1111



Substitution of Fe by tiny amounts of Mn
→ Drastic suppression of superconductivity

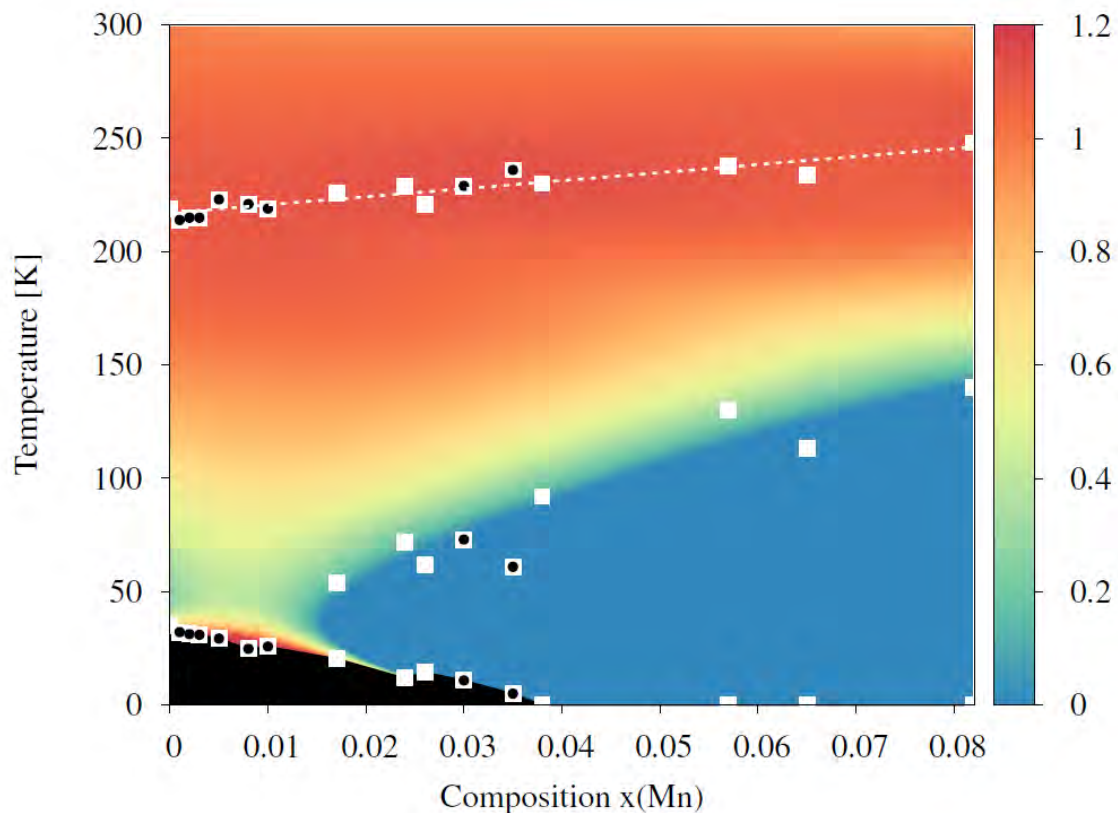
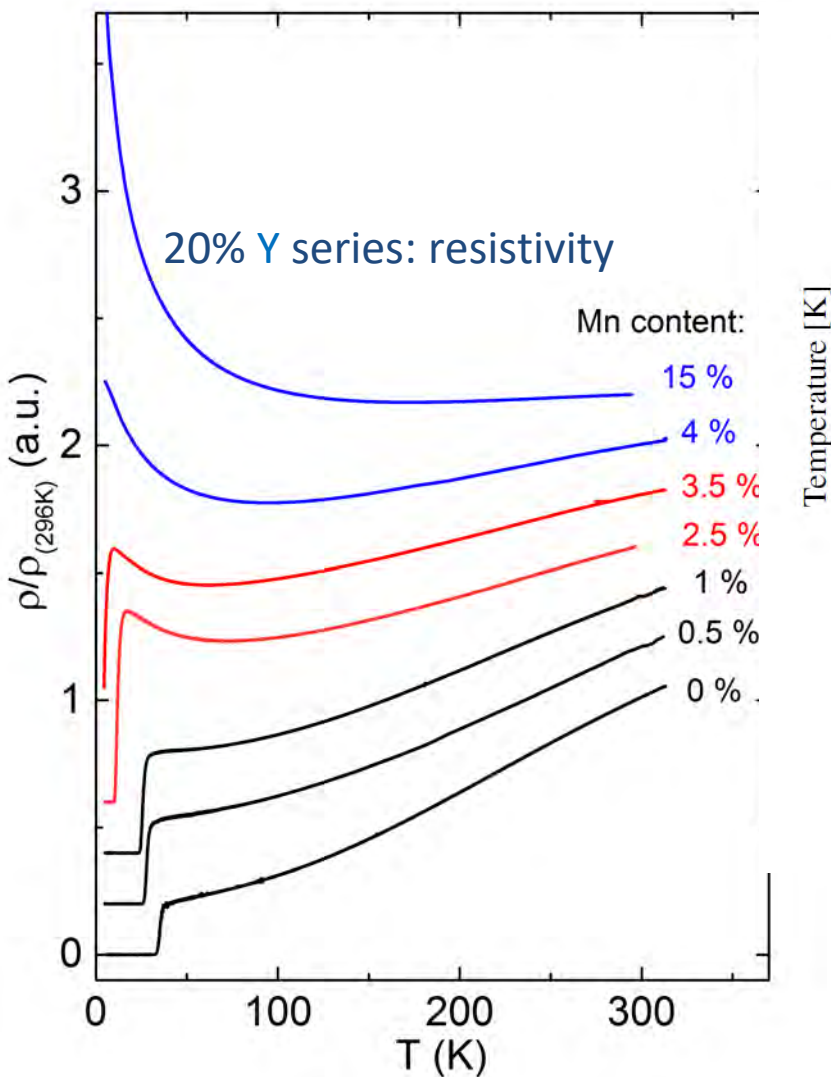
M. Sato et al. , J. Phys. Soc. Jpn. 2010



Suppression is stronger
for $\text{La} > (\text{La}, \text{Y}) > \text{Sm}$

F. Hammerath P. Carretta, BB et al.
Phys. Rev. B(R) 2015

Poisoning effect of Mn doping in La 1111



Substitution of Fe by tiny amounts of Mn

→ drastic suppression of superconductivity

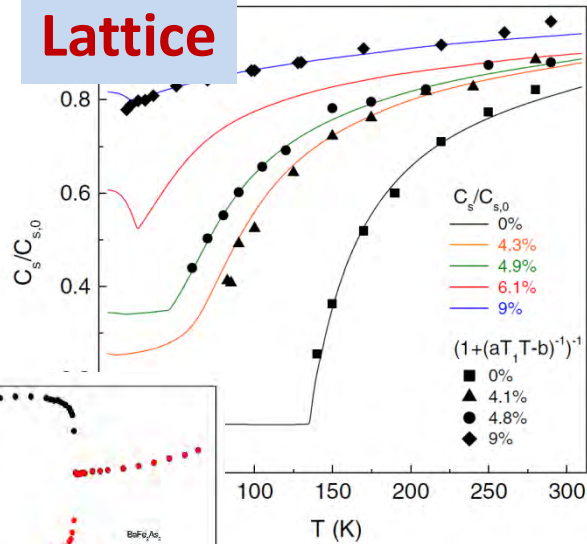
→ localisation of electrons

OUTLINE

- **Doped LaOFeAs: an „extraordinary“ Fe based SC**
- **Magnetic & nematic transitions in LaOFeAs**
- **Phase diagram of Co-doped LaOFeAs**
- **Nematic fluctuations in (doped) LaOFeAs**

Nematic order in Fe based SC

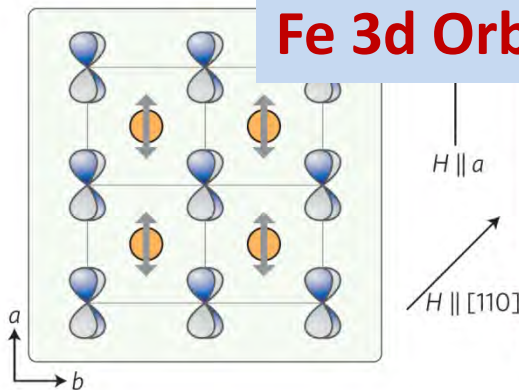
Lattice



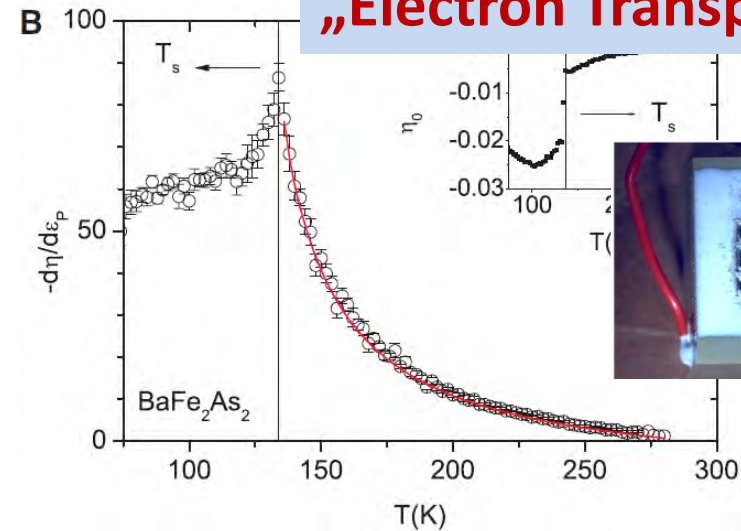
Comparison between the relative shear modulus lines, from Ref. [8]) and the rescaled NMR $1/T_1T$ (closed symbols, from Ref. [3]) for different “effective” Co concentrations in $\text{Ba}(\text{Fe}_{1-x}\text{Co}_x)_2\text{As}_2$. The

R.M. Fernandes, A.E. Böhmer, C. Meingast, and J. Schmalian, PRL 2013

Fe 3d Orbitals

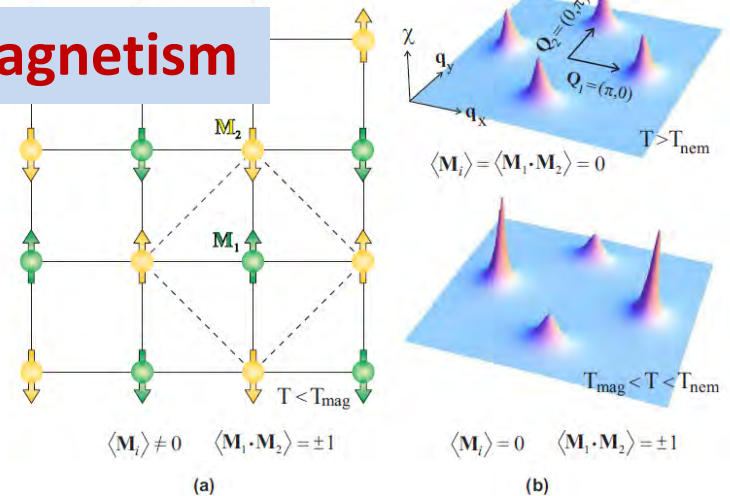


„Electron Transport“



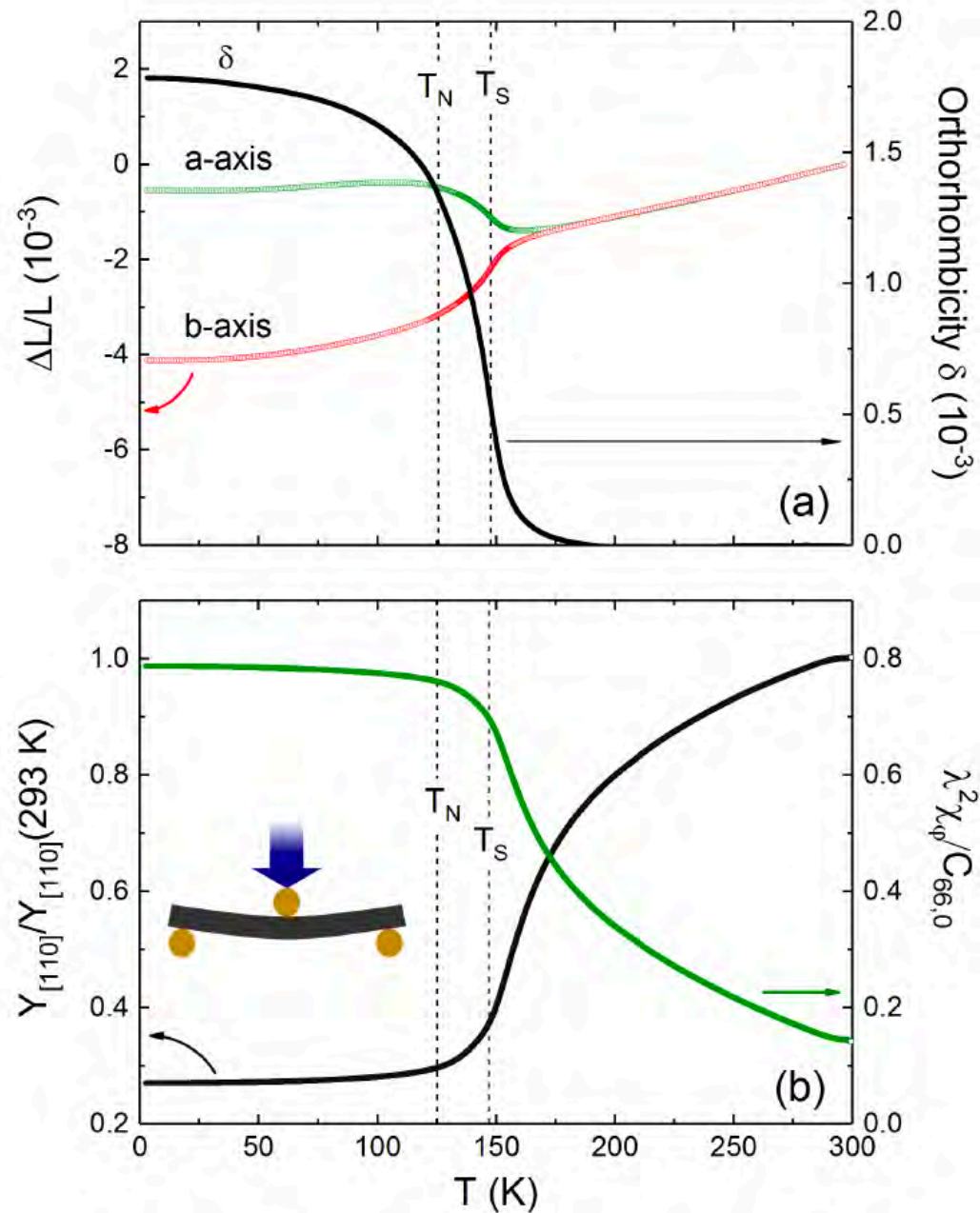
Chu et al. Science 2012

Magnetism

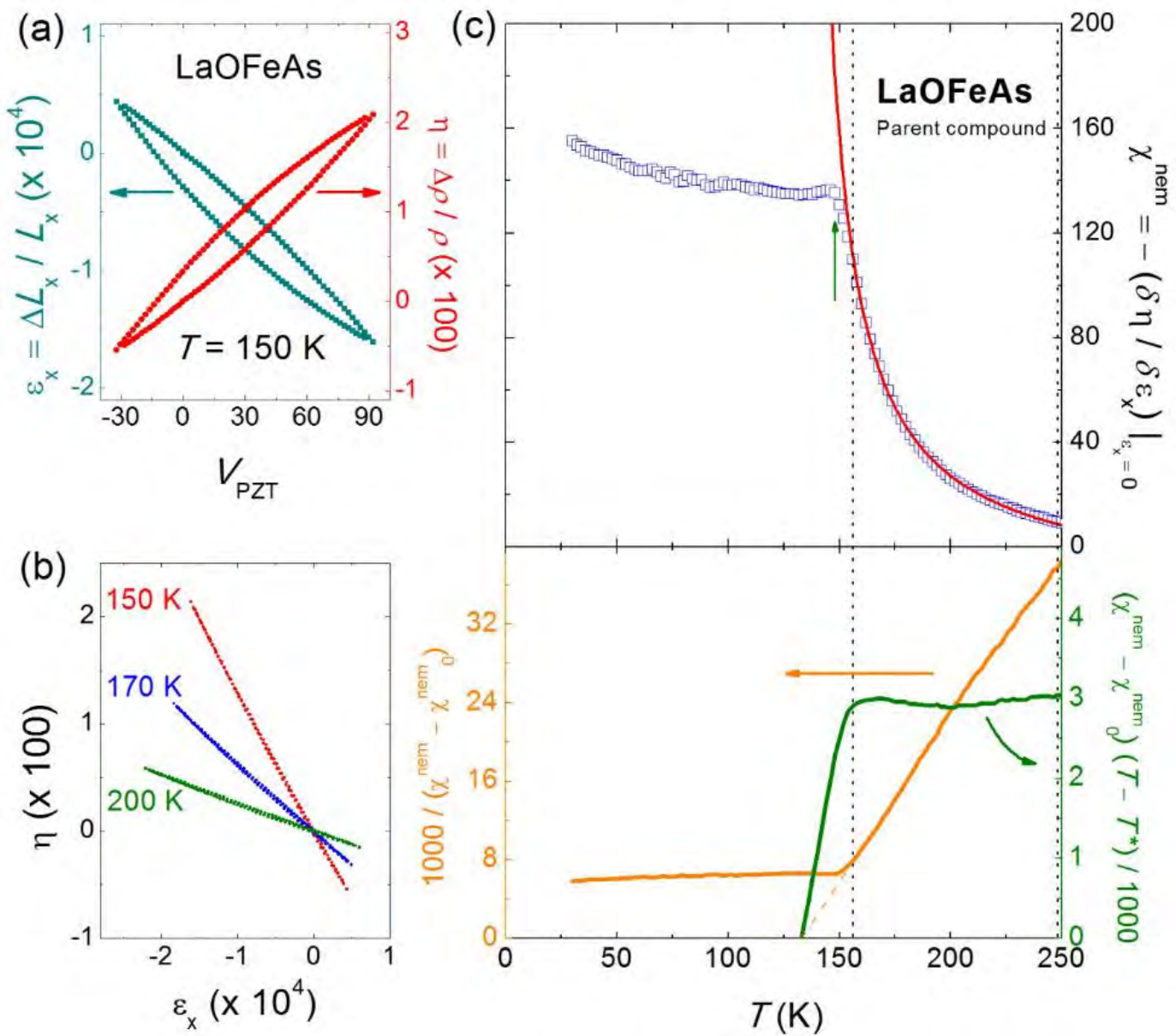
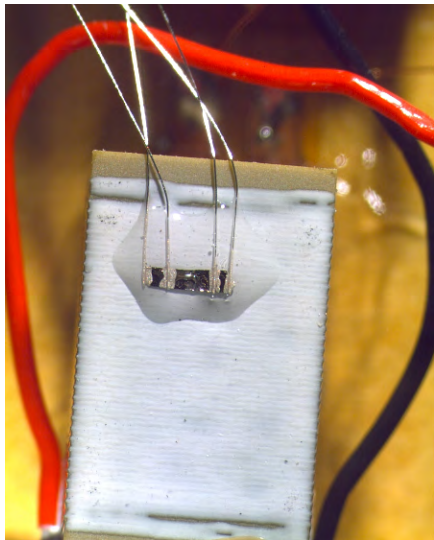


R. Fernandes, A. Chubukov, J. Schmalian Nat. Phys. 2014

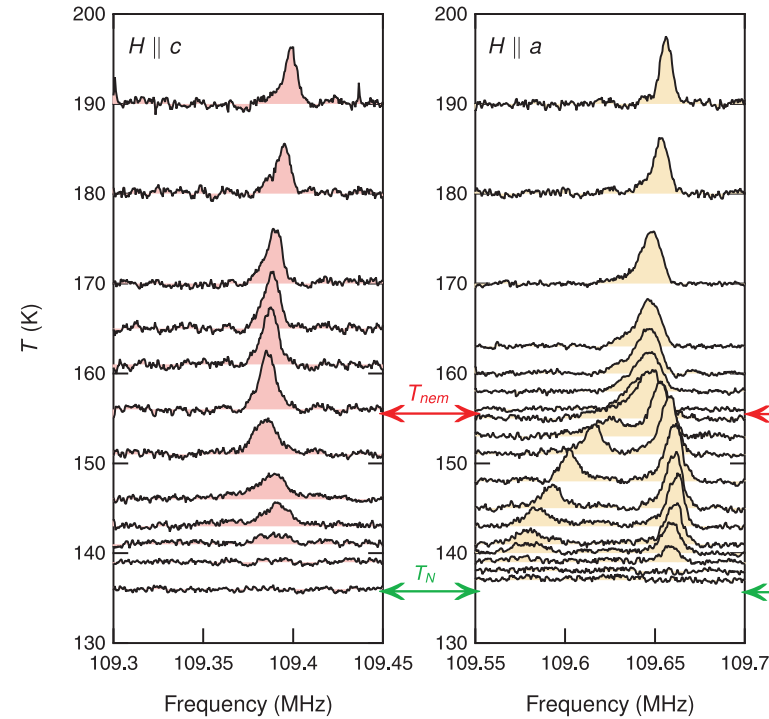
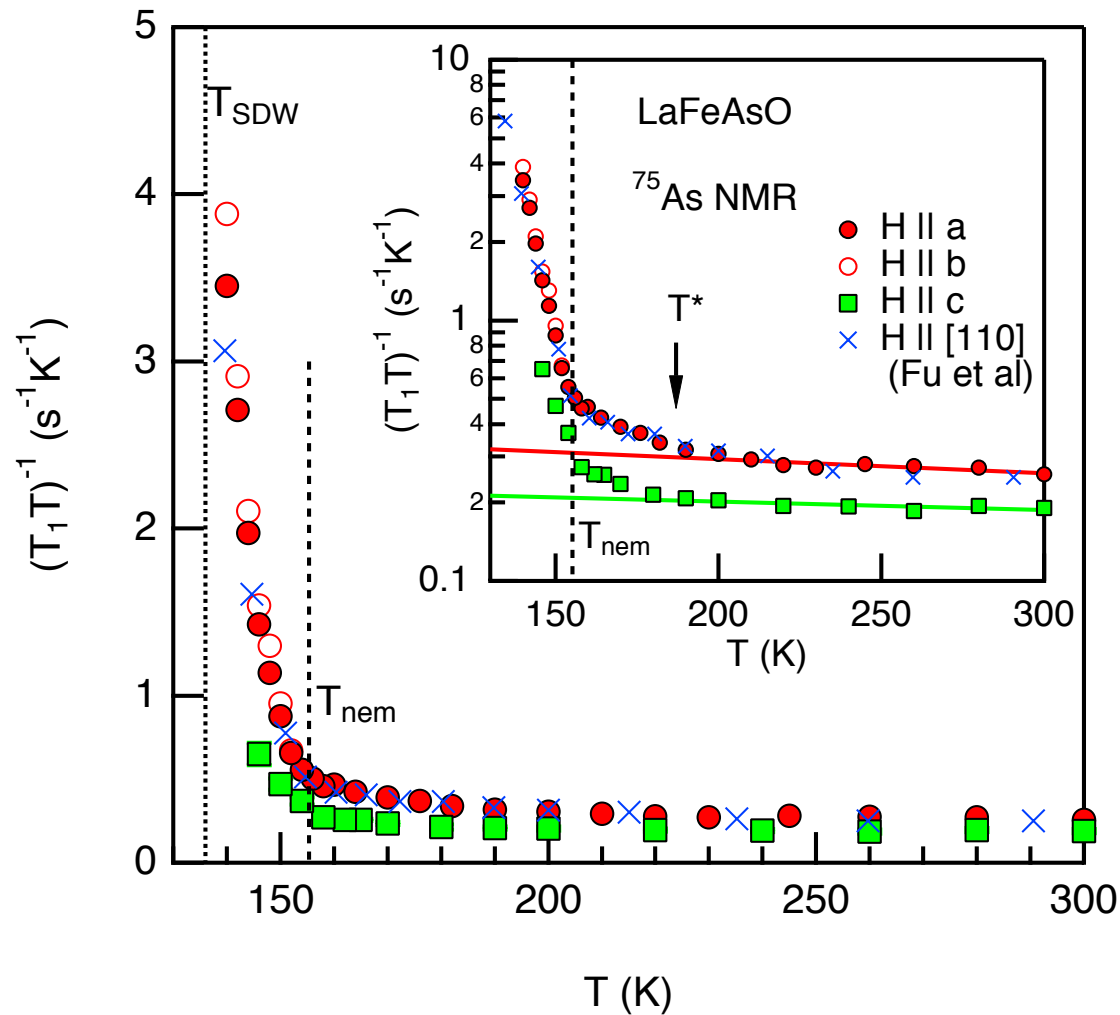
Nematic order in LaOFeAs: Structure, elastic constant



Nematic susceptibility of Co doped LaOFeAs



Nematic order in LaOFeAs: NMR



S. Baek, BB et al., Phys. Rev. B 2018

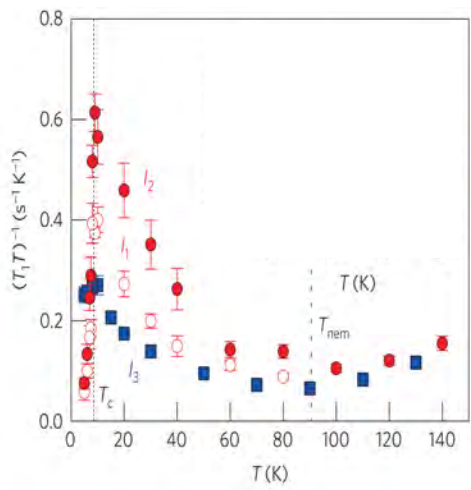
No clear evidence for magnetic instability above T_s

Strong (\gg FeSe) enhancement of slow spin fluctuations at T_s

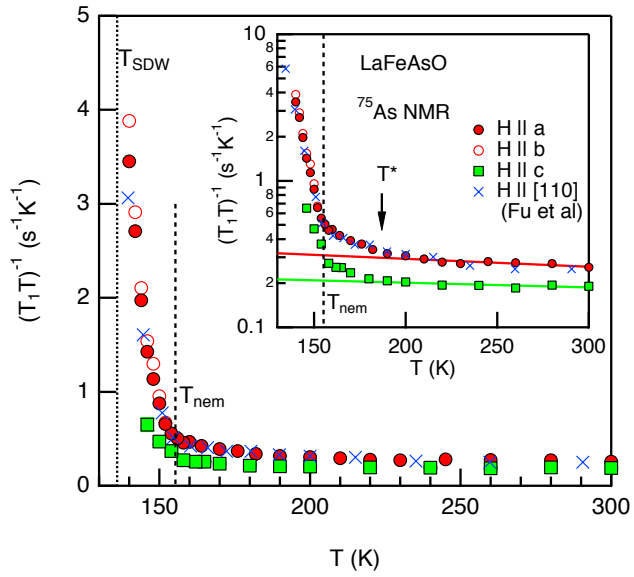
Nematic transitions of Fe based SC

Coupling between orbitals/lattice and (slow) spin fluctuations (NMR)

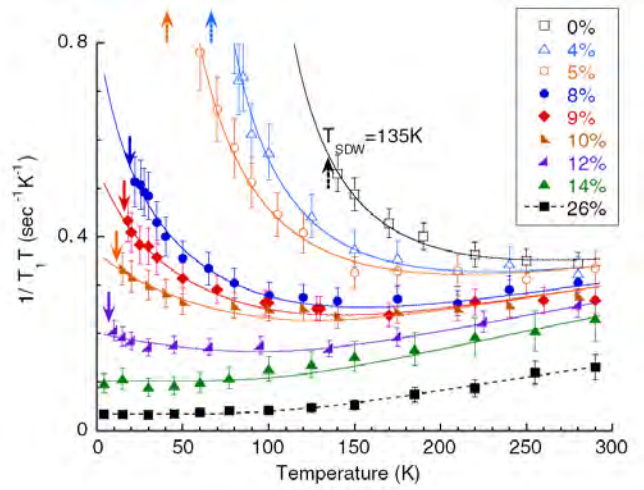
FeSe $T_N = 0$	LaOFeAs $T_N < T_S$	BaFe₂As₂ $T_N = T_S$
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S. Baek, BB et al., Nat. Mat. 2015

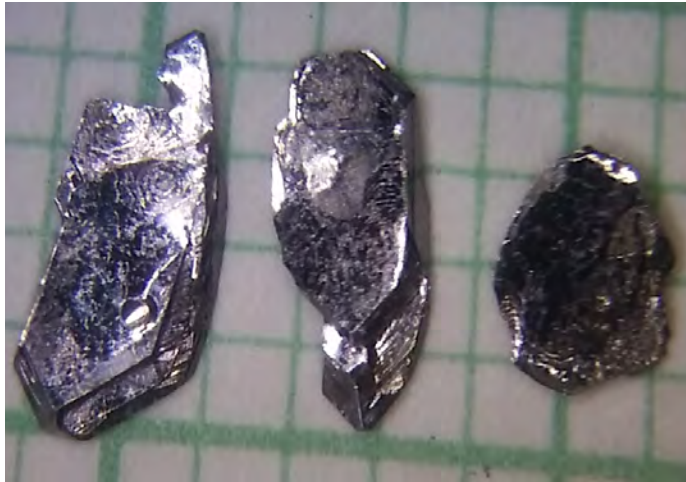


S. Baek, BB et al., Phys. Rev. B 2018



Ning et al. PRL 104, 037001 (2010)

Crystals of Co doped $\text{LaO}(\text{Fe},\text{Co})\text{As}$

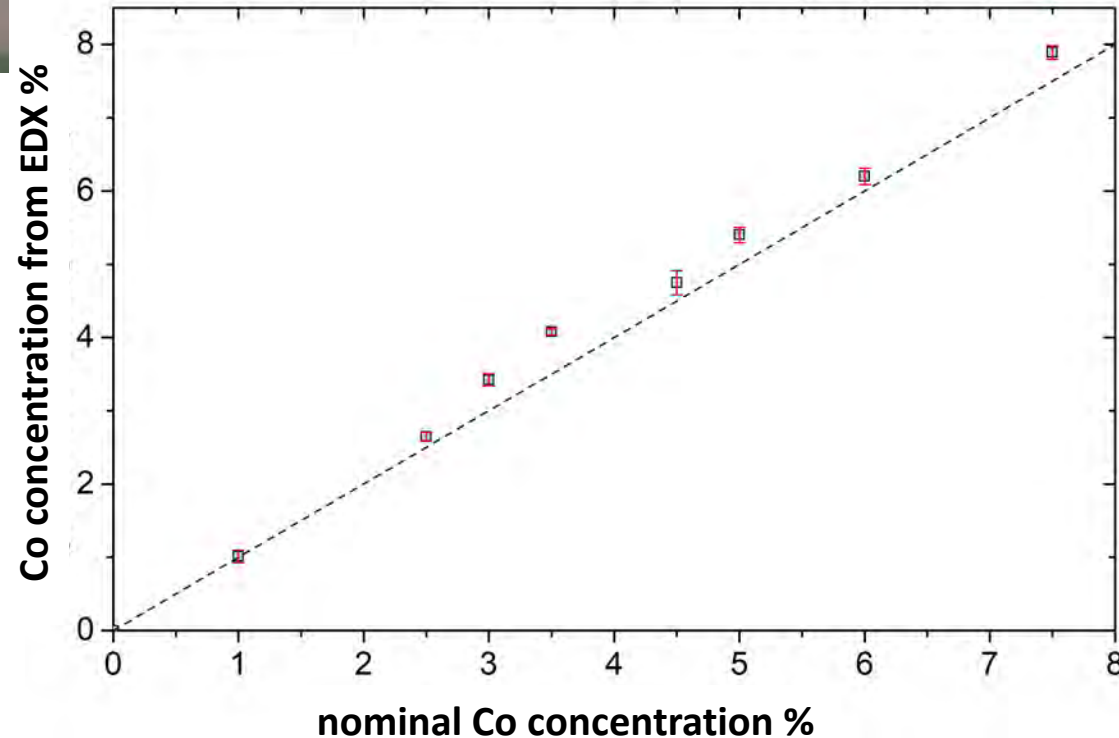


Co doping:

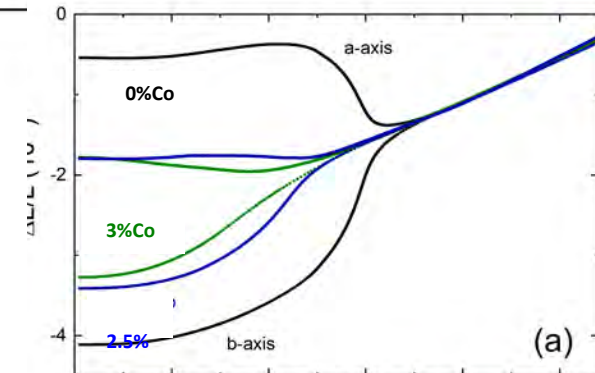
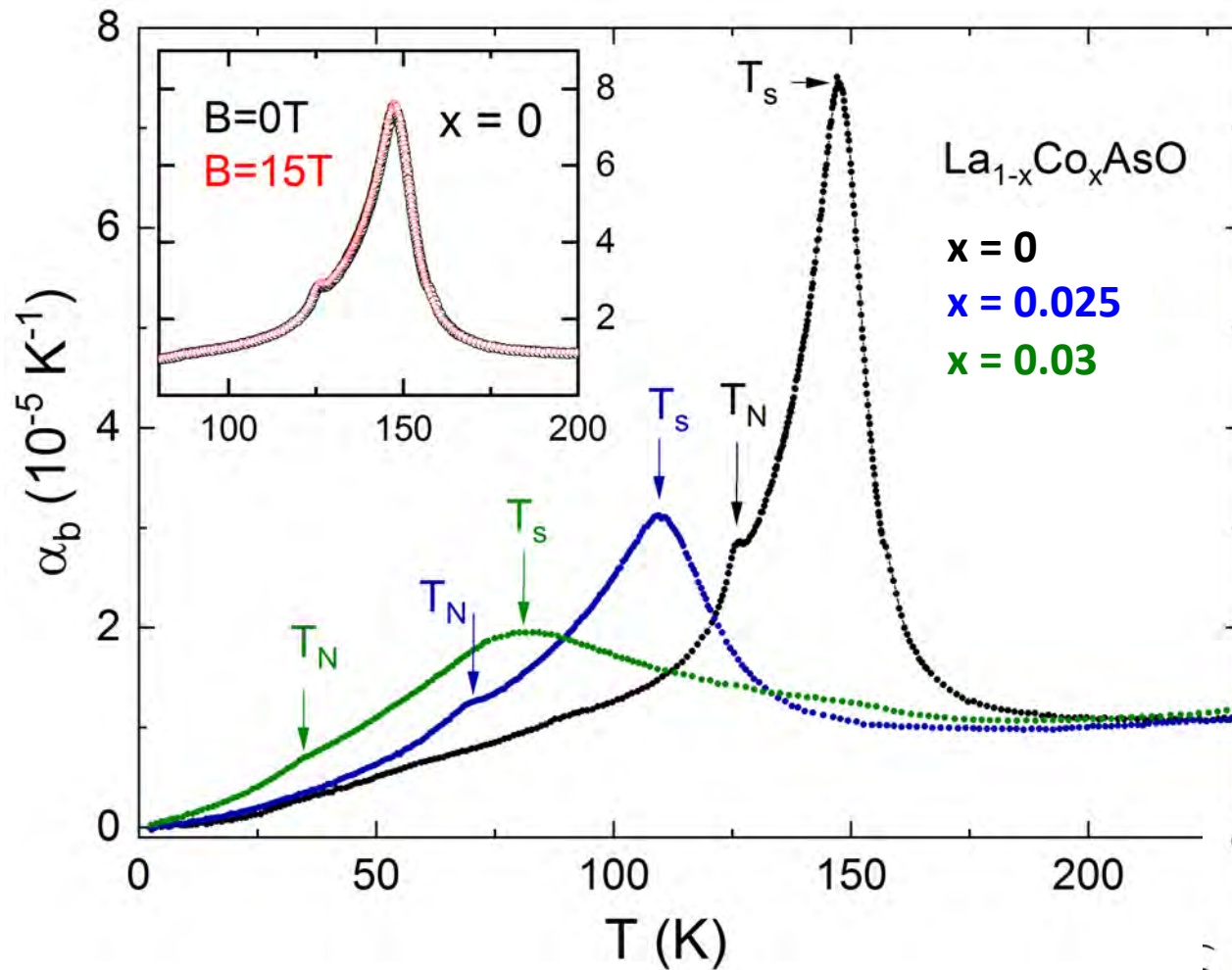
- electron doping
- impurities

work in progress

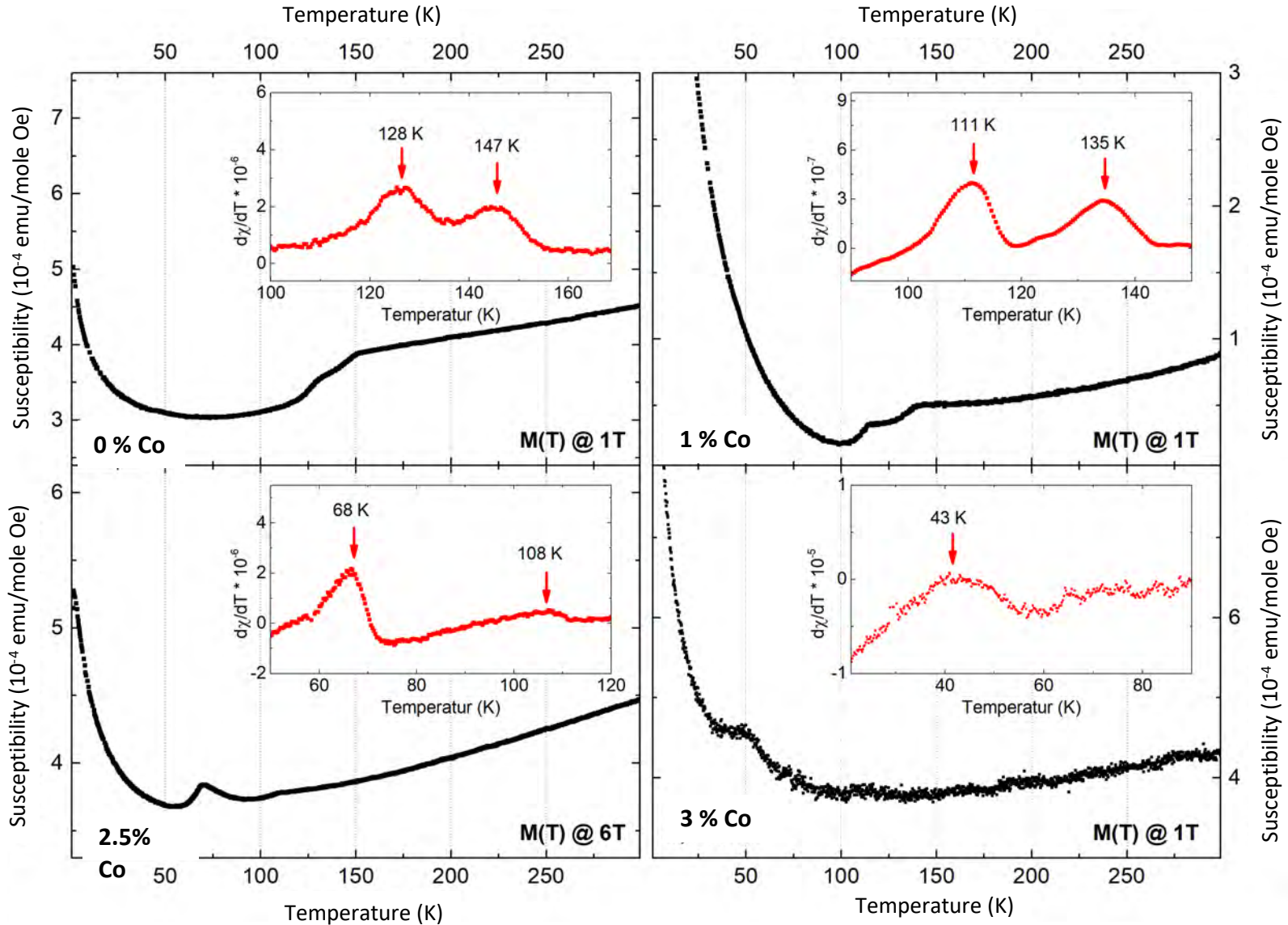
- fluorine doping
- Sm 1111
- Ce 1111
- ...



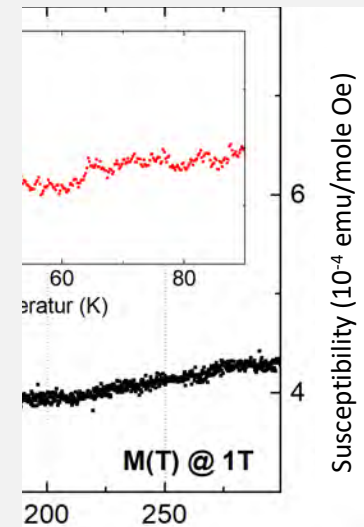
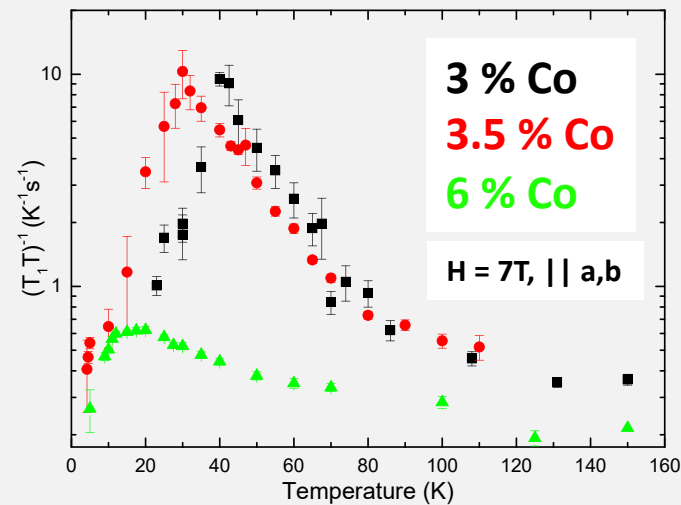
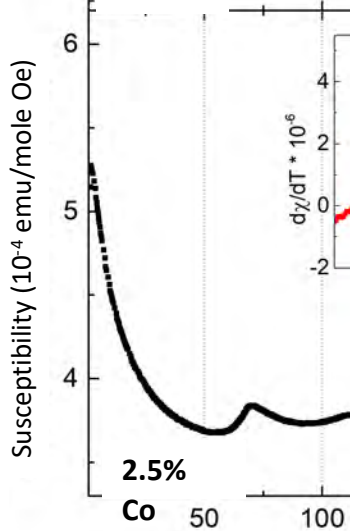
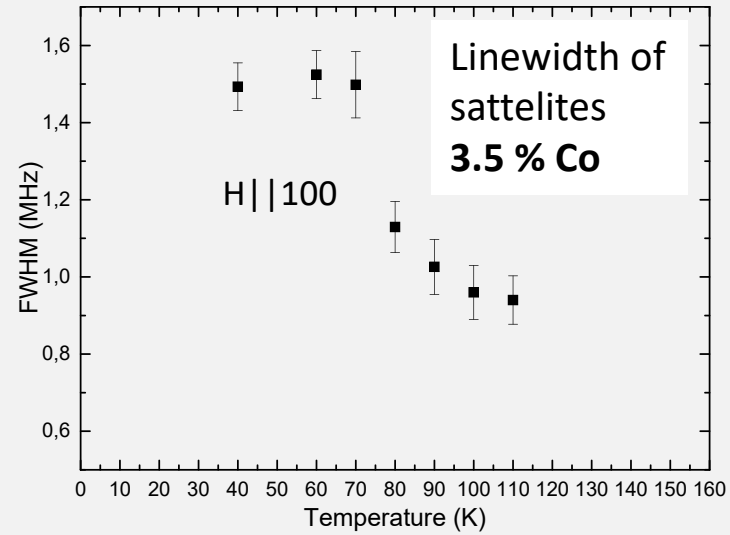
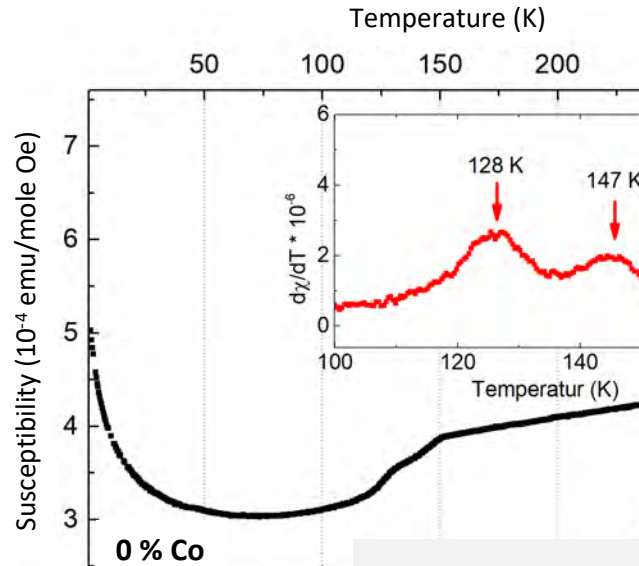
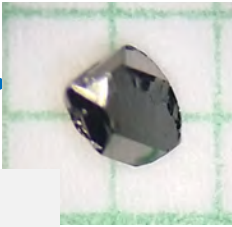
Phase diagram of Co-doped La 1111 revisited ...



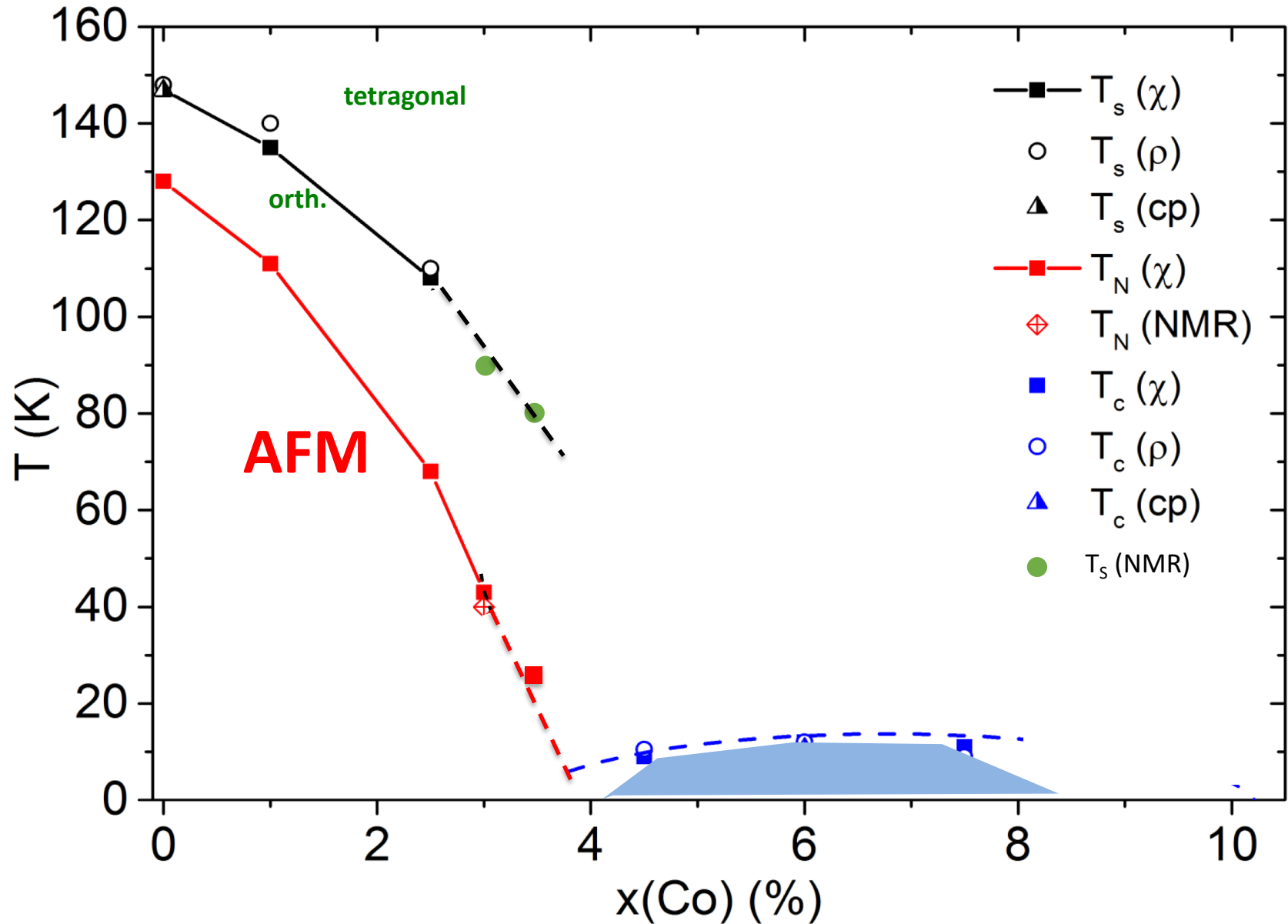
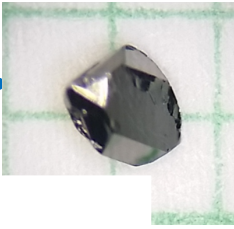
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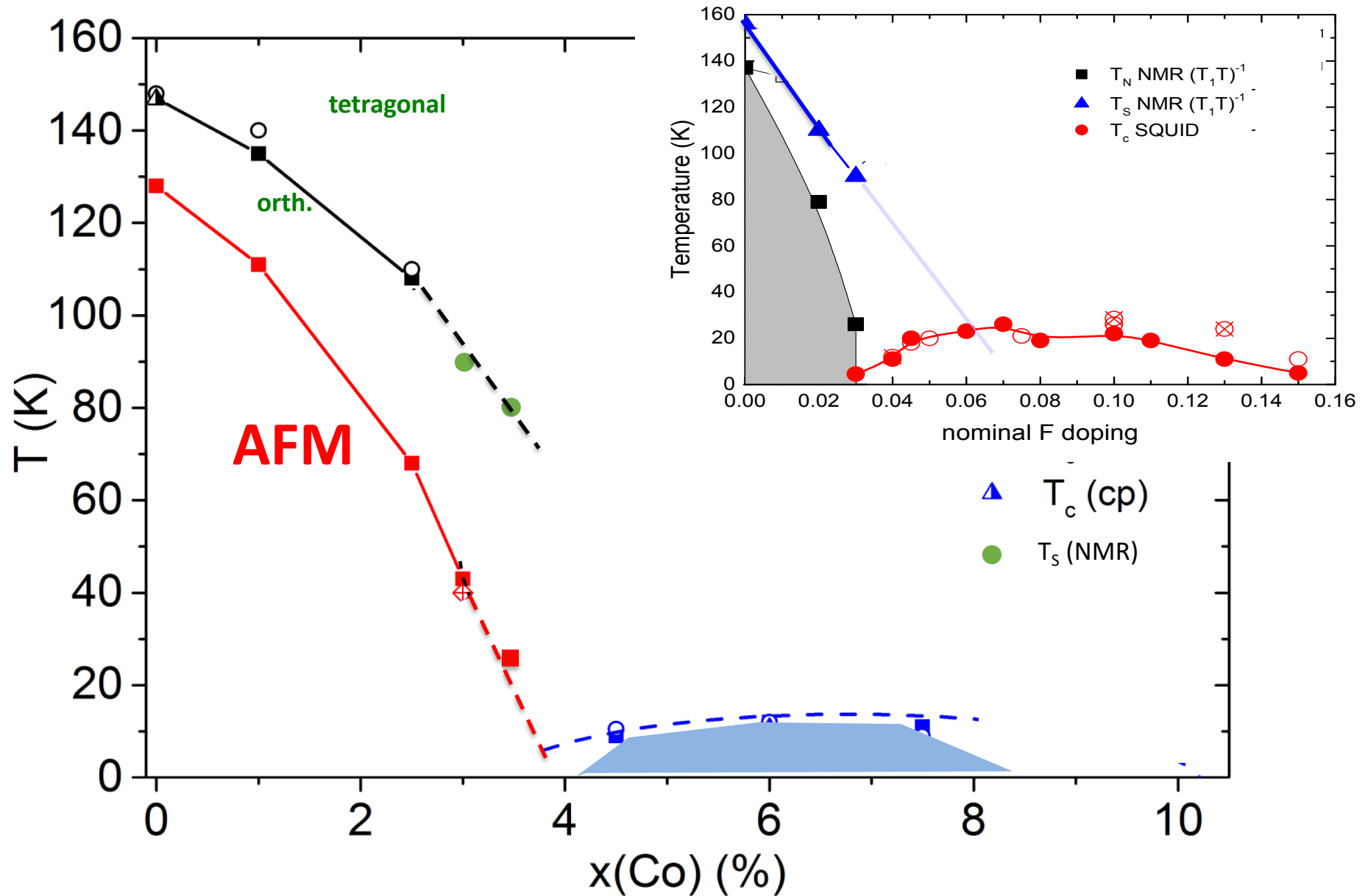
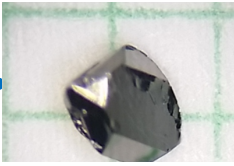
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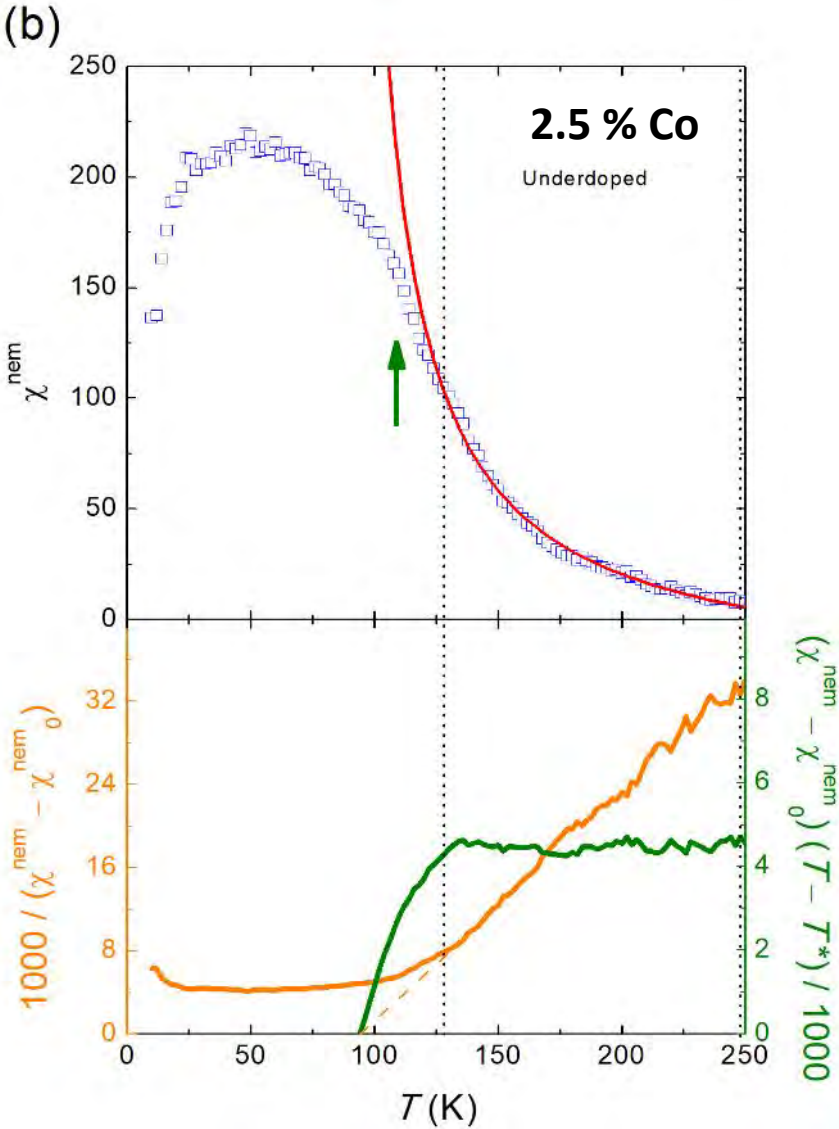
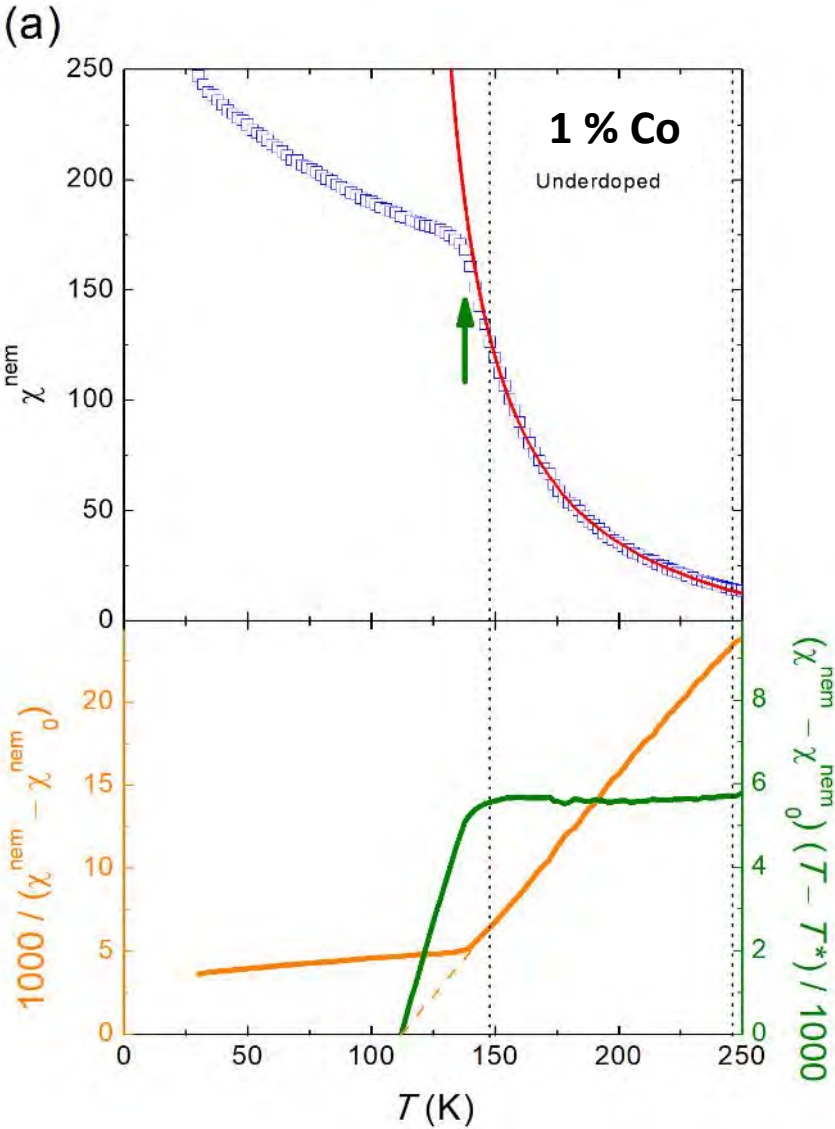
Phase diagram of Co-doped La 1111 revisited ...



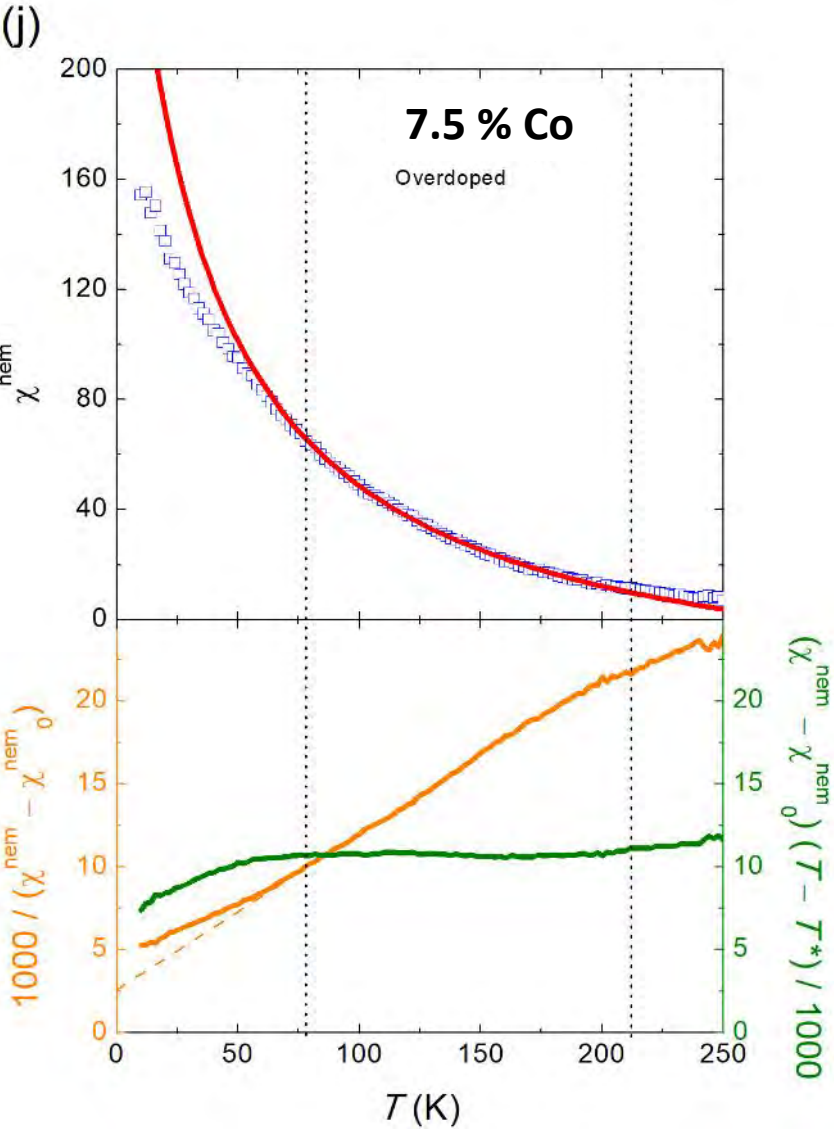
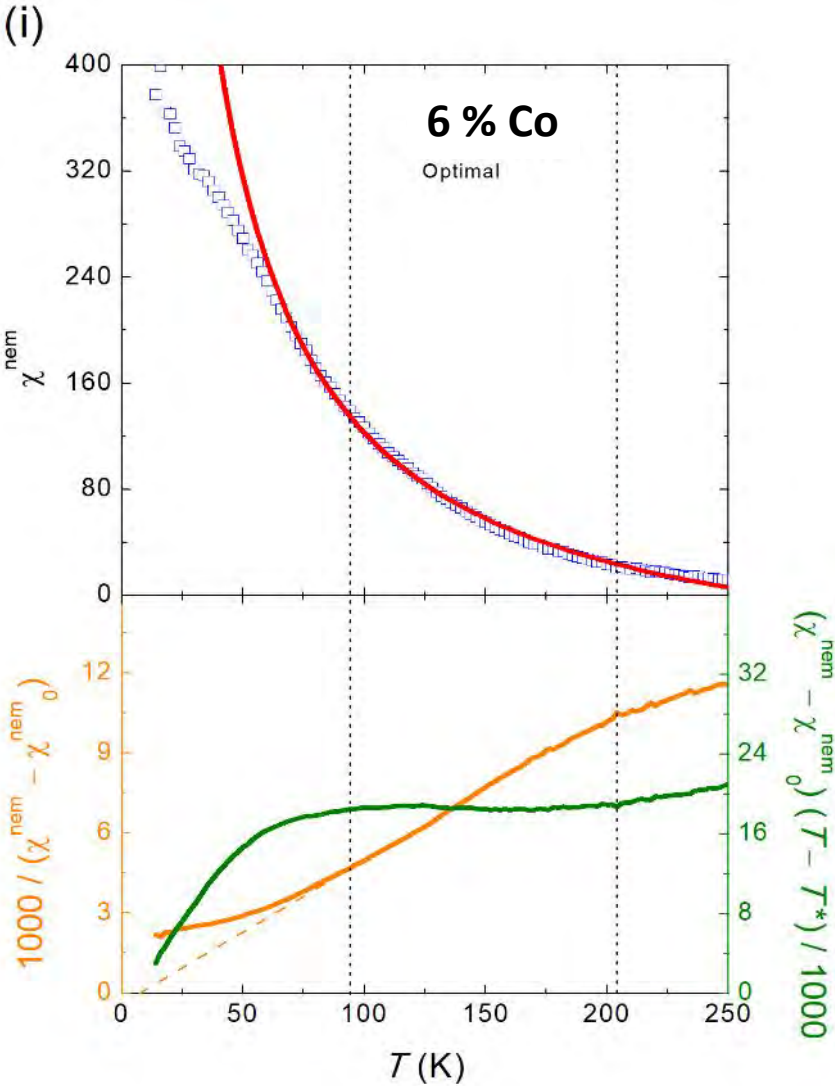
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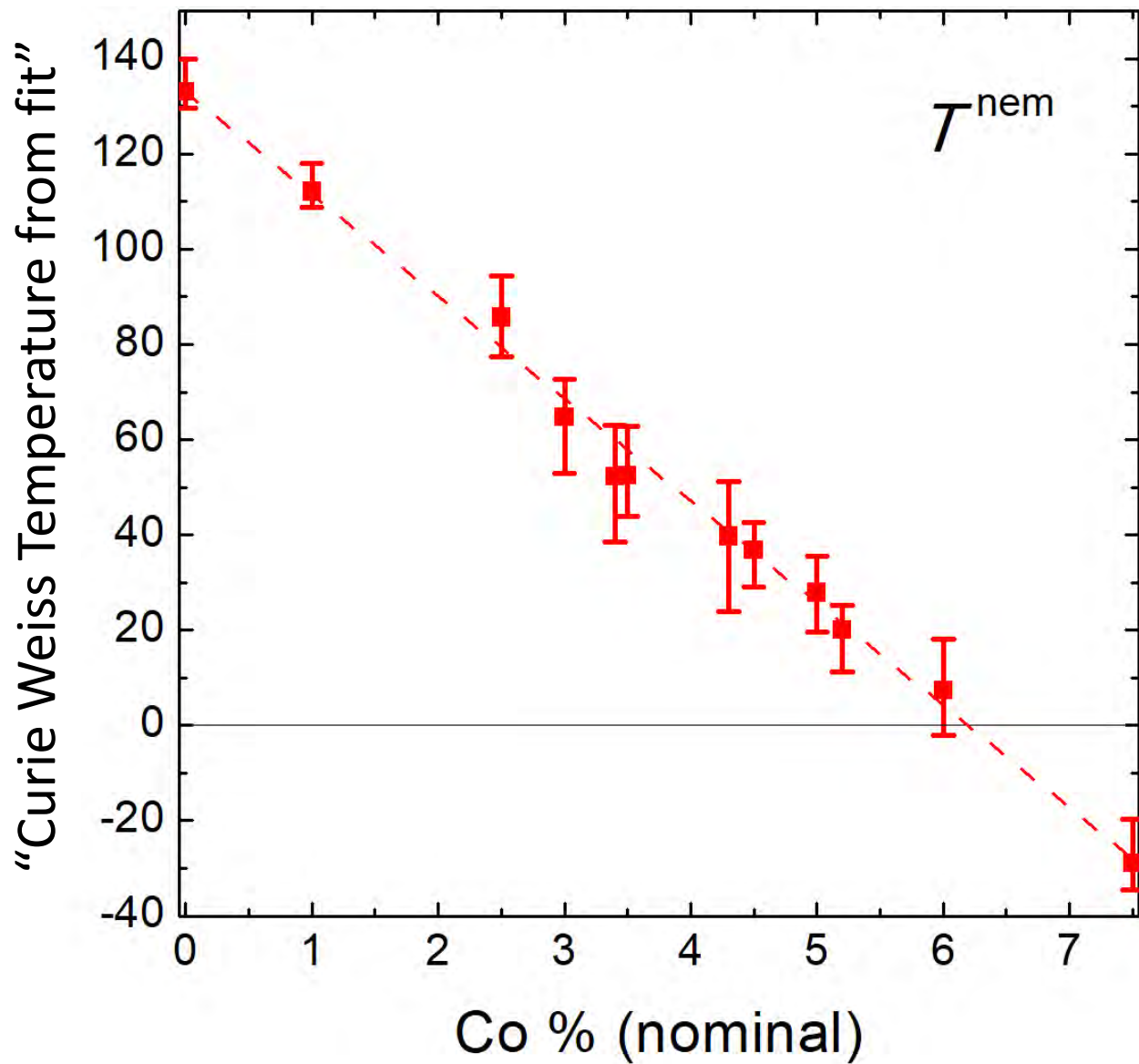
Nematic susceptibility of Co doped LaOFeAs



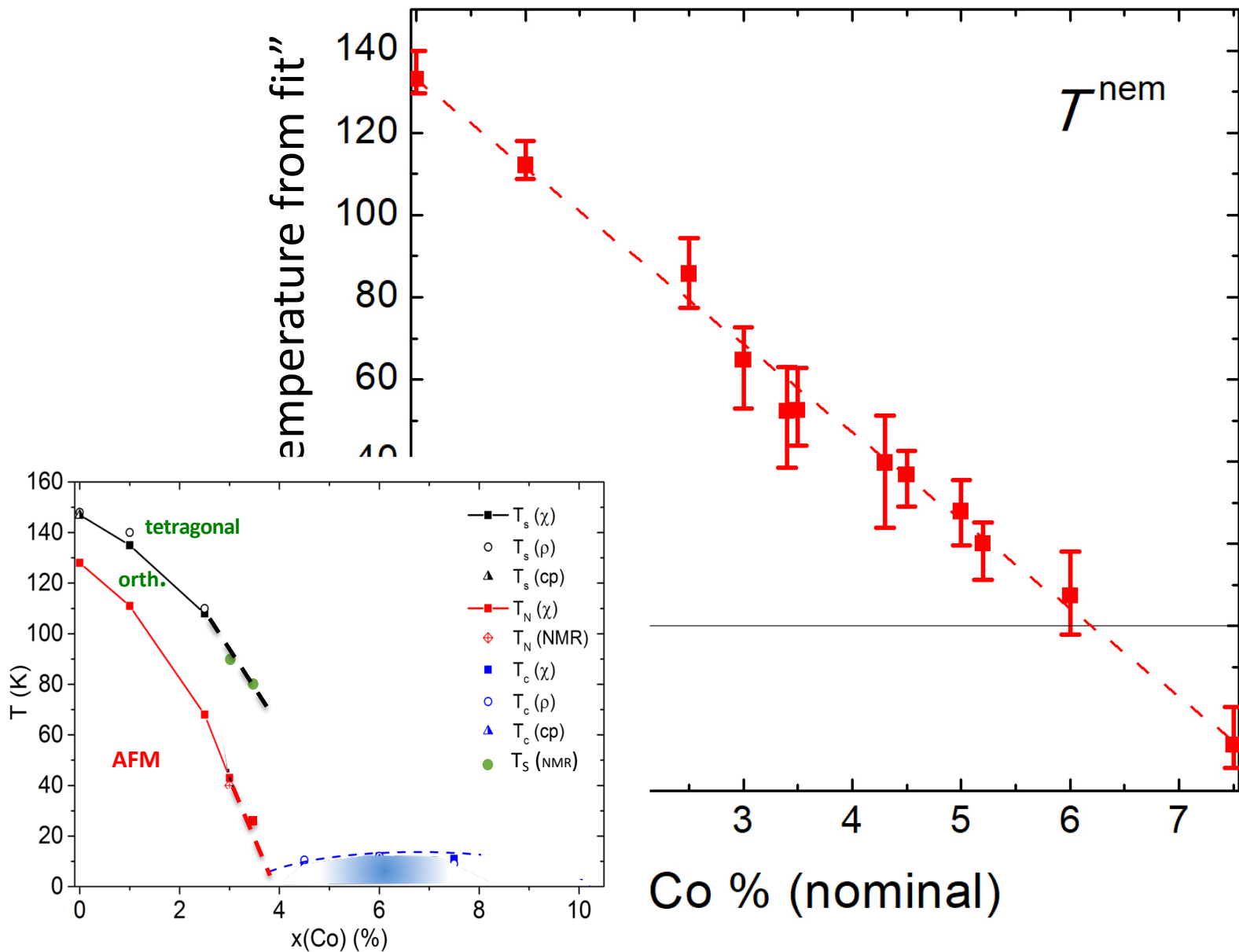
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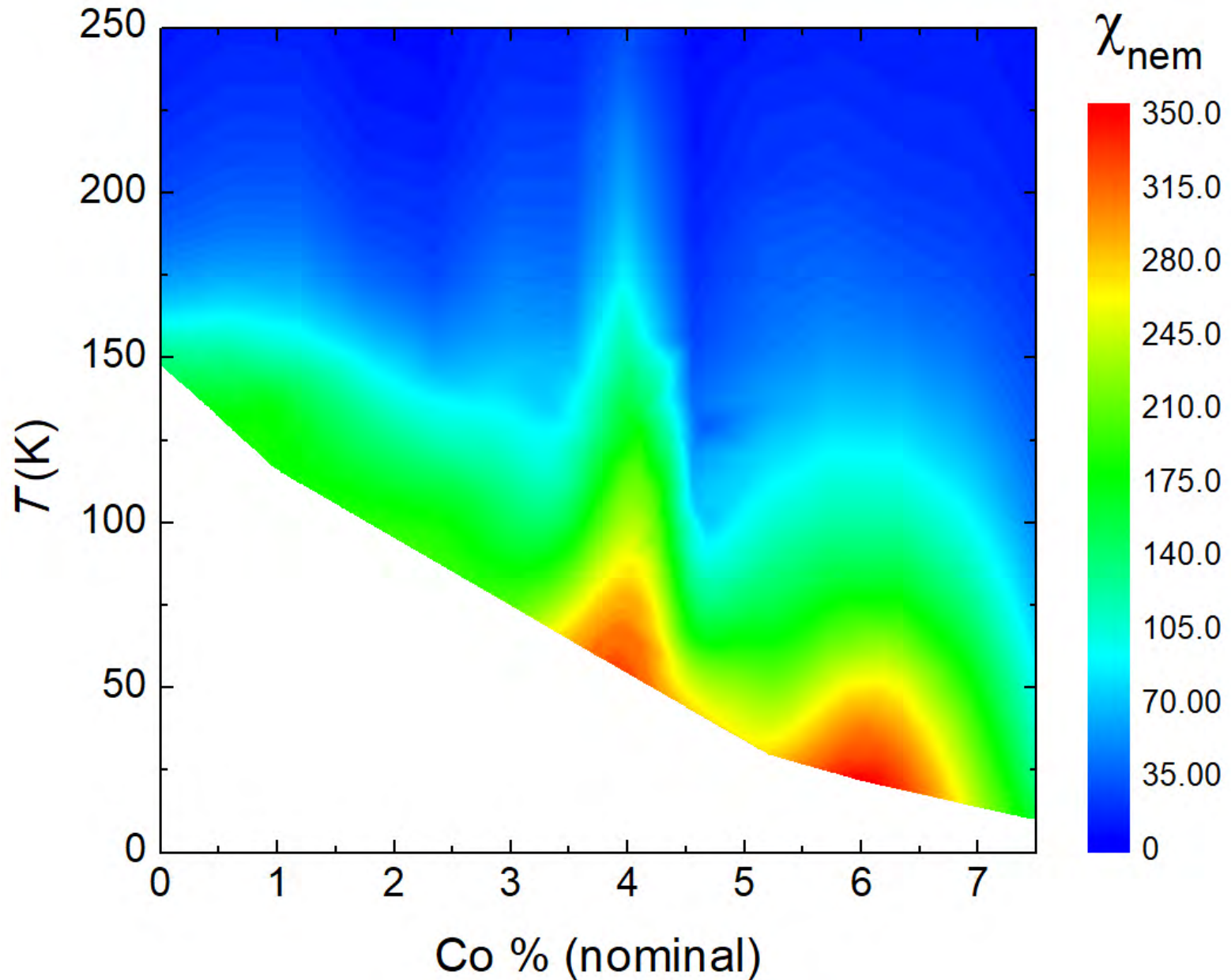
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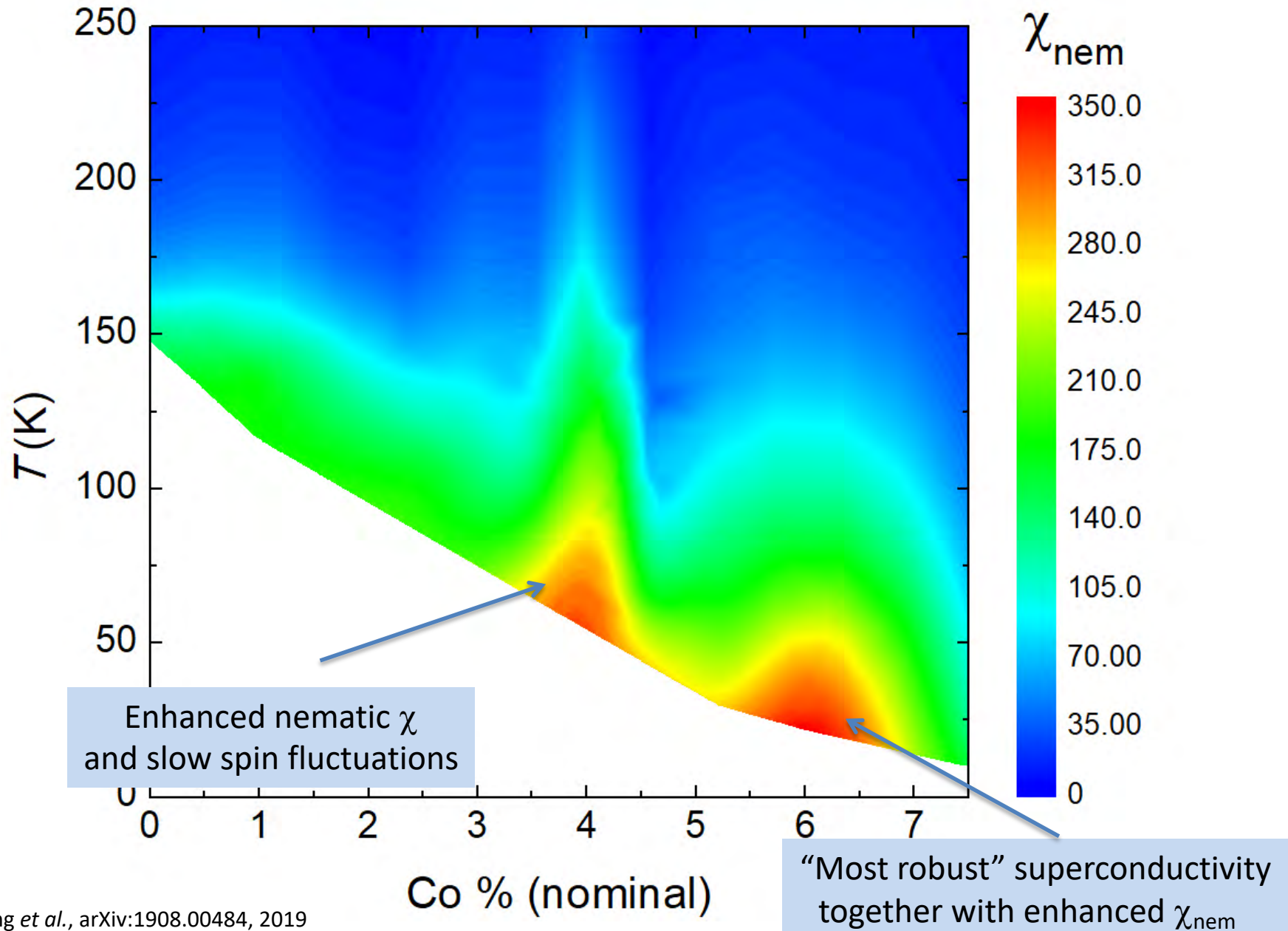
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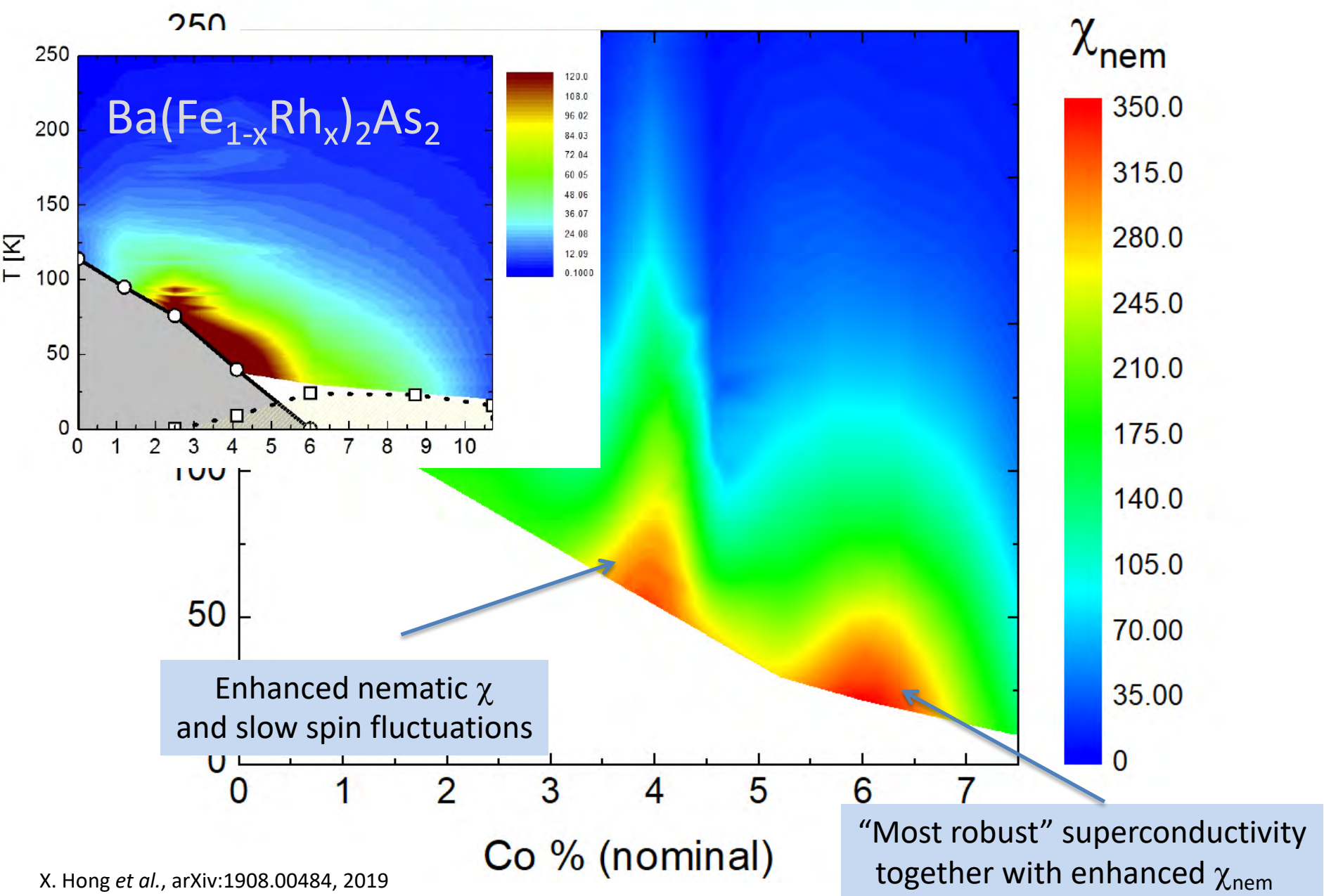
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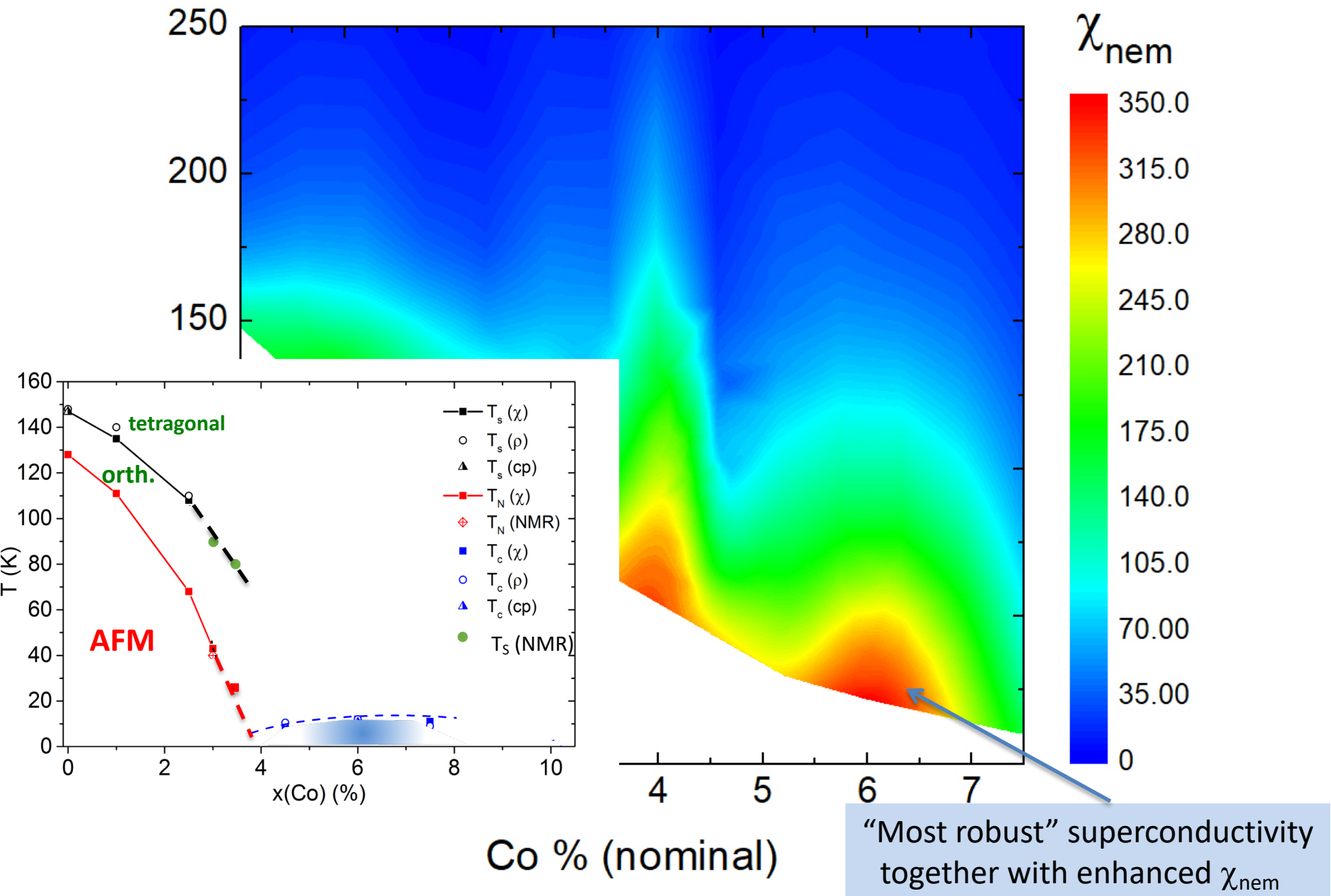
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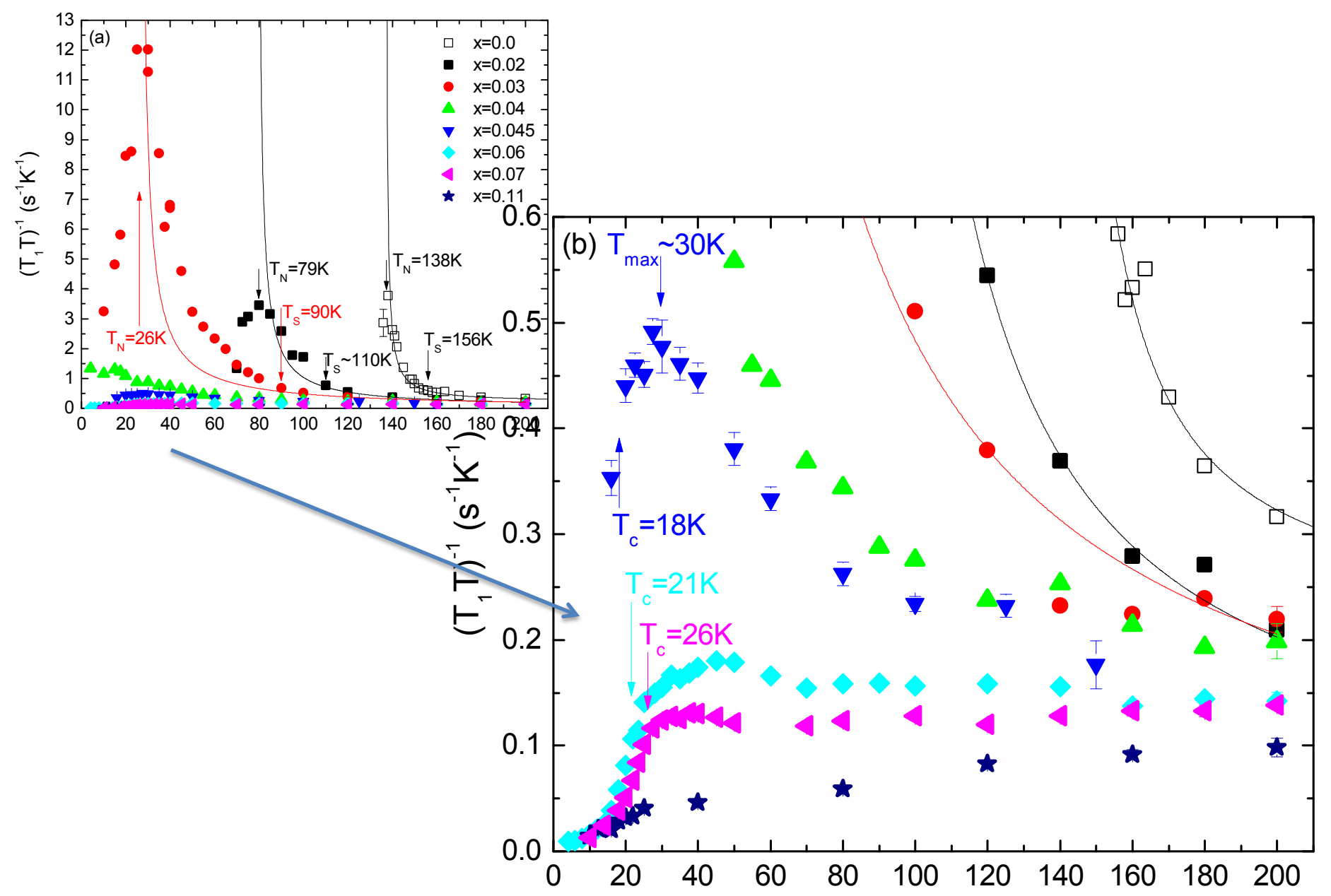
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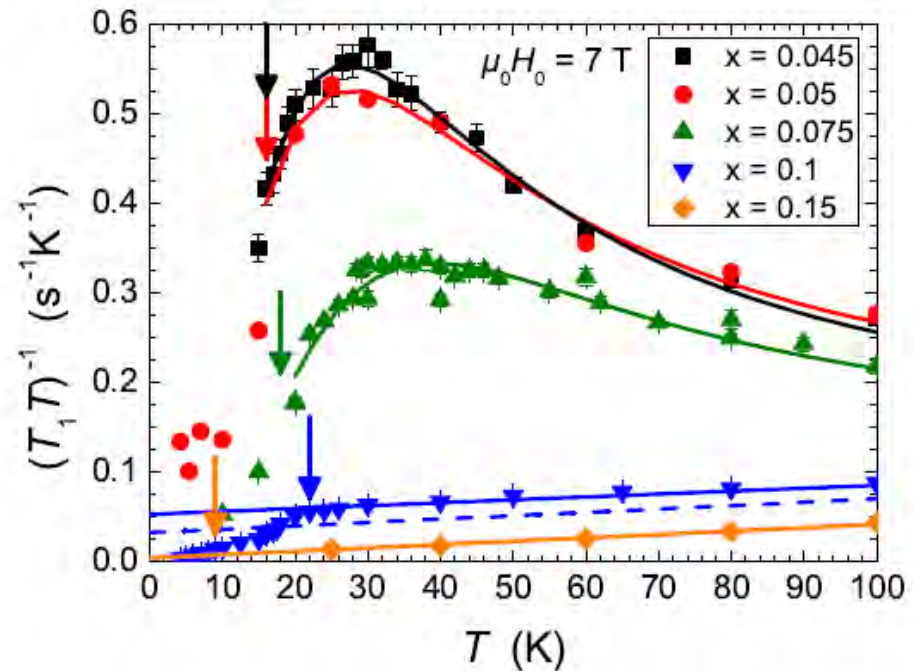
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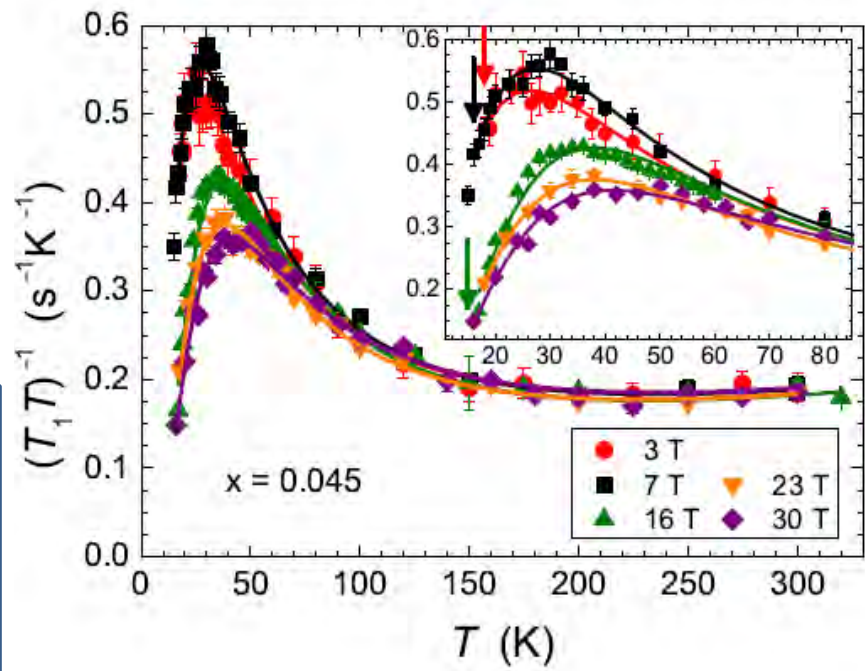
Anomalous slow spin fluctuations in underdoped $\text{LaO}_{1-x}\text{F}_x\text{FeAs}$



Anomalous slow spin fluctuations in underdoped LaOFeAs



NMR on underdoped 1111:
No long range
magnetic order



Bloembergen-Purcell-Pound (BPP) model

$$T_{1,BPP}^{-1}(T) = \gamma^2 h_{\perp}^2 \frac{\tau_c(T)}{1 + \tau_c^2(T) \omega_L^2}$$

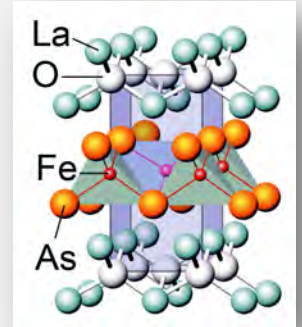
Peak in $1/T_1$ if correlation time of spin fluctuation τ_c equals the inverse (H dep.) Larmor frequency, i.e. for

$$\tau_c \sim 1/\omega_L$$

OUTLINE

Nematic fluctuations in doped La1111 crystals

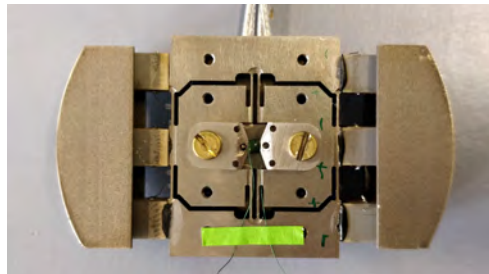
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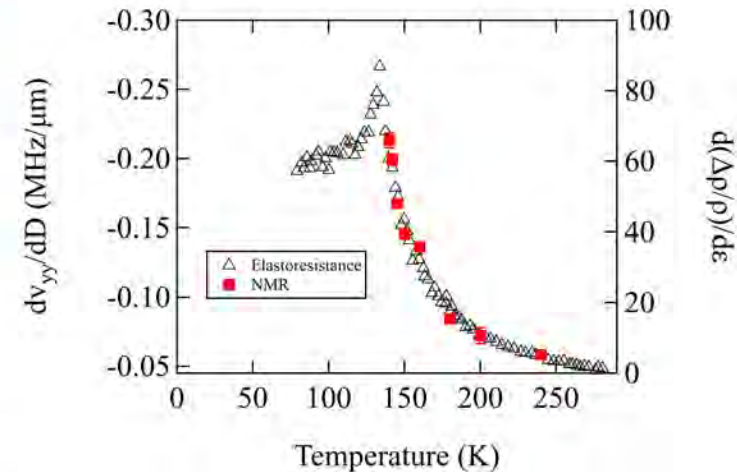
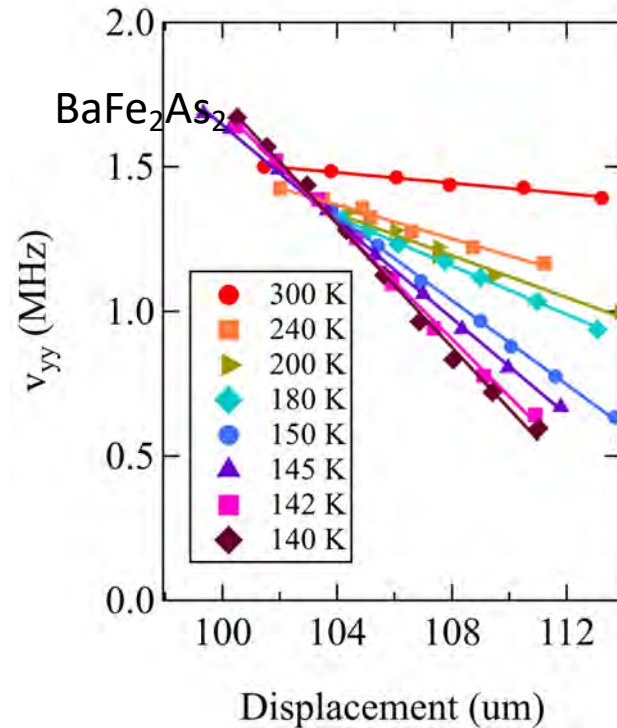
(Development of) methods for strain dependent ...

- Strain dependent NMR on BaFe_2As_2 ; strain up to $(-0.86\%; 0.42\%)$
- Elasto-Seebeck effect on Fe based superconductors
- Elasto-Nernst effect on Fe based superconductors
- ARPES@1³ beamline under strain (ongoing)

Electric Field Gradient (EFG) vs strain



In-situ strain control
Measure same sample
for $H \parallel a,b$ & $H \parallel c$
Min = -0.86 % strain
Max = 0.42 % strain

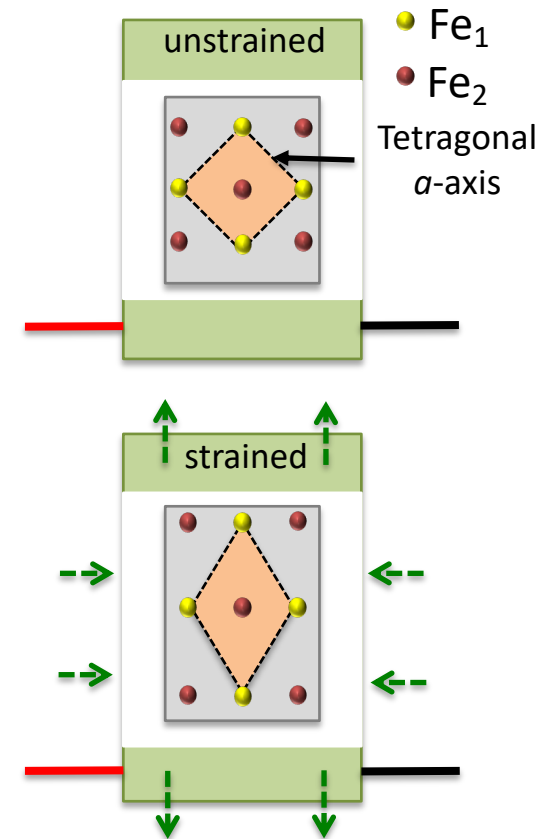
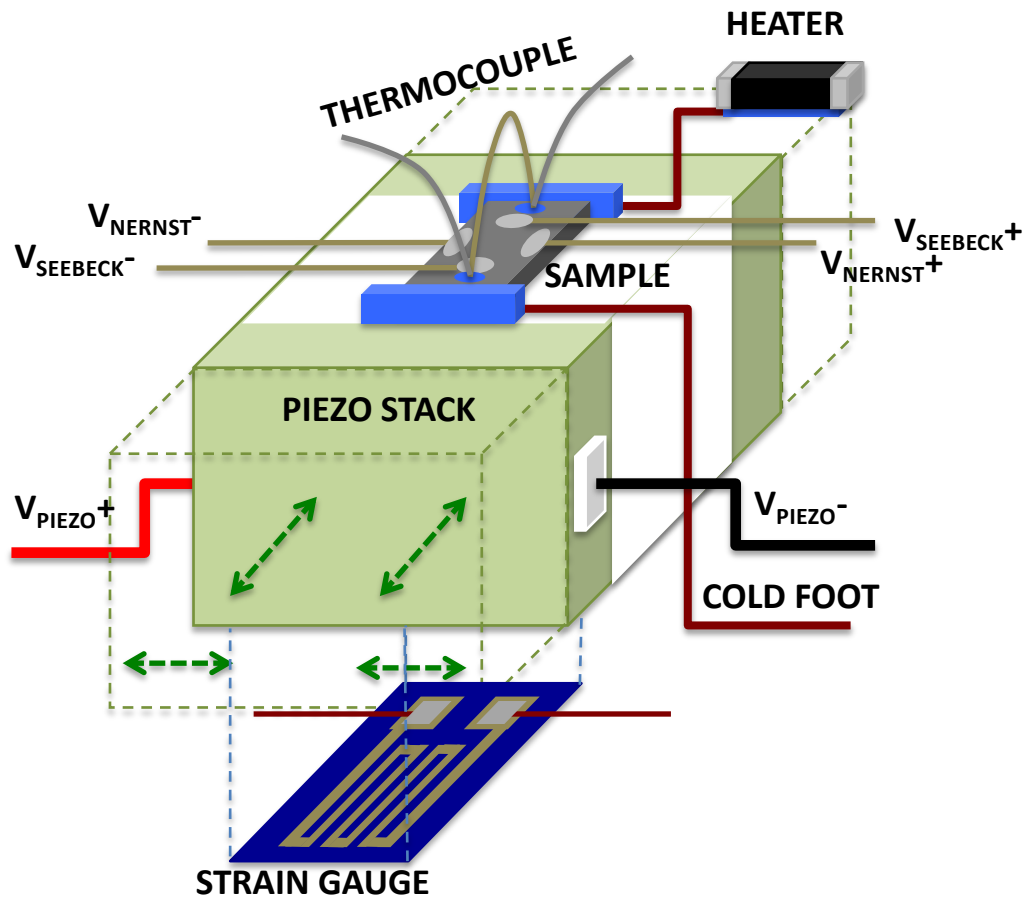


Chu et al., Science, 337(6095), 710 (2012)

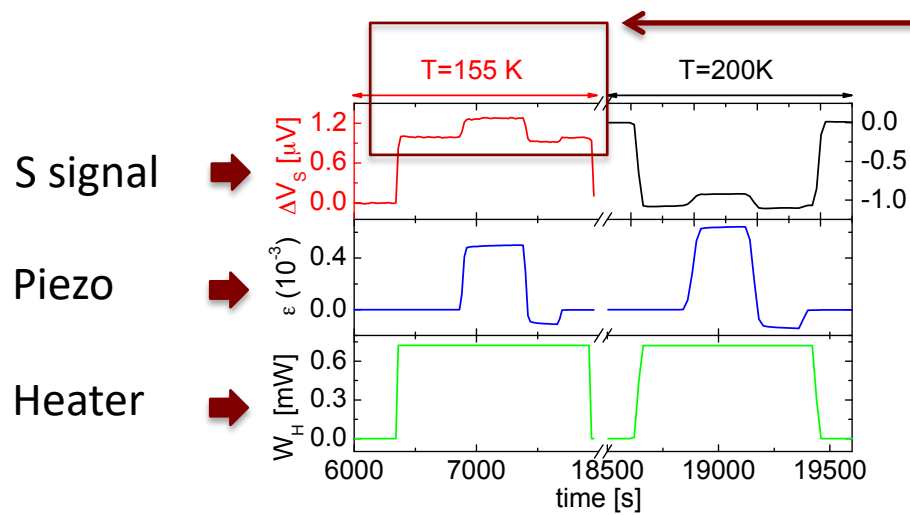
- Extract EFG from NMR spectral measurements vs strain
- EFG, $d\eta/d\varepsilon \sim \chi_{\text{nem}}$; As p - and Fe d -orbitals hybridize
→ **Quadrupolar NMR = Local probe of nematic susceptibility**

Strain-derivative of thermoelectric coefficients

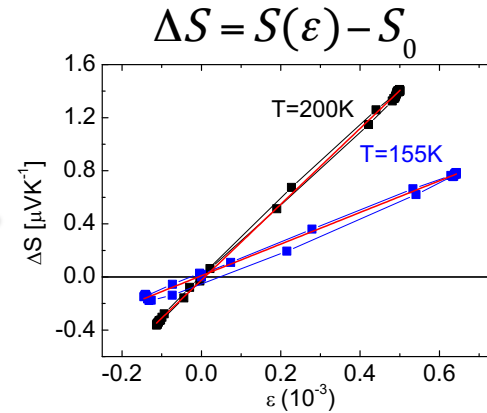
The experimental setup



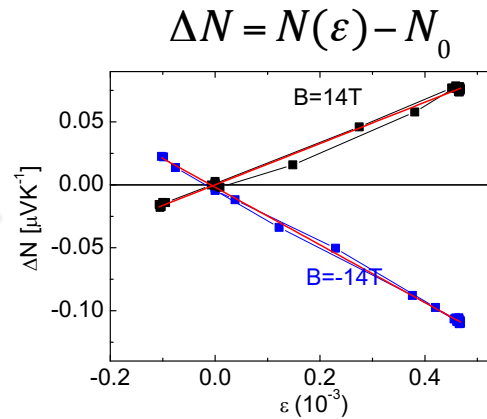
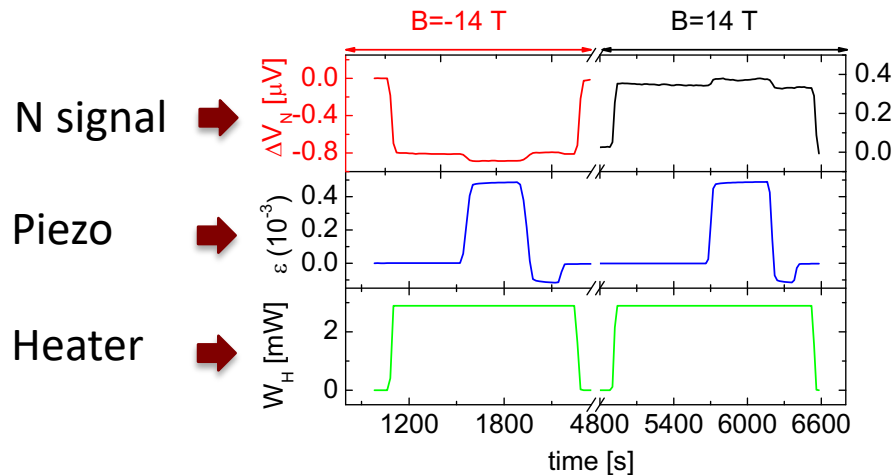
The strain-derivative of S and N



Large effect with tiny strain

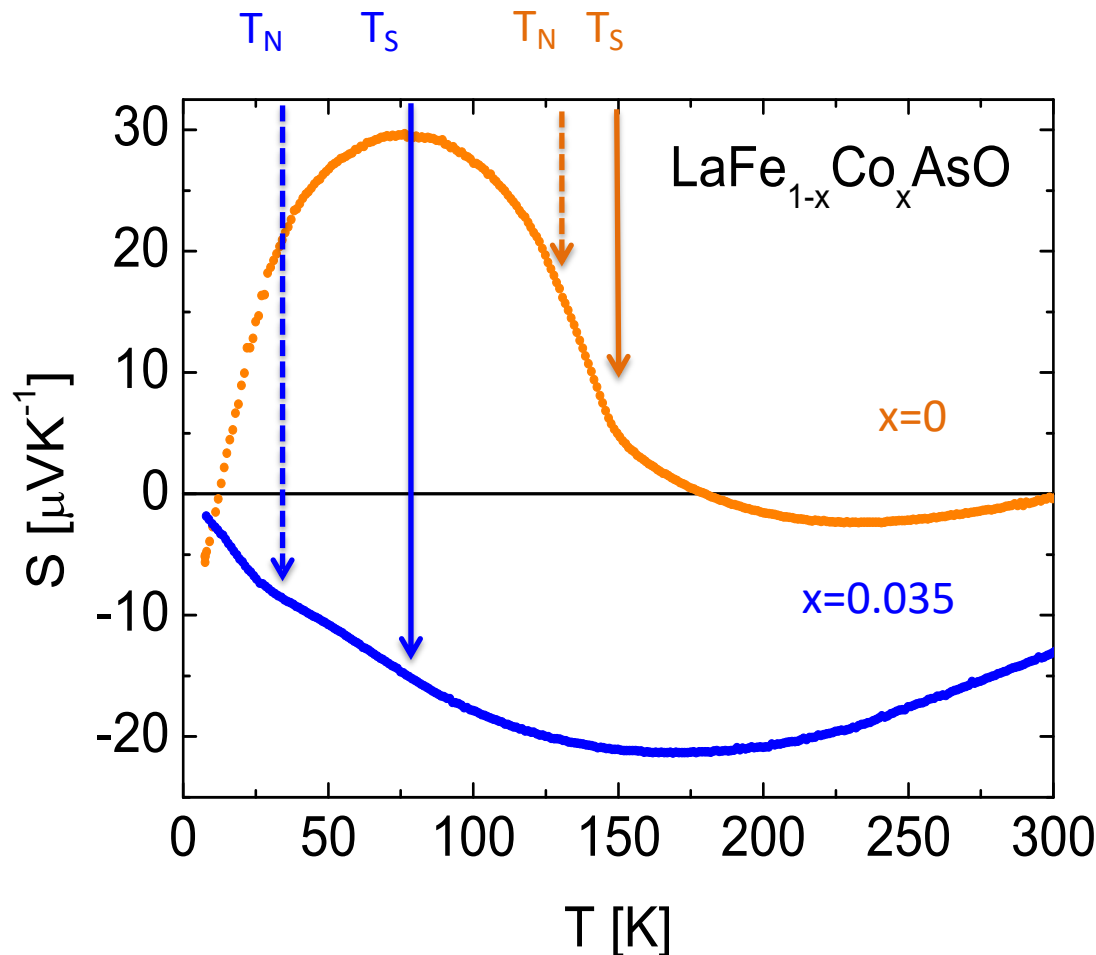


$$\frac{\delta(\Delta S)}{\delta \epsilon}$$



$$\frac{\delta(\Delta N)}{\delta \epsilon}$$

Seebeck effect $S(T)$ in $\text{LaFe}_{1-x}\text{Co}_x\text{AsO}$



$$S = \frac{E_x}{\nabla_x T}$$

Mott formula

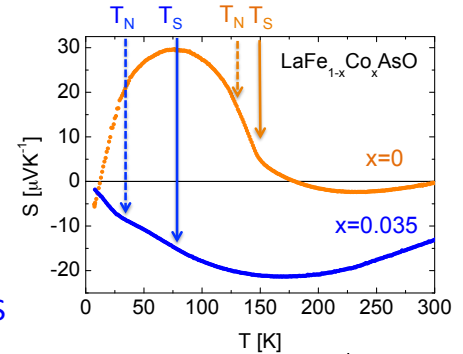
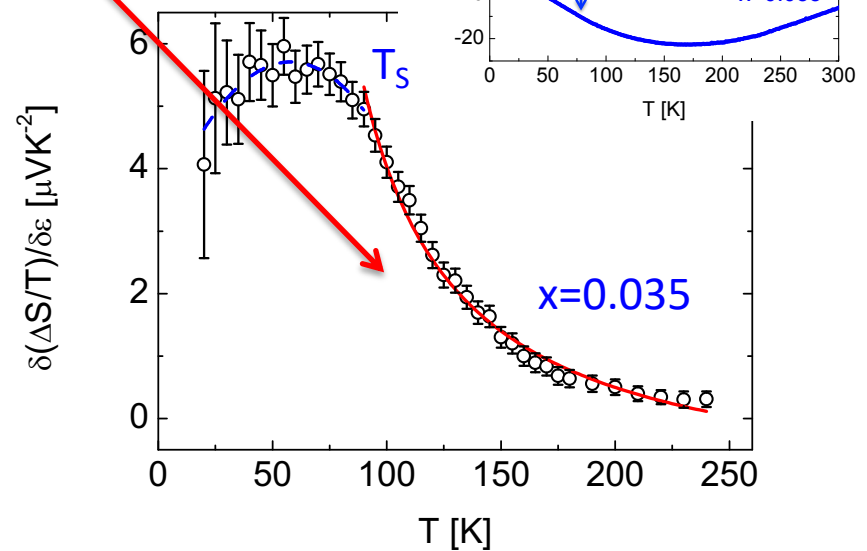
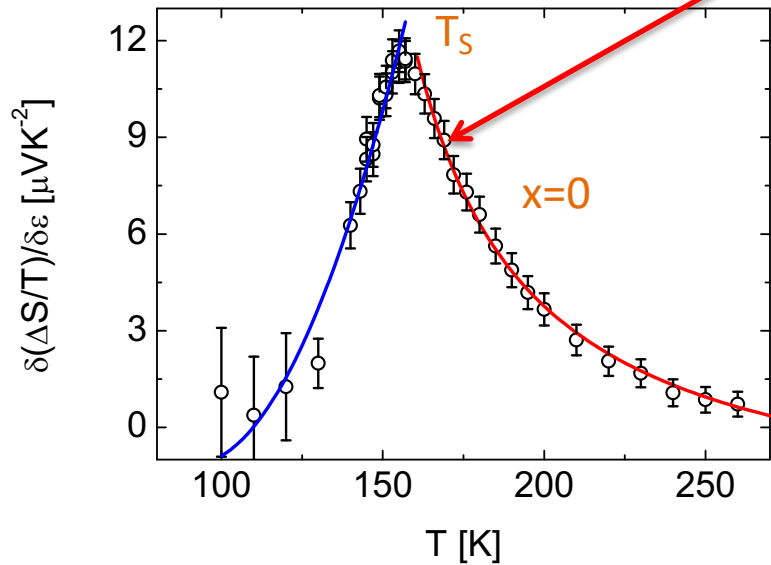
$$S = -\frac{\pi^2}{3} \frac{k_B^2 T}{e} \left(\frac{\partial \ln \sigma(\epsilon)}{\partial \epsilon} \right)_{\epsilon_F}$$

Energy derivatives of
density and mobility

- S changes sign: multi-band, electron & holes
- e-doping: increase of S with negative sign

Strain dependent Seebeck

$$\frac{\delta(\Delta S / T)}{\delta \varepsilon} = k + \frac{C}{T - T^*}$$

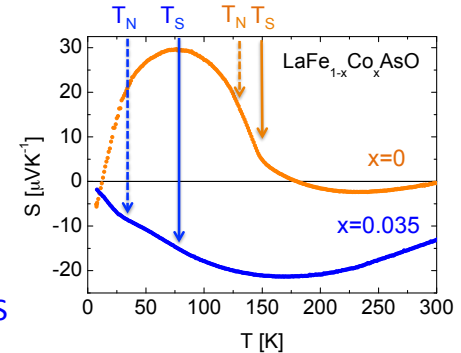
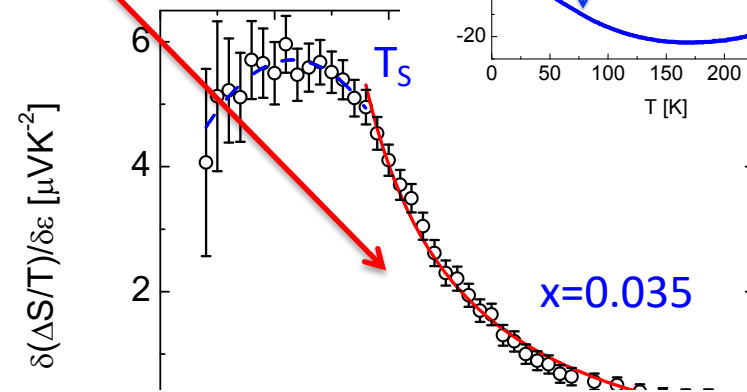
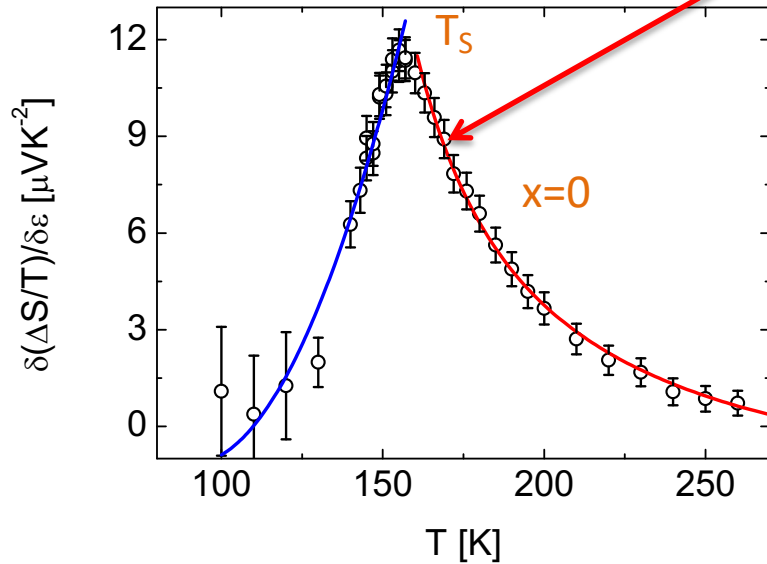


BaFe_2As_2

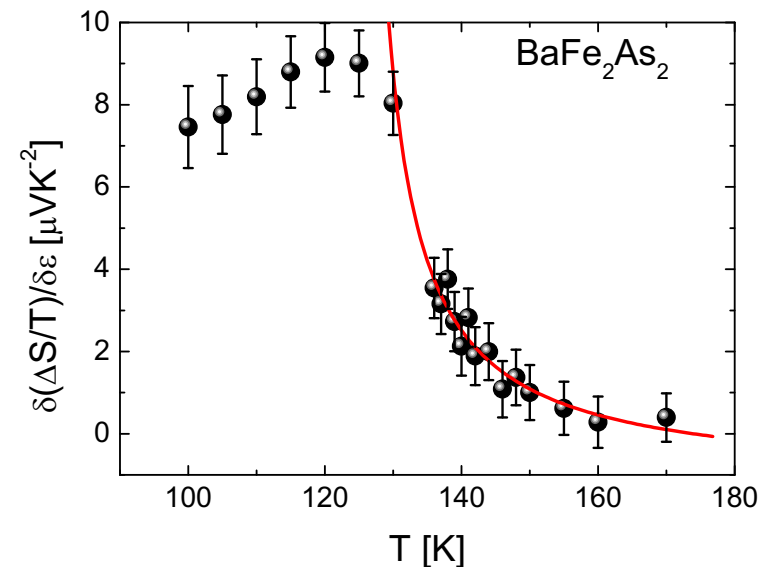
- Anomaly of $\delta S/\delta \varepsilon$ at T_S and not at T_N
- $\delta S/\delta \varepsilon$ Independent on the sign of S ➔ Band selectivity of nematic fluctuations?
- Curie-Weiss like behaviour in the tetragonal phase, $T^* \approx T^*(\rho)$

Strain dependent Seebeck

$$\frac{\delta(\Delta S/T)}{\delta\epsilon} = k + \frac{C}{T - T^*}$$



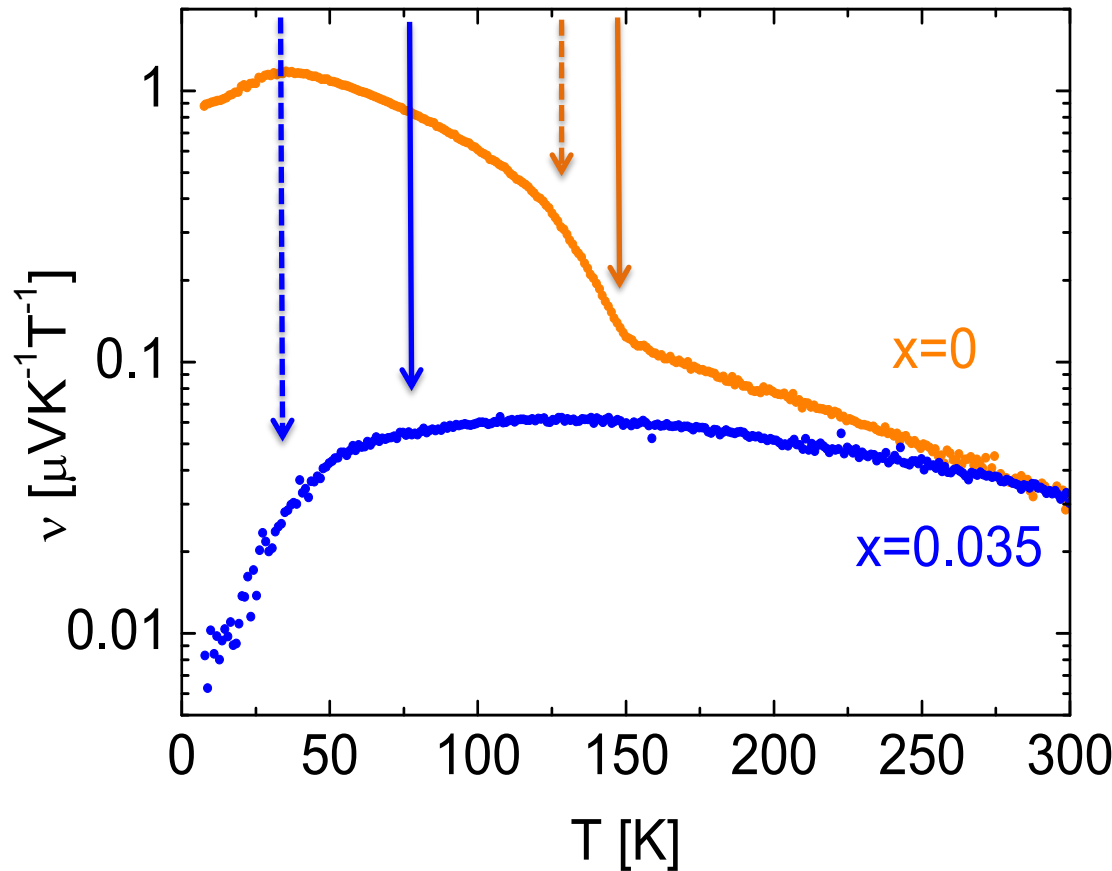
- Anomaly of $\delta S/\delta\epsilon$ at T_S and not at T_N
- $\delta S/\delta\epsilon$ Independent on the sign of S
- Curie-Weiss like relaxation in the tetragonal phase, $T^* \approx T^*(\rho)$



ns?

Nernst effect in $\text{LaFe}_{1-x}\text{Co}_x\text{AsO}$

T_N T_S T_N T_S



$$N = -\frac{E_y}{\nabla_x T}$$

Sonheimer formula

$$N = \frac{\pi^2}{3} \frac{k_B^2 T}{e} \frac{\partial \Theta_H}{\partial \epsilon} \Big|_{\epsilon_F}$$

N : energy derivative of the Hall angle $\Theta_H = \frac{\sigma_{xy}}{\sigma_{xx}}$

Simple metals (large ϵ_F): $N \approx 0$

If $N \neq 0$ "often": $N \sim \mu_H / \epsilon_F$

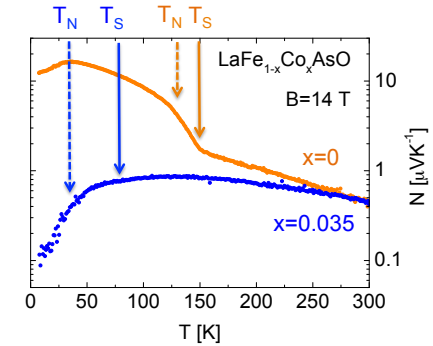
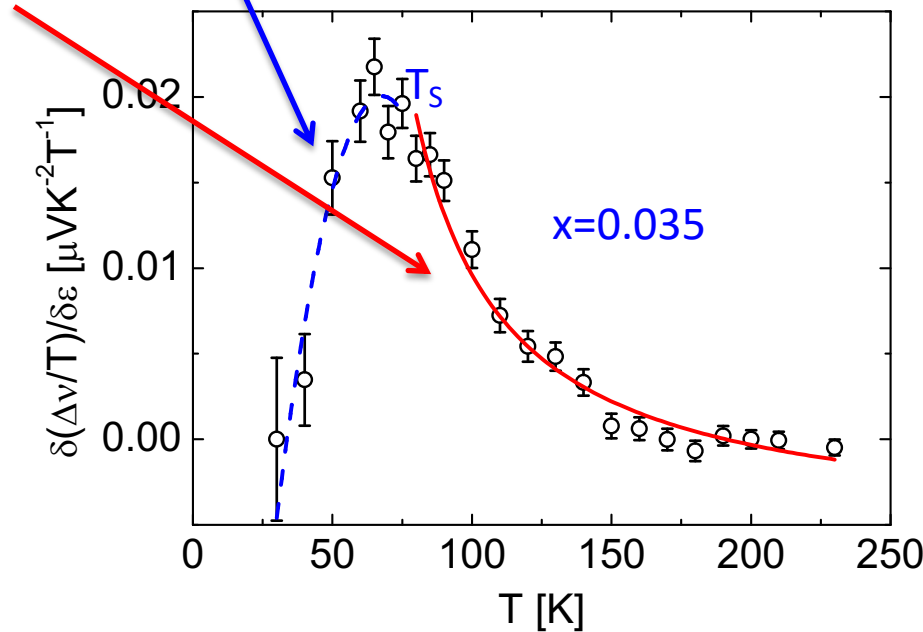
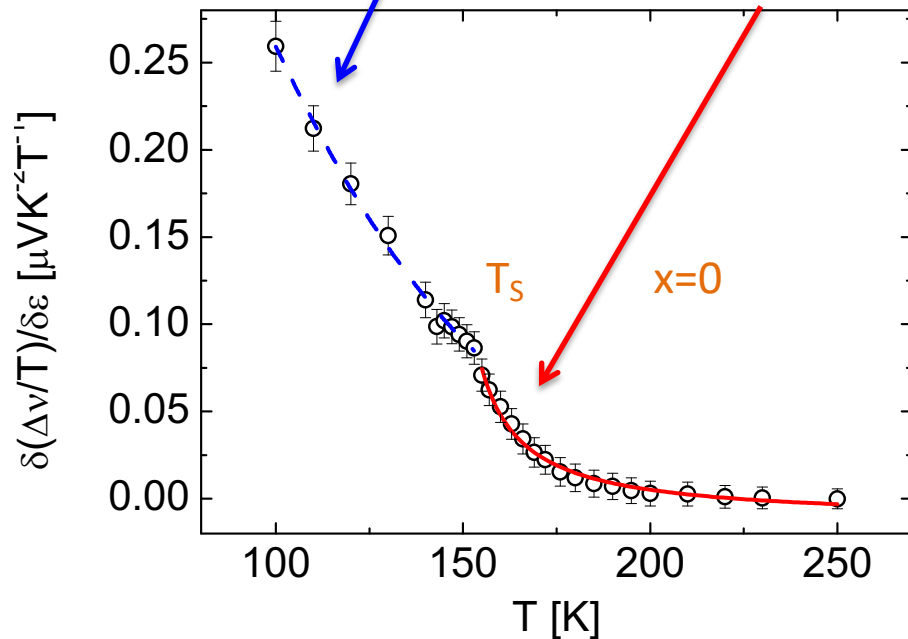
- **x=0: Strong increase below T_S**
- **X= 3.5 % : Decrease at low T (below T_N ?)**
- **$T > T_S$: similar behaviour of N for $x = 0$ and 3.5%**

Strain dependent Nernst effect

Strong increase below T_S

$$\frac{\delta(\Delta v / T)}{\delta \varepsilon} = k_v + \frac{C}{T - T^*}$$

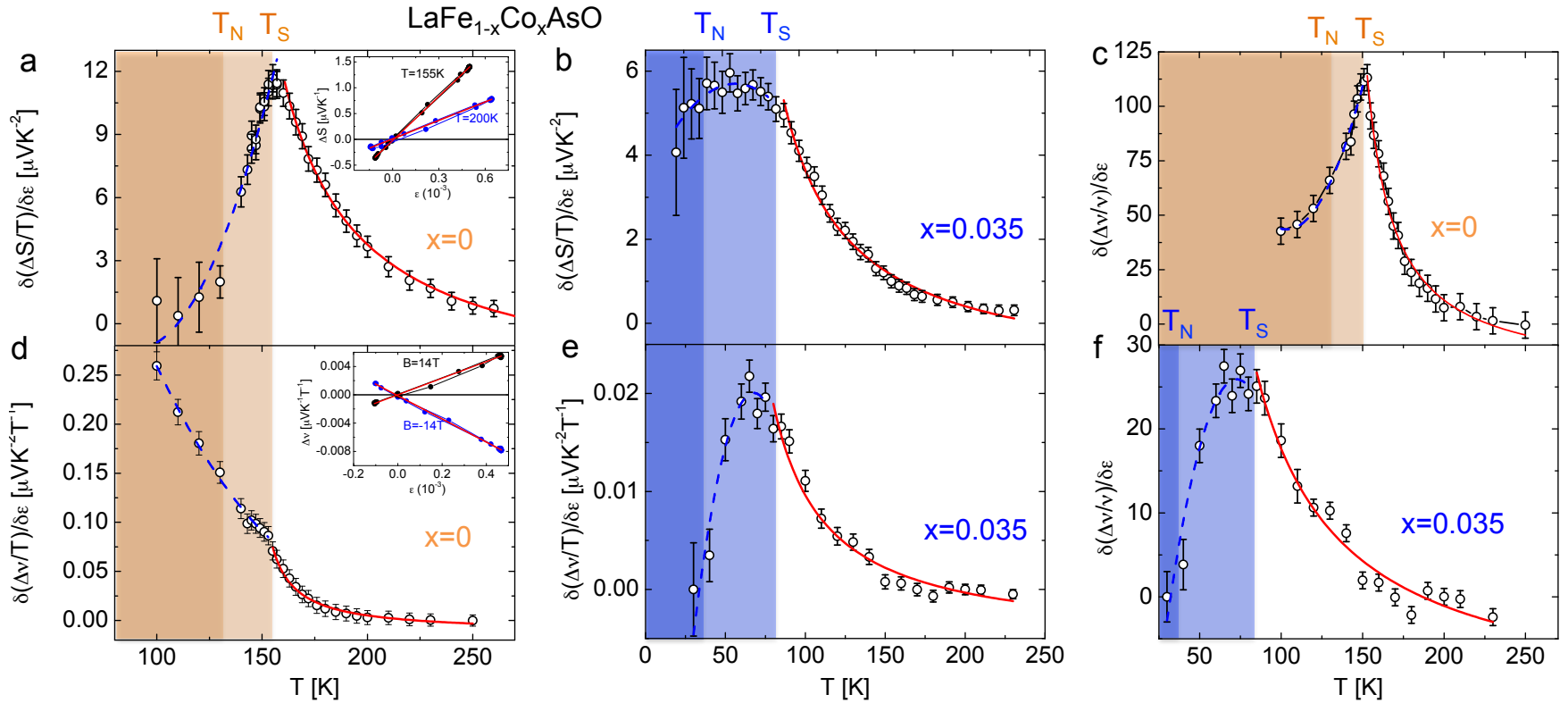
Decrease below T_S



Curie-Weis behaviour for $T > T_S$

absolute value much larger for $x = 0$ (in contrast to $\delta\rho/\delta\varepsilon$)

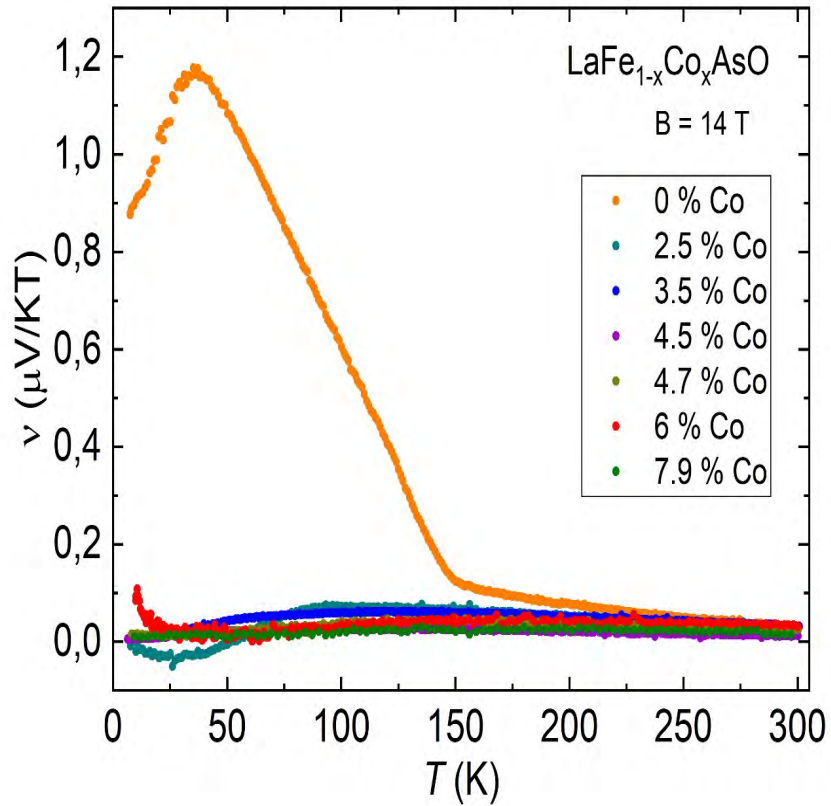
Nernst and Seebeck effect under strain in LaOFeAs



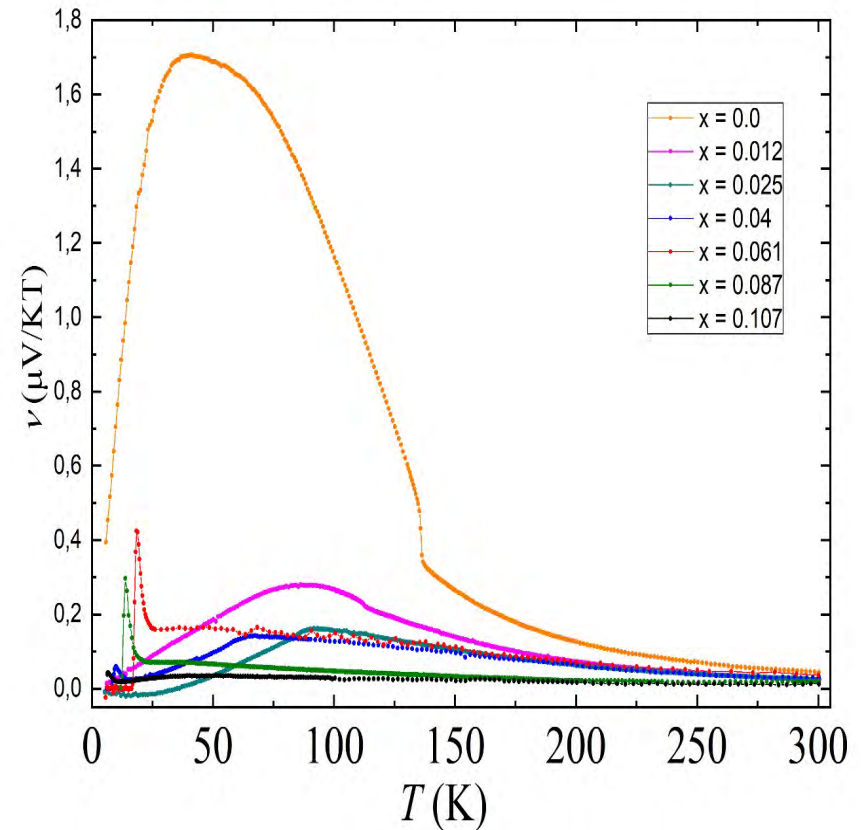
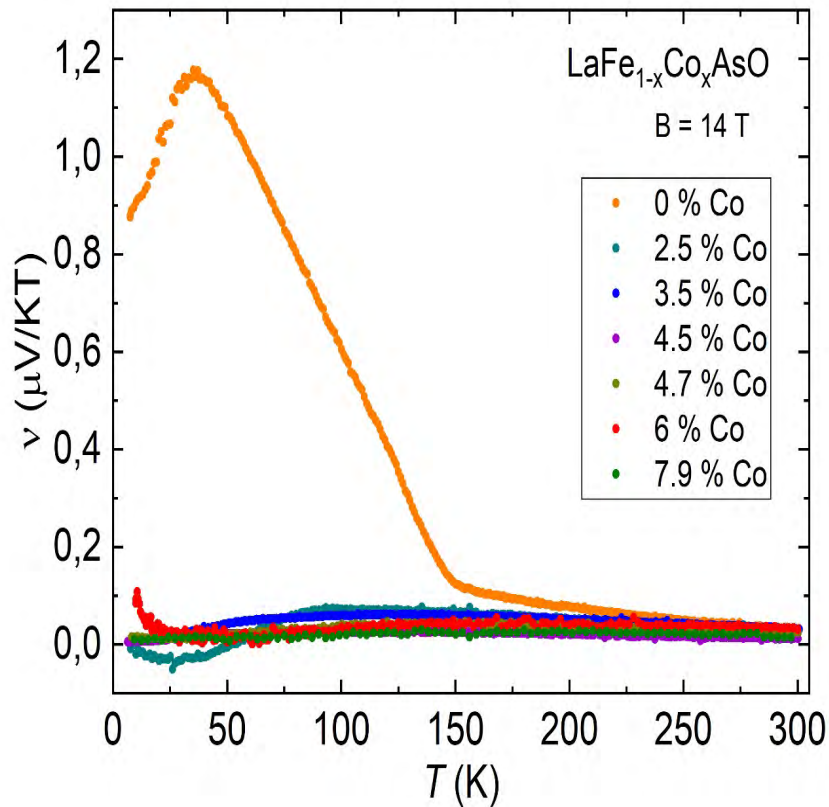
- Nematic fluctuations/strain derivative of transport related to T_S and not to T_N
- Strain dependence of transport band selective (different signs of S)
- Universal Curie-Weiss behaviour of strain derivative for all transport properties
- Elasto-thermoelctric transport and elasto-resistivity not equivalently representative for nematic susceptibility!!

(scattering, Fermi surface, different pockets ...)

Nernst effect of $\text{LaFe}_{1-x}\text{Co}_x\text{AsO}$

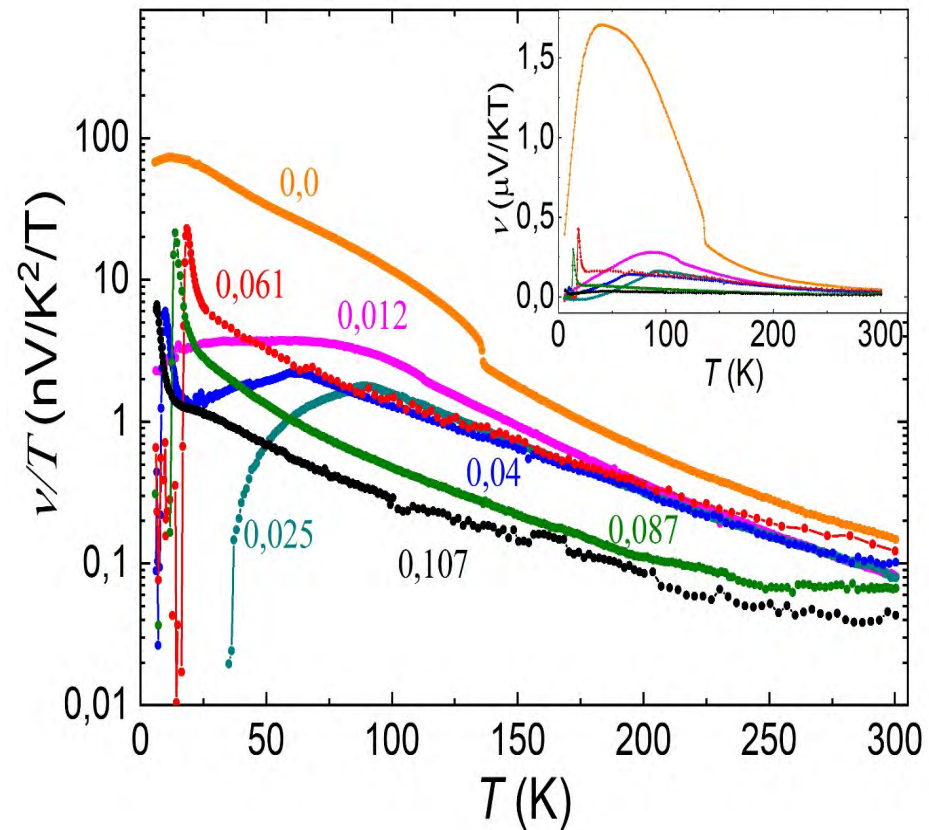
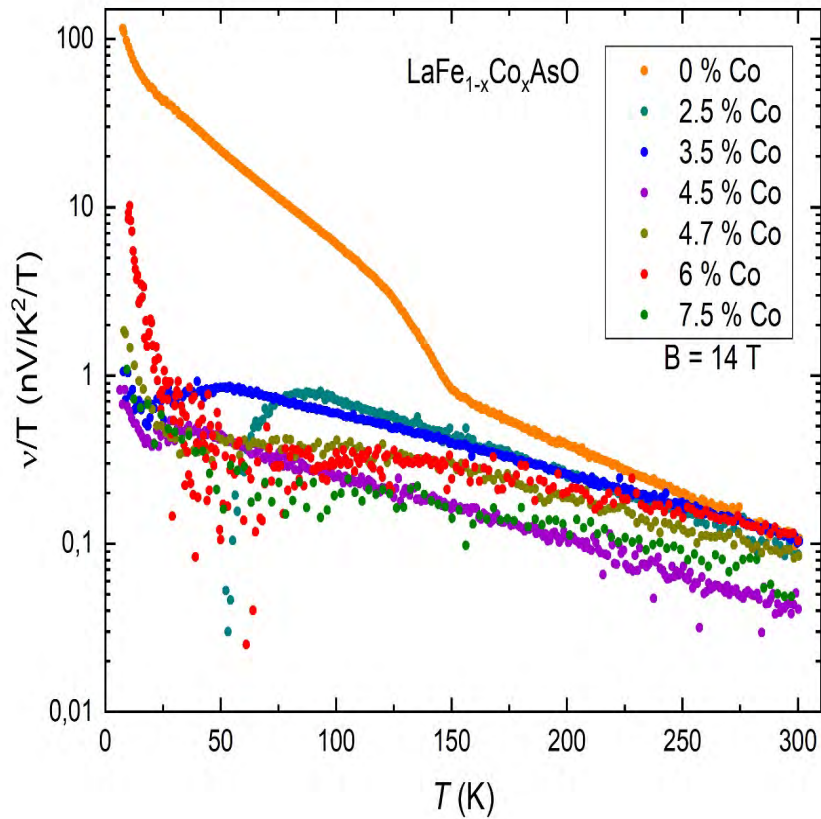


Nernst effect of $\text{LaFe}_{1-x}\text{Co}_x\text{AsO}$ and $\text{Ba}(\text{Fe}_{1-x}\text{Rh}_x)_2\text{As}_2$

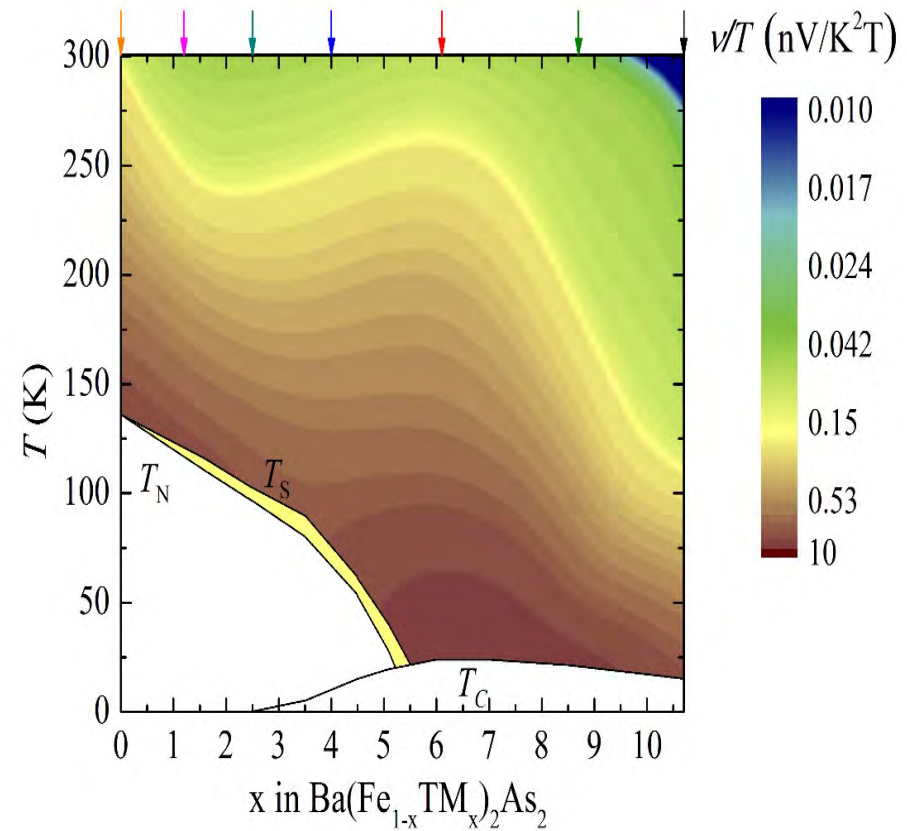
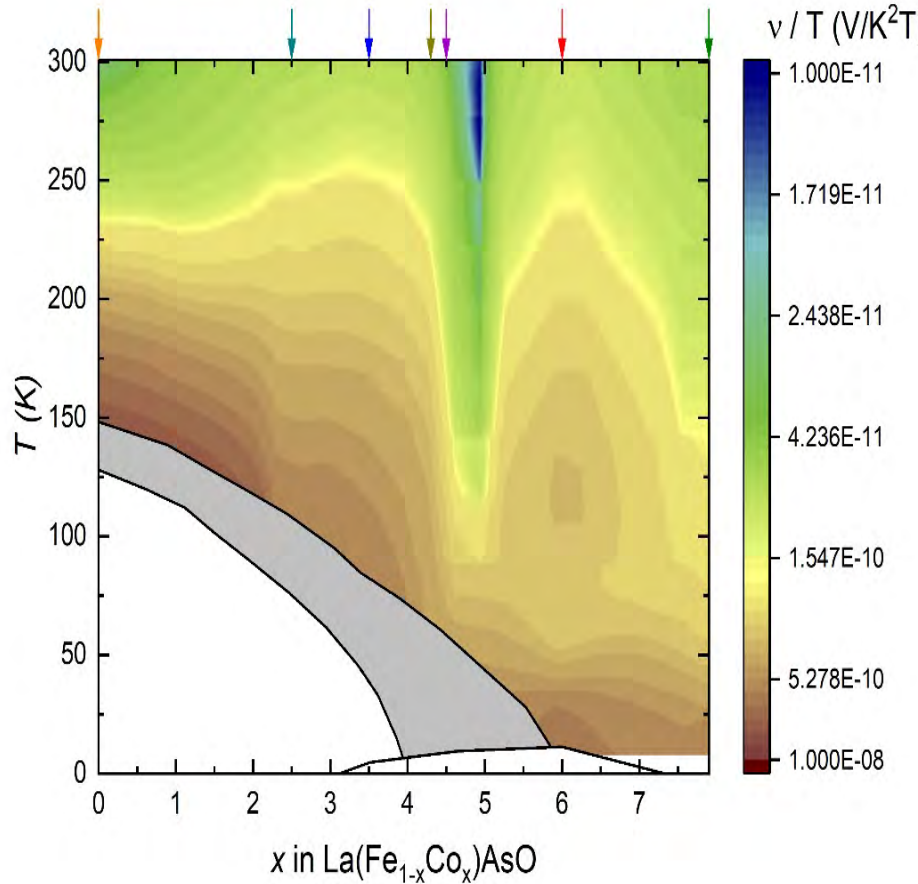


- Huge Nernst effect in nematic/magnetic phase of parent compounds
- Strikingly similar behaviour in LaOFeAs and BaFe_2As_2
- **Peculiar “electronic state” independent on defects, dimensionality, ...**
but drastic suppression as a function of doping

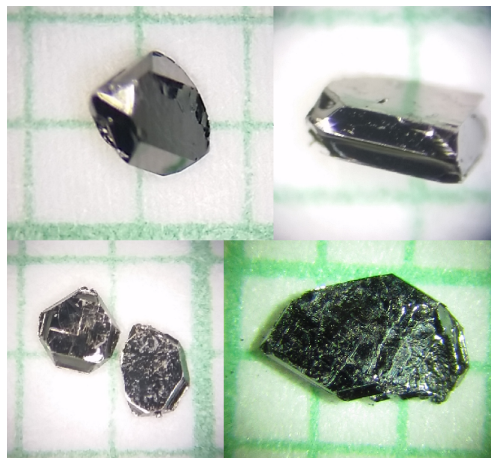
Nernst effect of $\text{LaFe}_{1-x}\text{Co}_x\text{AsO}$ and $\text{Ba}(\text{Fe}_{1-x}\text{Rh}_x)_2\text{As}_2$



Nernst effect of $\text{LaFe}_{1-x}\text{Co}_x\text{AsO}$ and $\text{Ba}(\text{Fe}_{1-x}\text{Rh}_x)_2\text{As}_2$

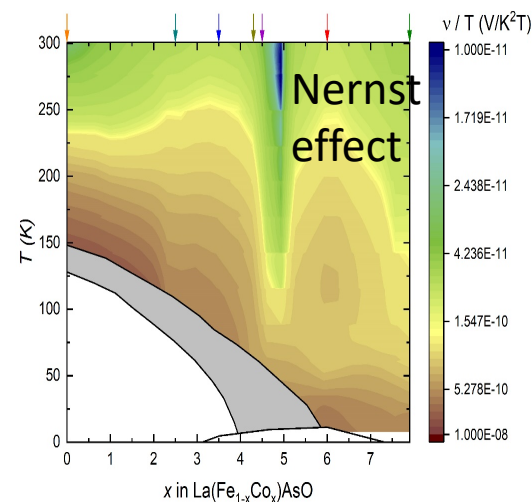
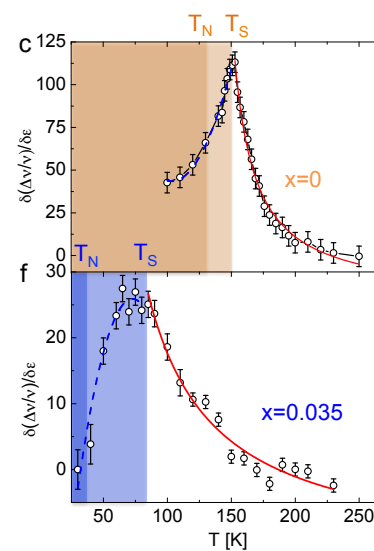
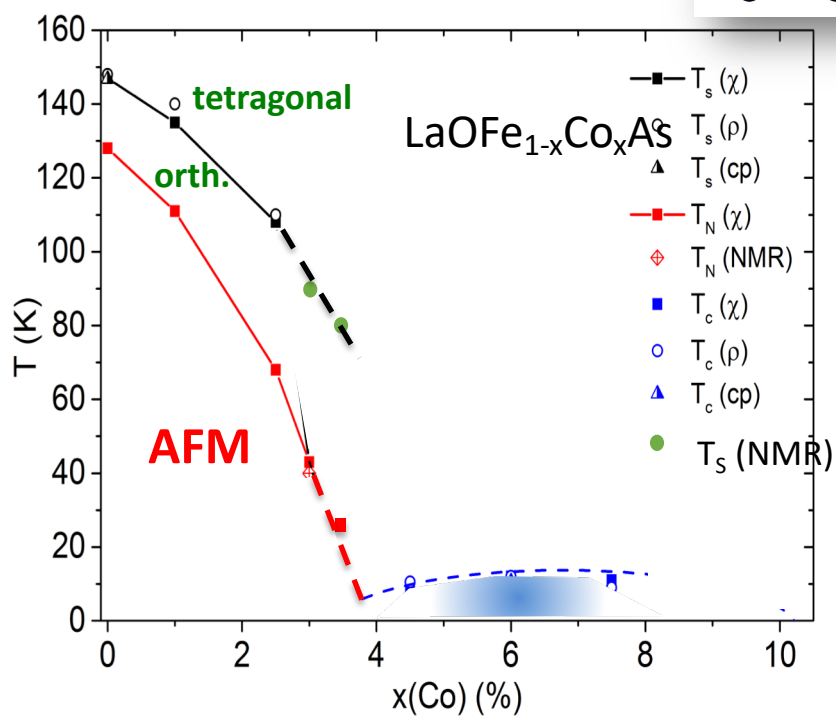
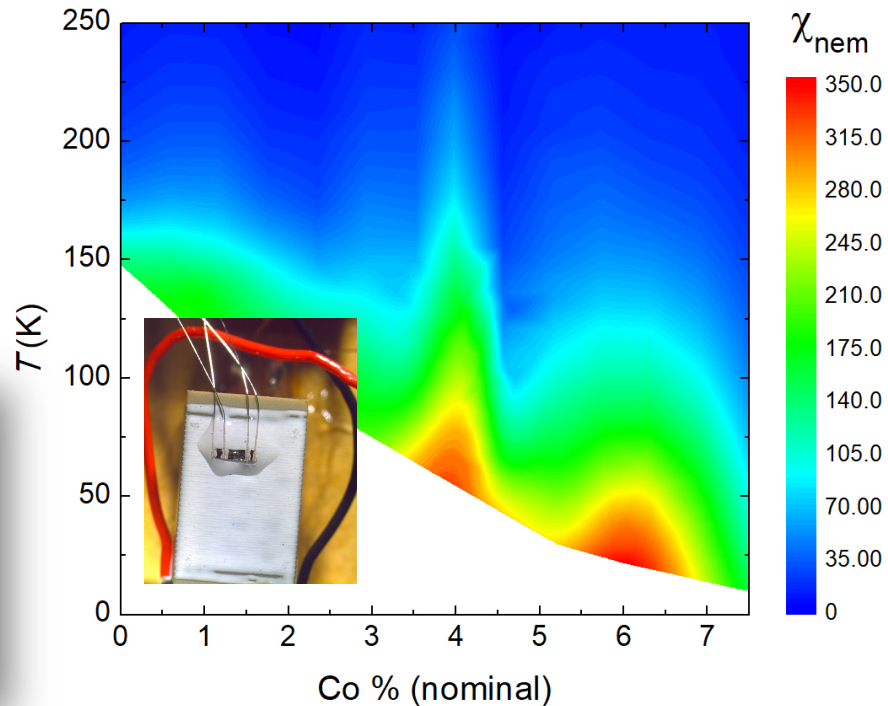
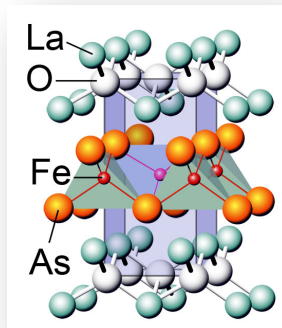


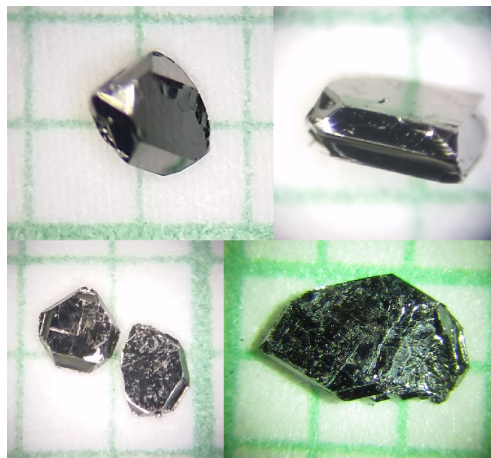
- Does the Nernst effect for $T > T_S$ measure nematic fluctuations?



work in progress

- fluorine doping
- Sm 1111
- Ce 1111
- ...





work in progress

- fluorine doping
- Sm 1111
- Ce 1111
- ...

