EXPERIMENTALLY TUNING THE GROUND STATE OF $BaFe_2As_2$ BY ORBITAL DIFFERENTIATION

<u>Priscila F. S. Rosa</u>[1,2], C. Adriano[1], T. M. Garitezi[1], T. M. Garitezi[1], T. Grant[2], Z. Fisk[2] and P. G. Pagliuso[1]

1. Institute of Physics “Gleb Wataghin”, UNICAMP, Campinas SP, 13083-970, Brazil

2. University of California, Irvine, California 92697, USA

GPOMS UNICAMP

CNPq

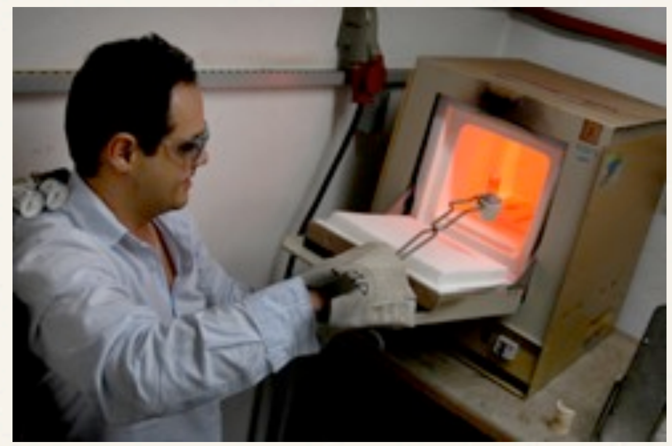
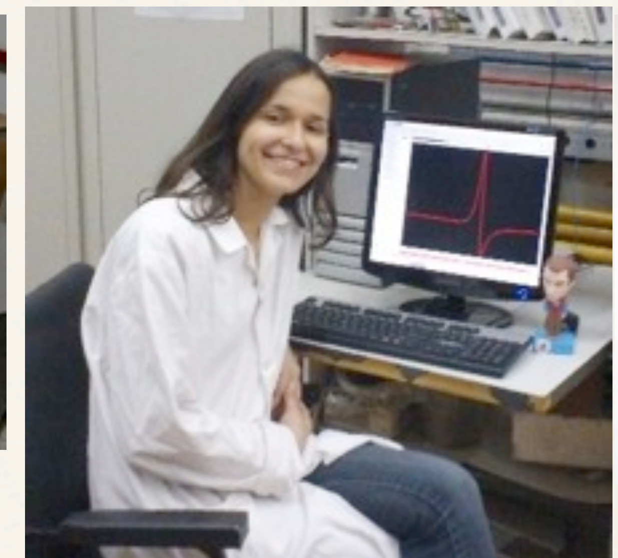
FAPESP

Magnetism, Bad Metals and Superconductivity: Iron Pnictides and Beyond

October 7, 2014

FeAs Team



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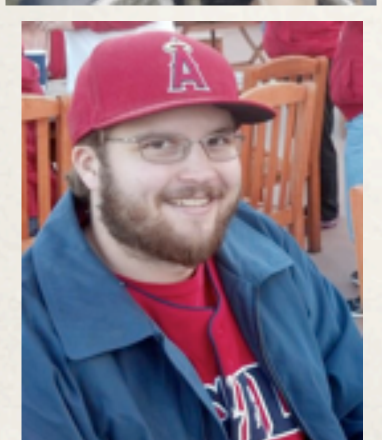

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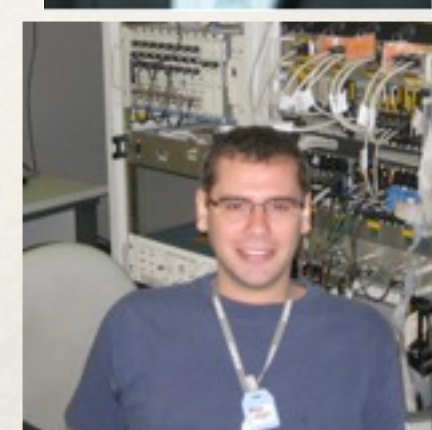

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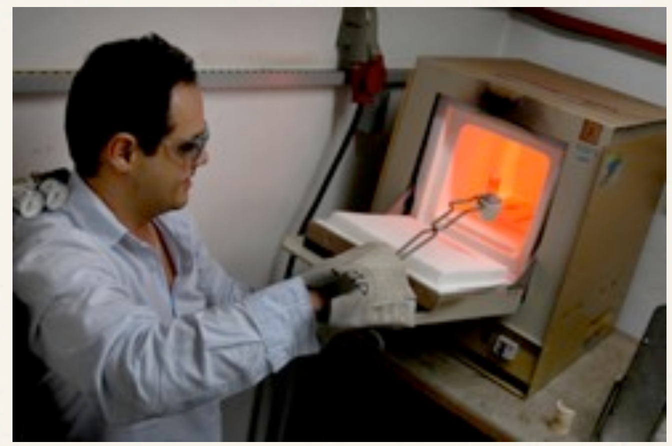



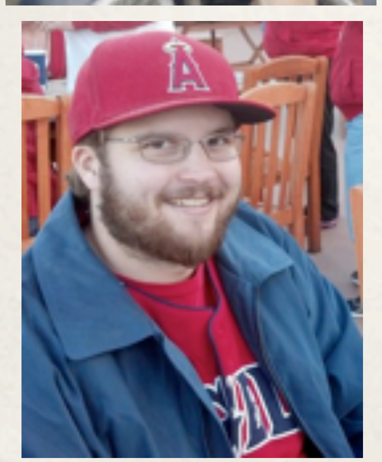

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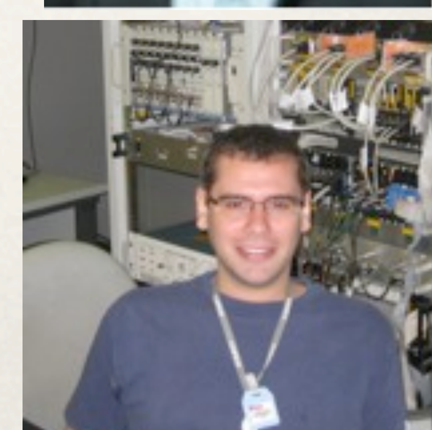

Outline

- Introduction and Motivation: Fe-based Superconductors

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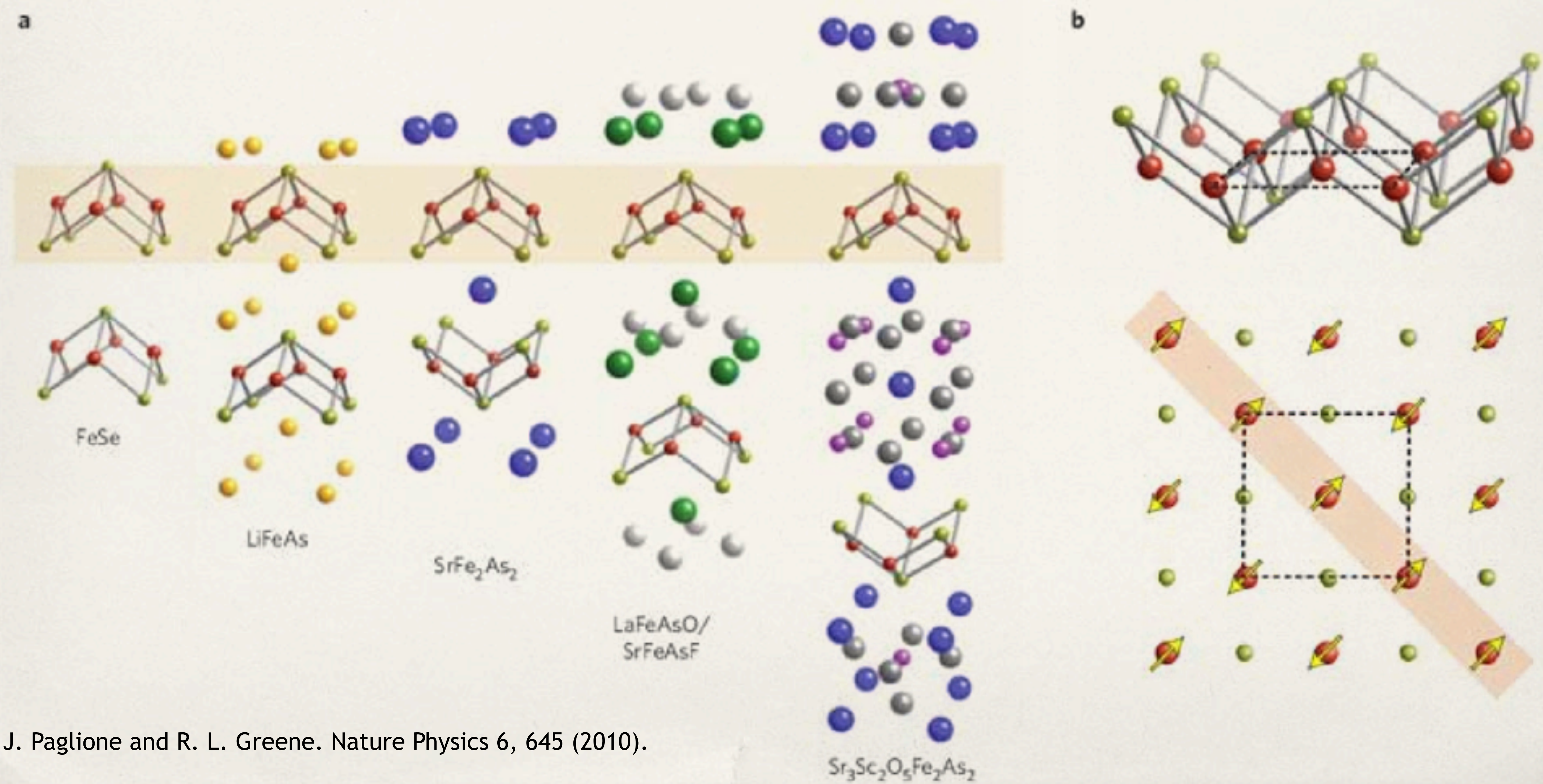
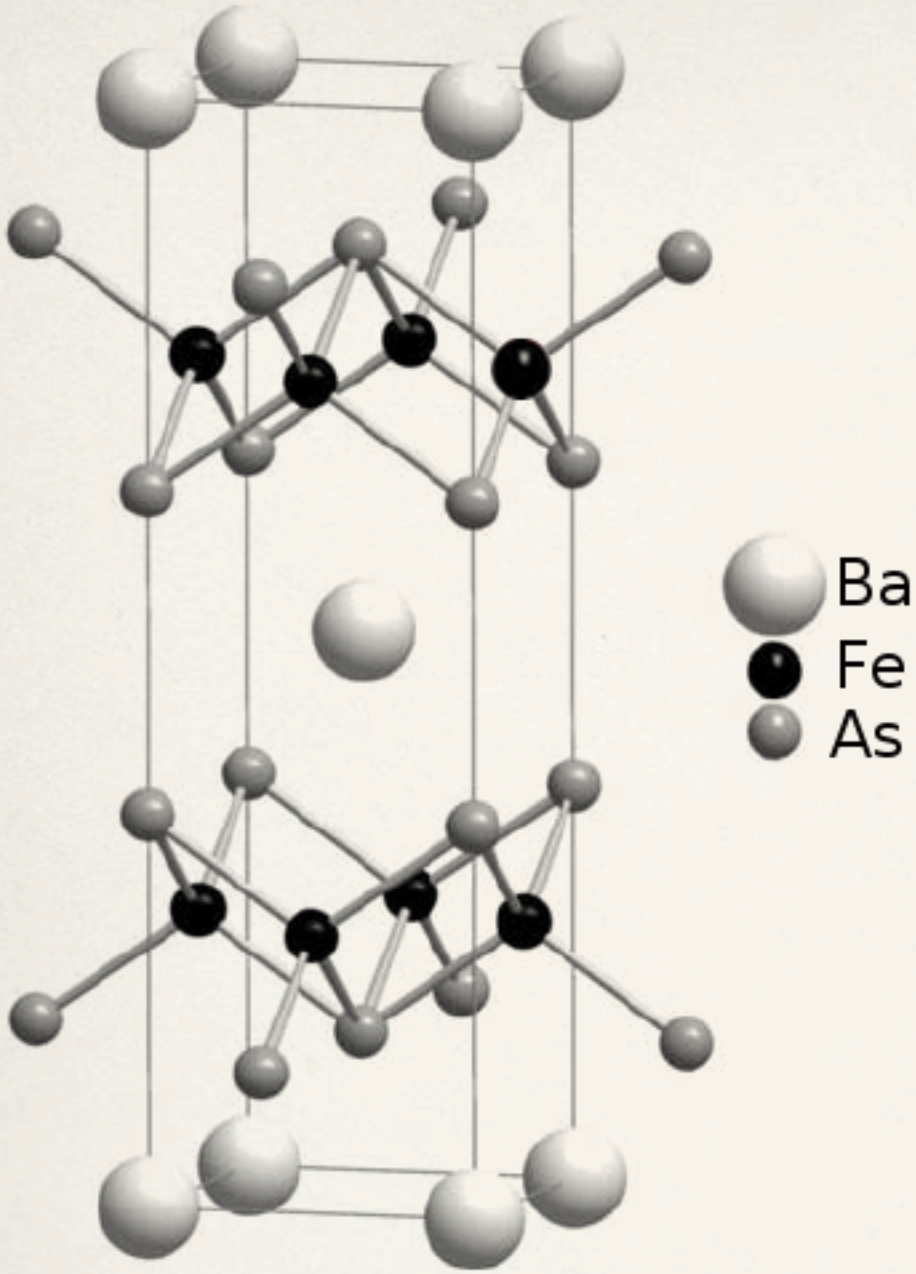
Fe-based superconductors

- Common Structural Parameter: $FeAs_4$ tetrahedra
- Common Electronic Parameter: Spin-Density Wave (SDW) magnetic instability.

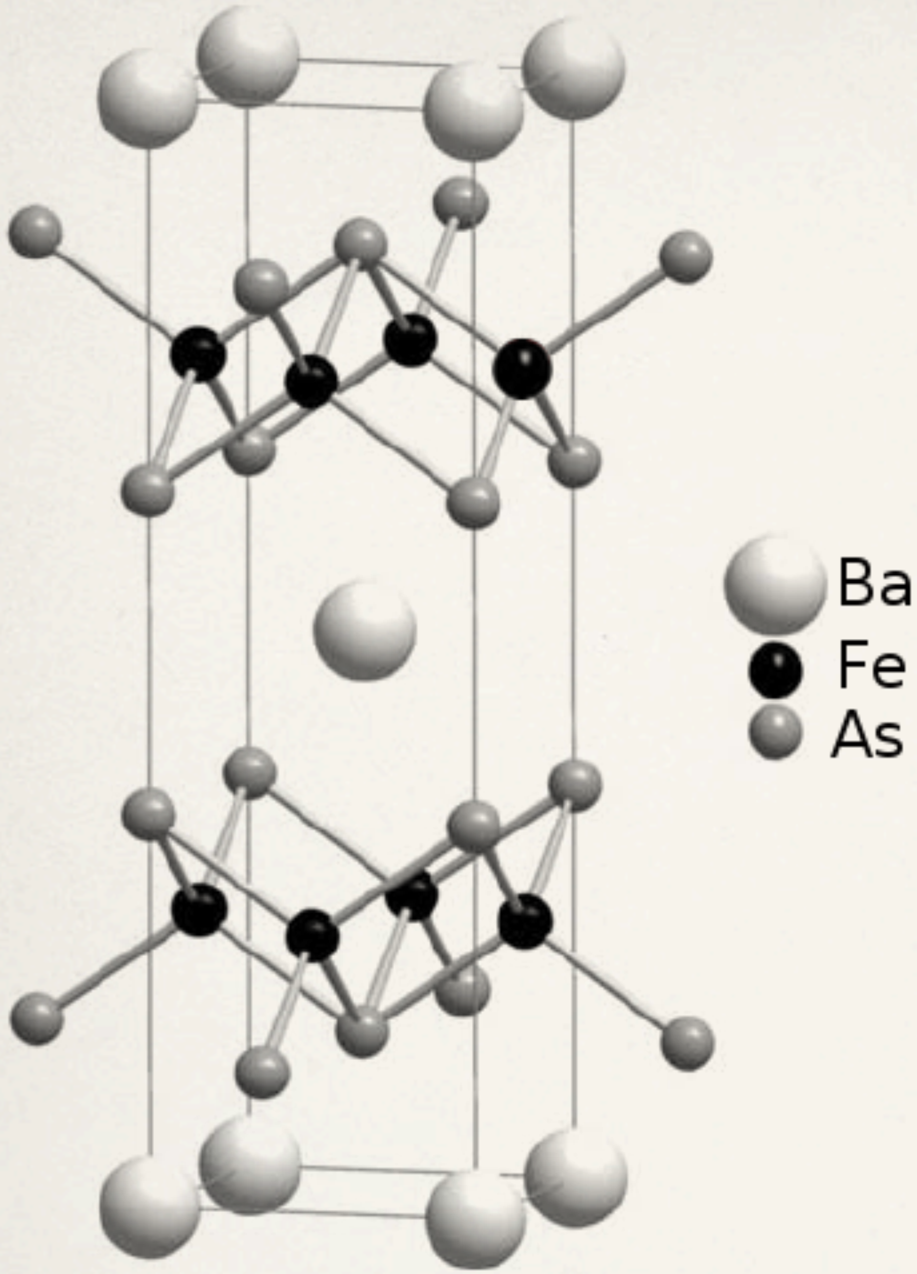


J. Paglione and R. L. Greene. Nature Physics 6, 645 (2010).



Good sample quality;

Variety of compounds.



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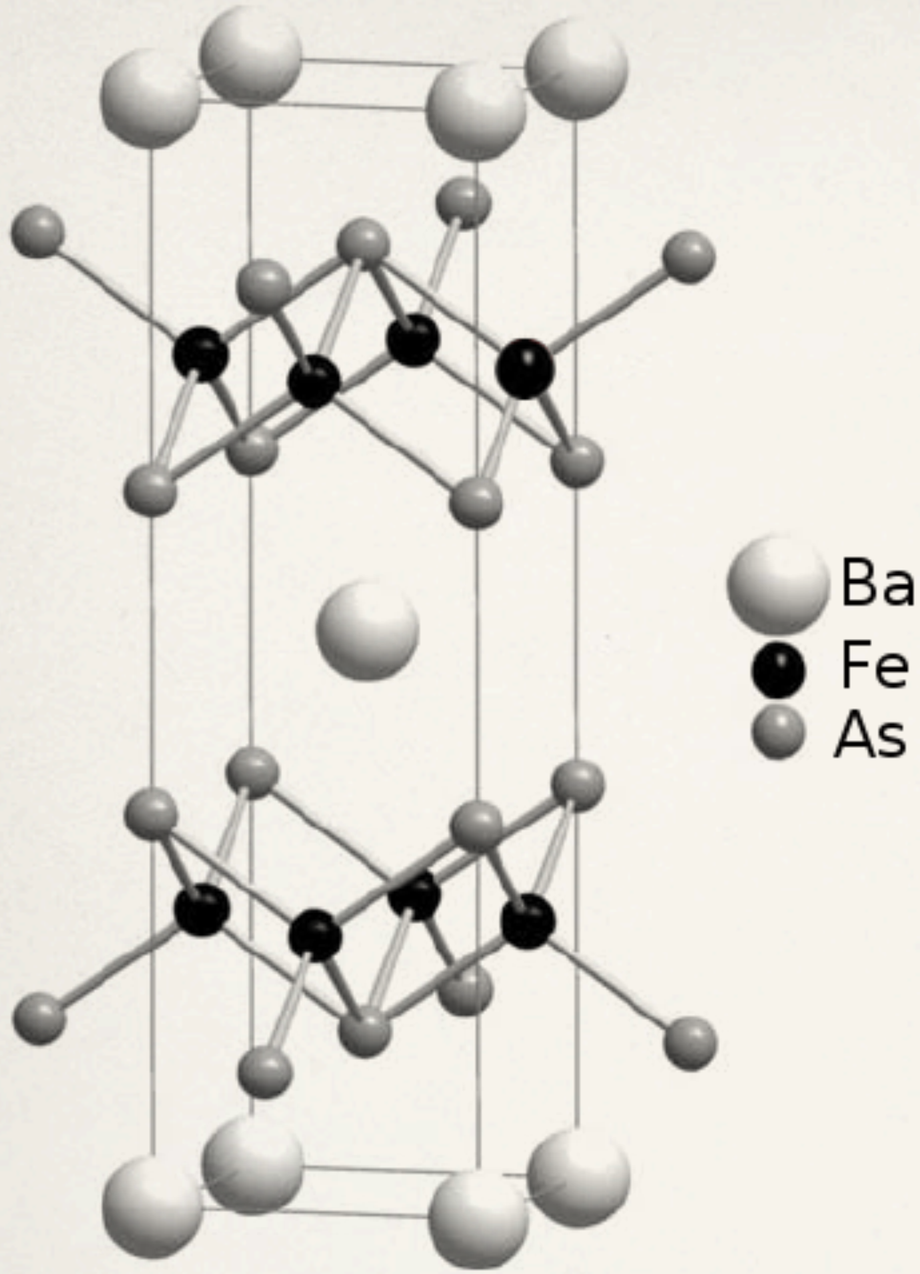

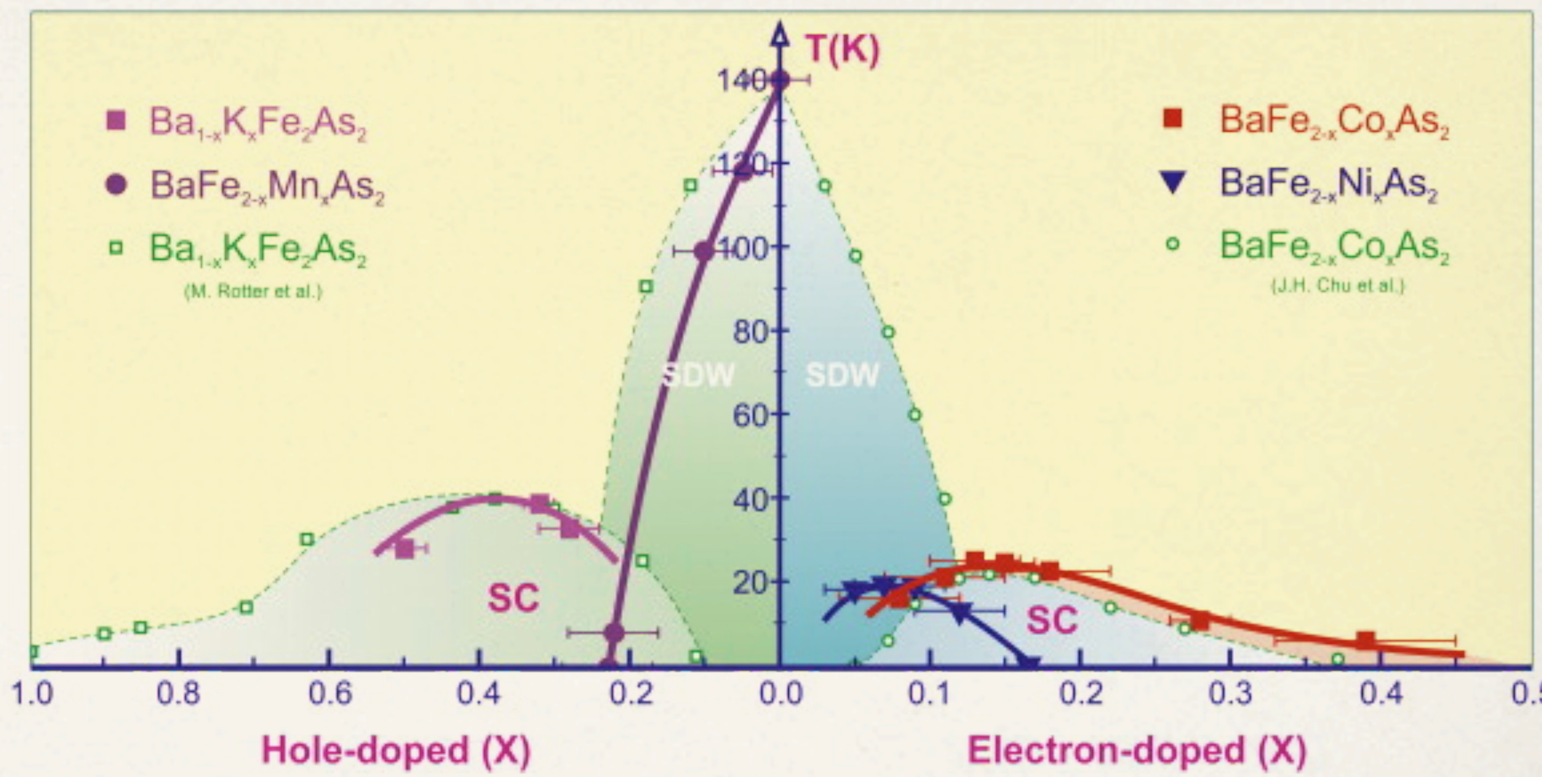

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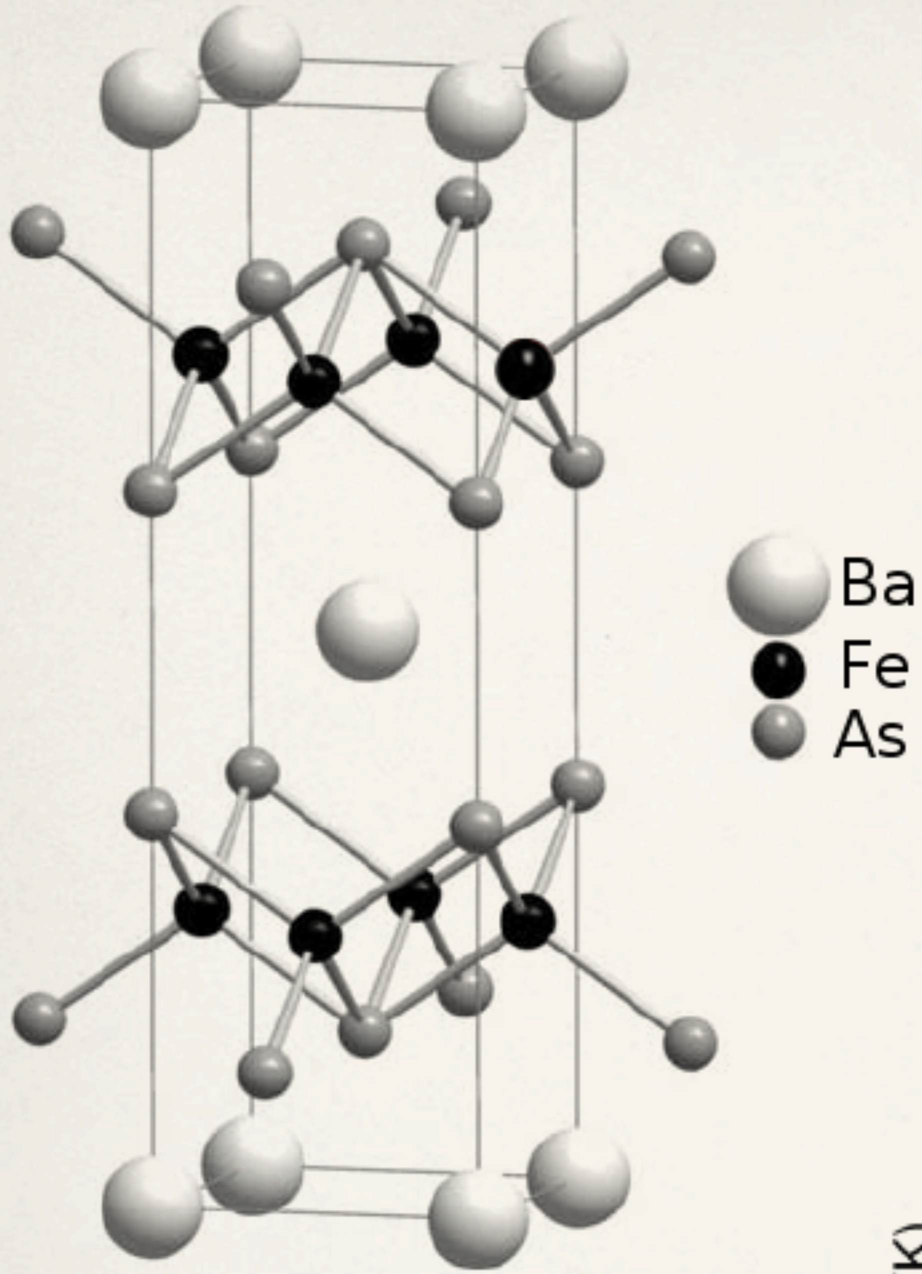

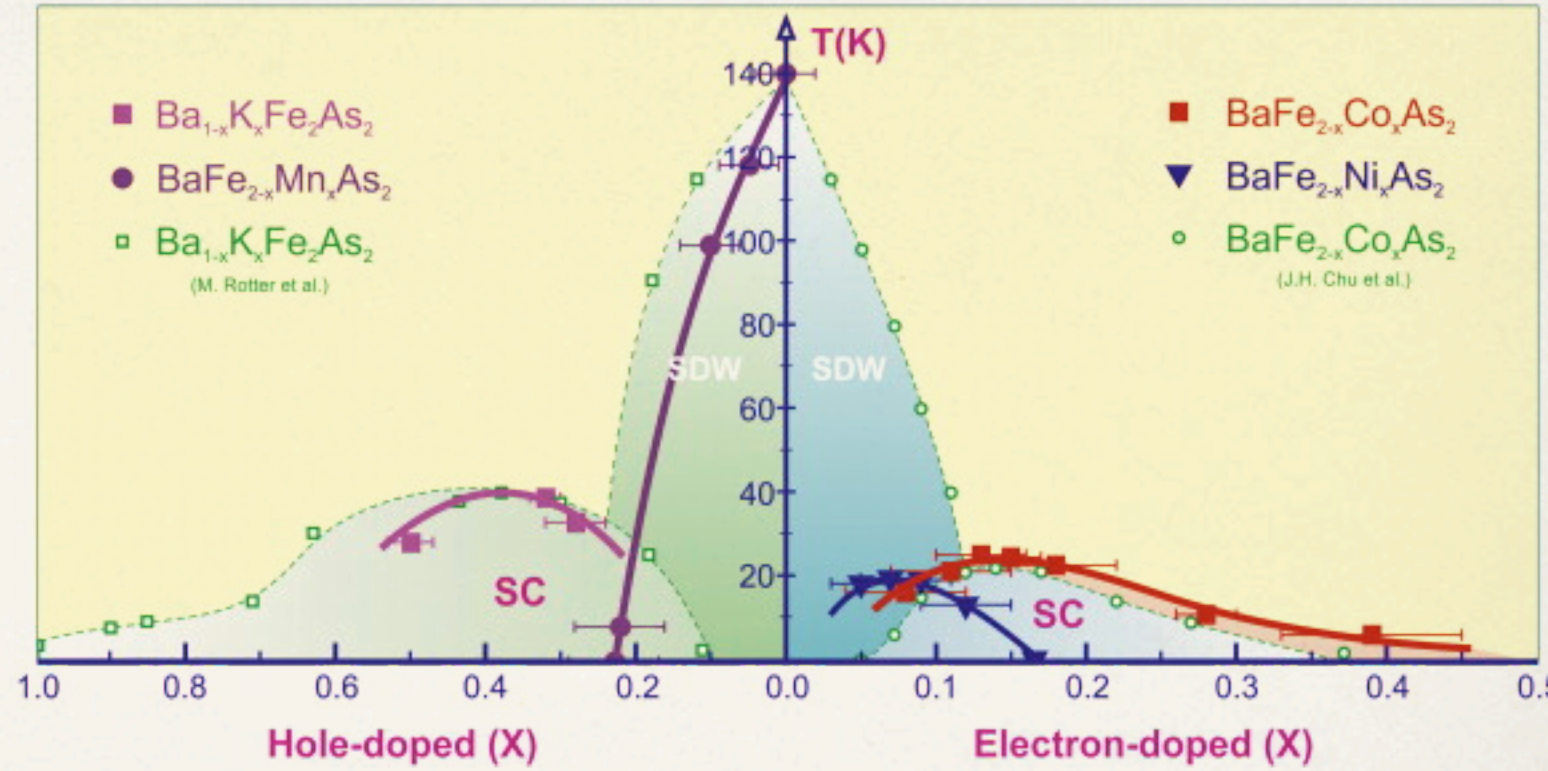

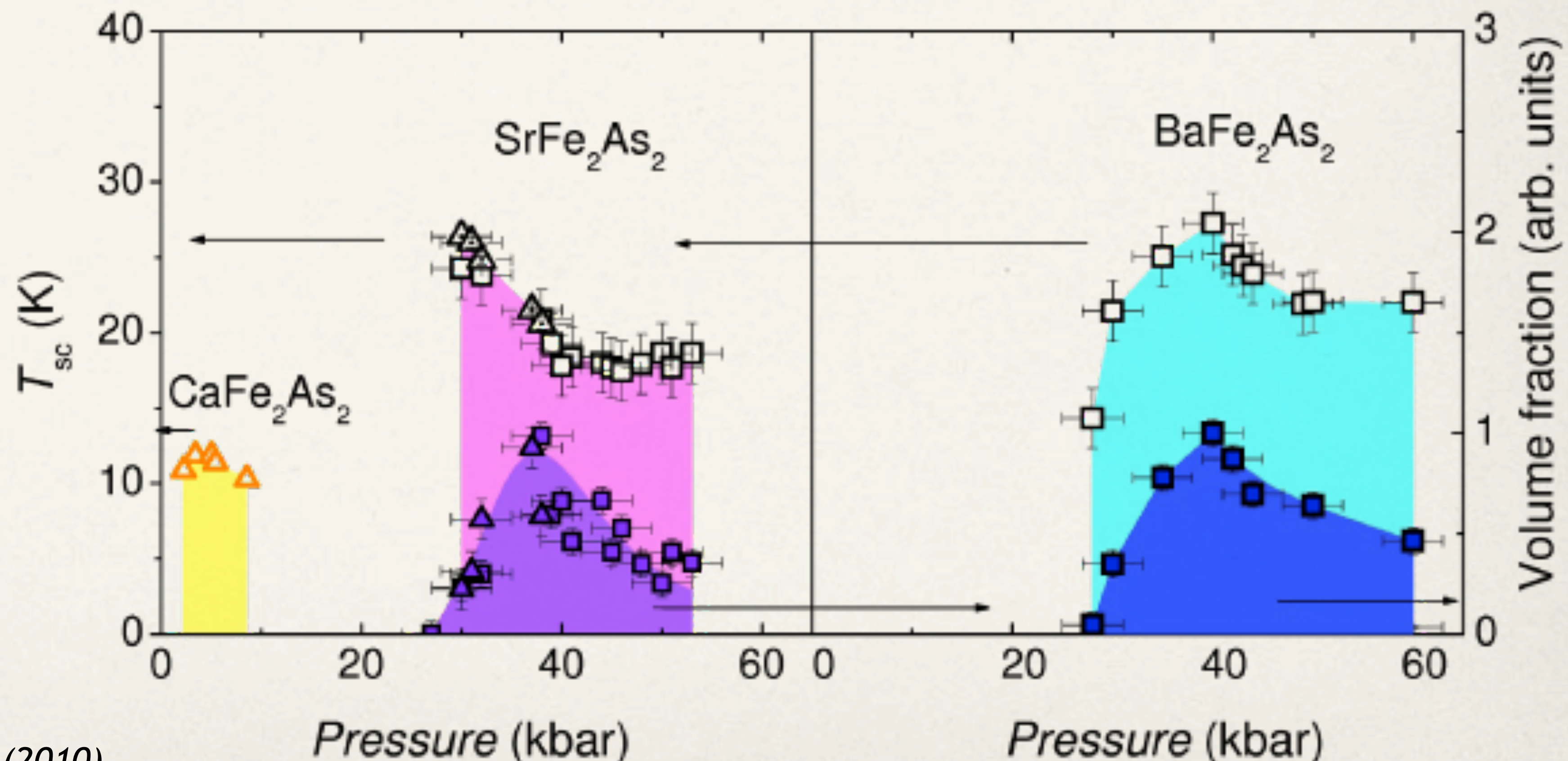

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How one can relate Fe-based superconductors to other unconventional superconductors?

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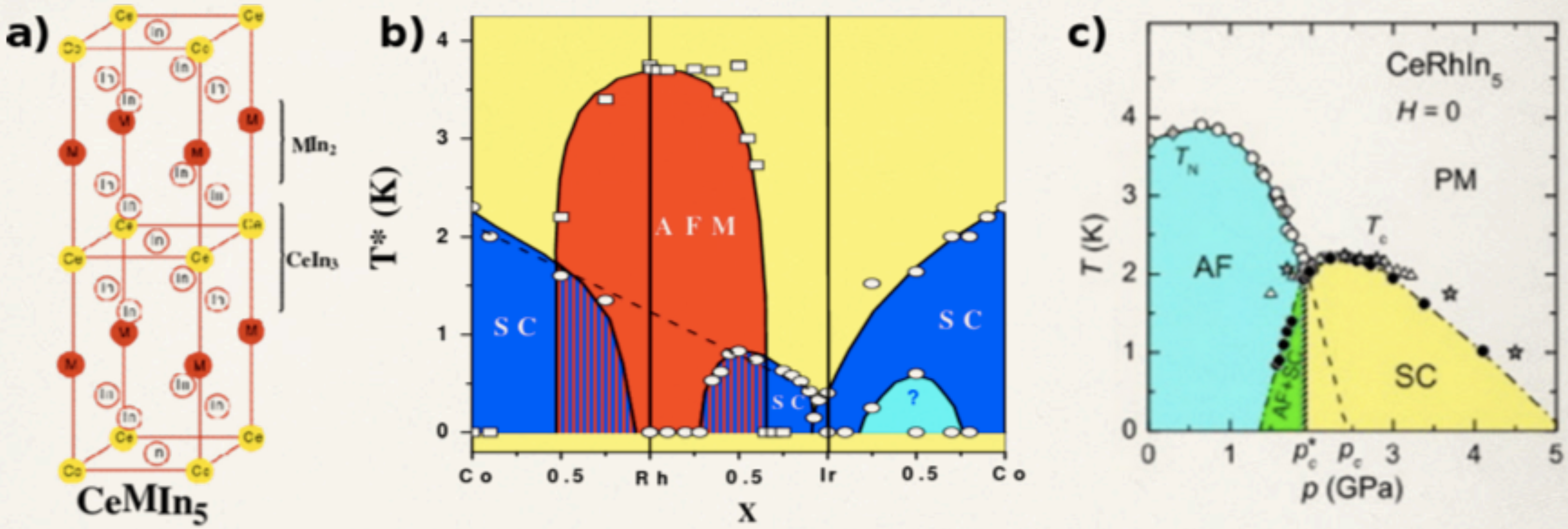
Heavy Fermions (*d-wave*)



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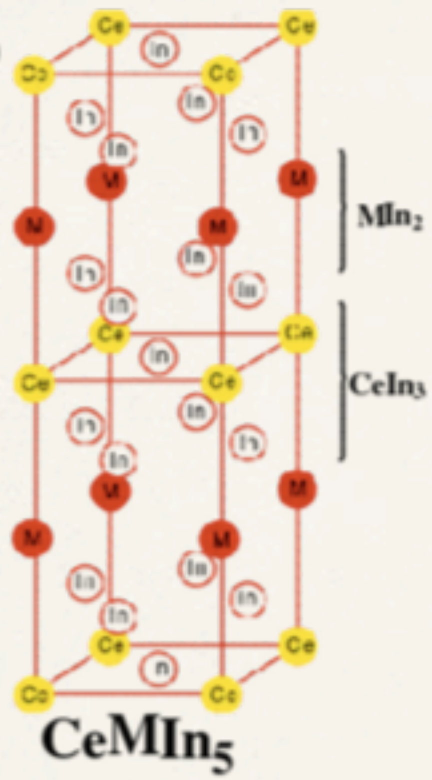

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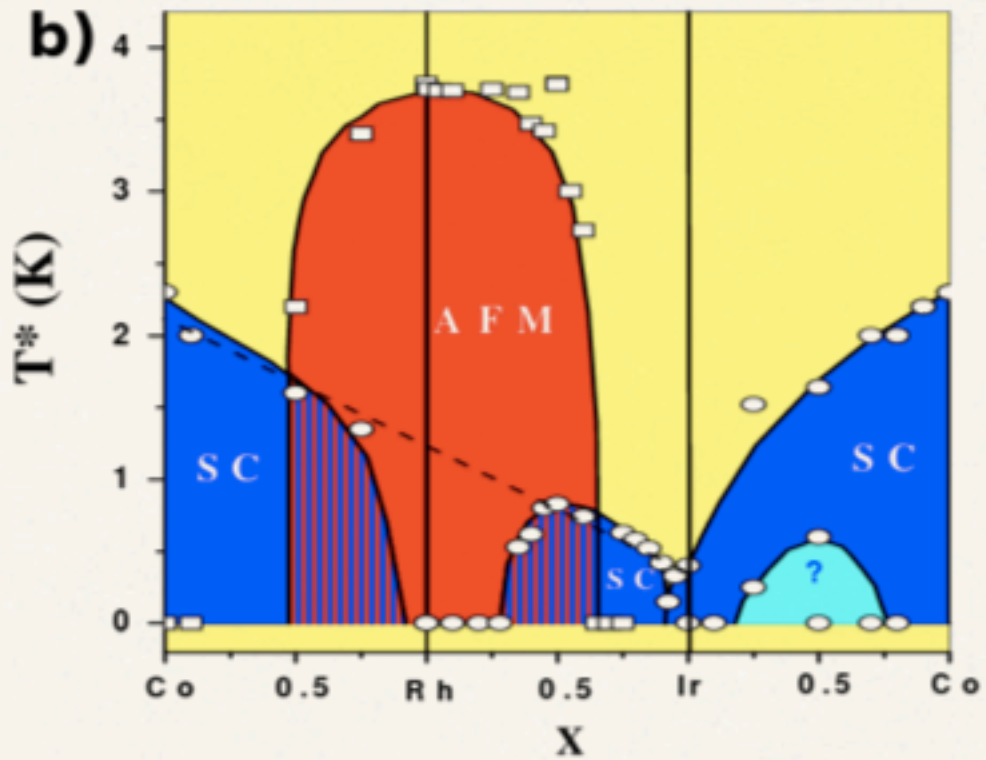
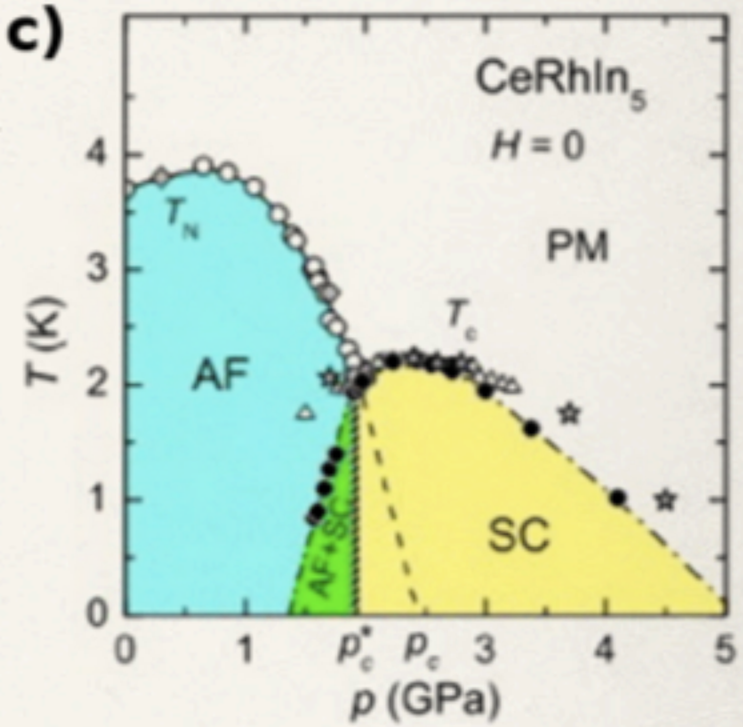
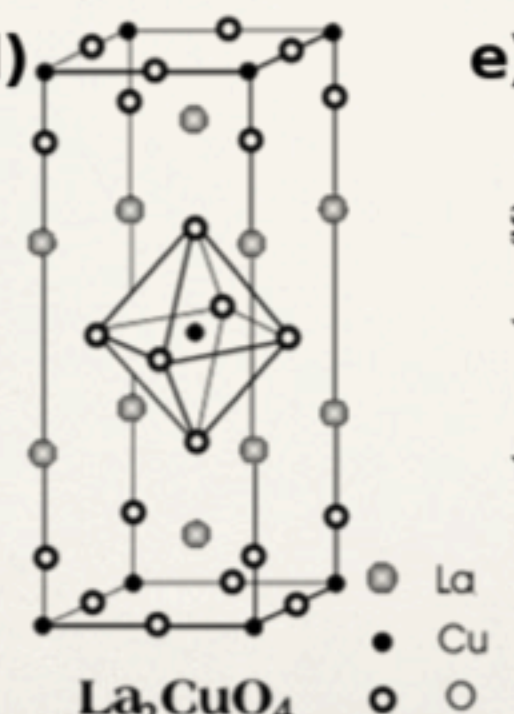


c)



Cuprates (*d-wave*)

d)



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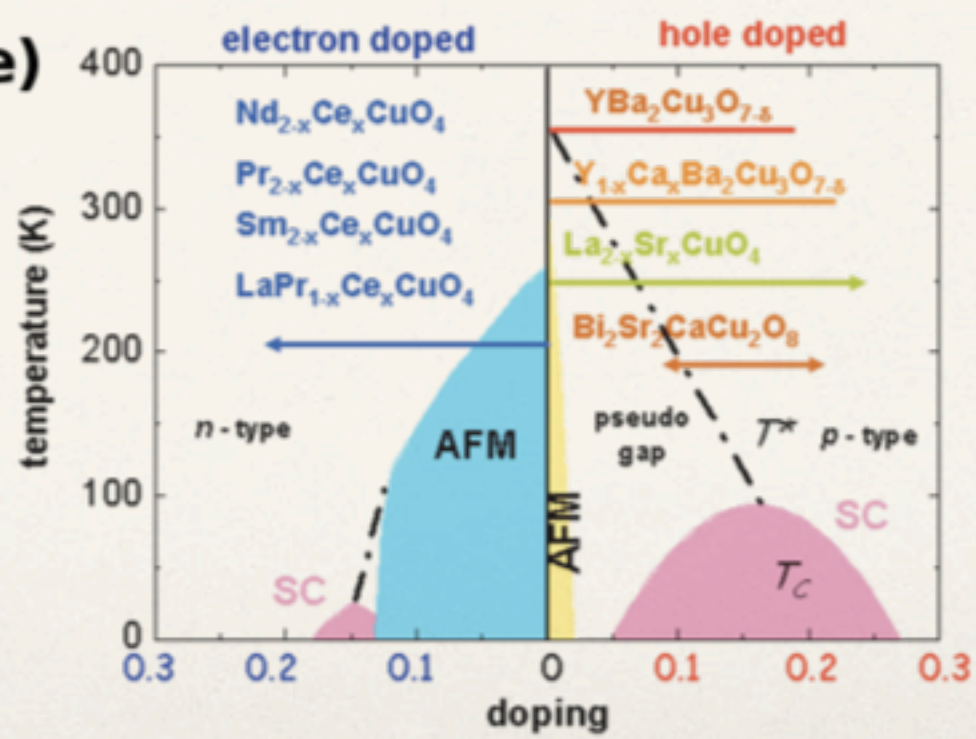

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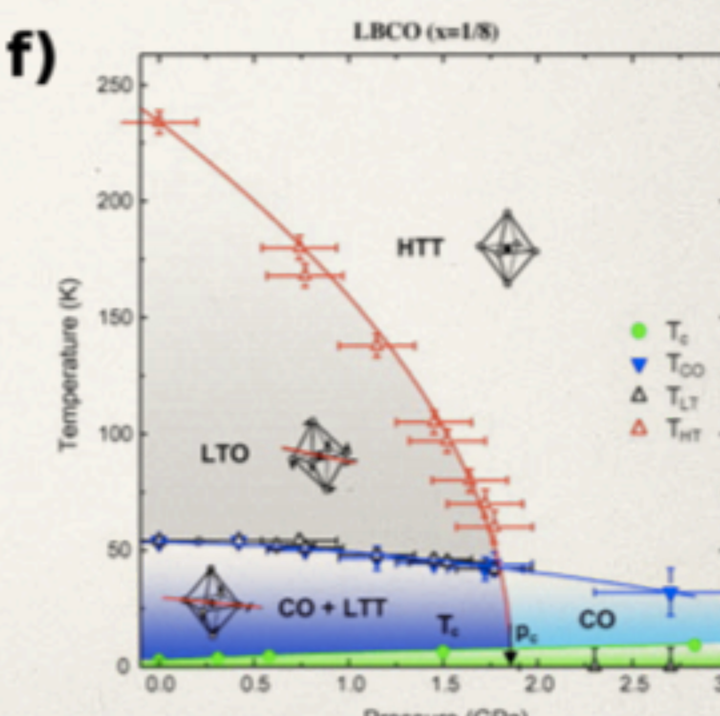

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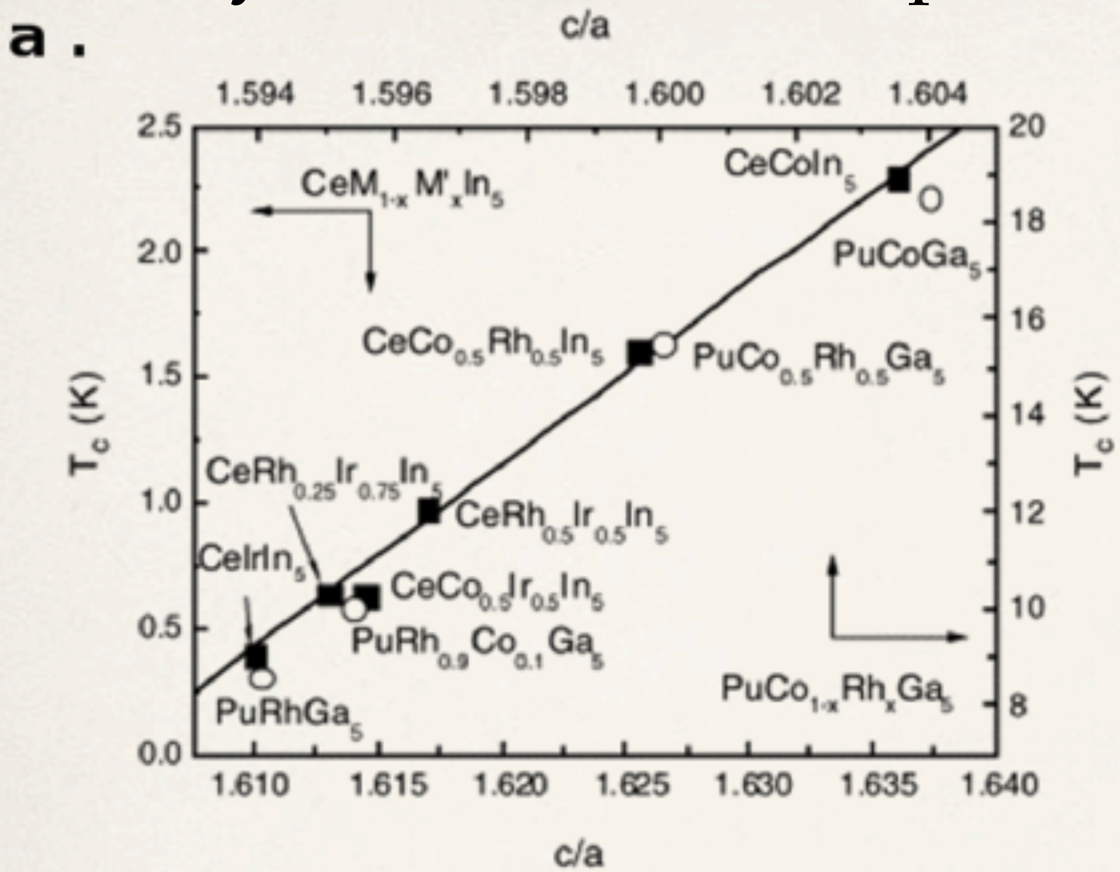
Structural Similarities

- Heavy Fermions and Cuprates



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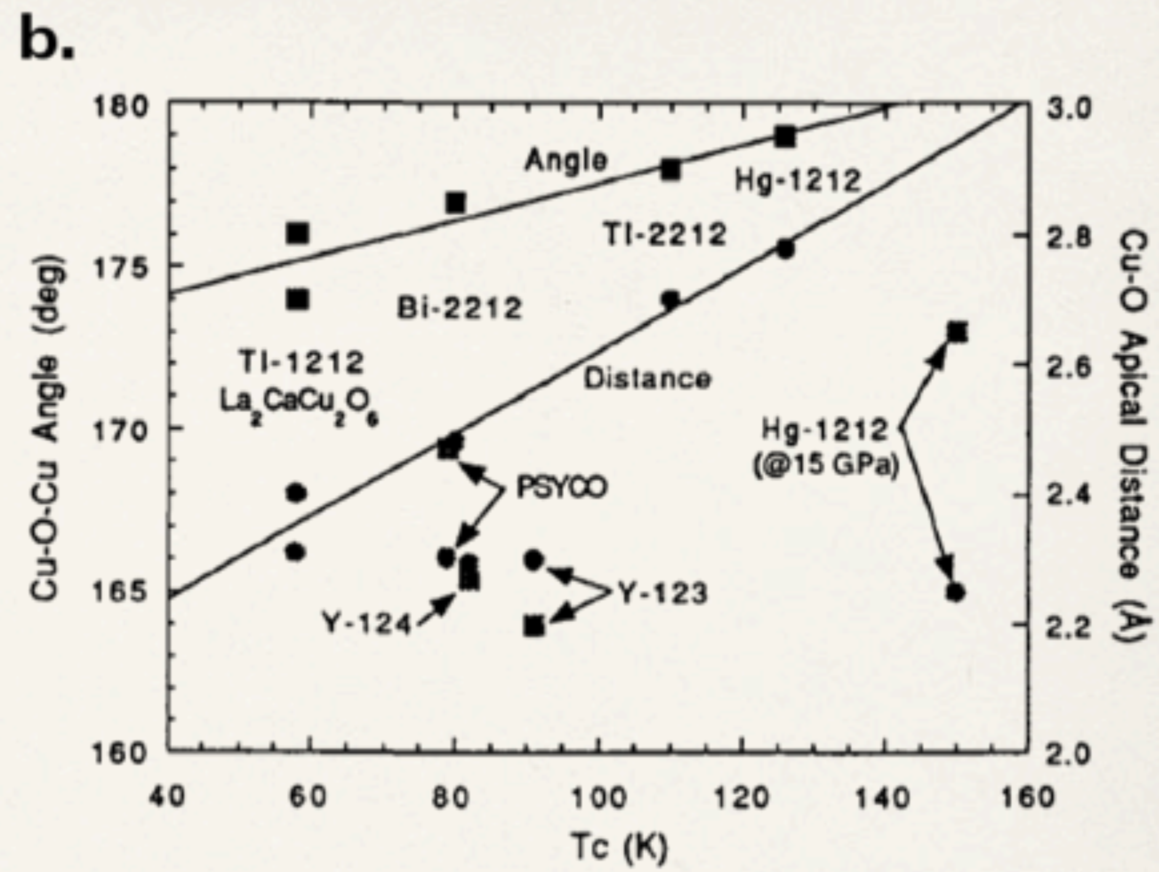

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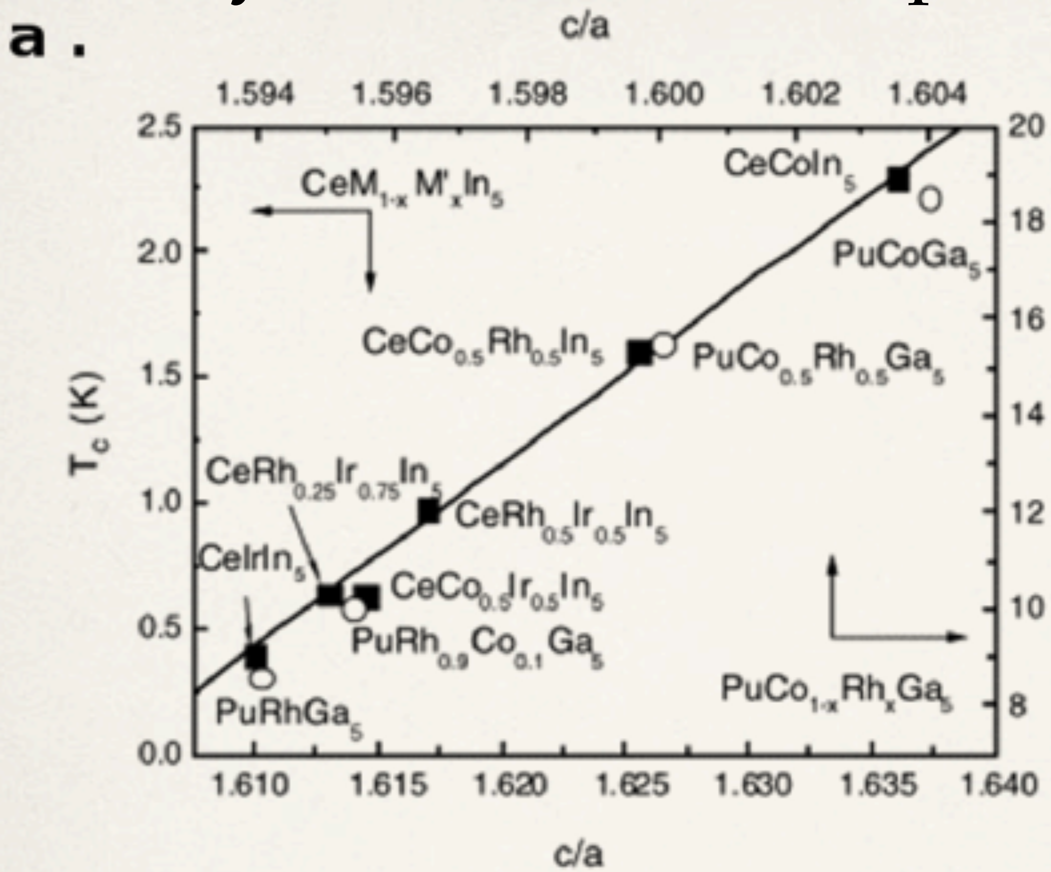

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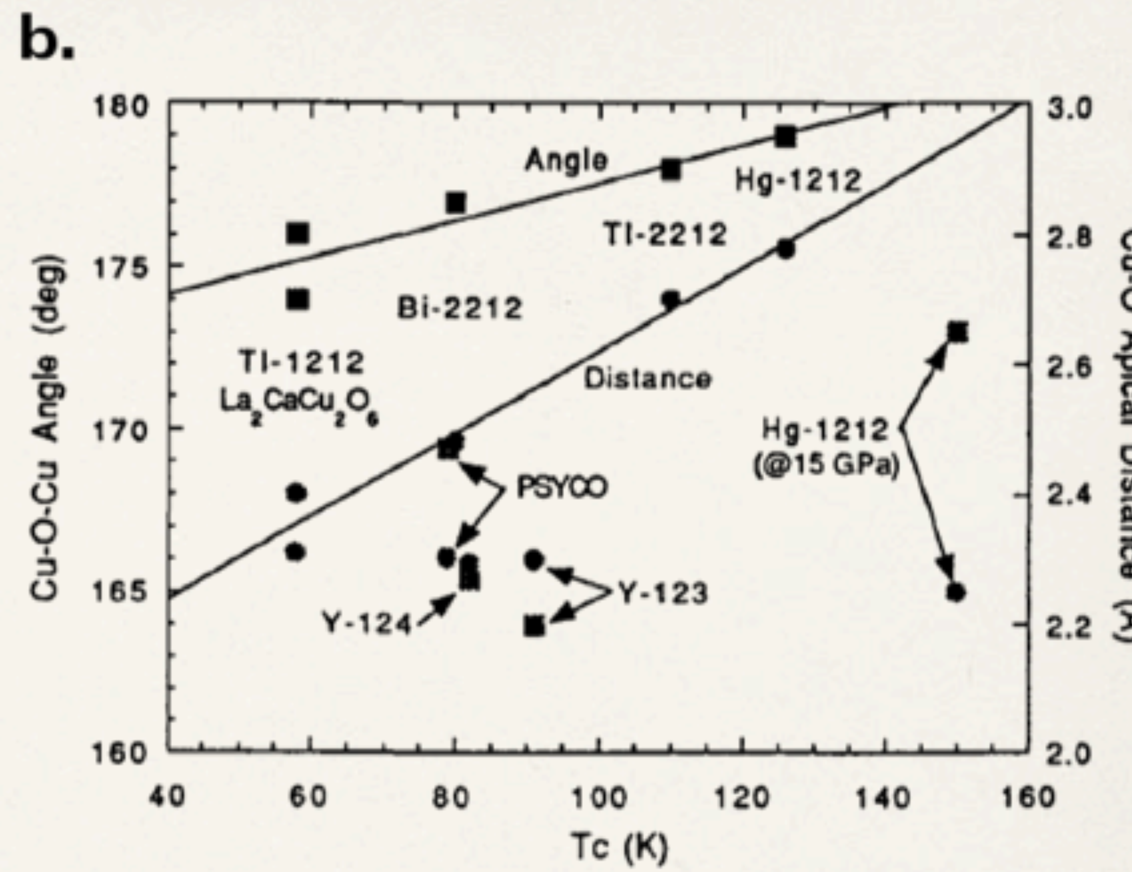

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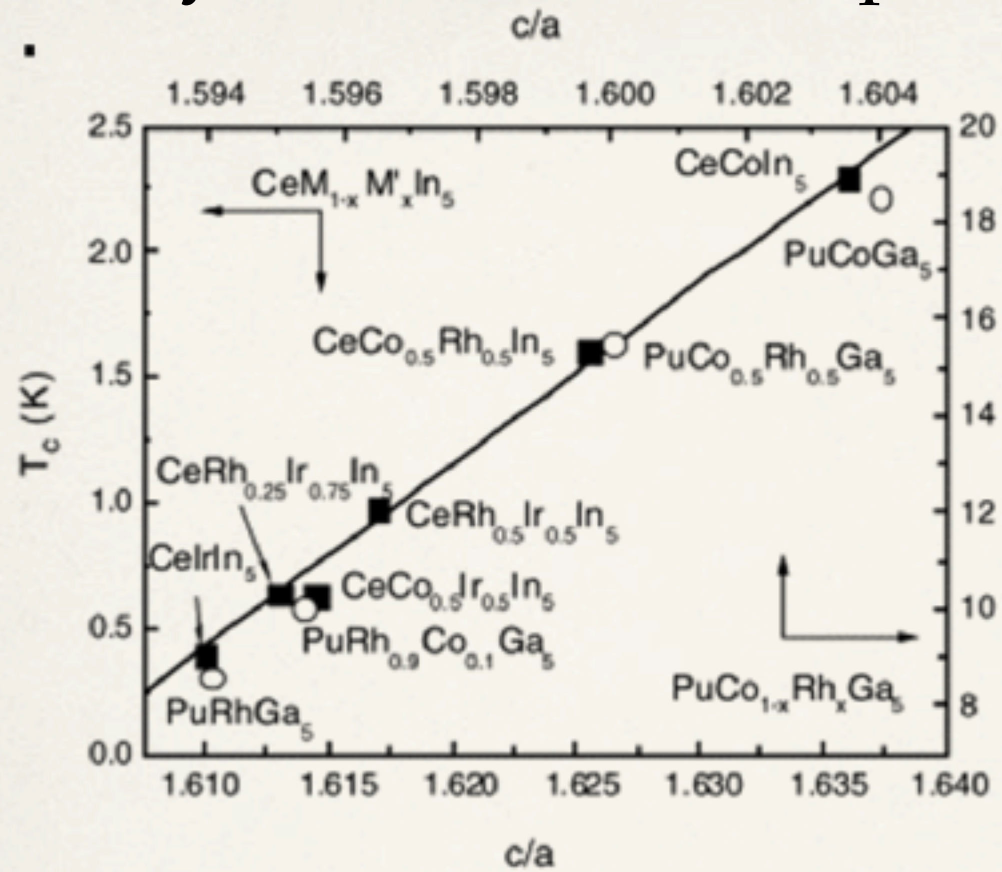

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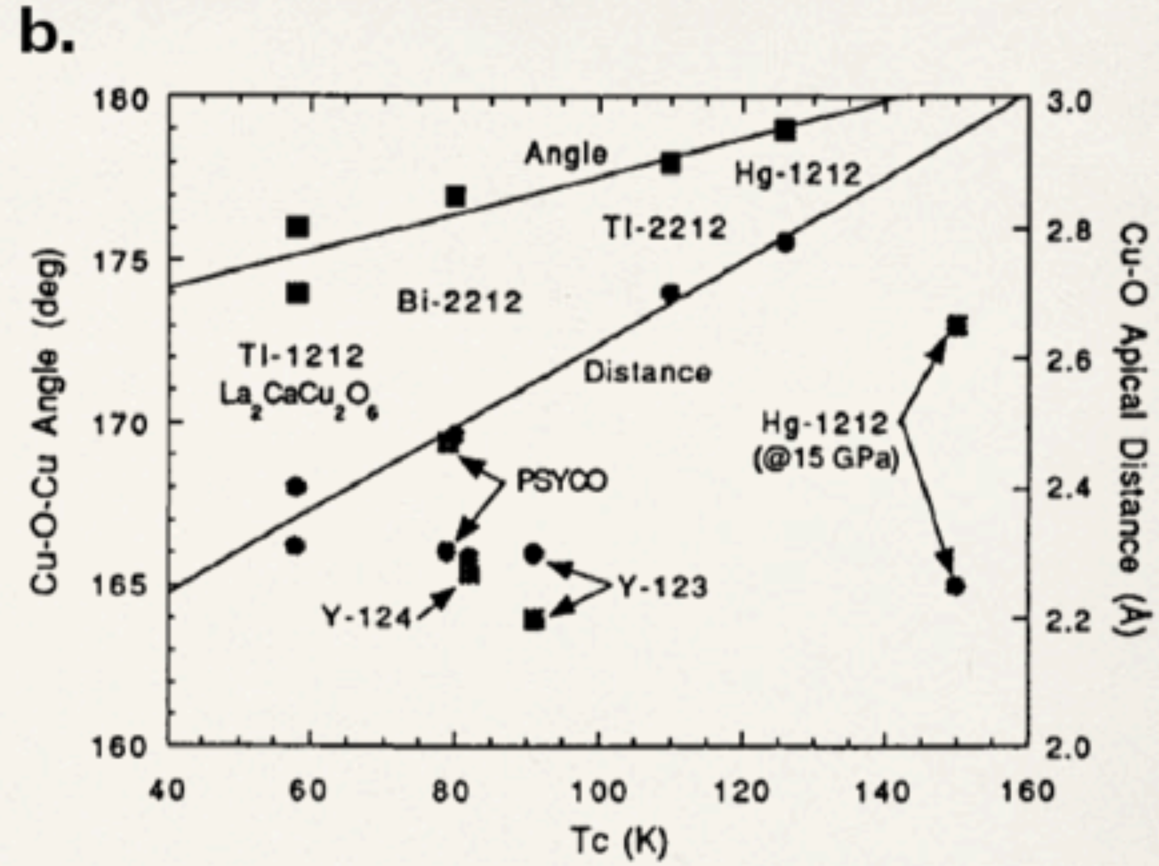

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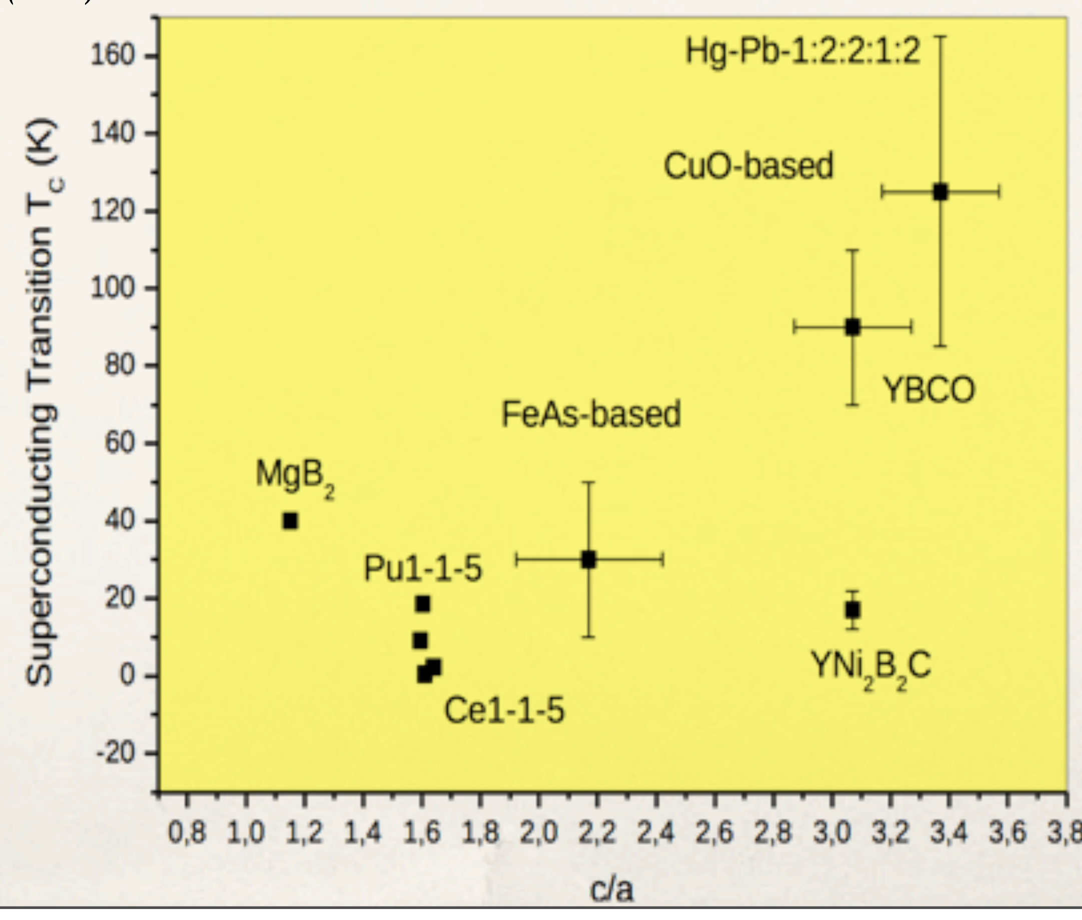

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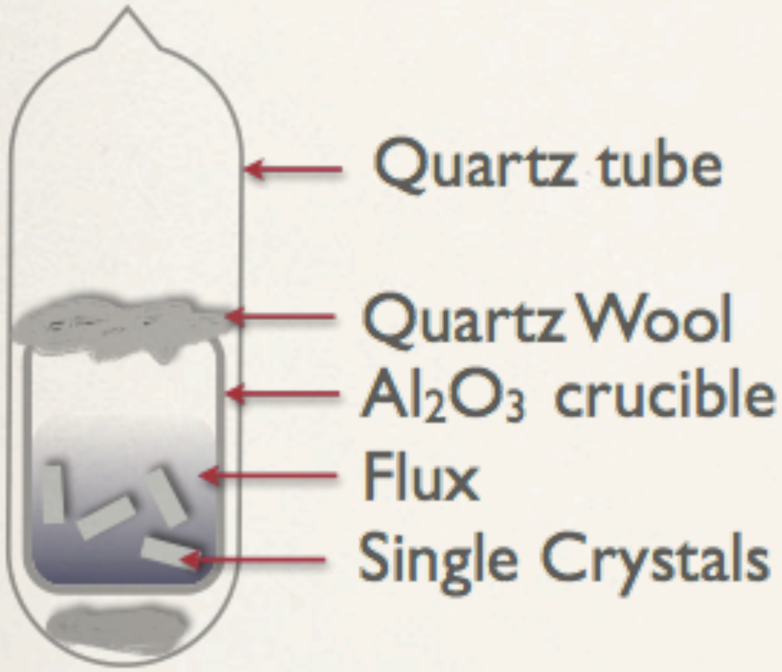
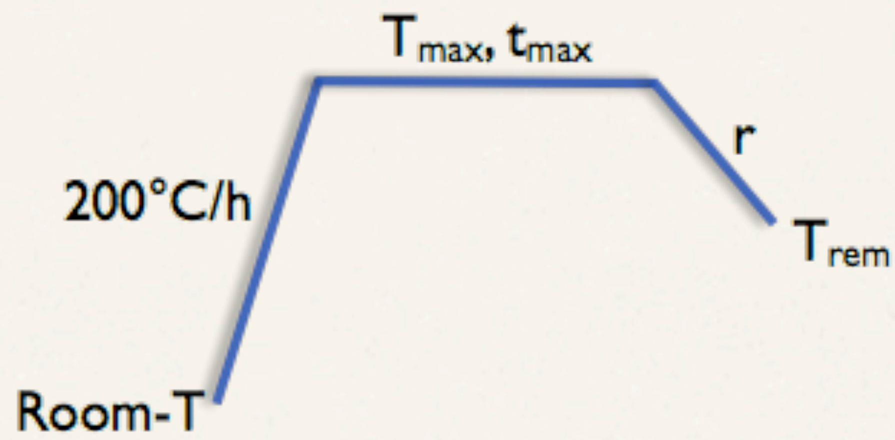
Single crystal growth by the metallic-flux technique





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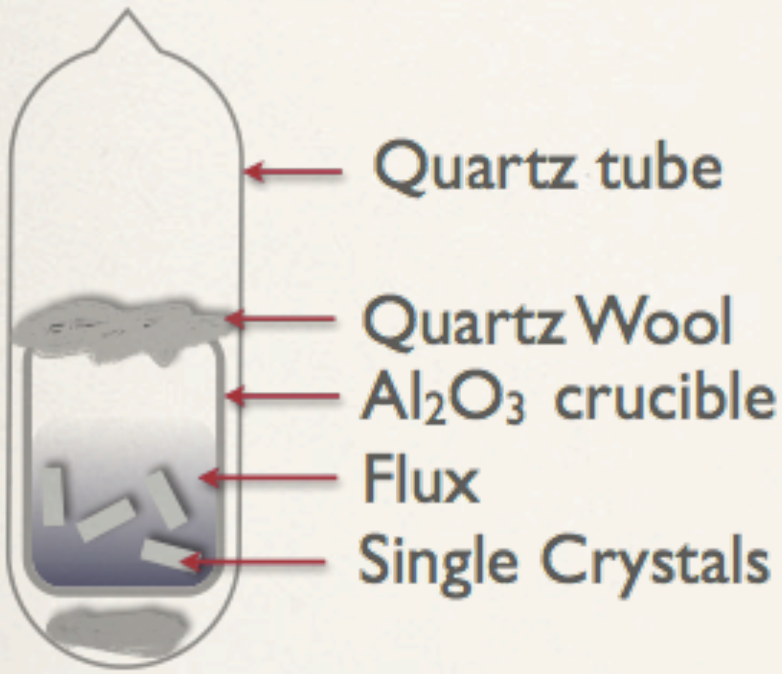

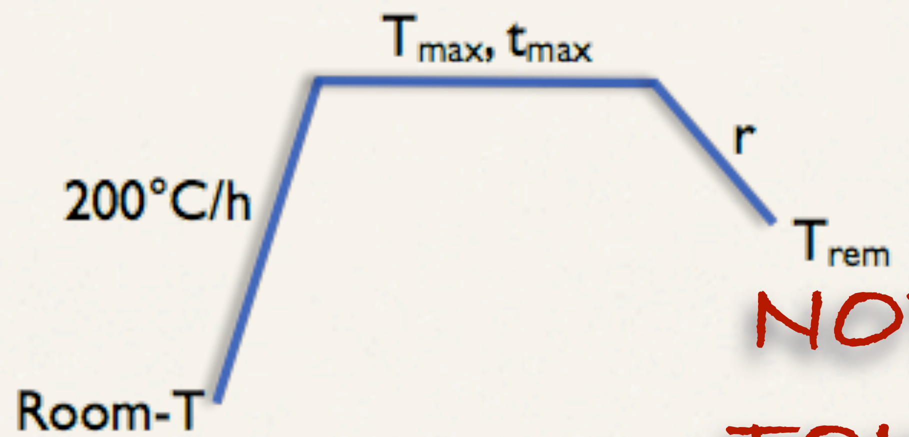

NOT A TOILET BOWL!!!

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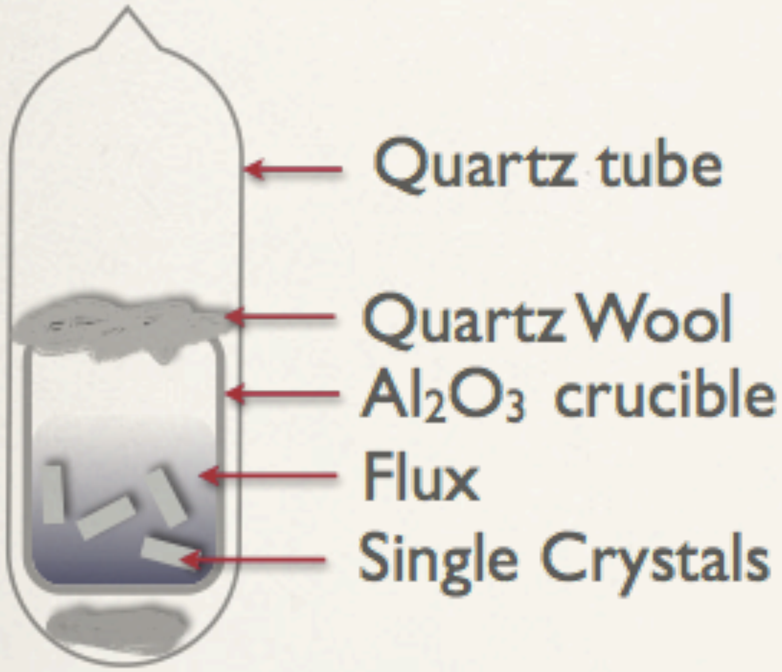

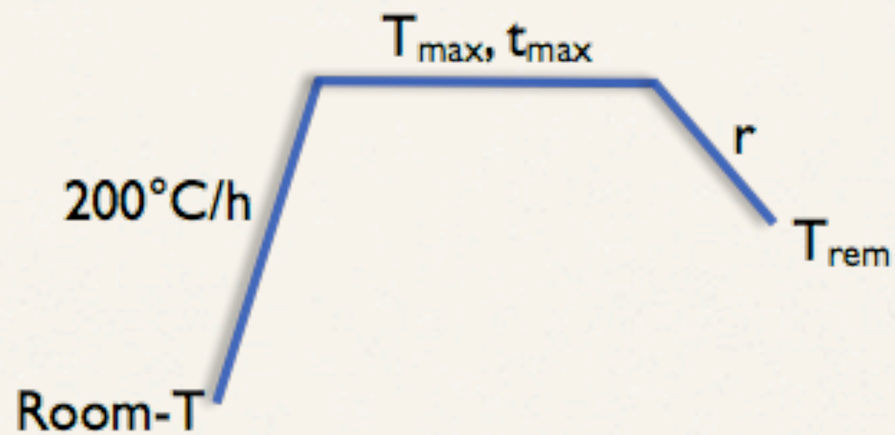

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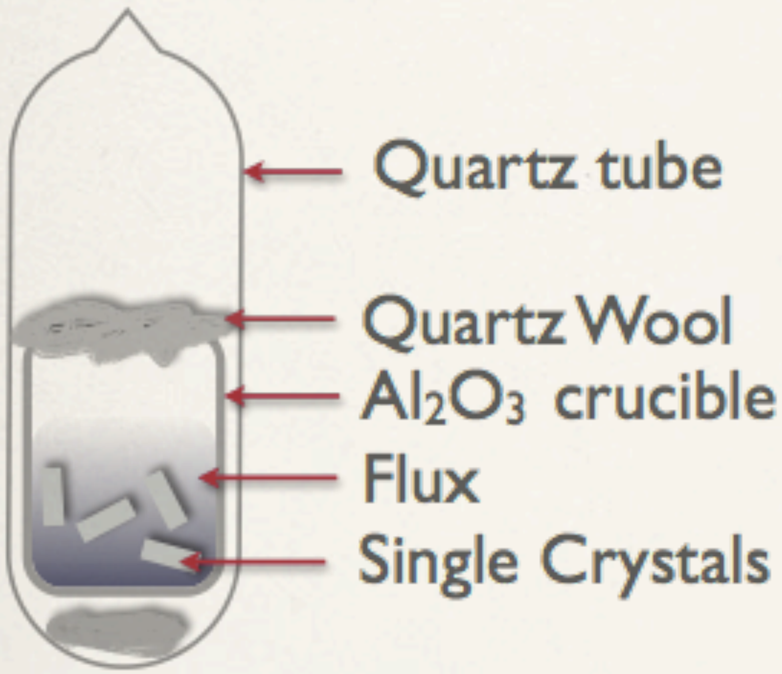

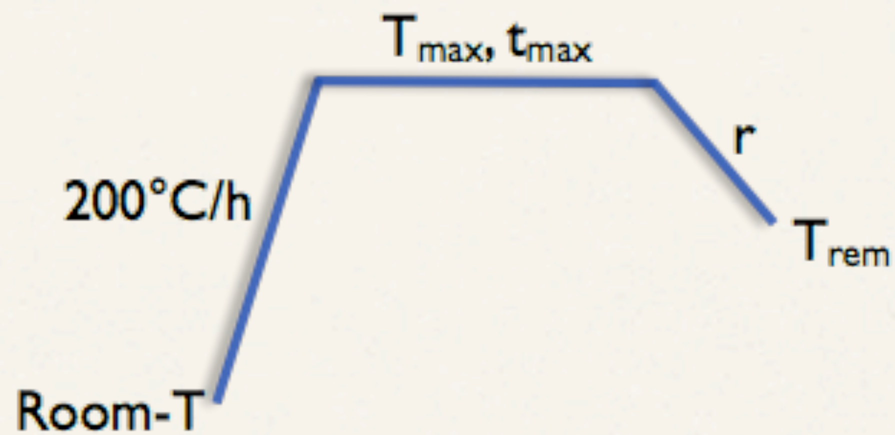

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- Current disadvantages: Sn-incorporation and possible non-stoichiometric 122 compounds using self-(FeAs-) flux.

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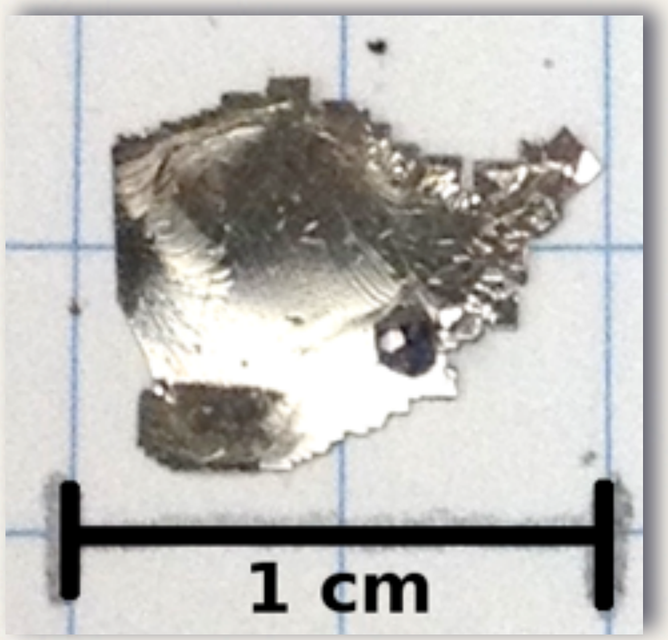
Indium flux → $BaFe_2As_2$



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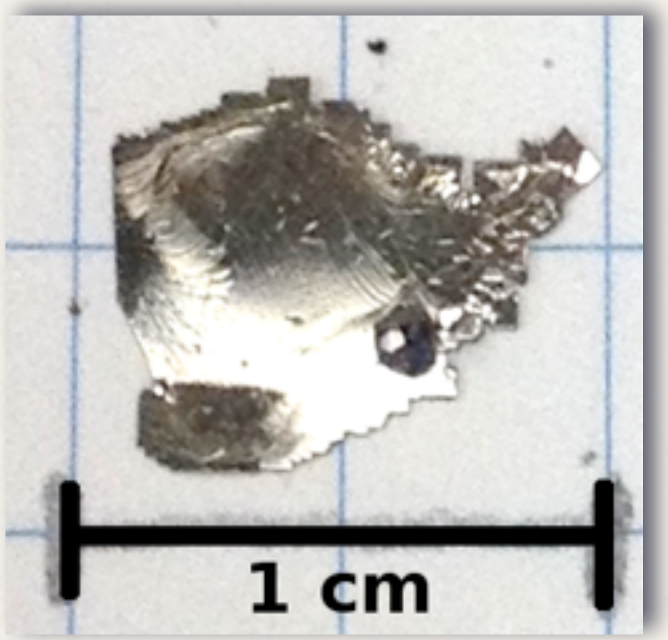

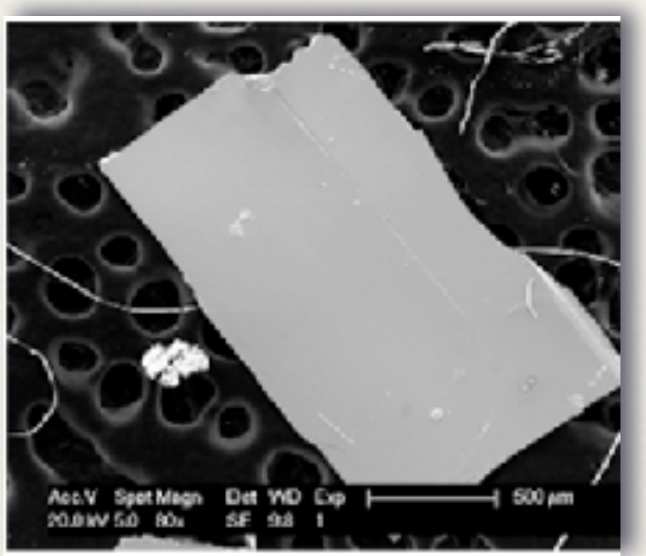

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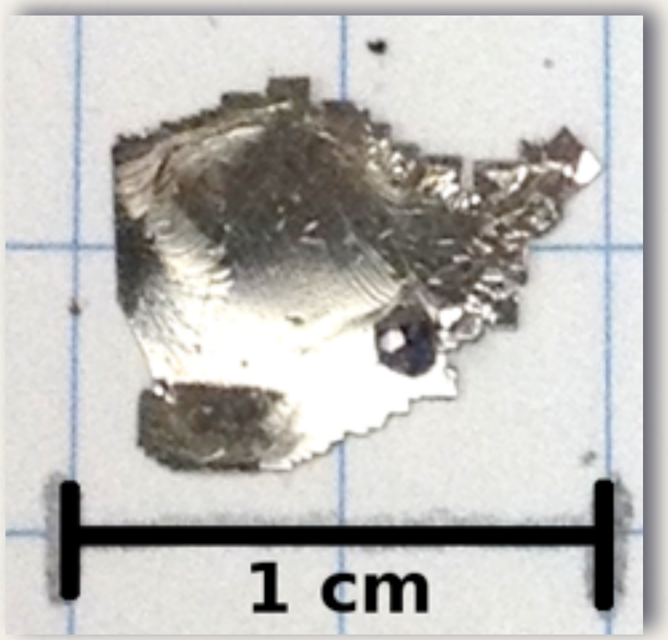
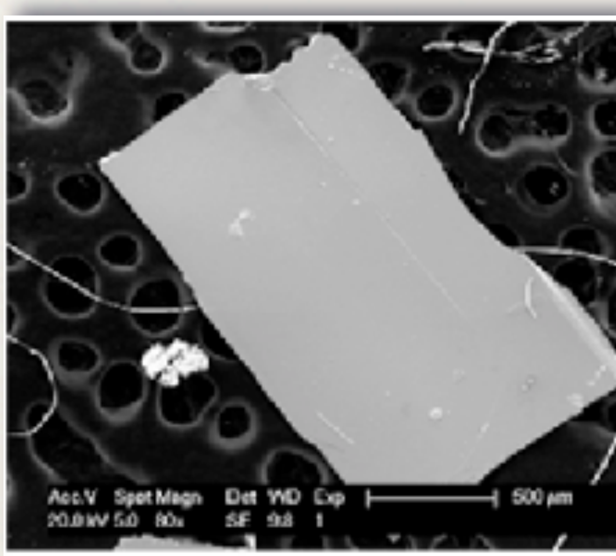
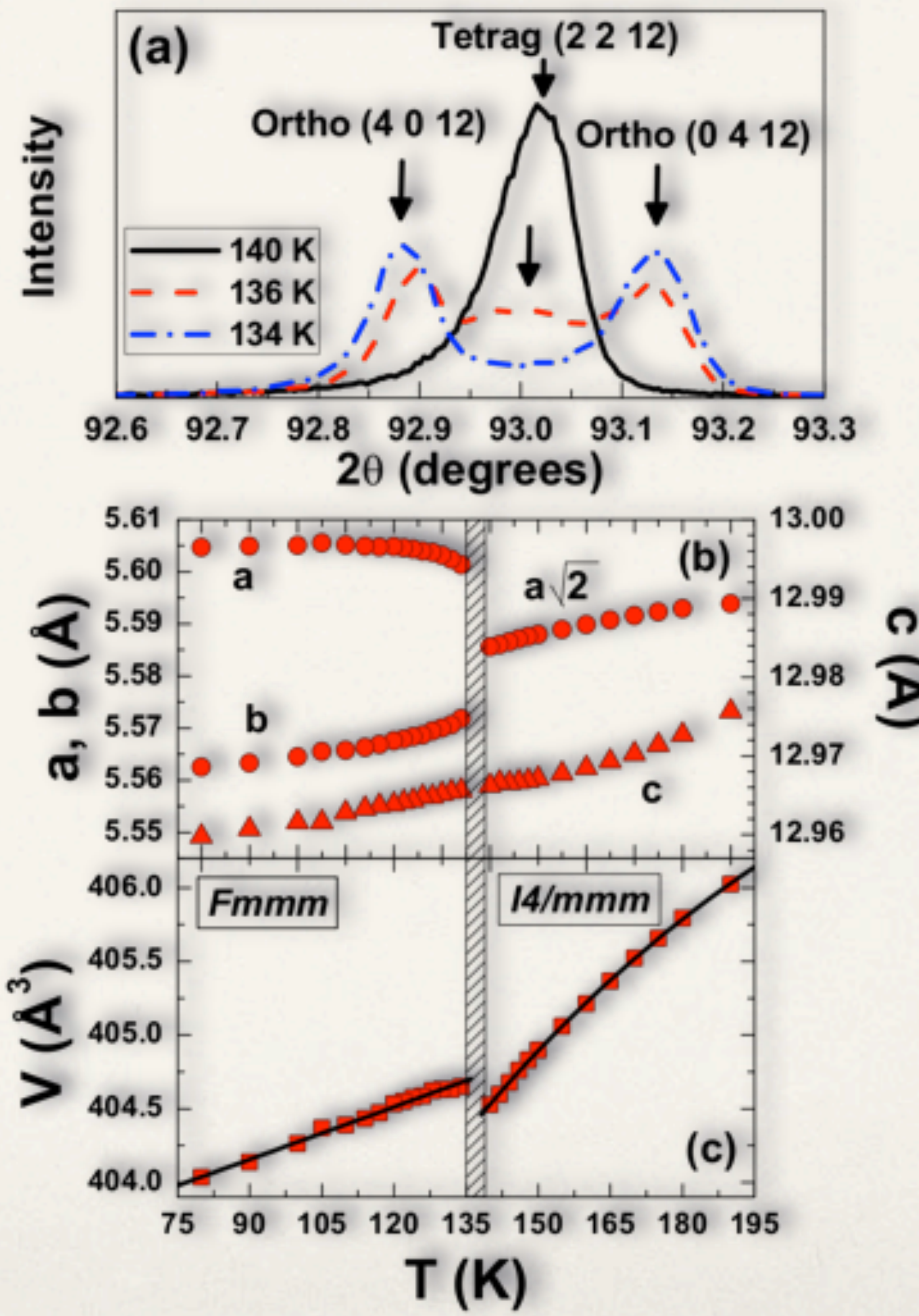
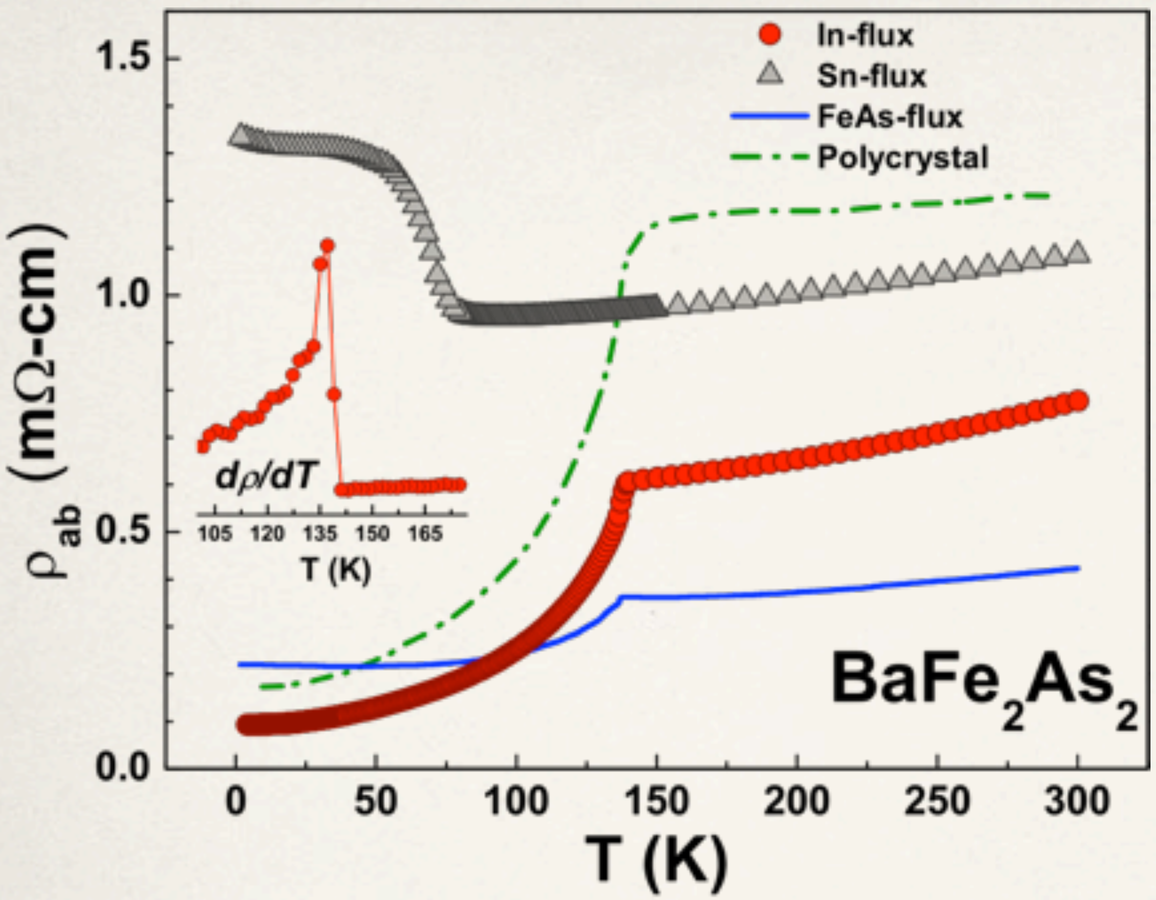






T. M. Garitezi, C. Adriano, P. F. S. Rosa et al. Brazilian Journal of Physics **43** (2013).

Macroscopic Properties and NMR



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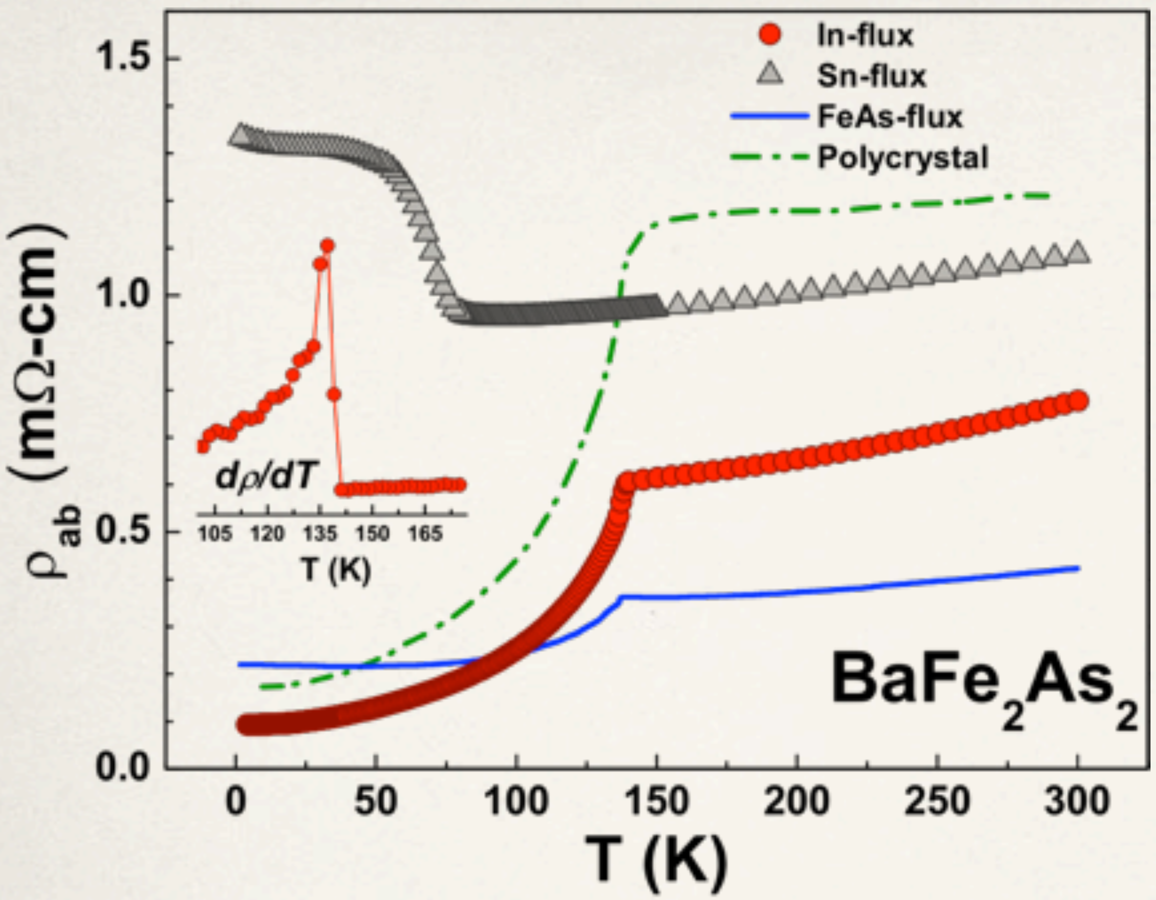

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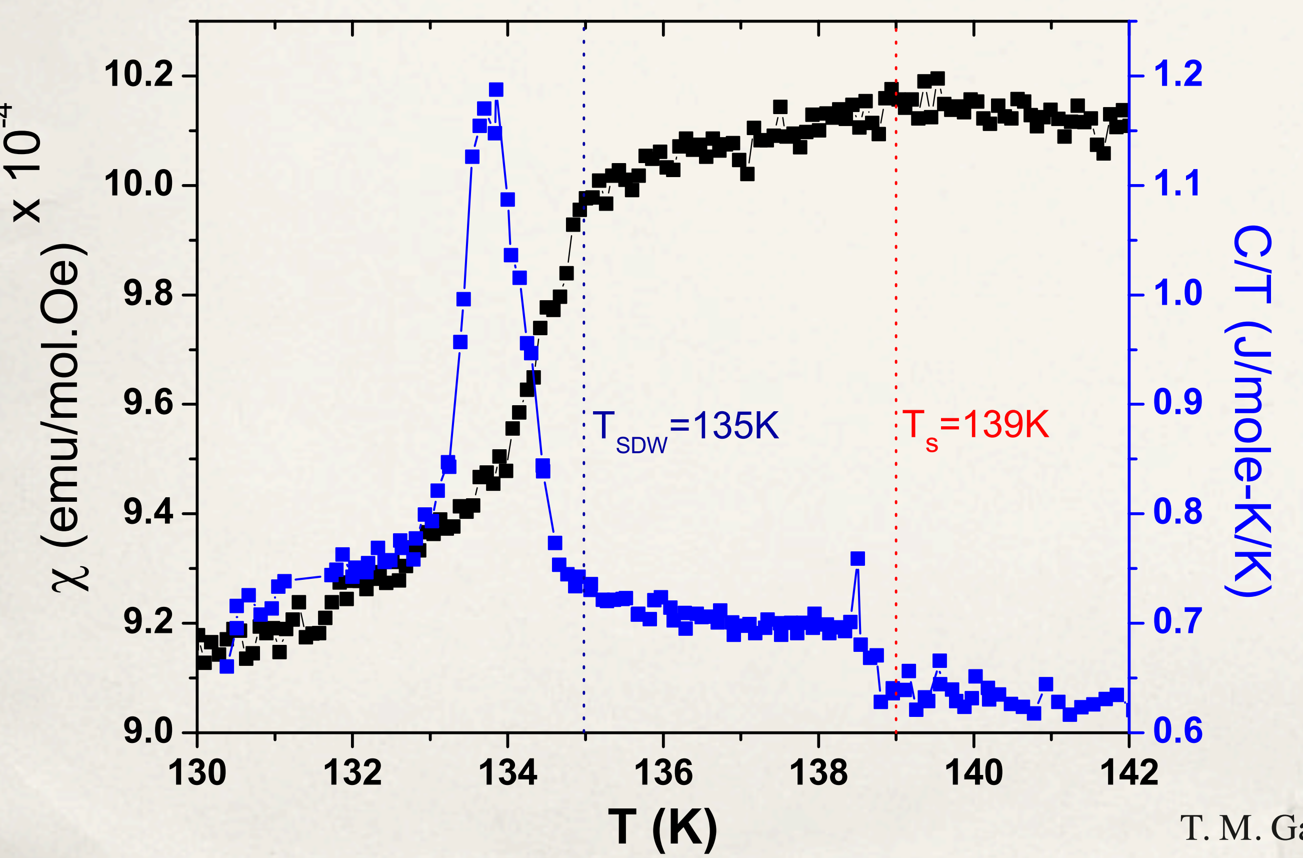

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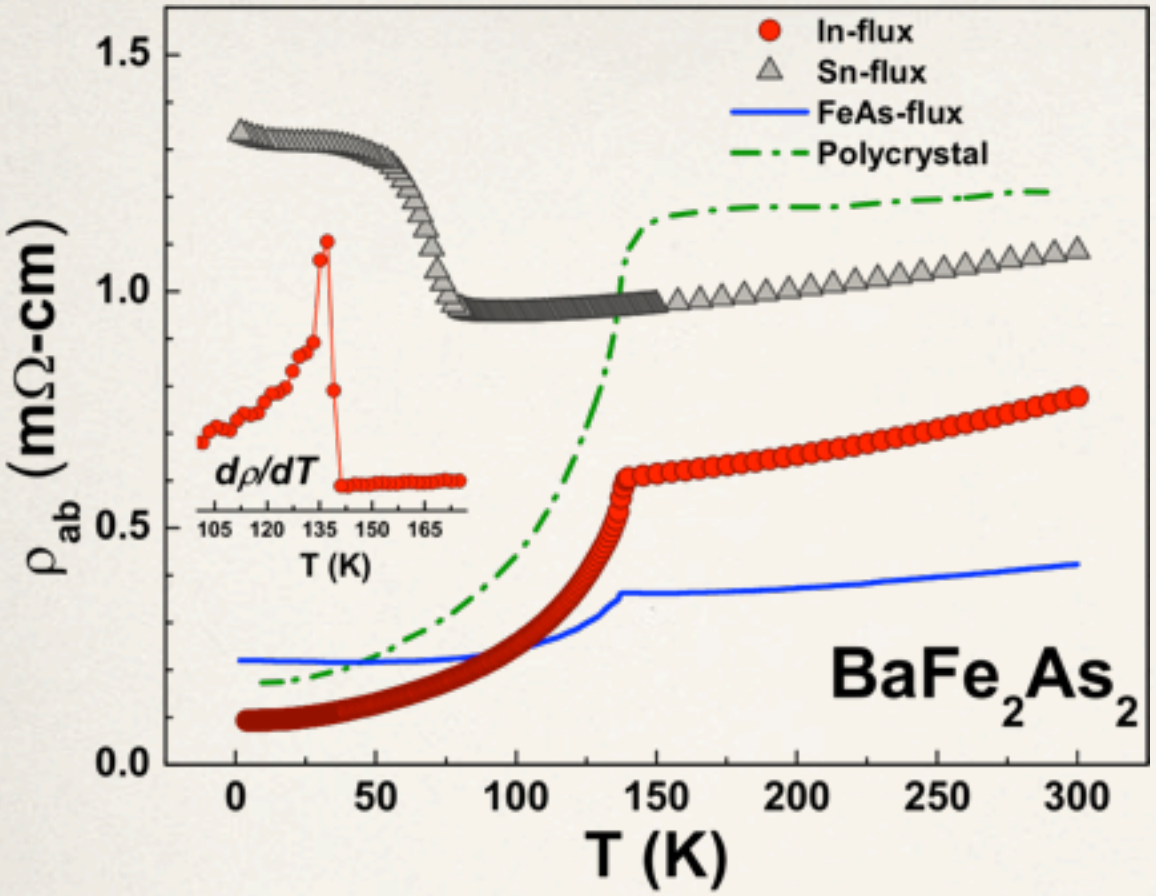

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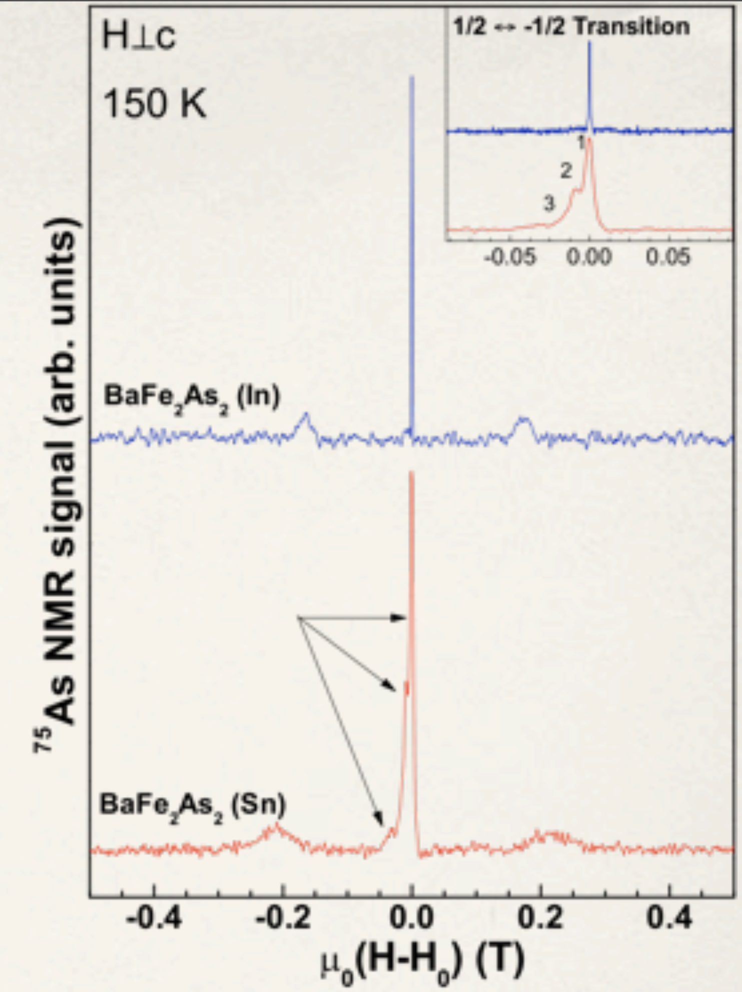

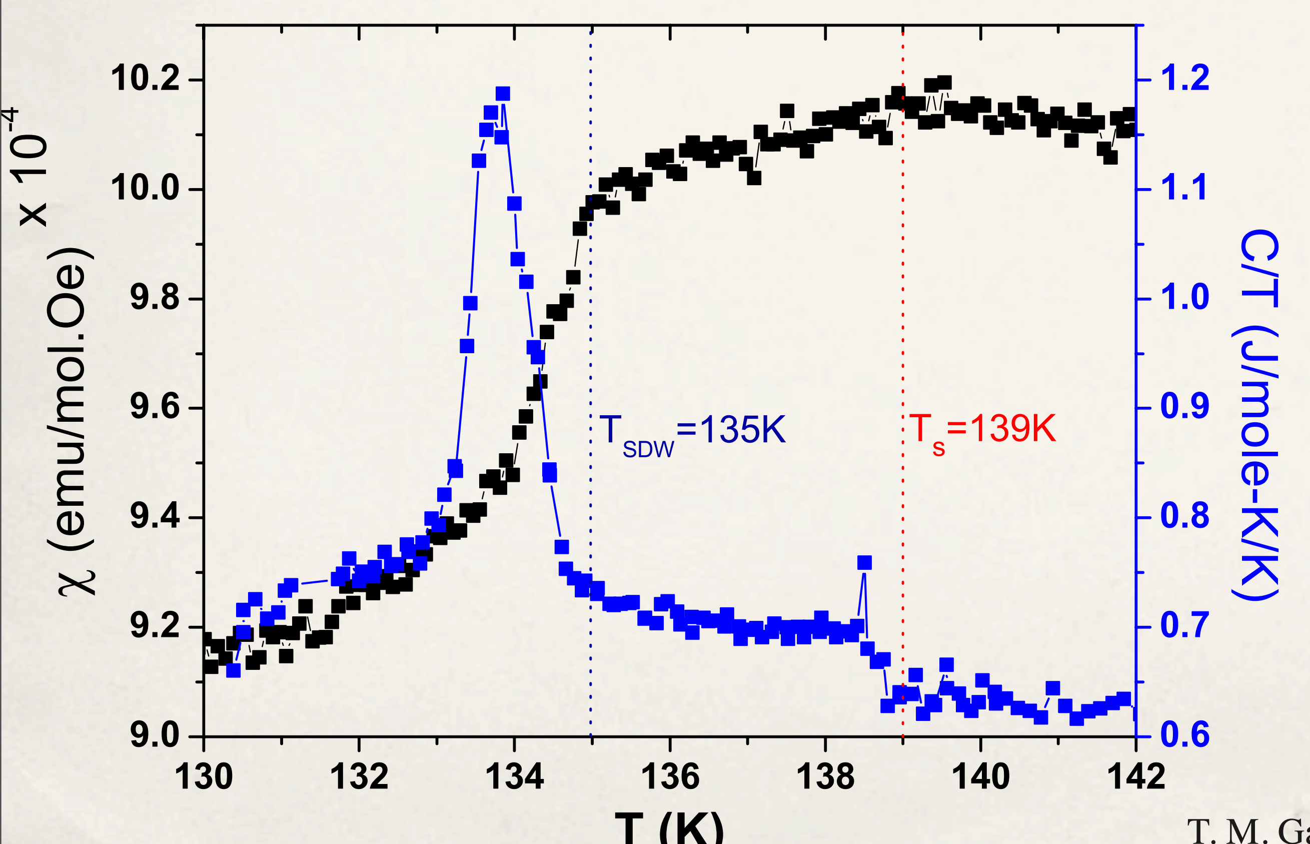

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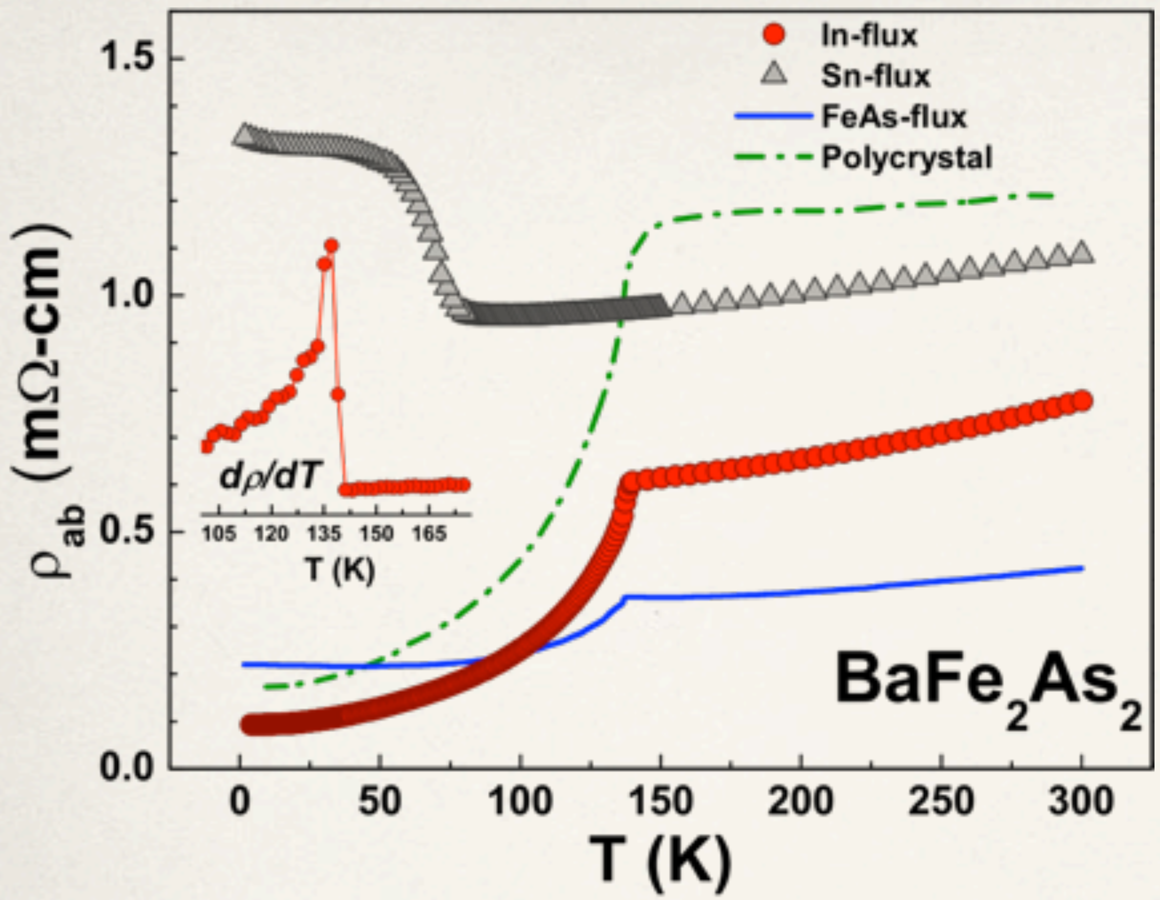

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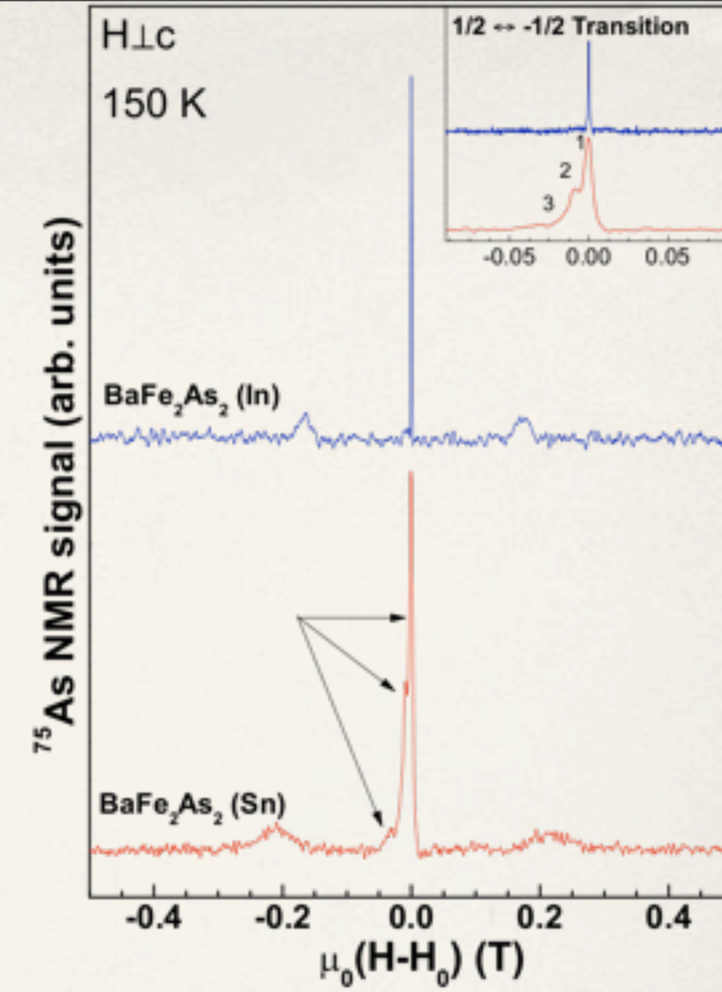

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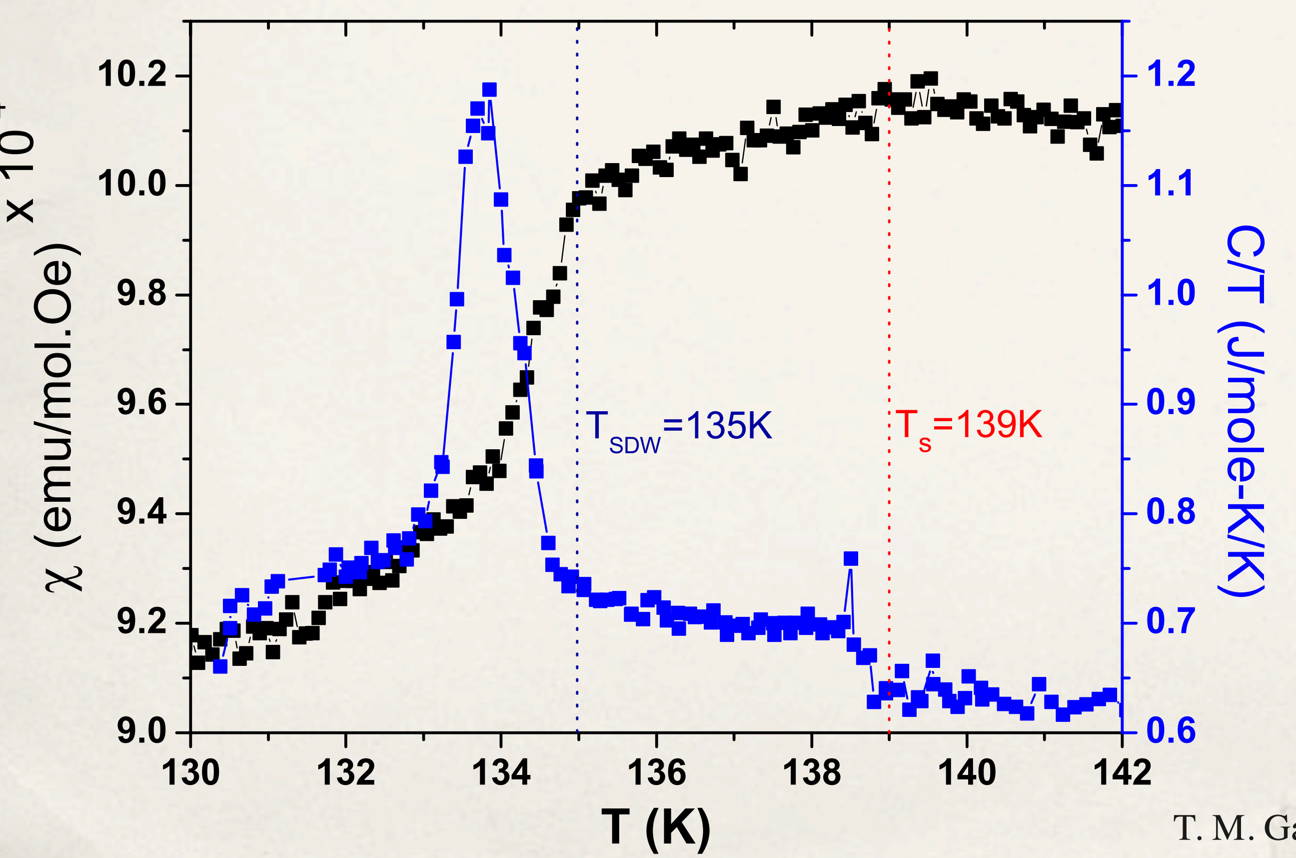

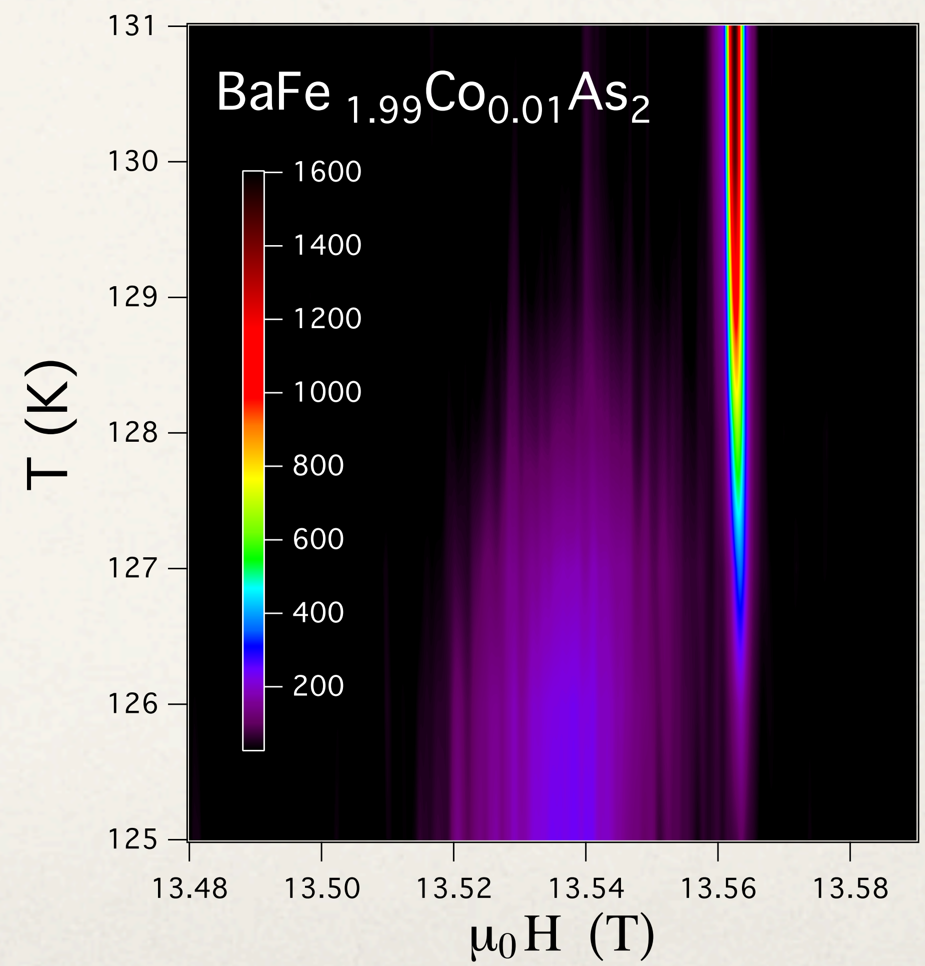

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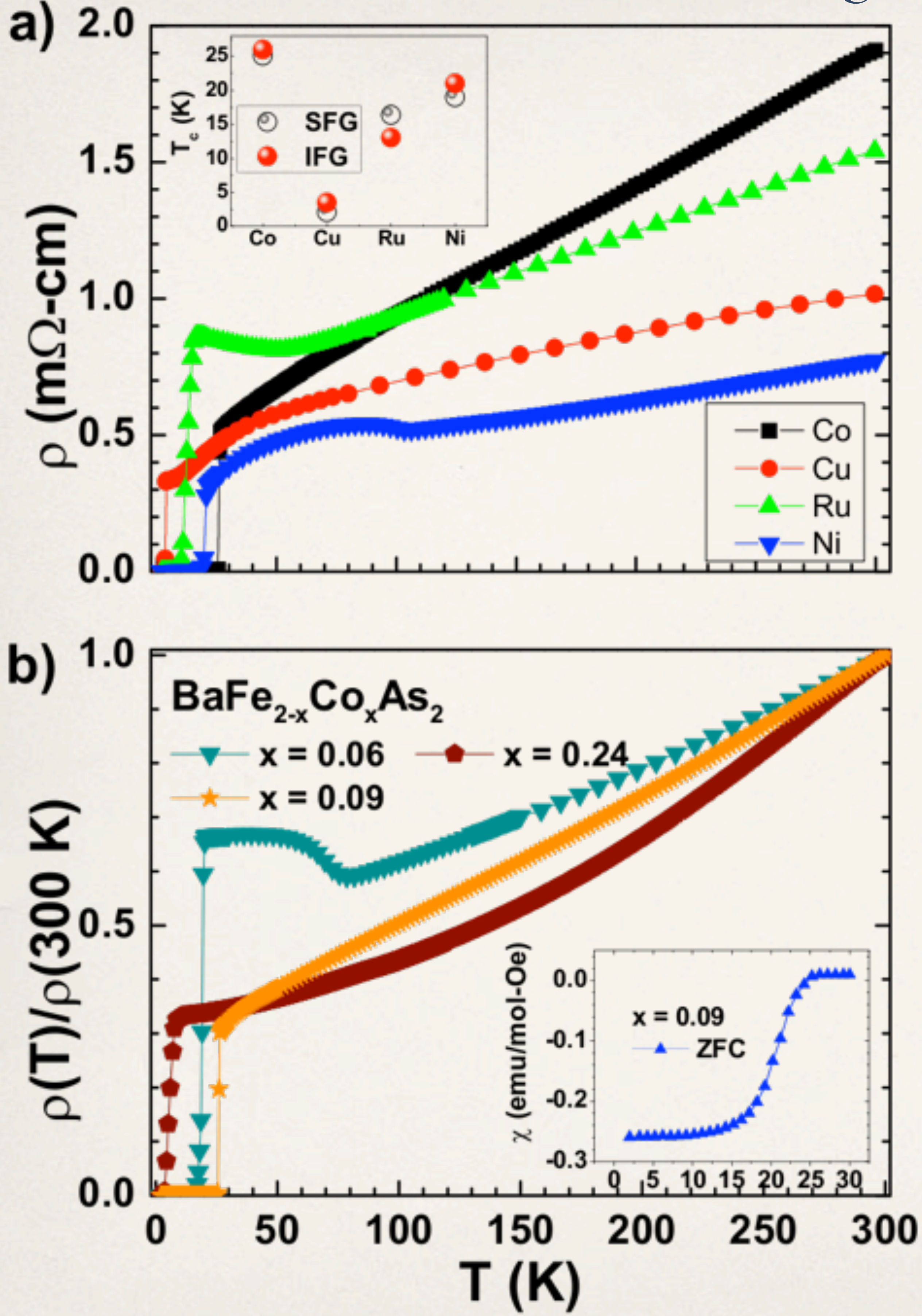
$BaFe_{2-x}M_xAs_2$: higher critical temperatures



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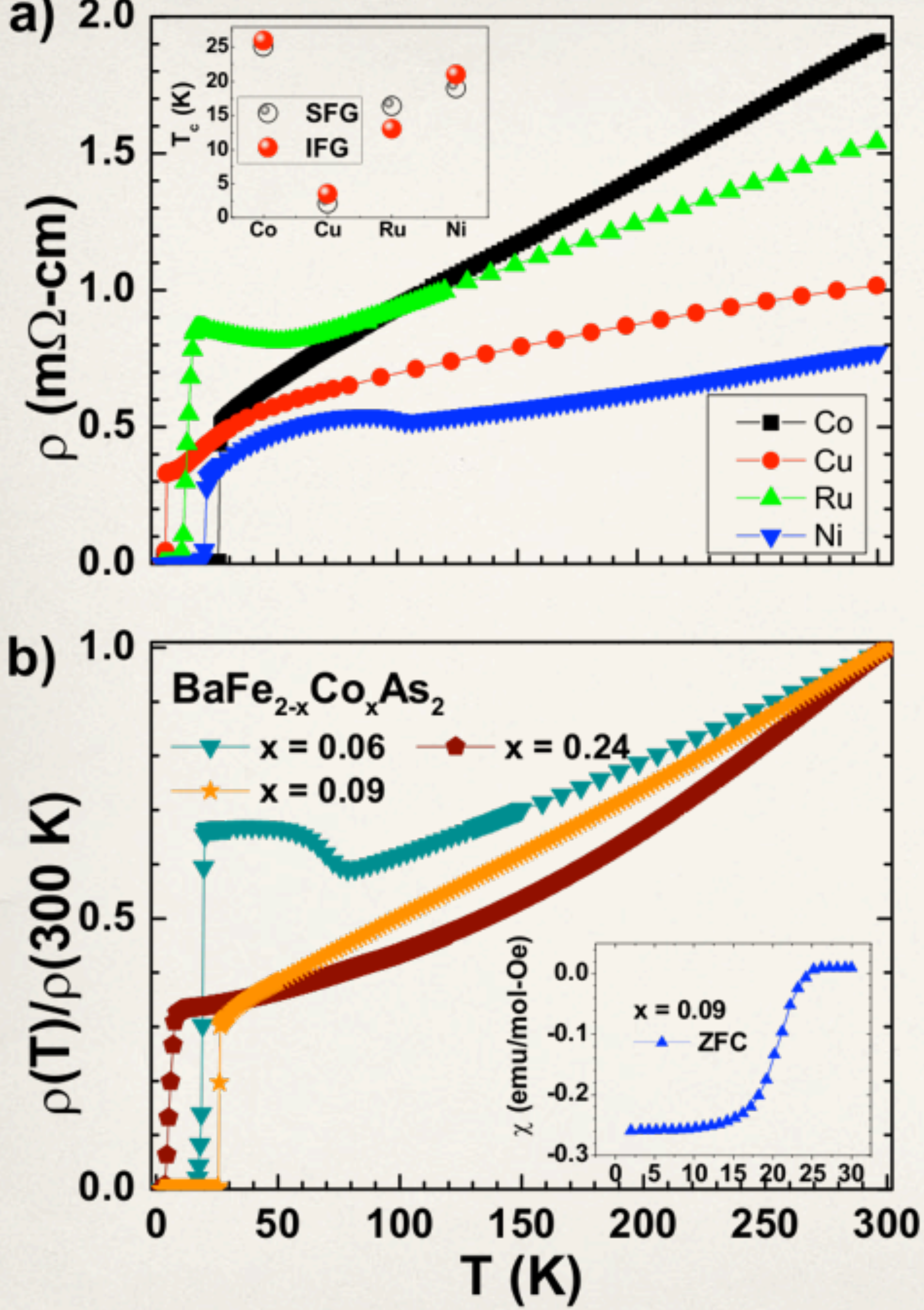
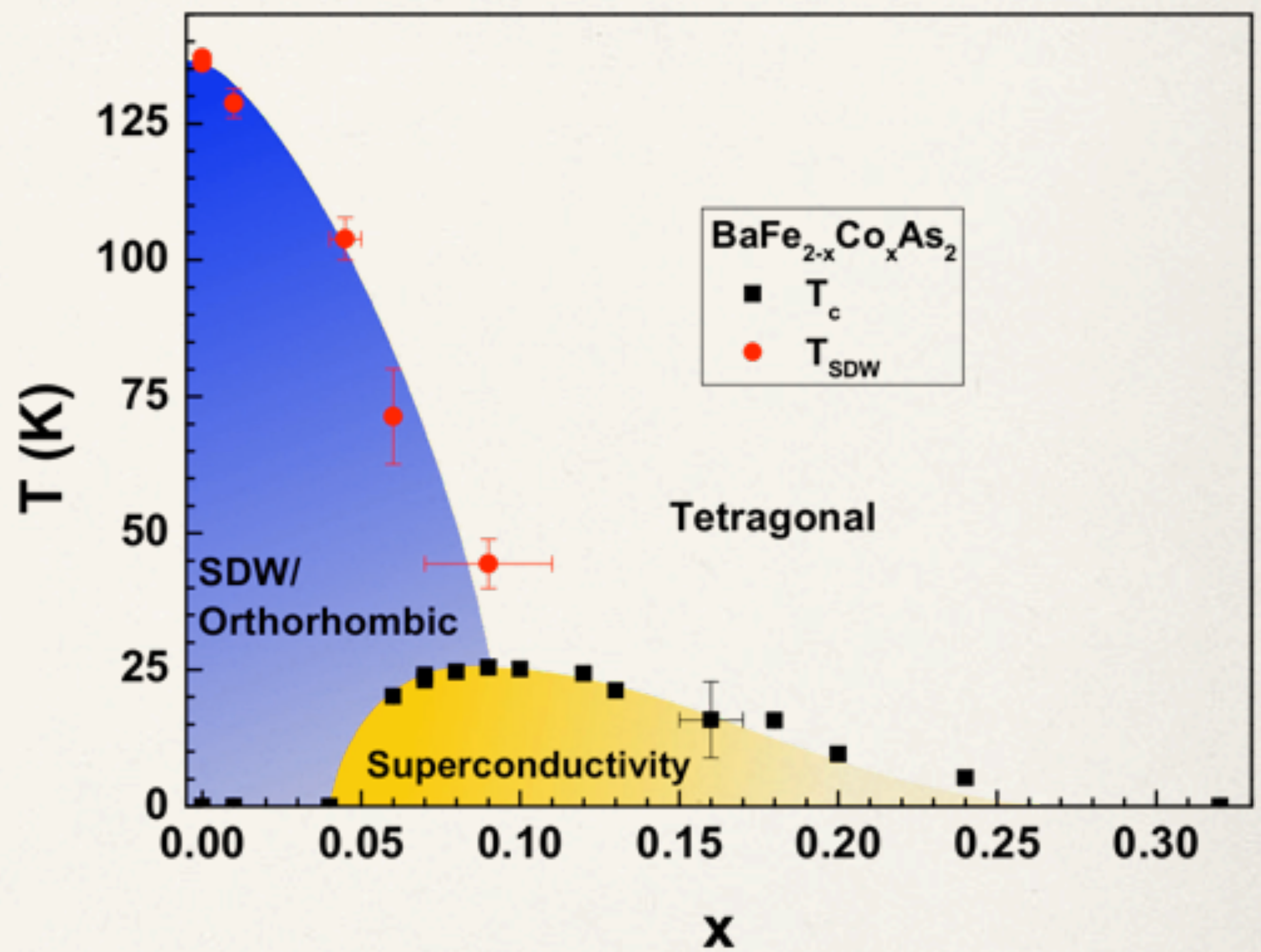
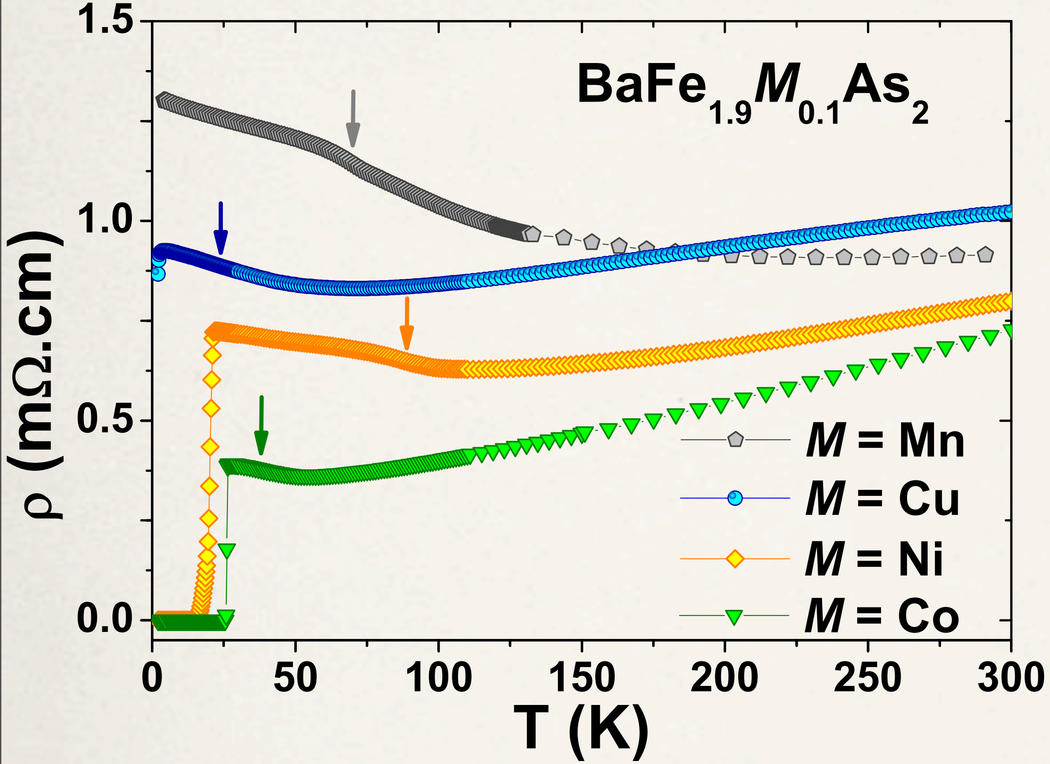


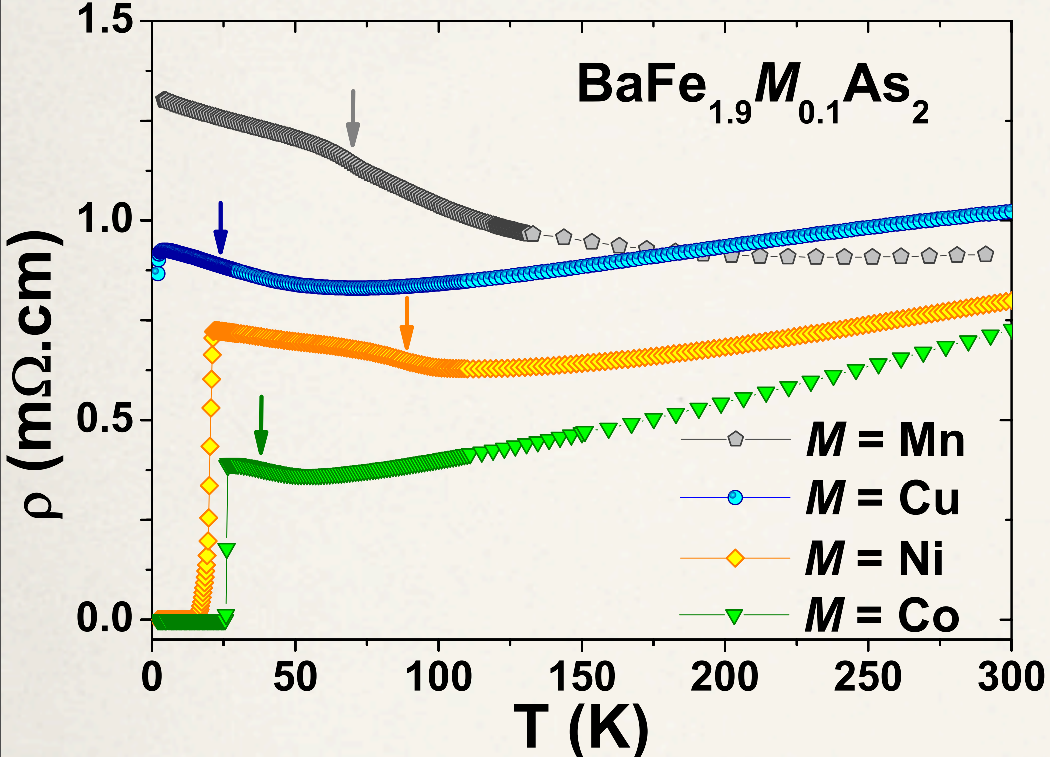


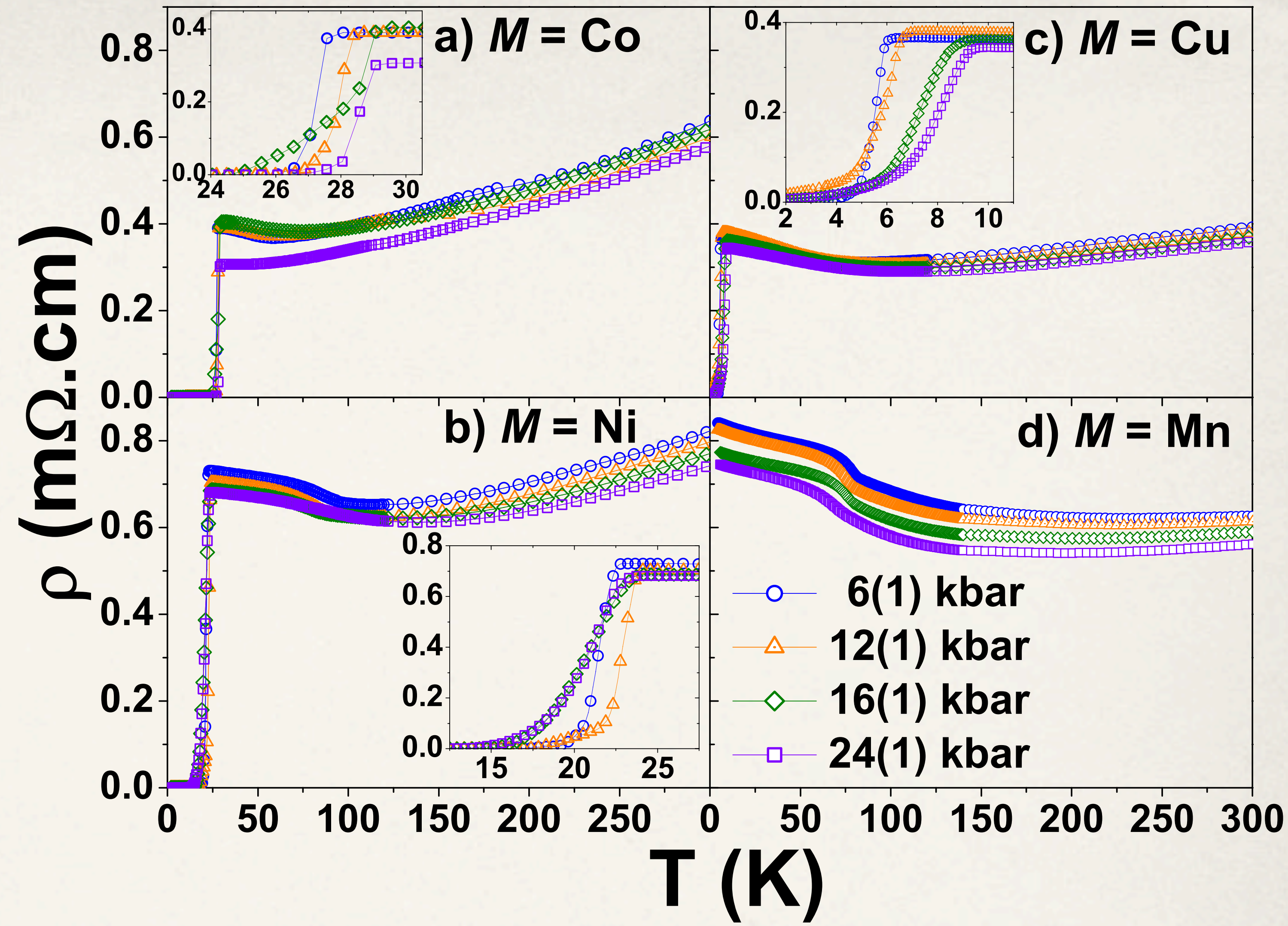
T. M. Garitezi, C. Adriano, P. F. S. Rosa et al. Brazilian Journal of Physics **43** (2013).

$BaFe_{2-x}M_xAs_2$: Tc-enhancement under pressure

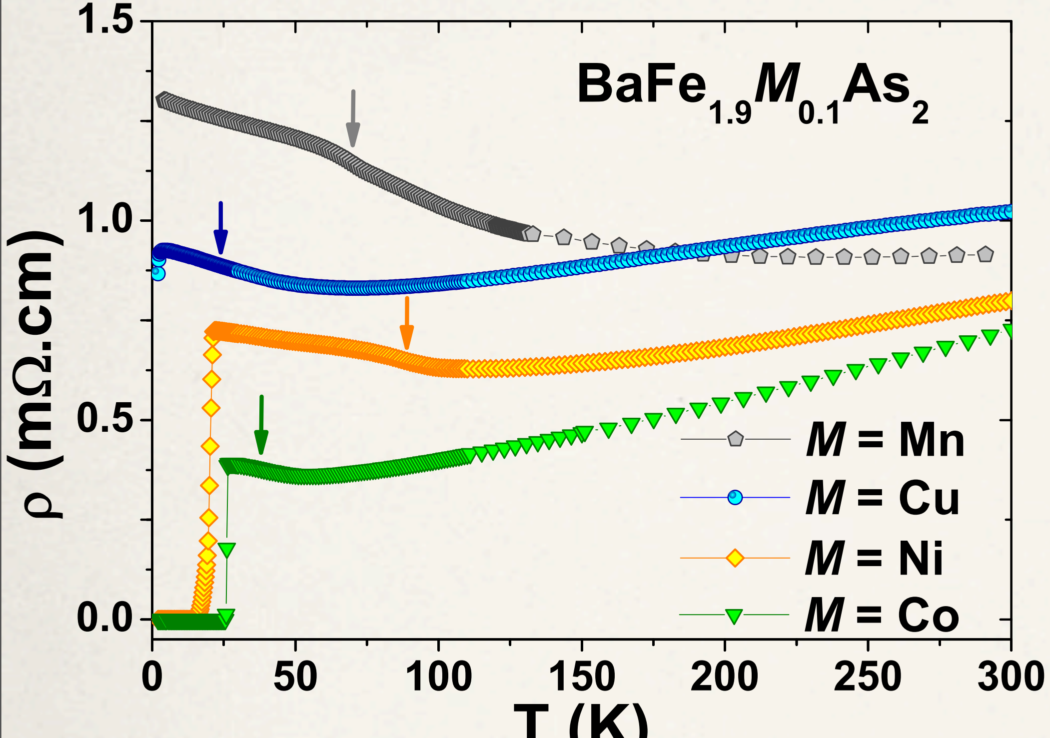


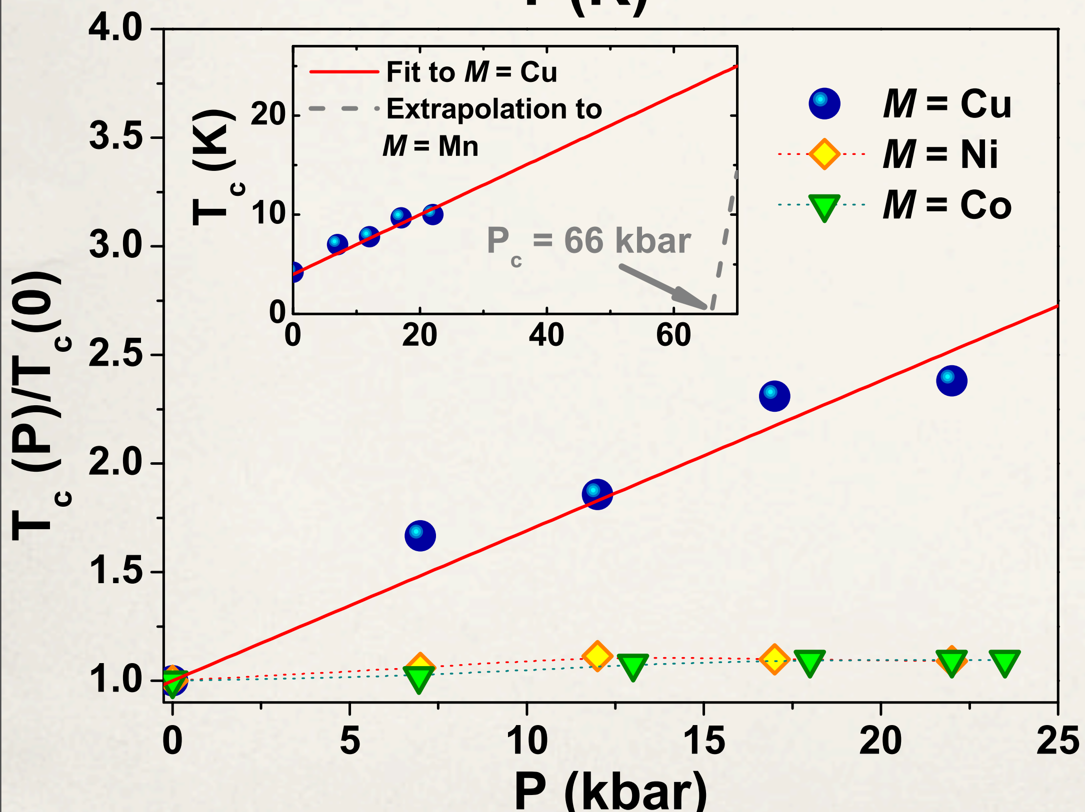
$BaFe_{2-x}M_xAs_2$: T_c-enhancement under pressure

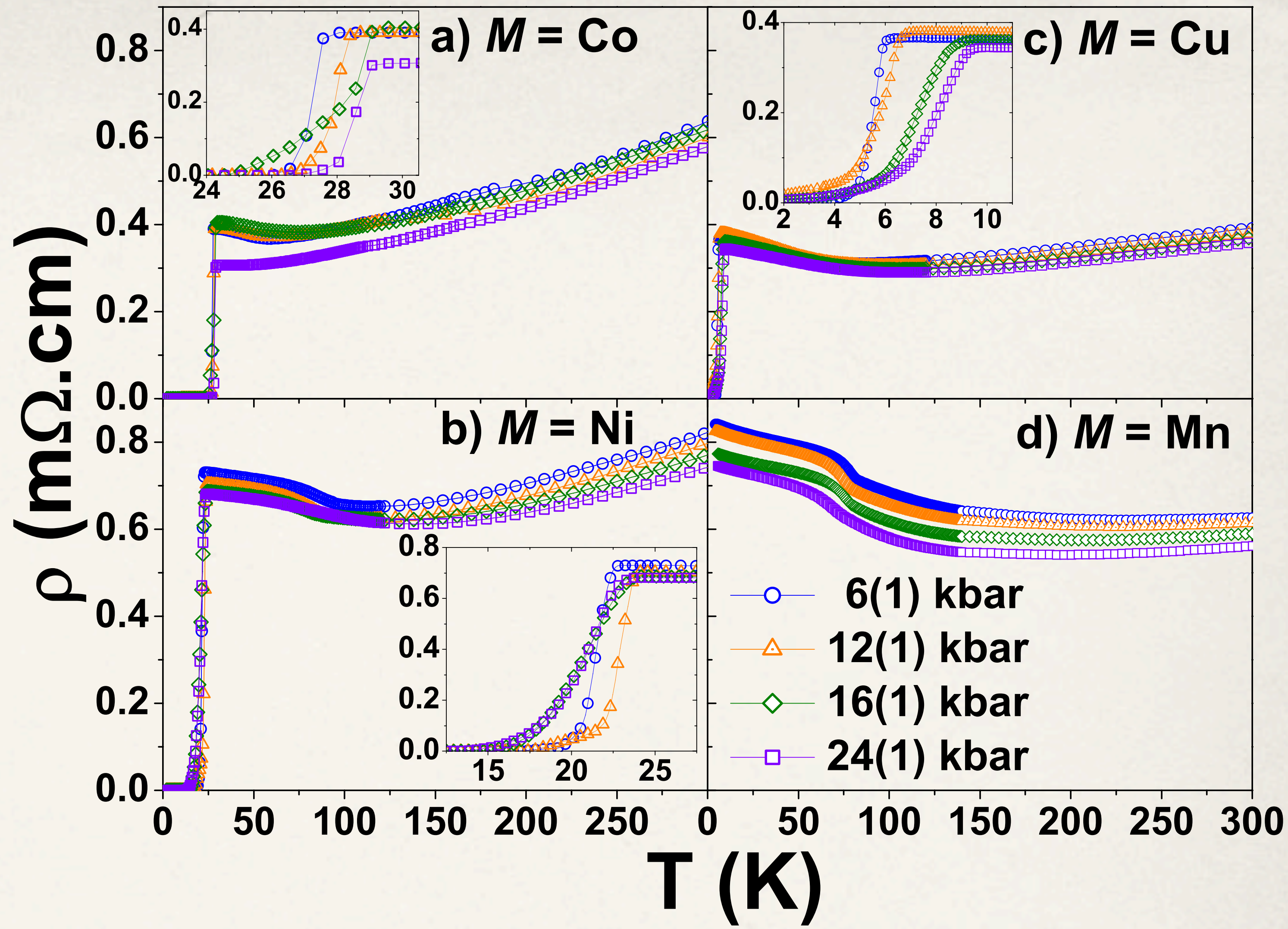




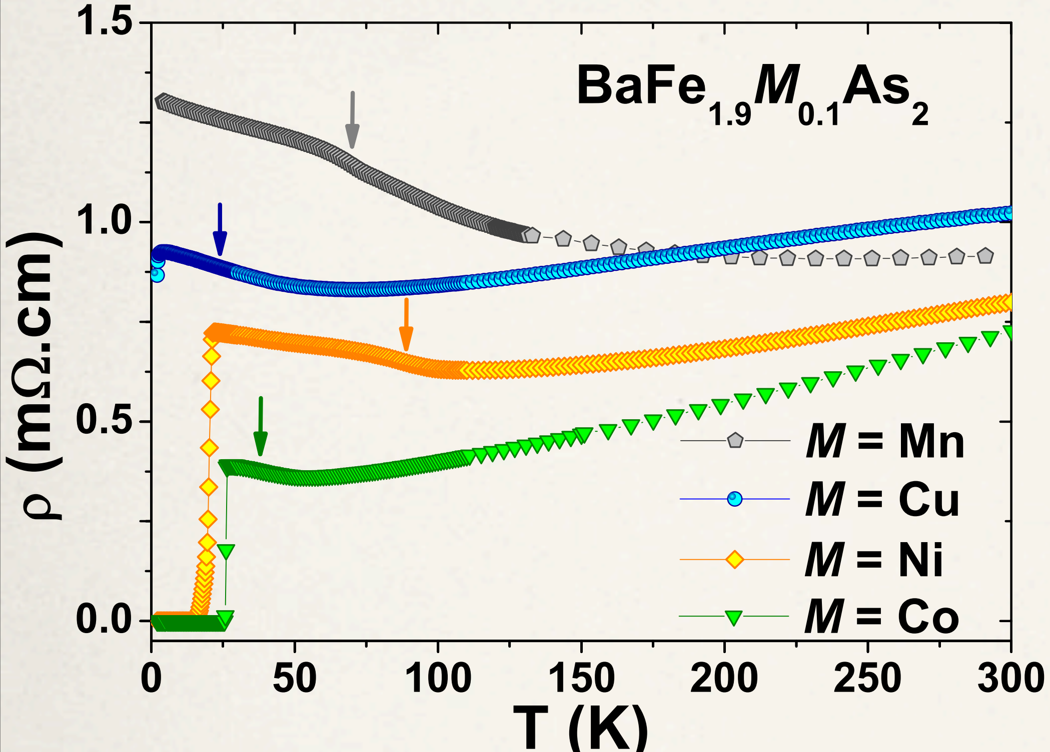
$BaFe_{2-x}M_xAs_2$: Tc-enhancement under pressure

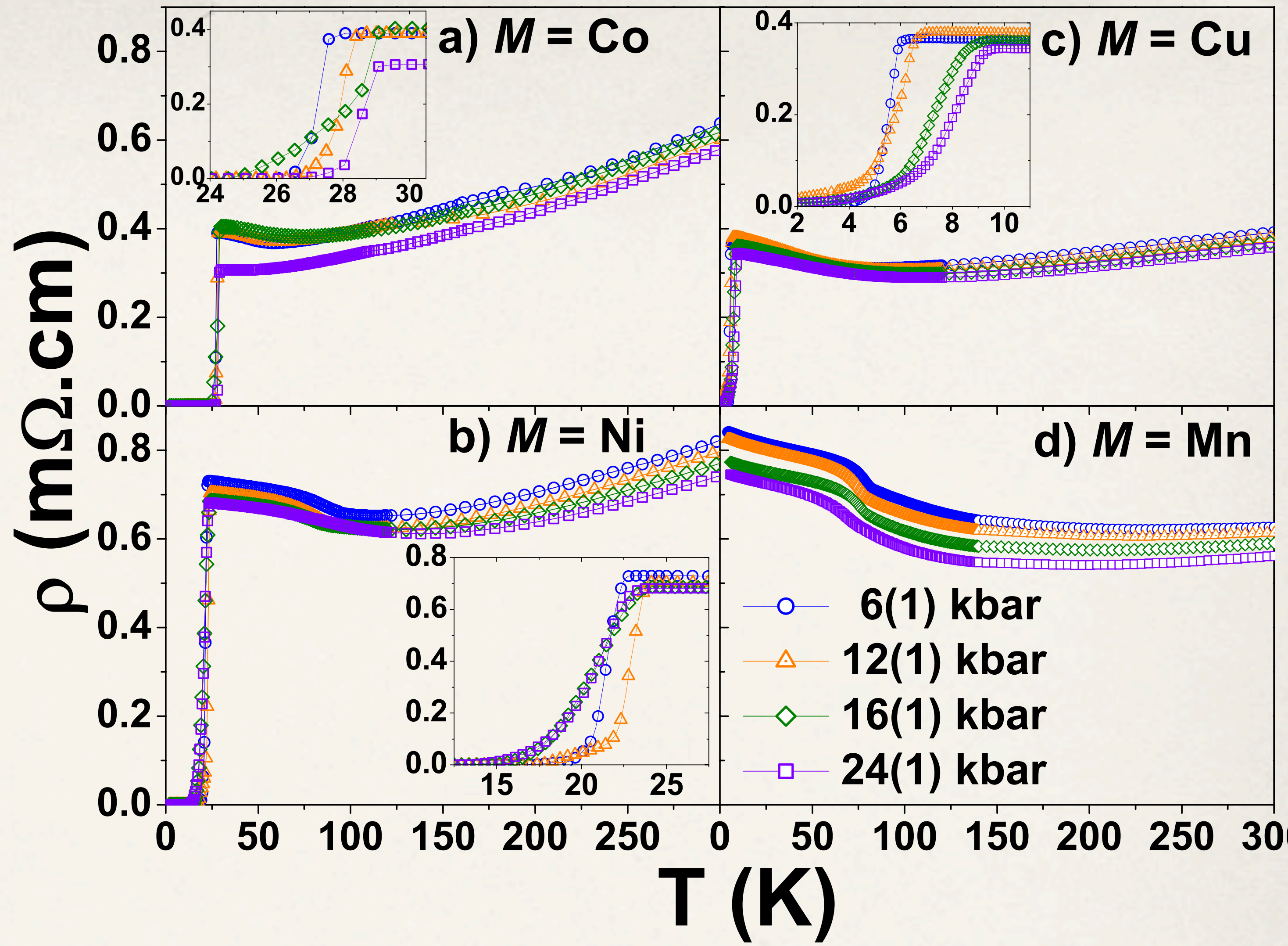


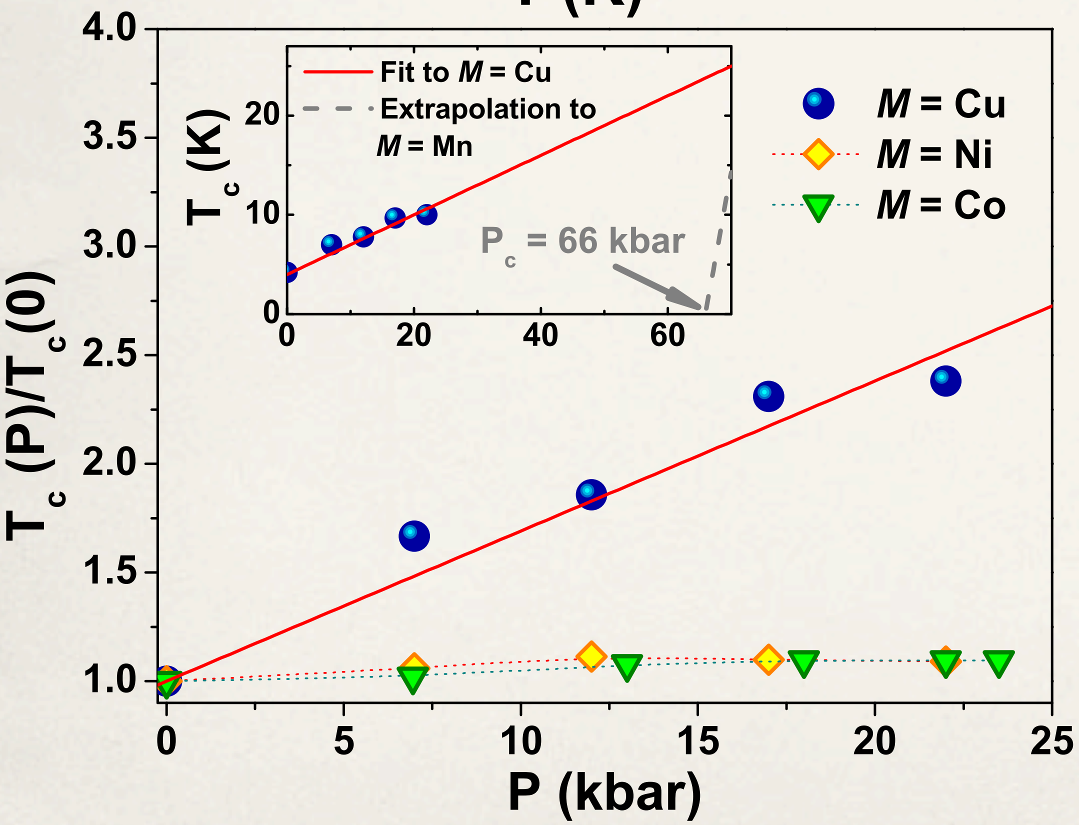


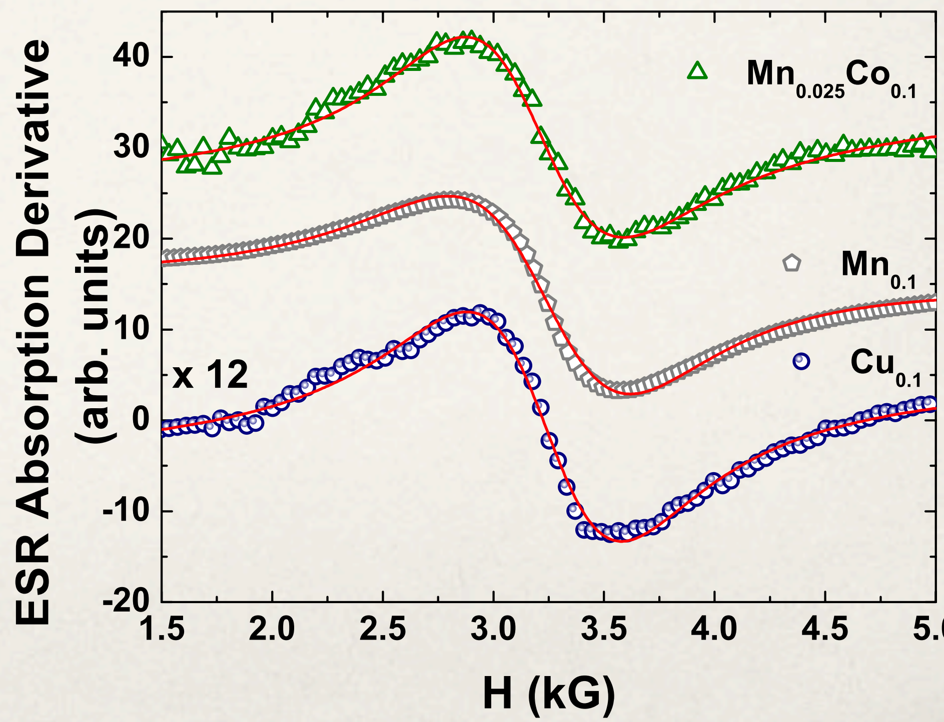


$BaFe_{2-x}M_xAs_2$: Tc-enhancement under pressure









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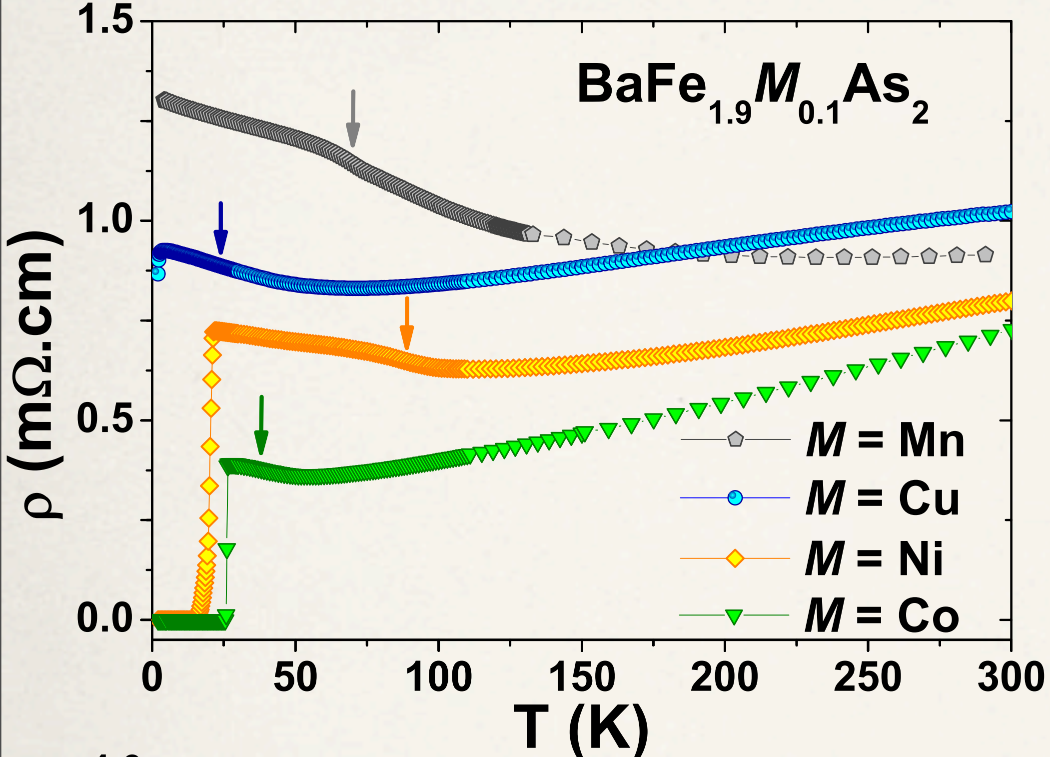
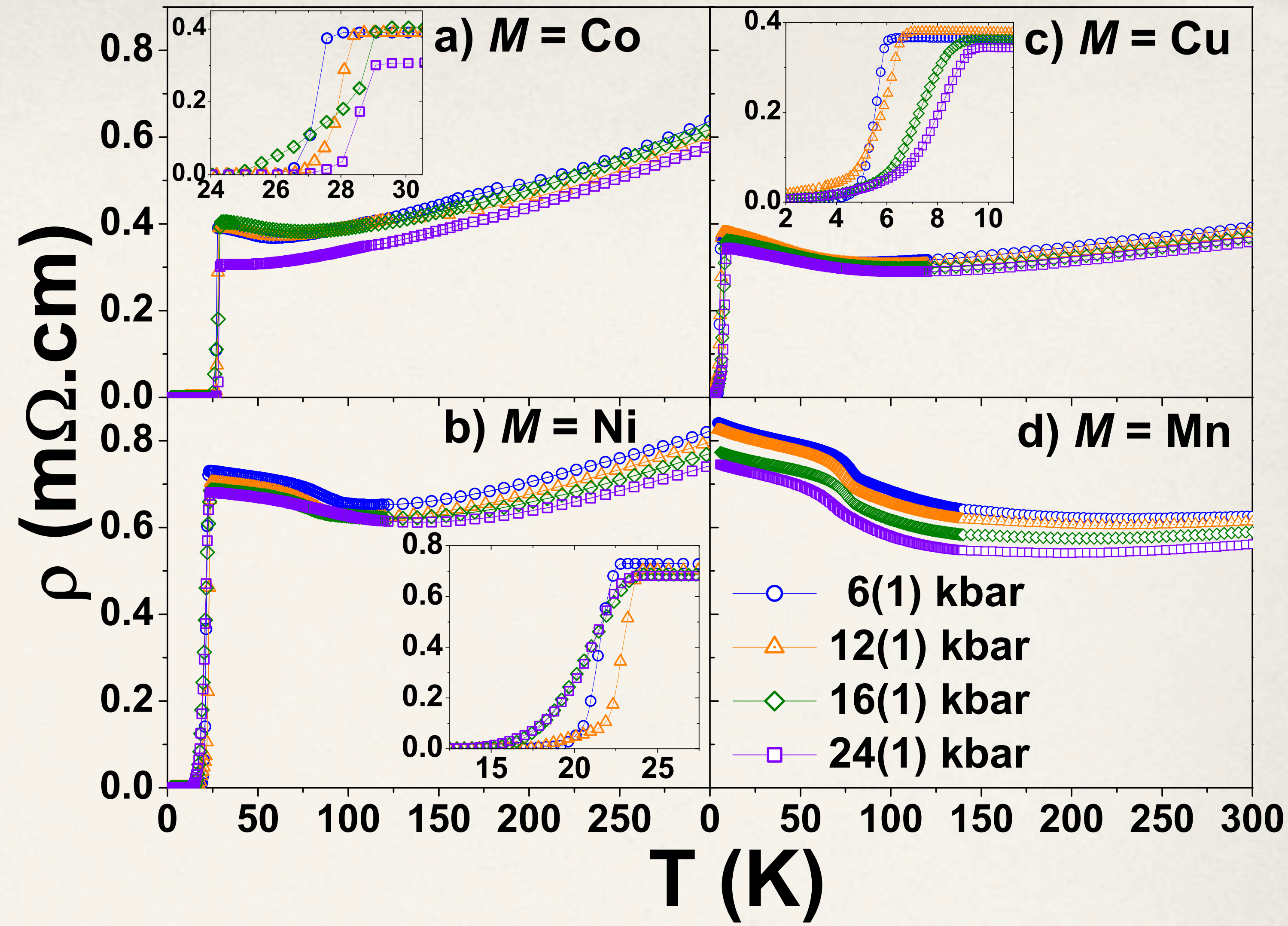
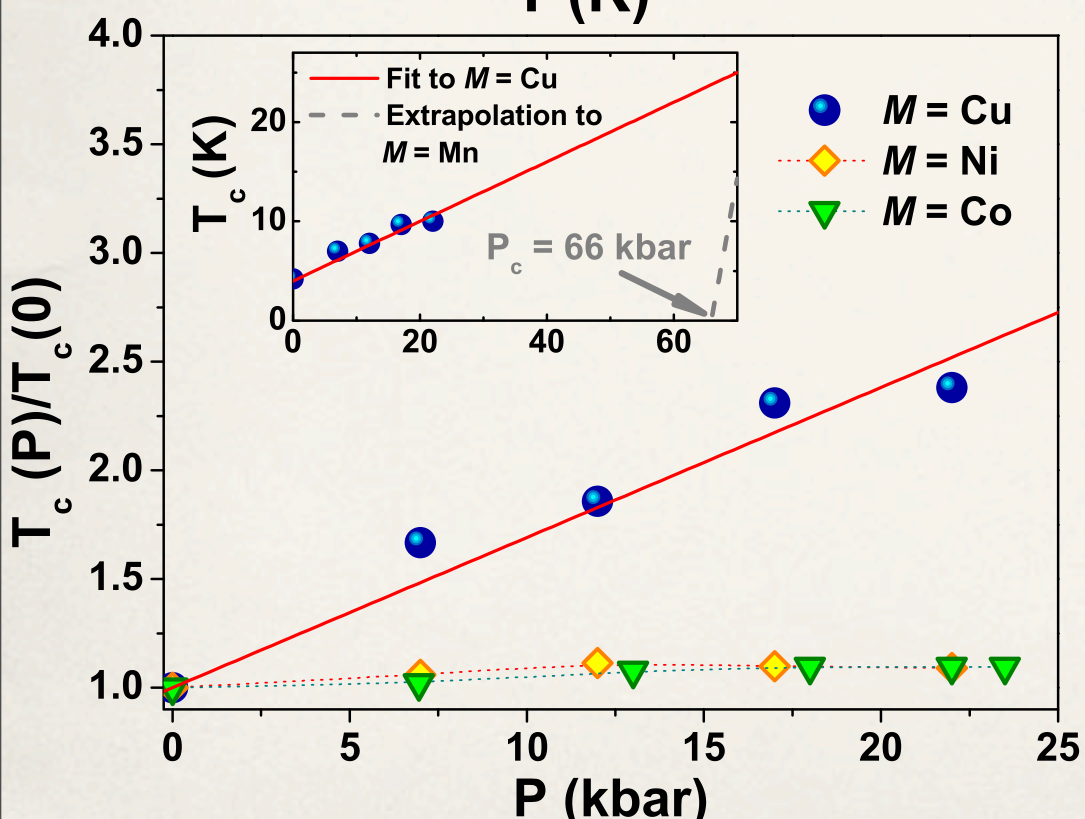
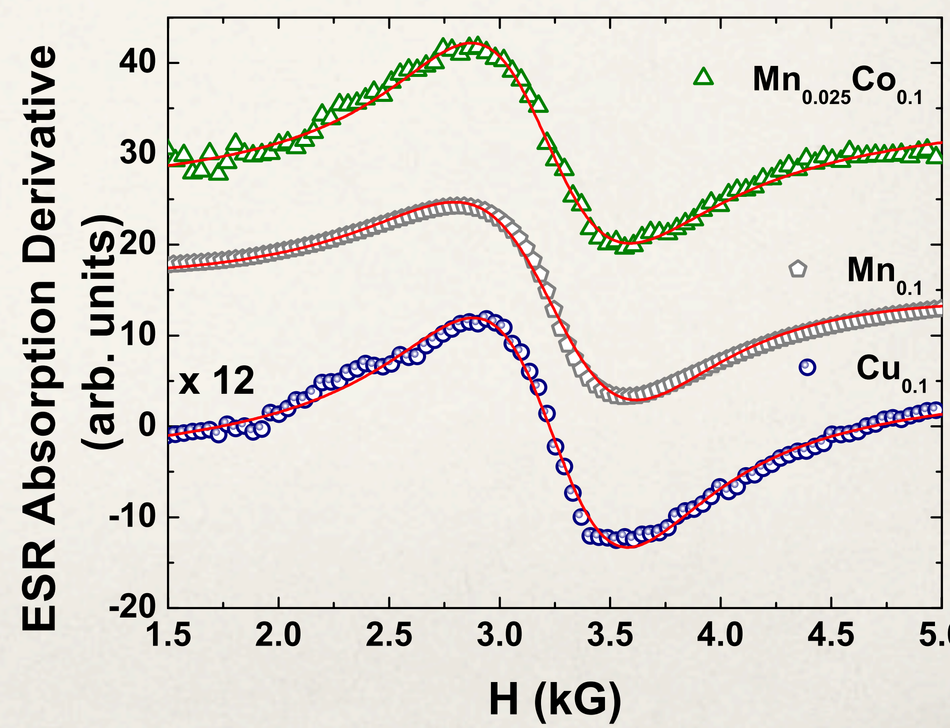






- Magnetic pair-breaking mechanism due to Cu^{2+} (S = 1/2) and Mn^{2+} (S = 5/2) local moments.



P. F. S. Rosa et al.Sci. Rep. 4, 6252; DOI:10.1038/srep06252 (2014).

Outline

- Introduction and Motivation: Fe-based Superconductors
- Alternative Single Crystal Growth and Macroscopic Properties
- Microscopic Investigation: X-Ray Absorption Spectroscopy (XANES and EXAFS) and Electron Spin Resonance (ESR)
- Conclusions and Perspectives

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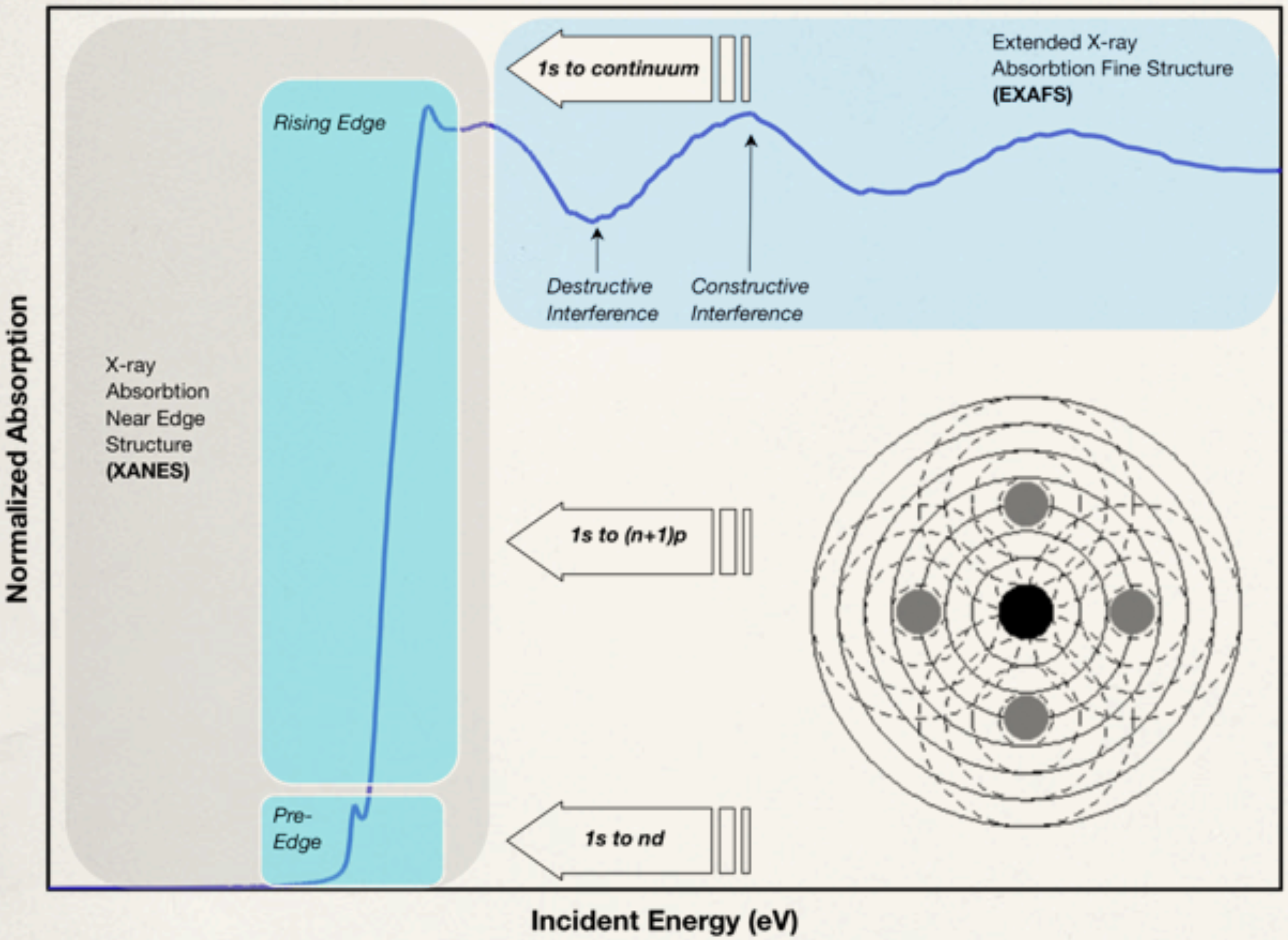
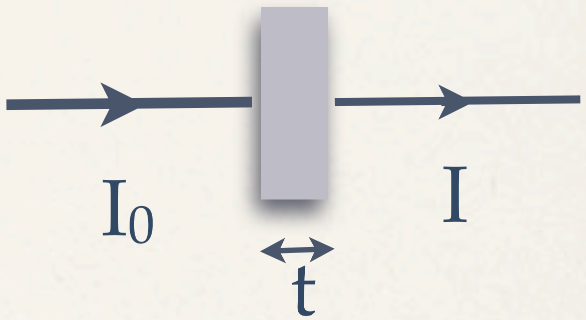
Microscopic Properties: Evolution of the FeAs distance

- X-Ray Absorption Spectroscopy



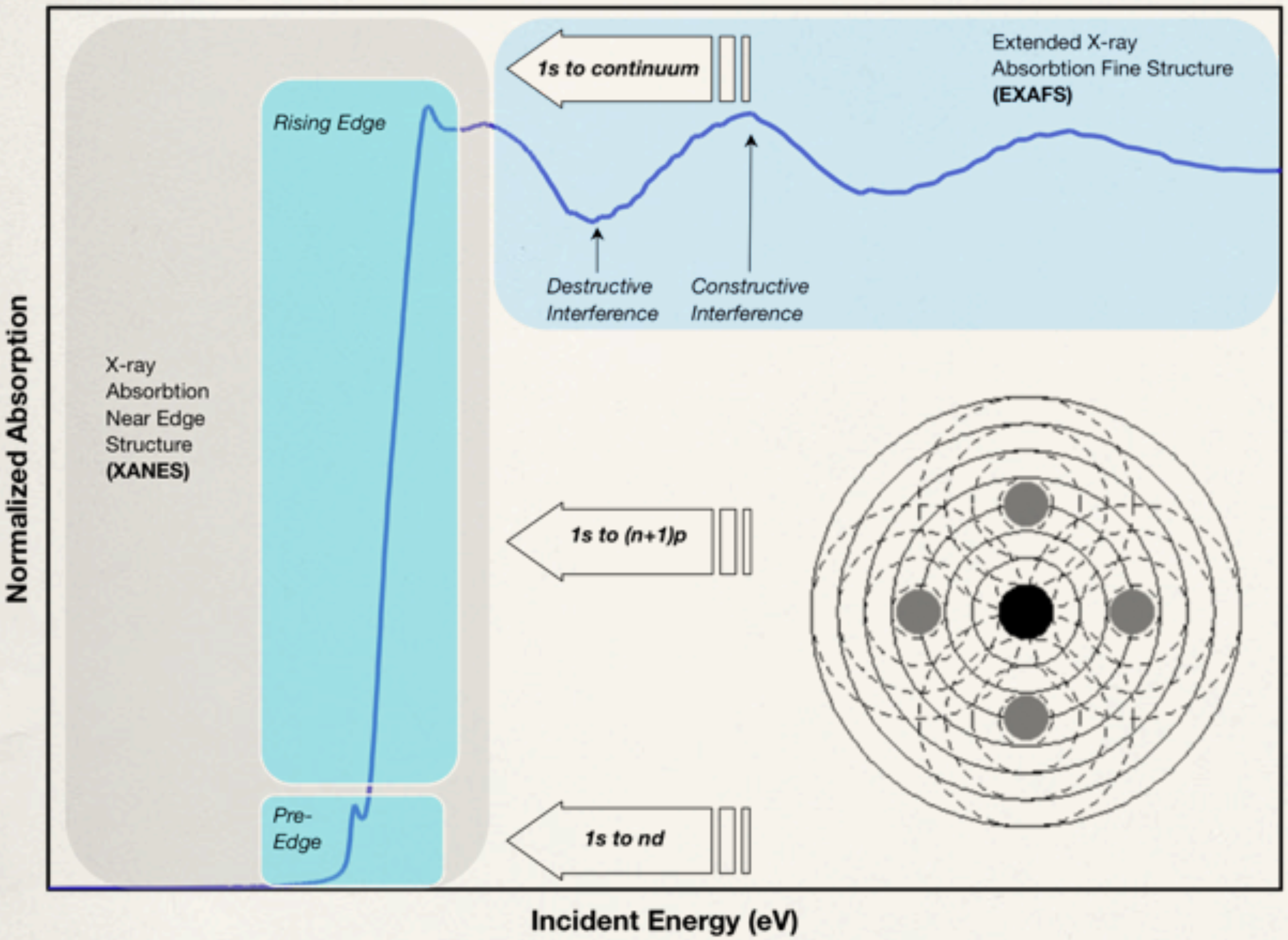
$$I = I_0 e^{-\mu(E)t}$$



For hv < 40 keV → photoelectron emission

Microscopic Properties: Evolution of the FeAs distance

- X-Ray Absorption Spectroscopy



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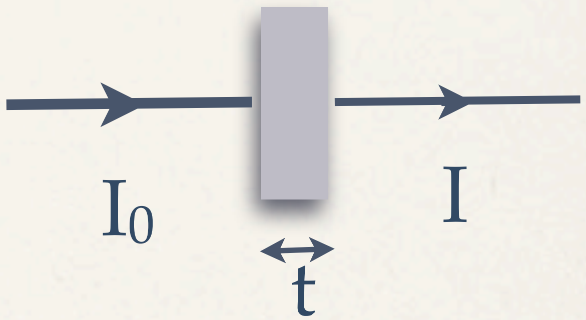
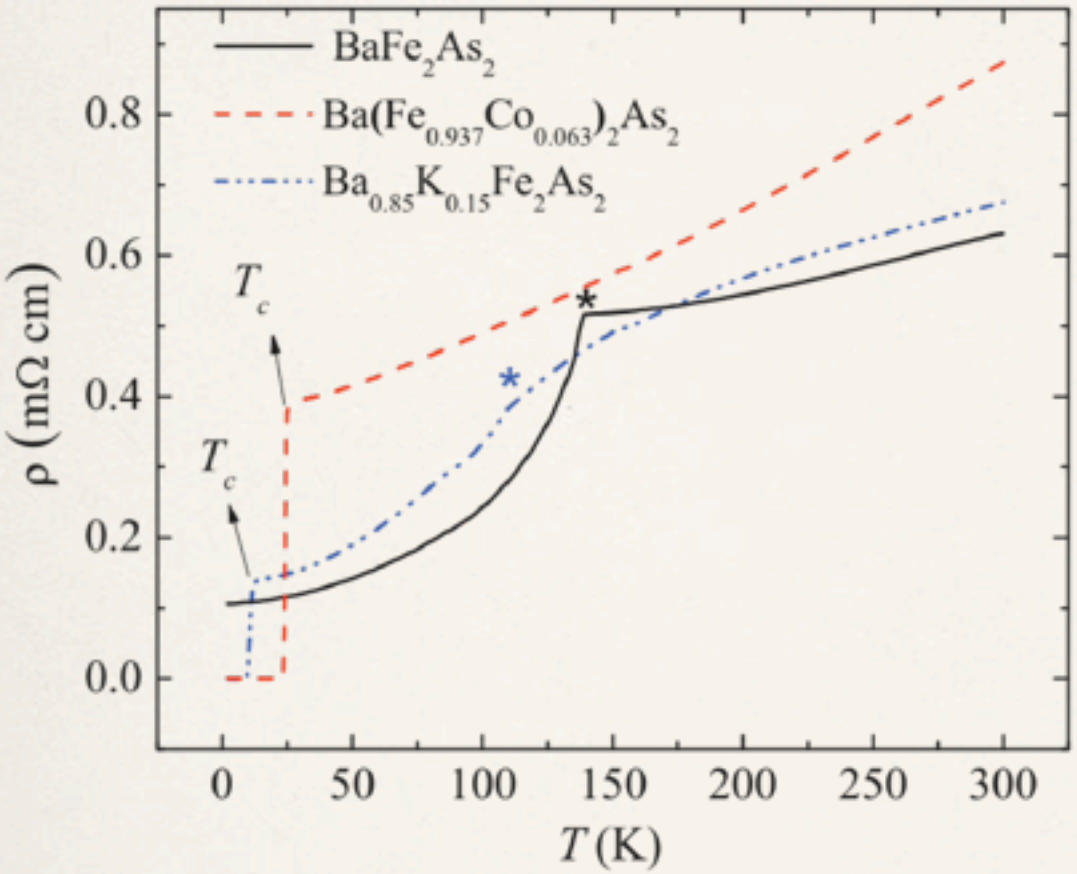


$$\chi(E) = \frac{\mu(E) - \mu_0}{\Delta\mu_0}$$

For hv < 40 keV → photoelectron emission

Microscopic Properties: Evolution of the FeAs distance

- EXAFS in the As *K* edge in transmission mode:



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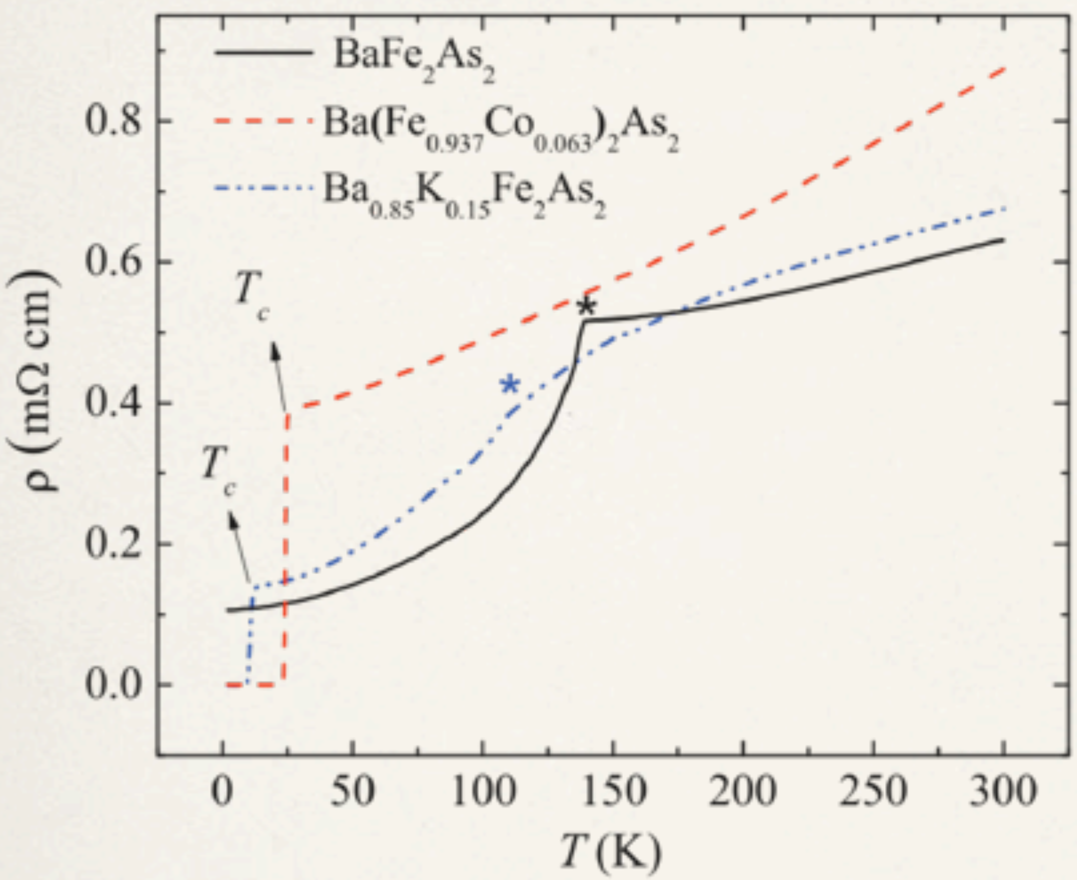

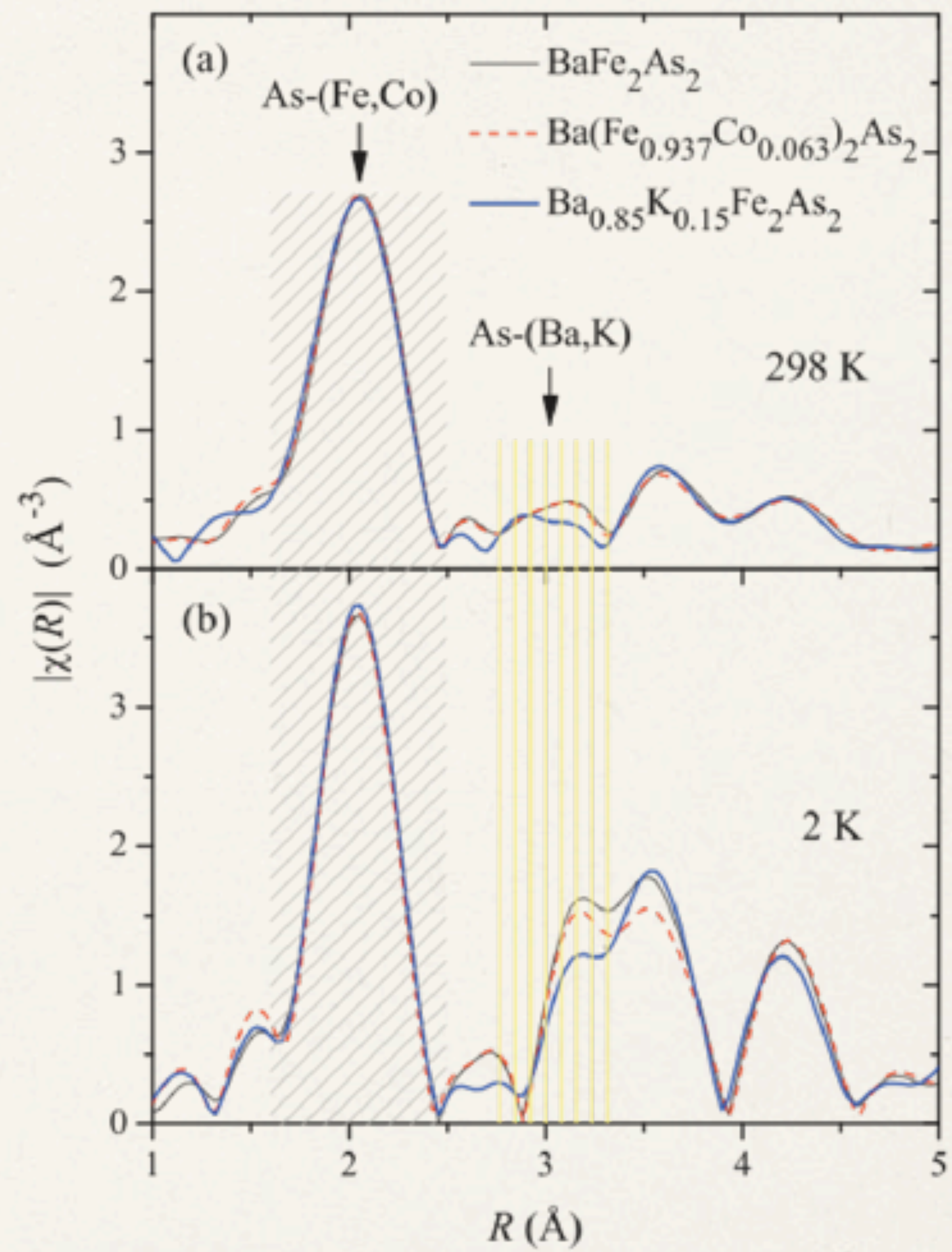

Experiments performed at XAFS2 beamline of the Brazilian Synchrotron Light Laboratory (LNLS).

Microscopic Properties: Evolution of the FeAs distance

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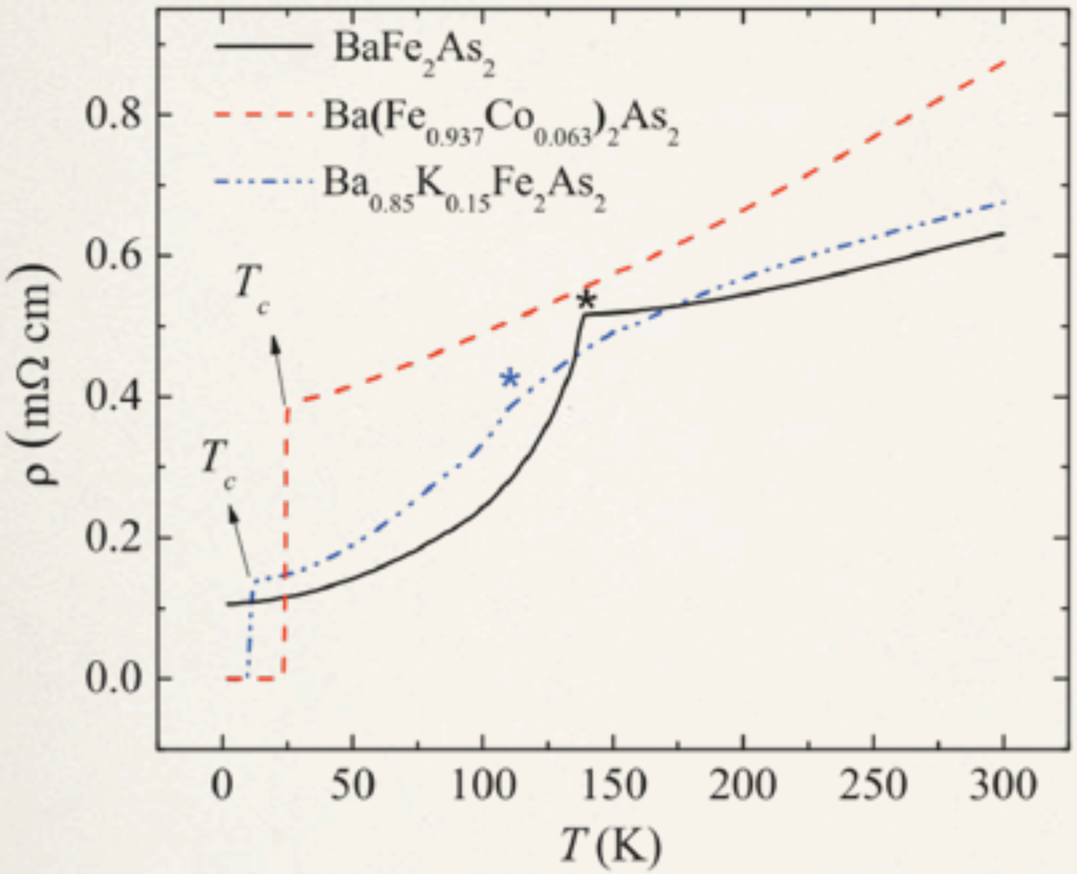
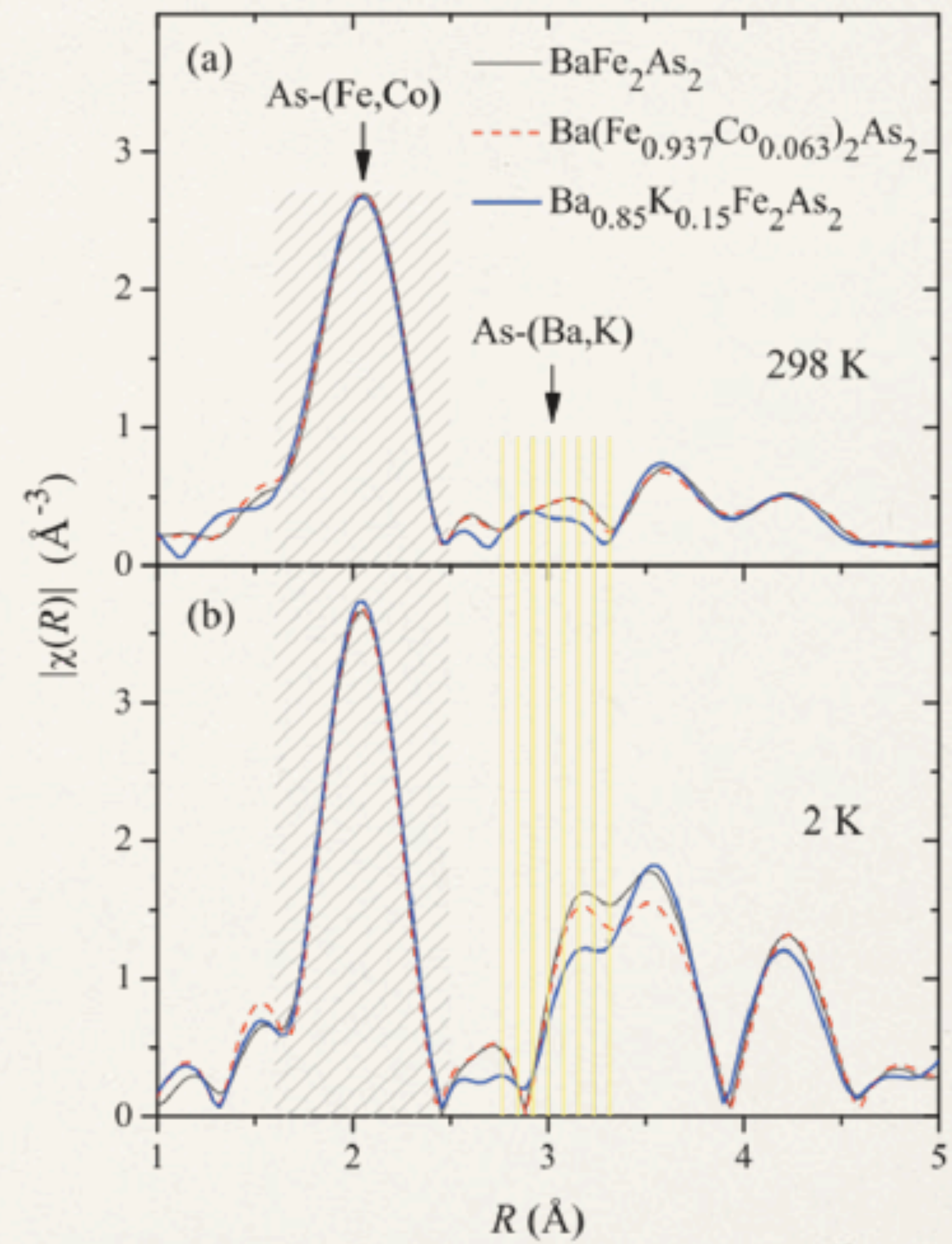


	$T = 2$ K	$T = 30$ K	$T = 298$ K
$BaFe_2As_2$			
d(As-Fe) (Å)	2.3915(12)	2.3914(7)	2.3985(14)
σ^2 (Å^2)	0.00266(12)	0.00250 (7)	0.00465(11)
$Ba[Fe_{0.937}Co_{0.063}]_2As_2$			
d[As-(Fe,Co)] (Å)	2.3833(12)	2.3838(9)	2.3951(12)
σ^2 (Å^2)	0.00262(12)	0.00268(9)	0.00466(9)
$Ba_{0.85}K_{0.15}Fe_2As_2$			
d(As-Fe) (Å)	2.3865(15)	2.3900(12)	2.3955(9)
σ^2 (Å^2)	0.00242(15)	0.00248(12)	0.00466(7)



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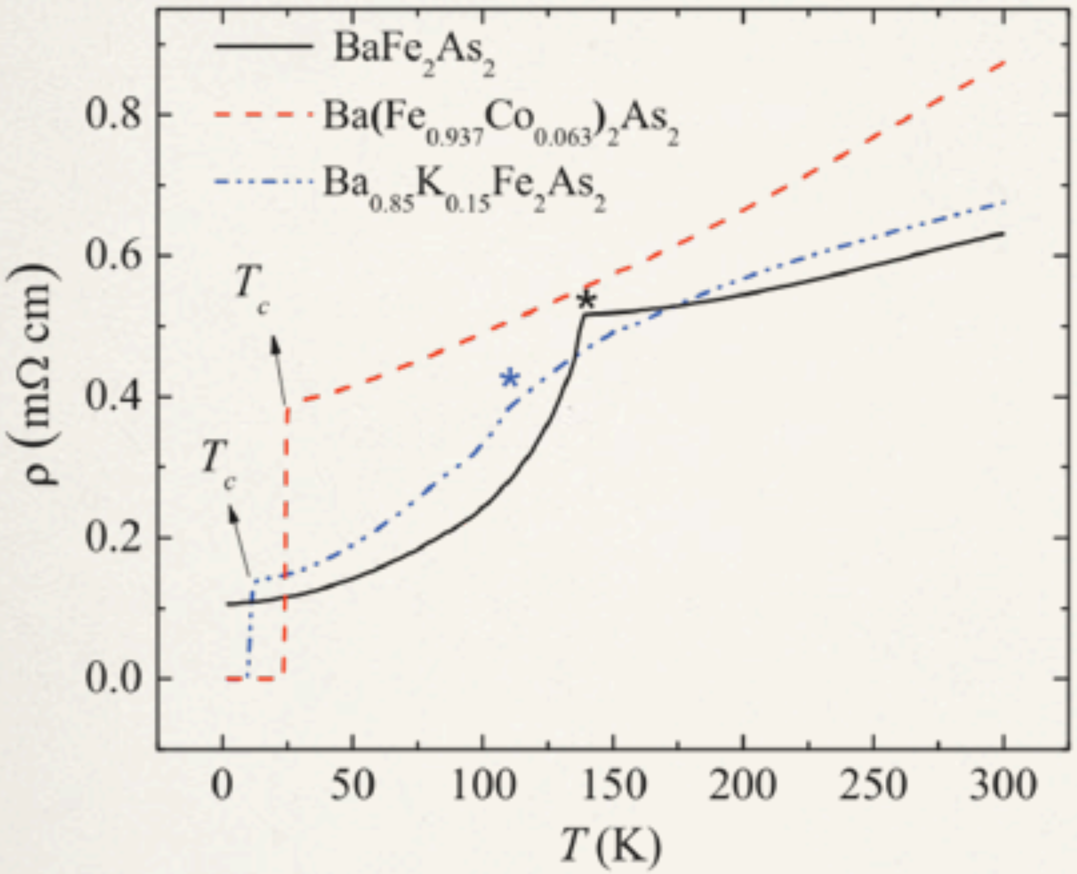

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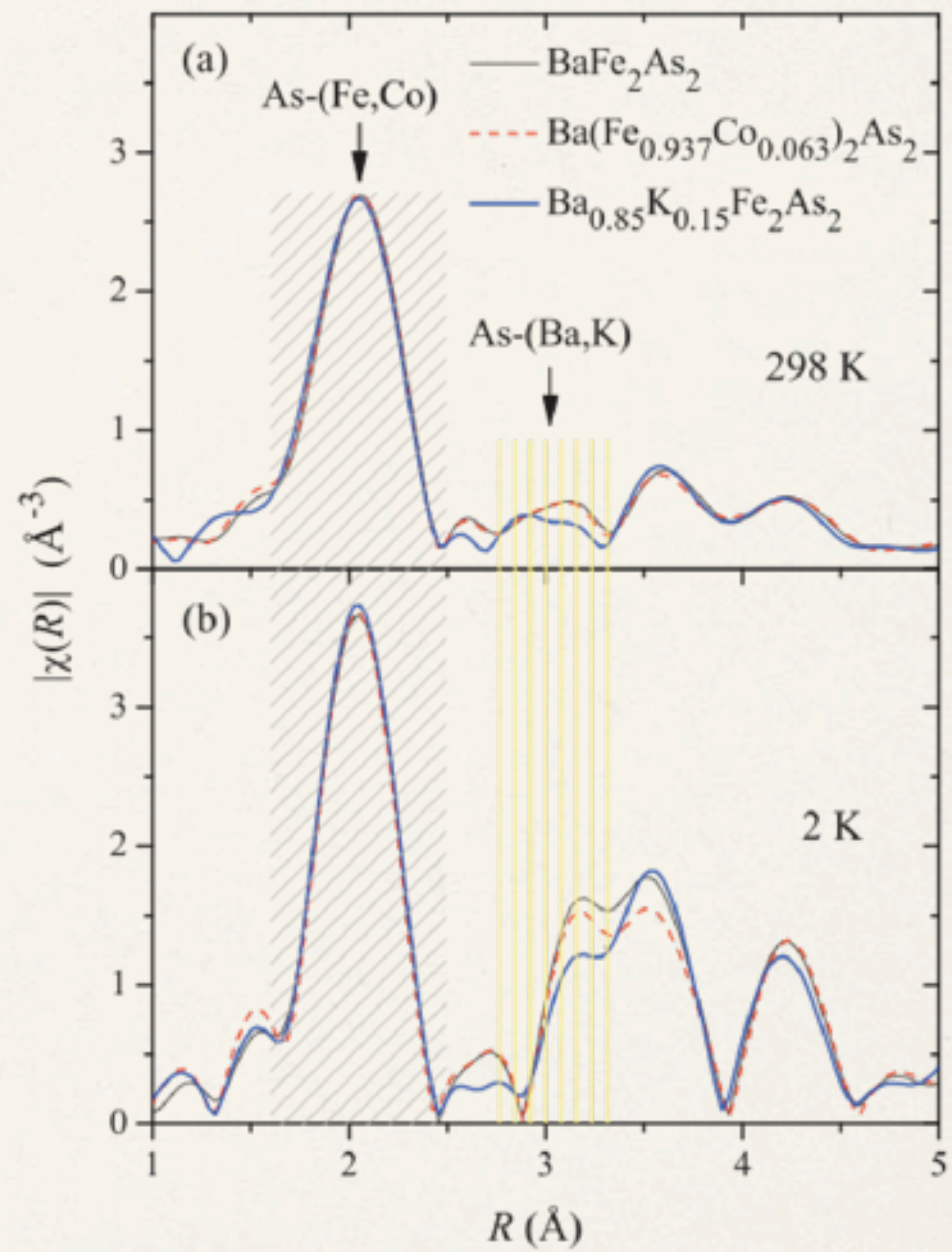
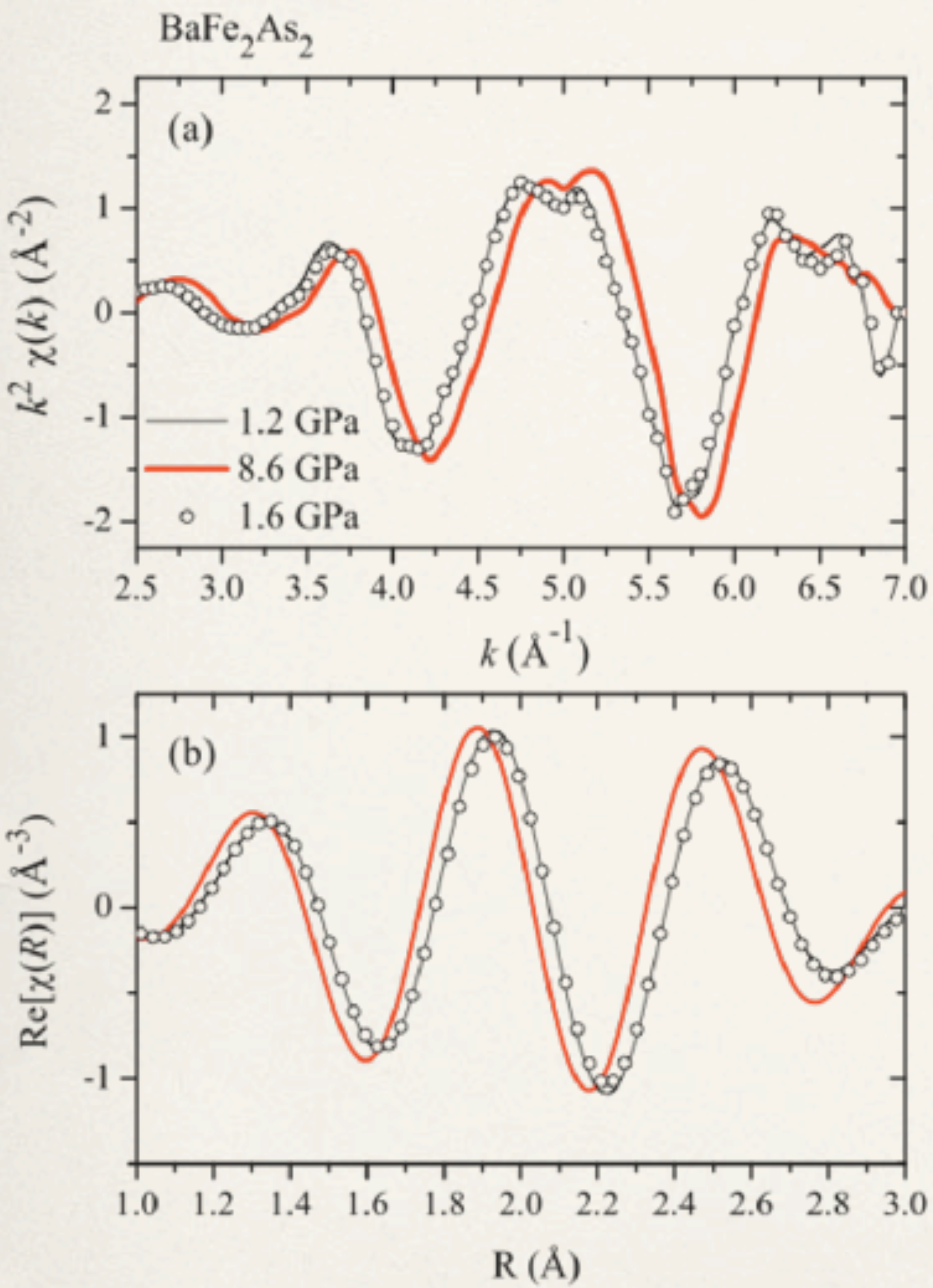
Decrease of FeAs distance with both K and Co substitution



Experiments performed at XAFS2 beamline of the Brazilian Synchrotron Light Laboratory (LNLS).

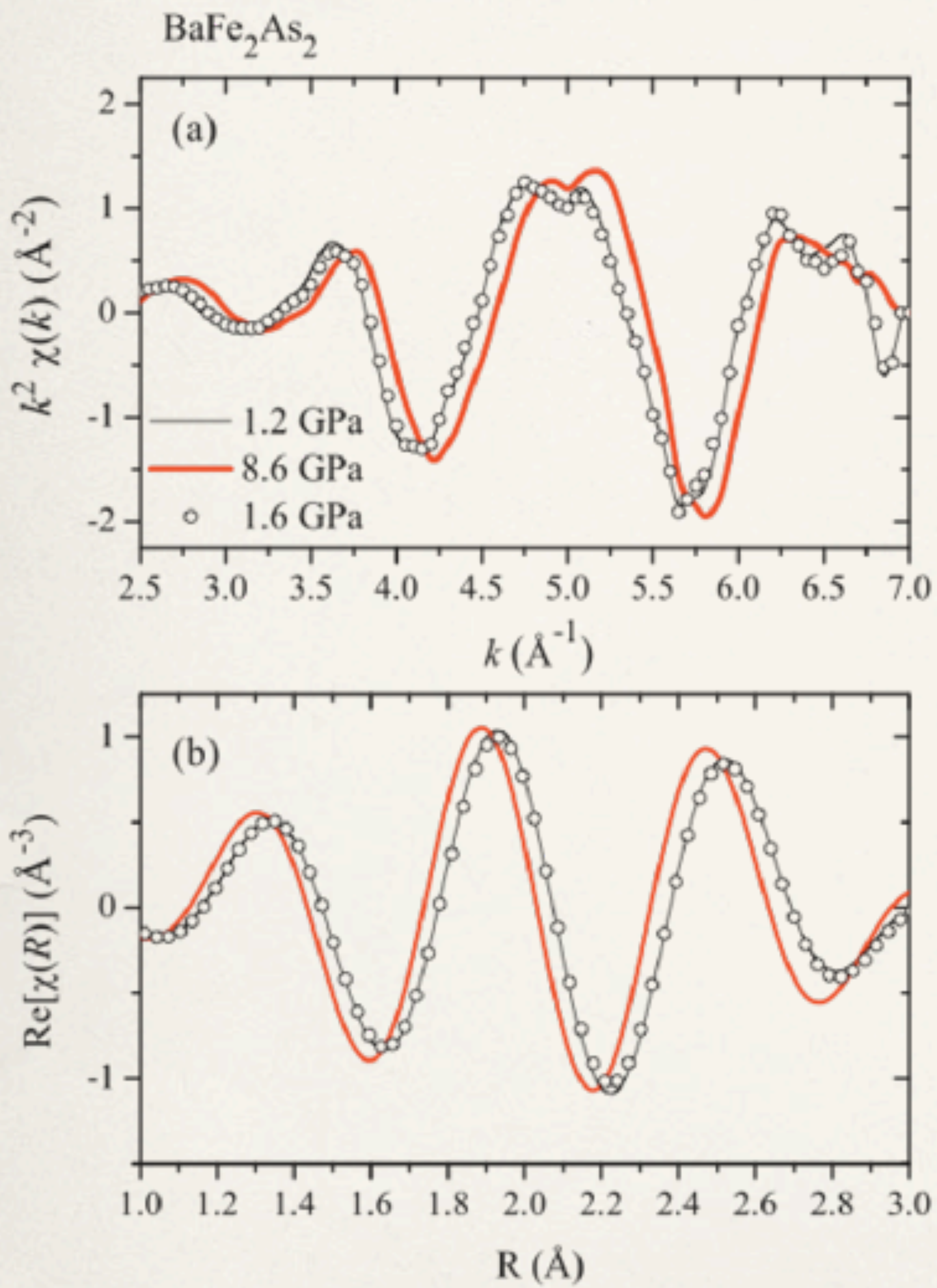
Microscopic Properties: Evolution of the FeAs distance

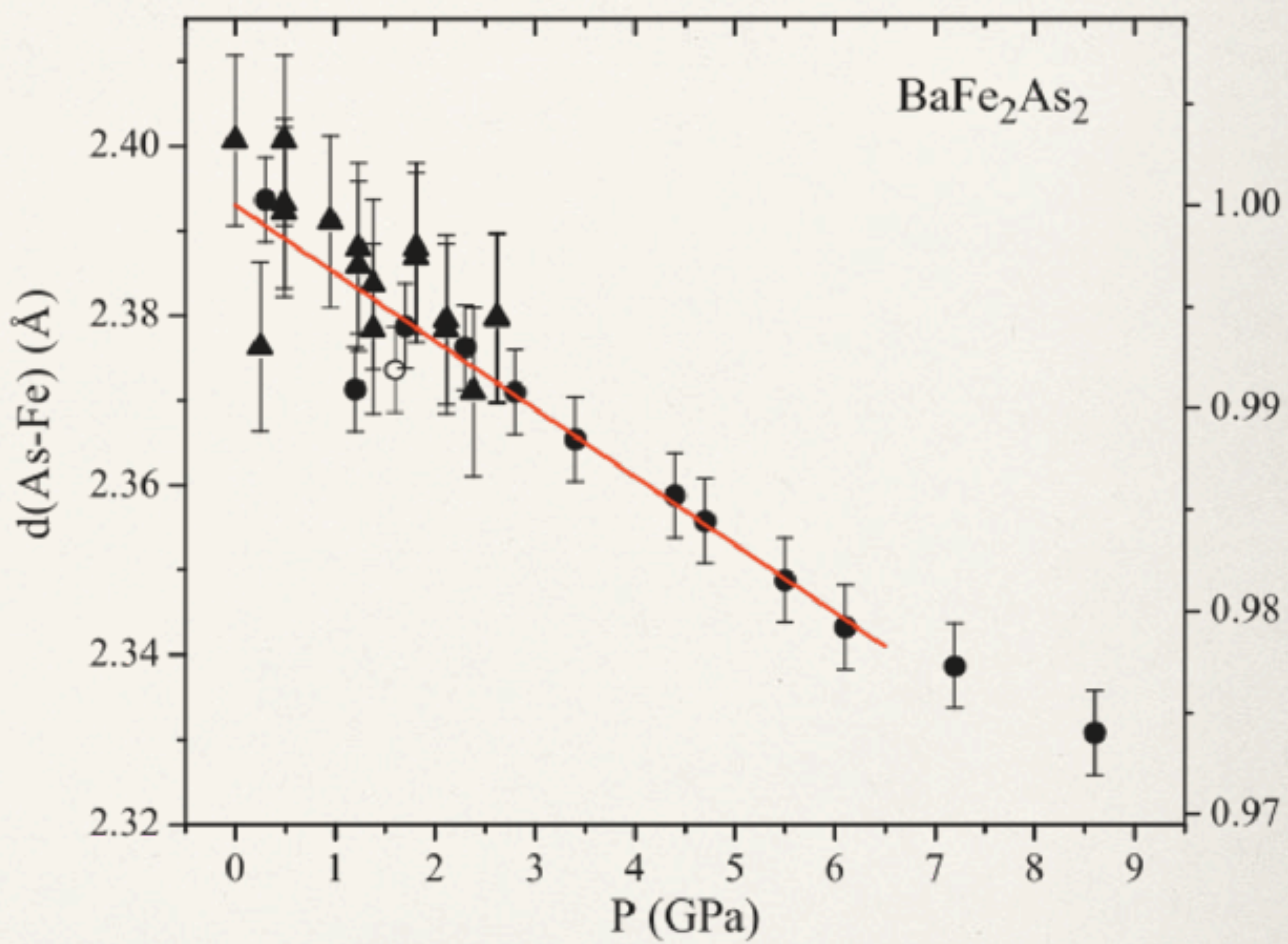
- Decrease of d(Fe-As) also with applied pressure.



Microscopic Properties: Evolution of the FeAs distance

- Decrease of d(Fe-As) also with applied pressure.



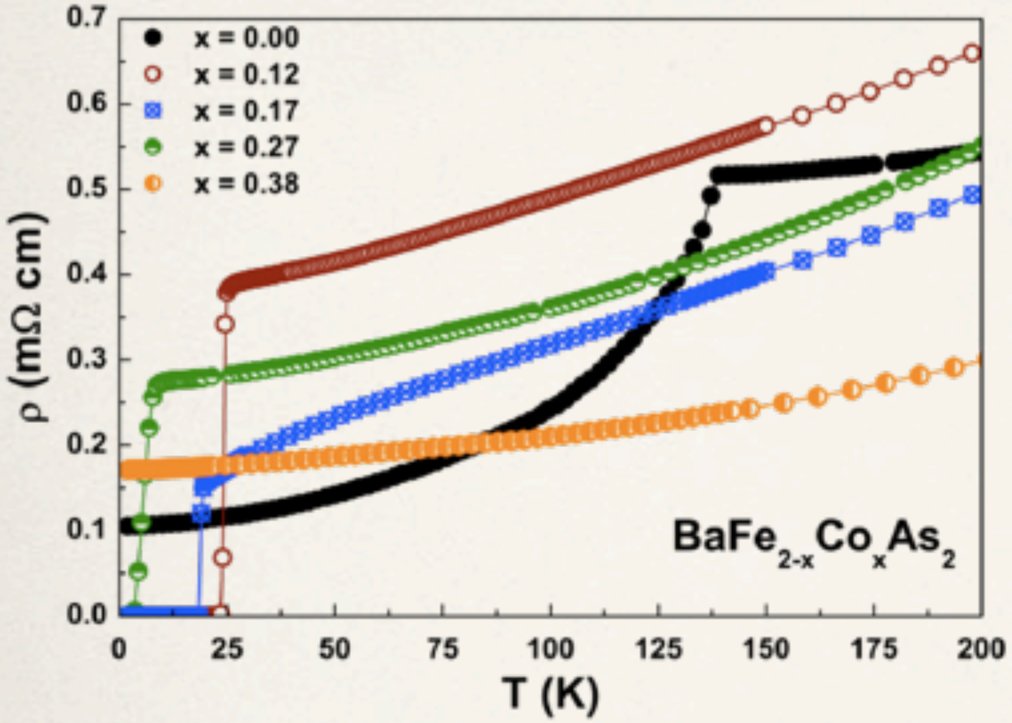


Experiments performed at DXAS beamline of the Brazilian Synchrotron Light Laboratory (LNLS).

E. Granado, L. Mendonça-Ferreira, F. Garcia, G. de M. Azevedo, G. Fabbris, E. M. Bittar, C. Adriano, T. M. Garitezi, P. F. S. Rosa *et al*. Phys. Rev. B **83,** 184508 (2011).

Microscopic Properties: Fe Valence (XANES)

- Is Cobalt an effective carrier doping?



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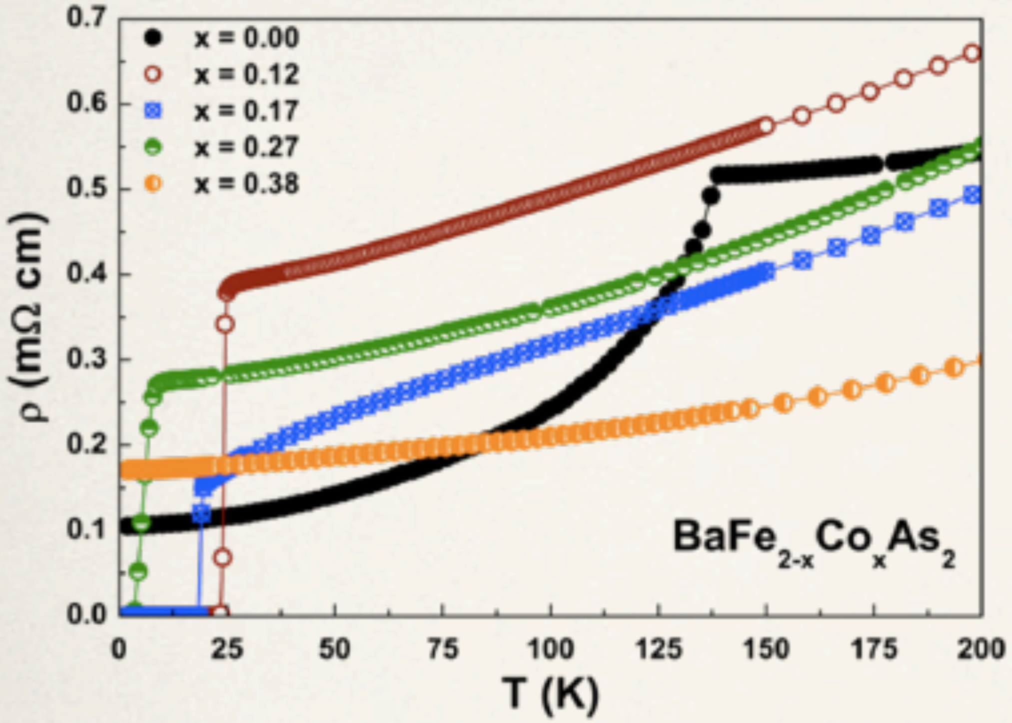

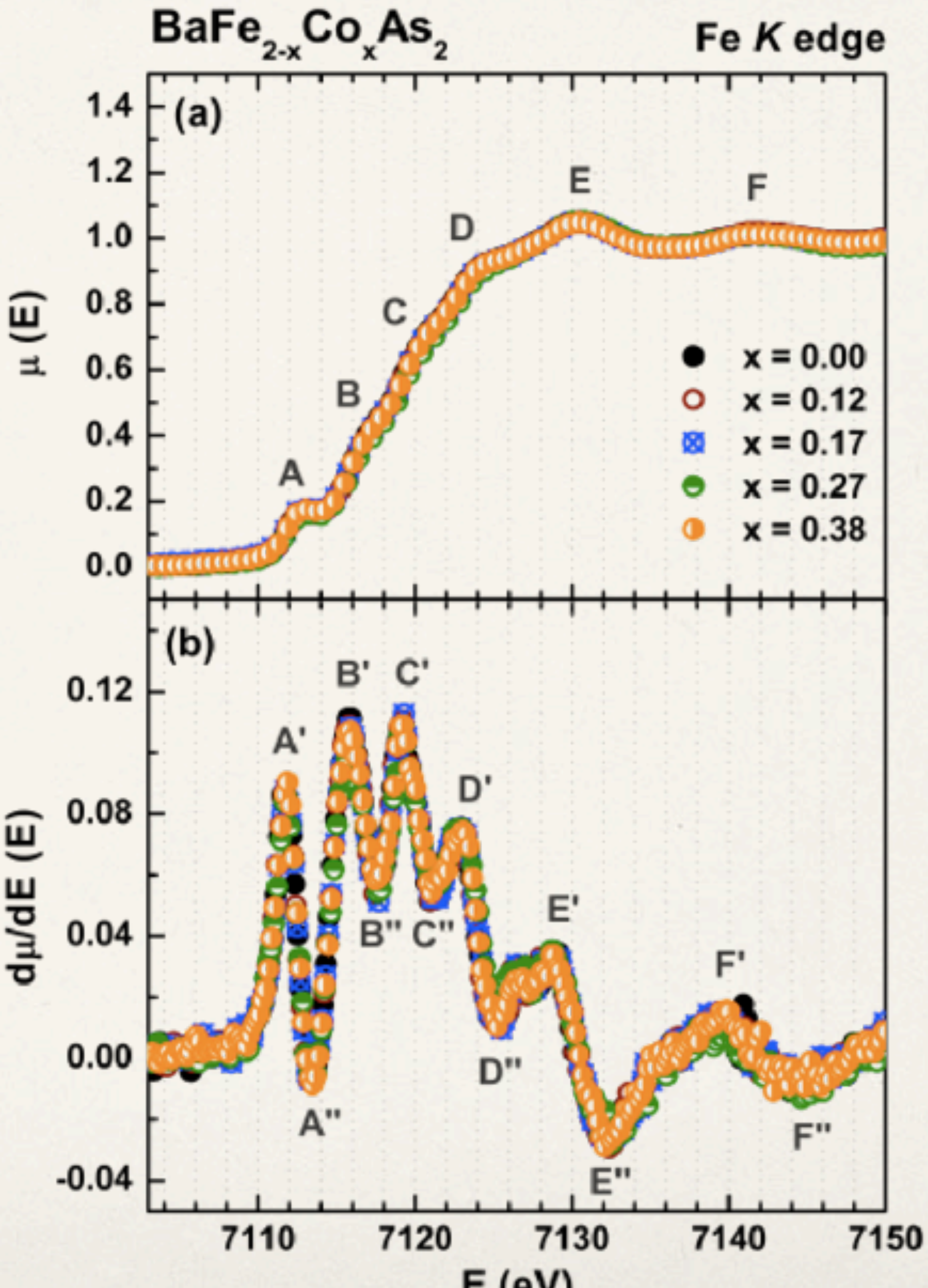

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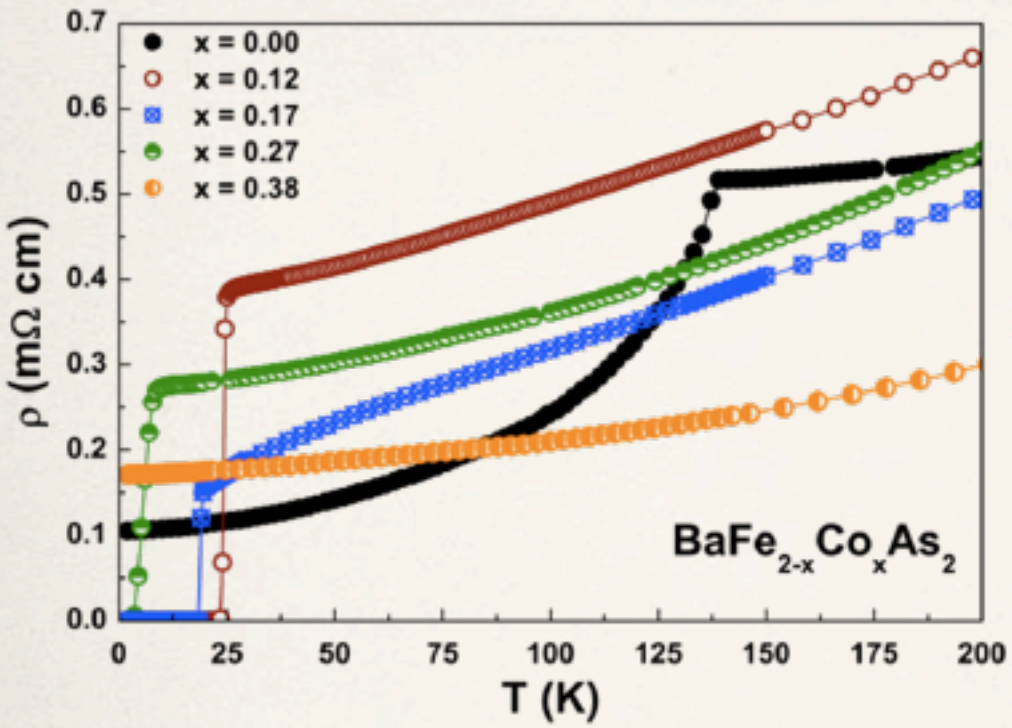
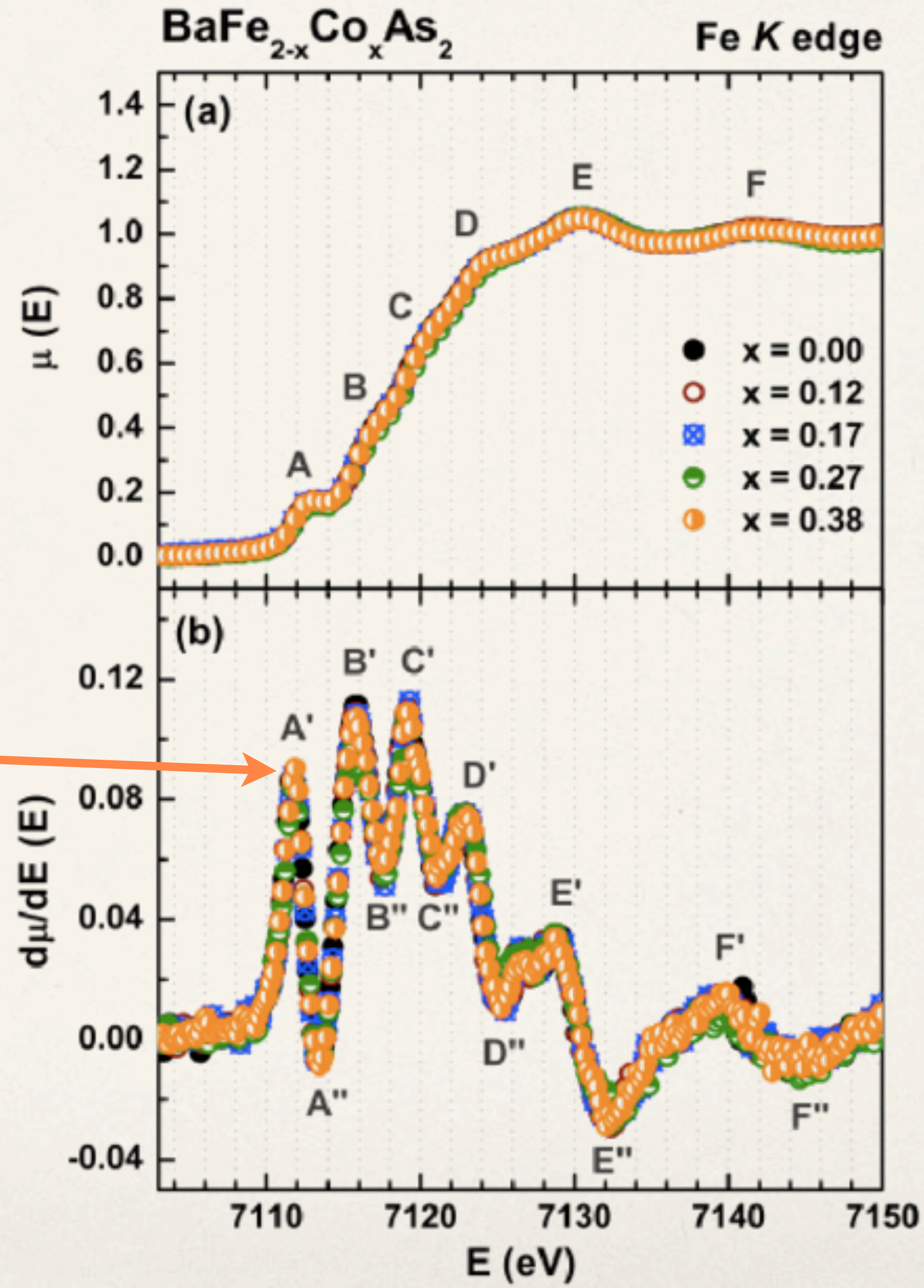
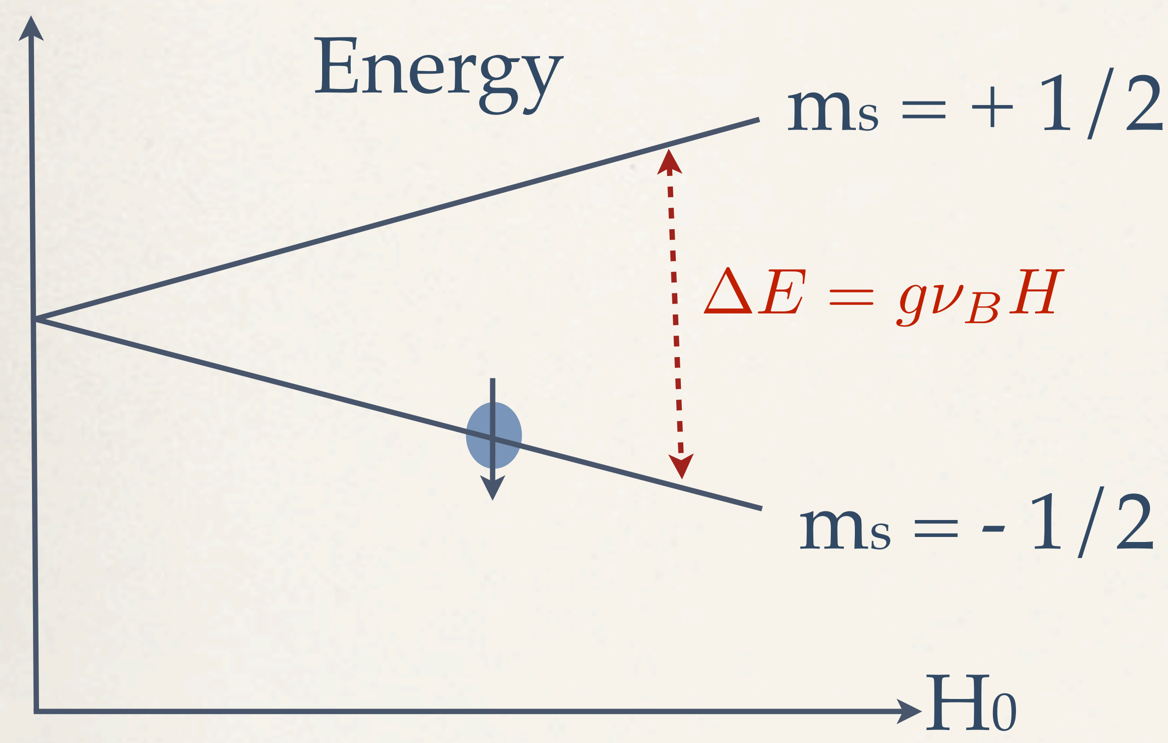




- No! There is no shift in the Fe *K*-edge absorption.

E. Bittar, C. Adriano, T. M. Garitezi, P. F. S. Rosa *et al*. Phys. Rev. Lett. **107,** 267402 (2011).

Electron spin resonance (ESR): Relaxation Mechanism in Metals



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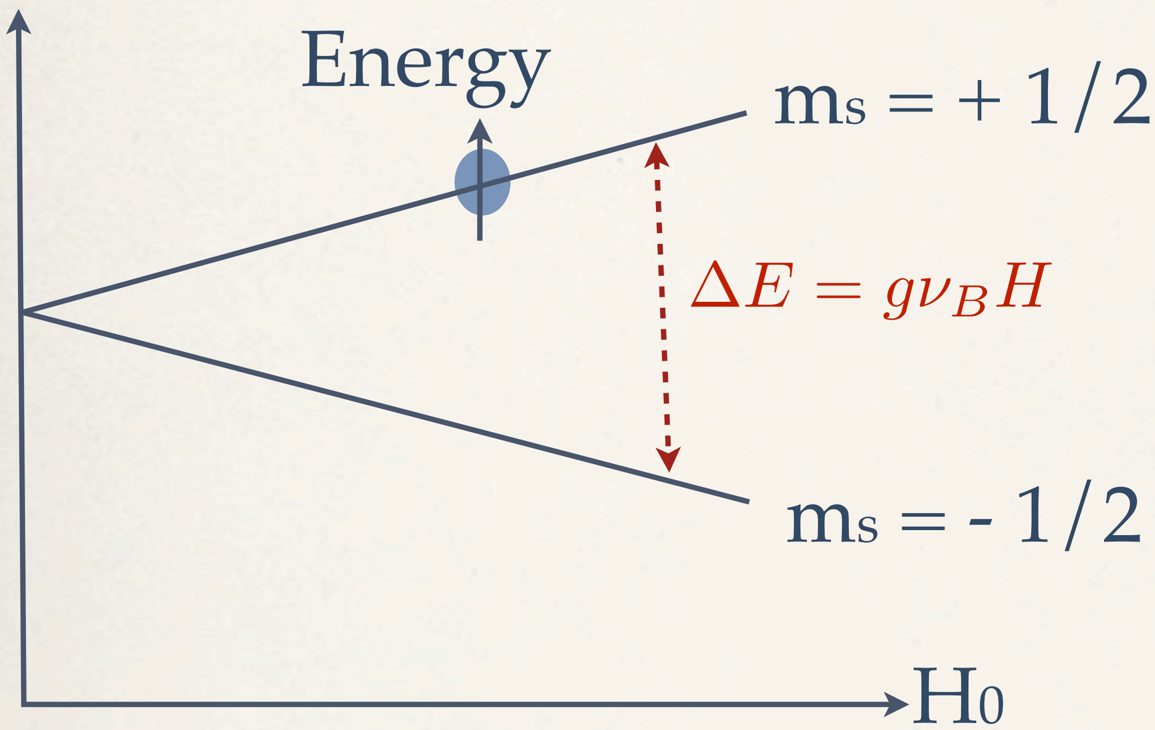

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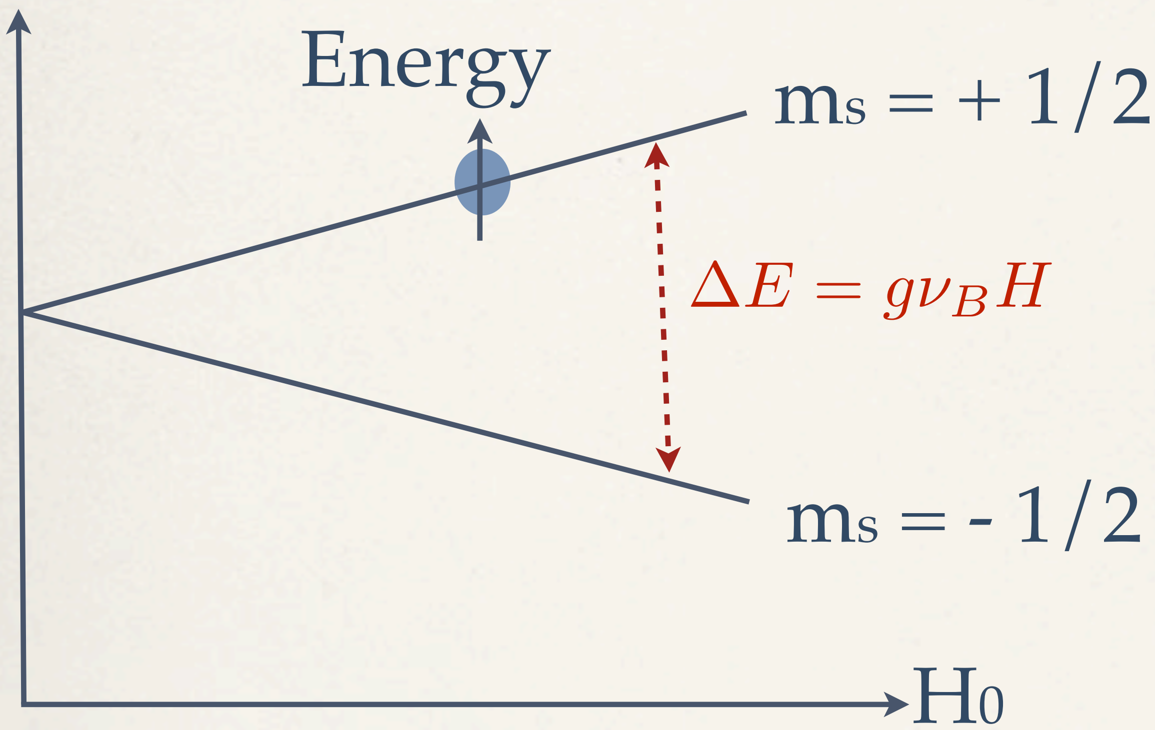

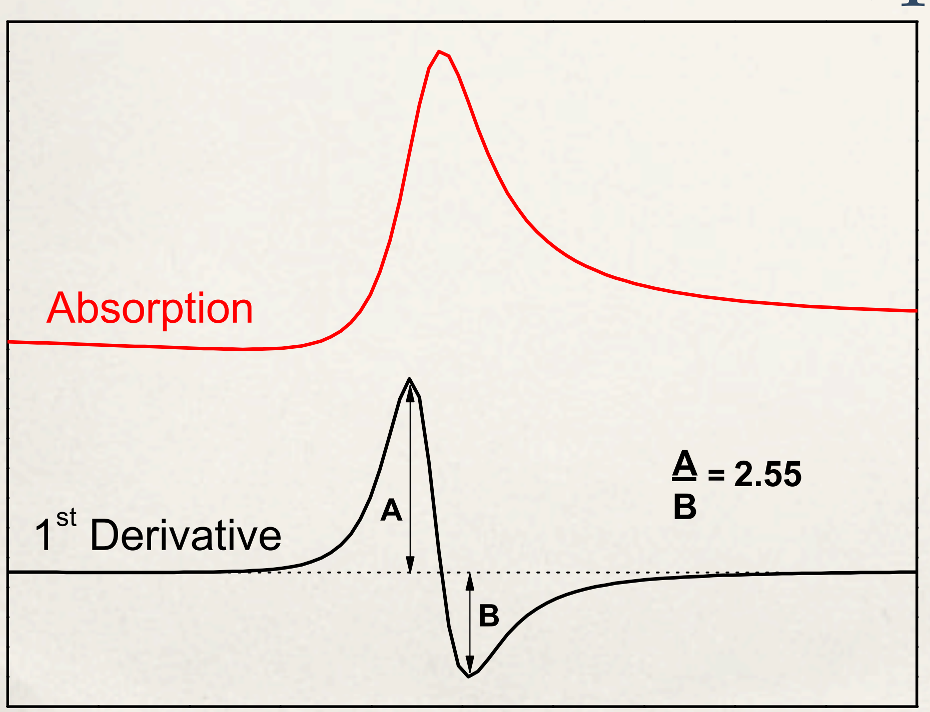

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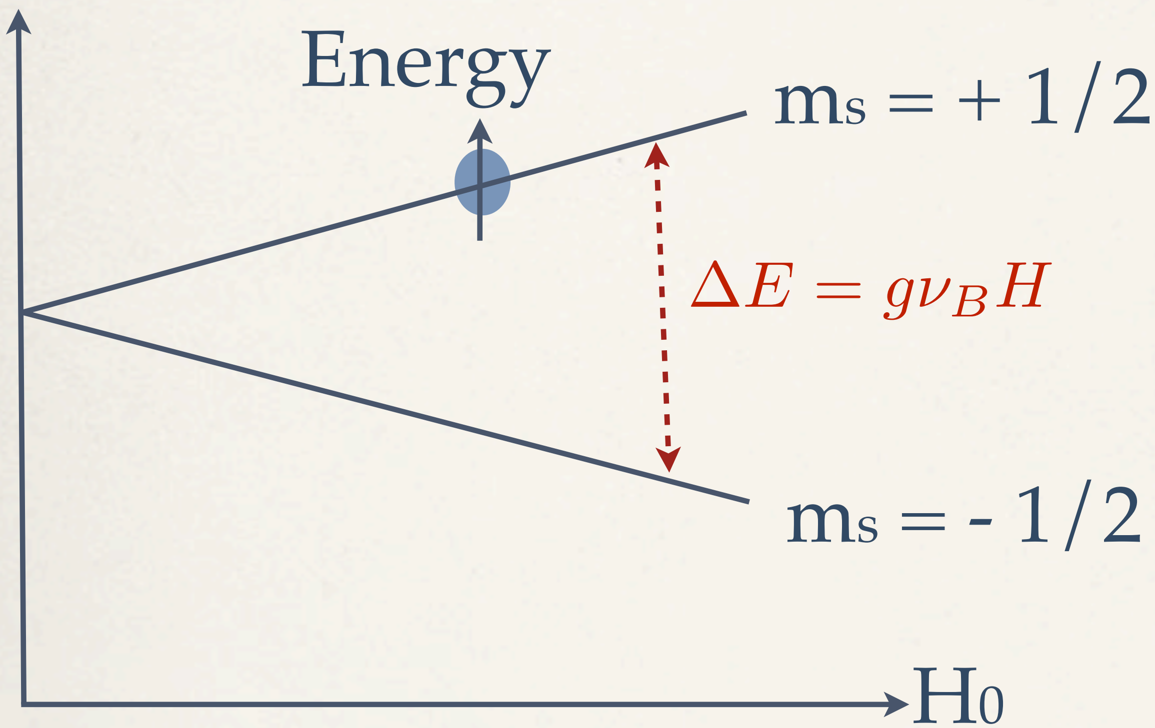
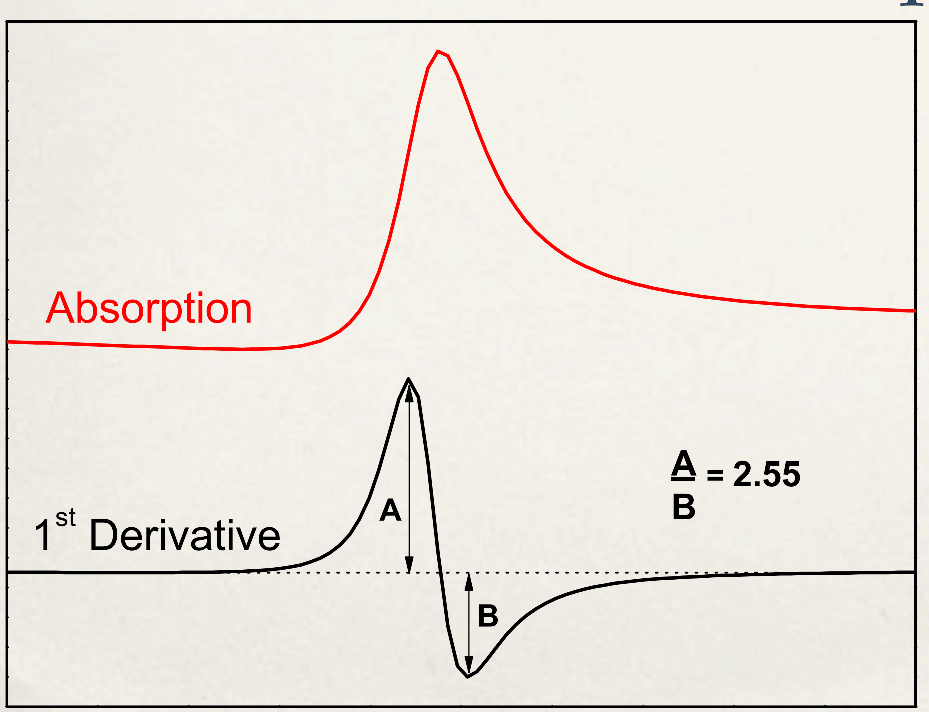


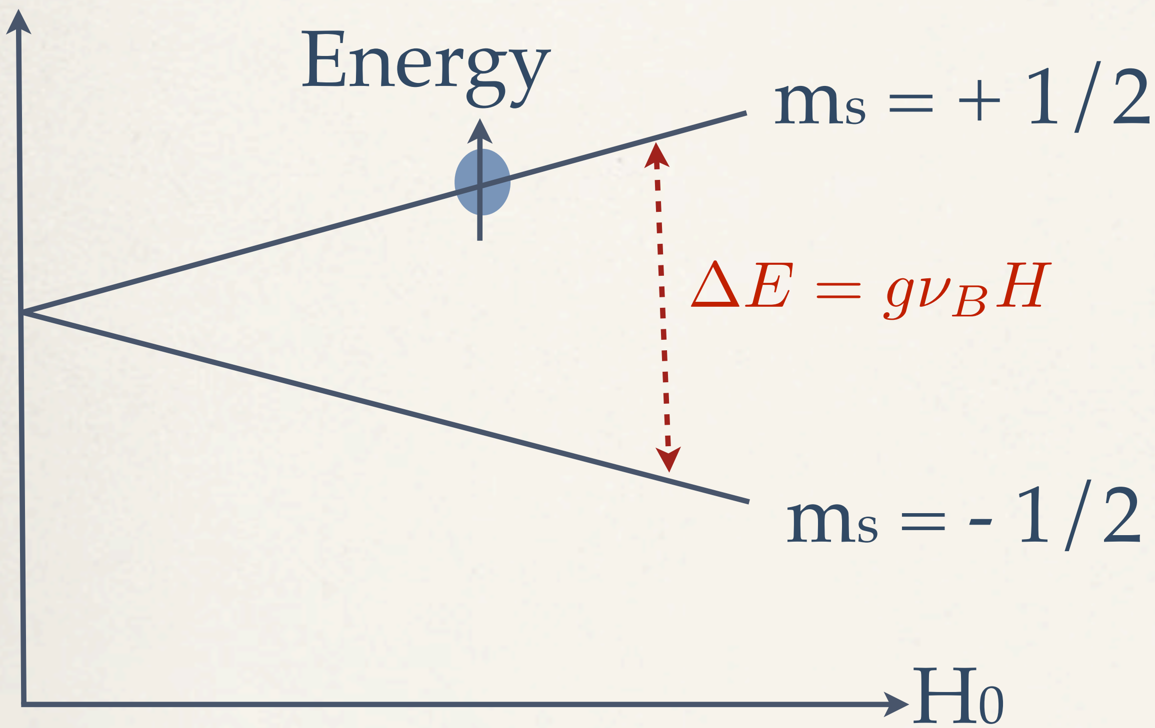


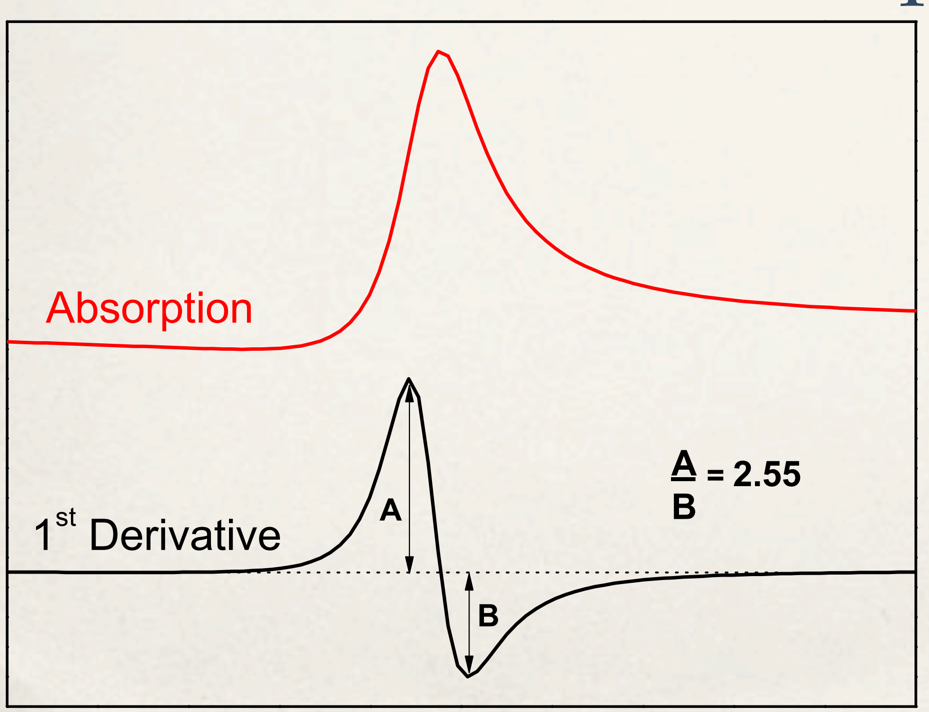
Conduction Electrons (e)

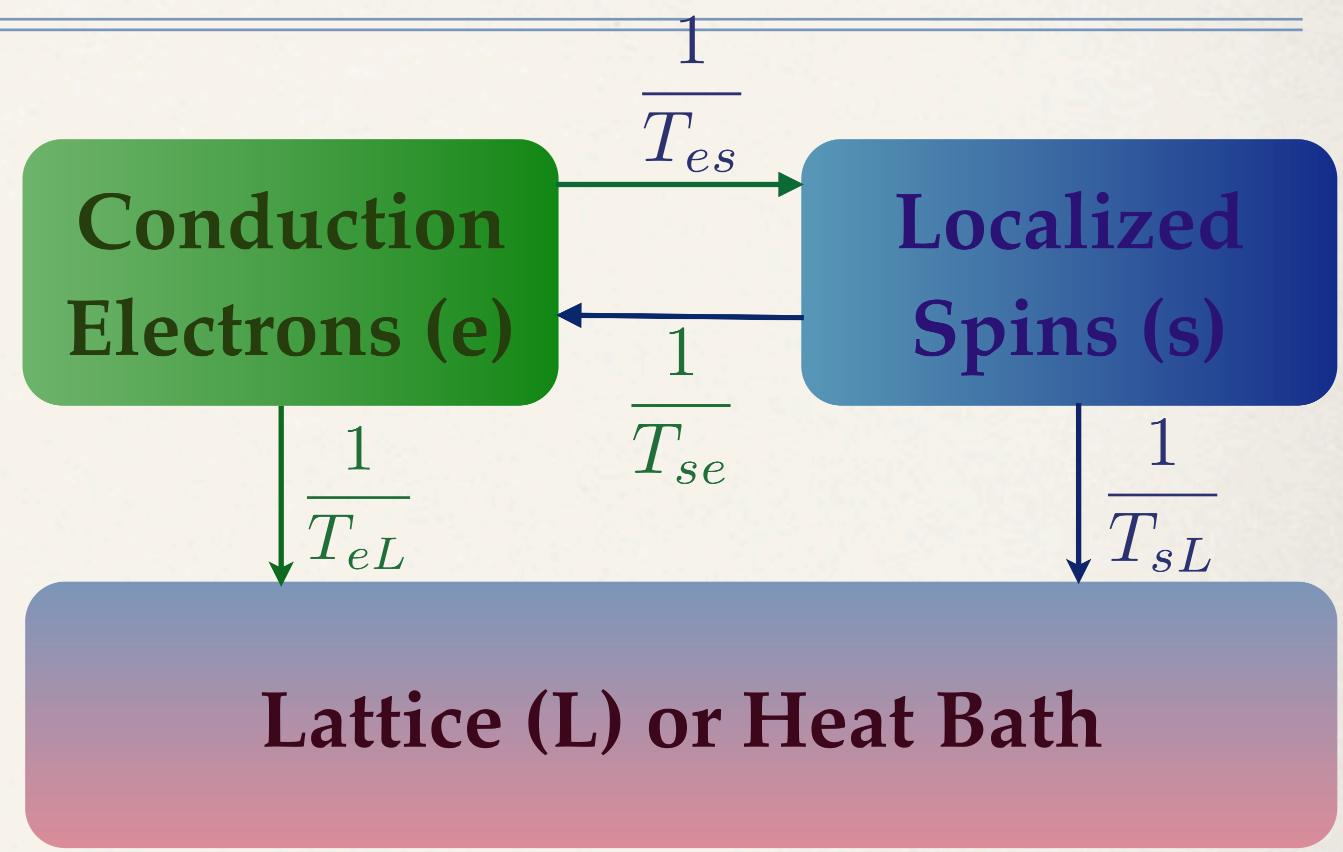
Localized Spins (s)

Lattice (L) or Heat Bath

Electron spin resonance (ESR): Relaxation Mechanism in Metals







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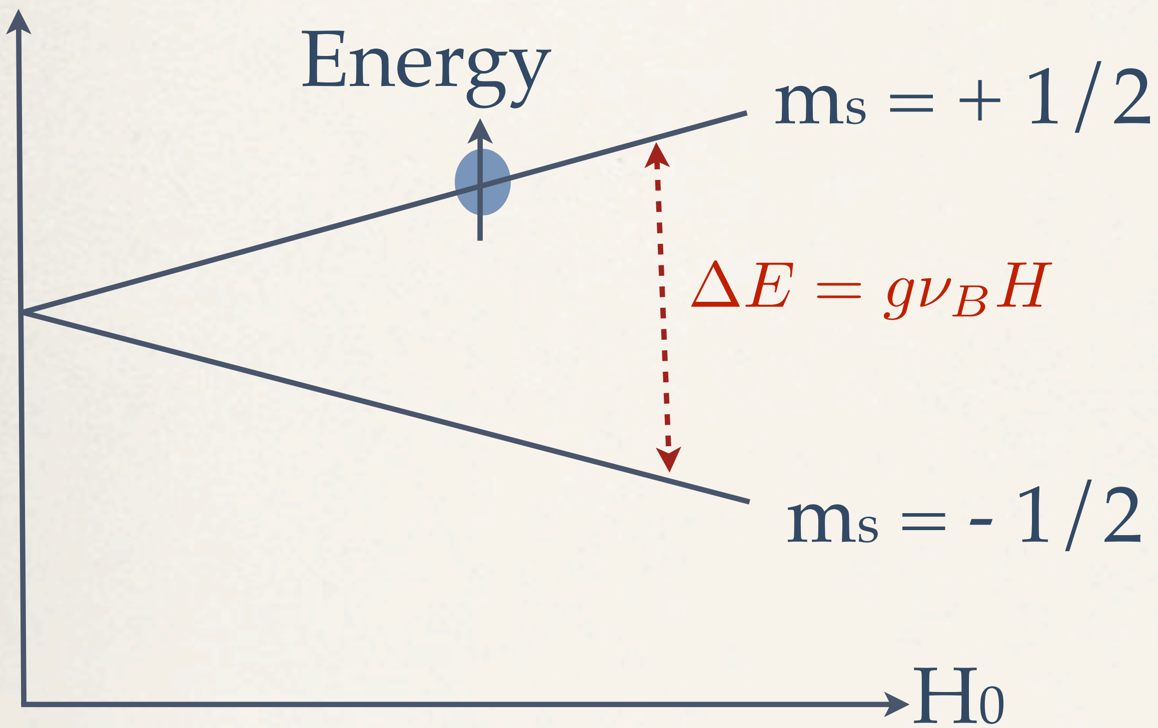

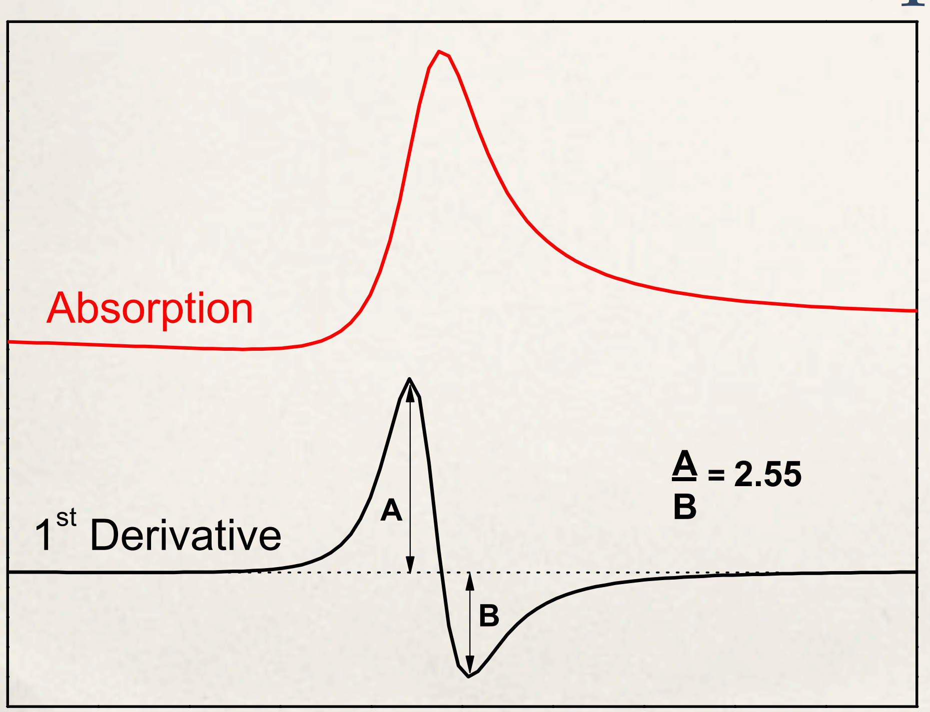

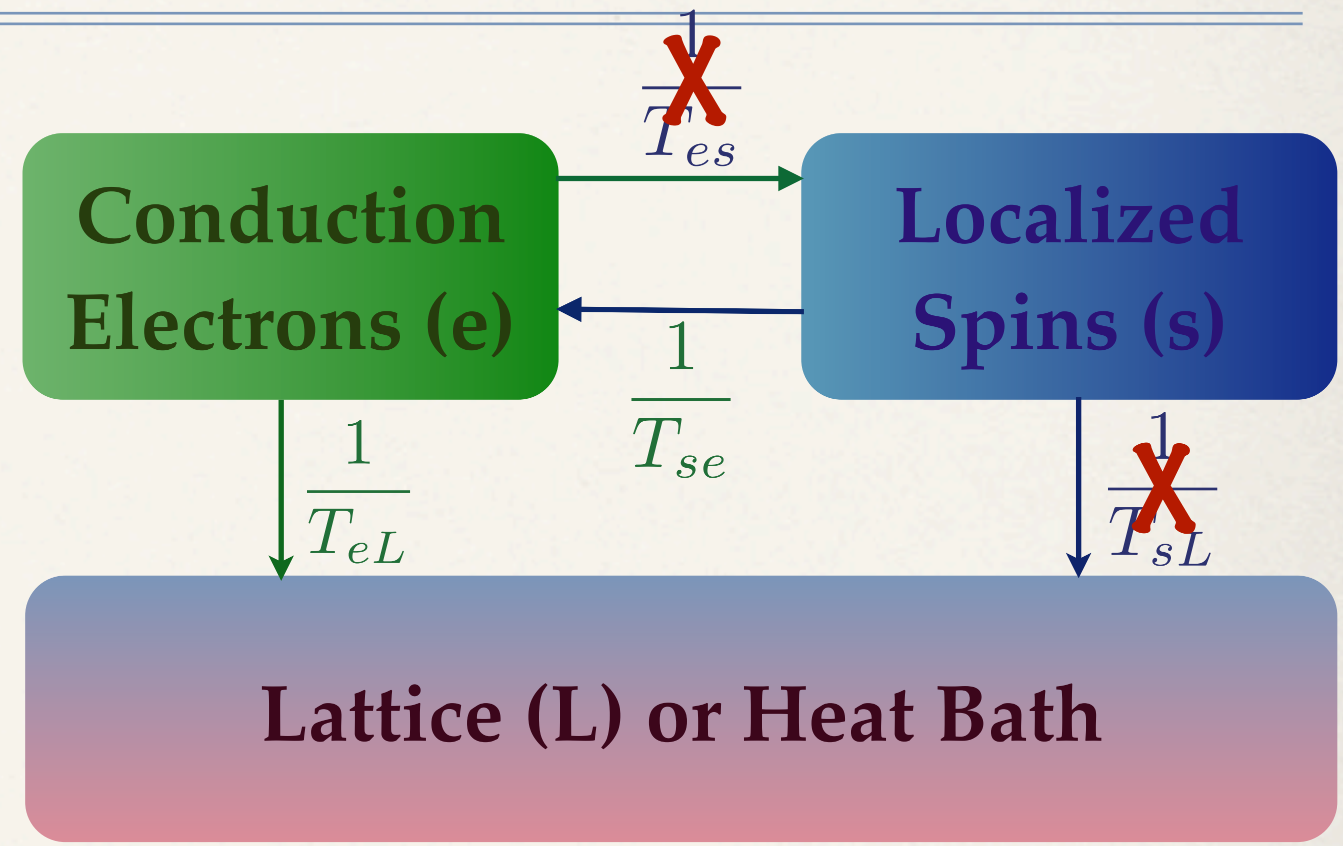

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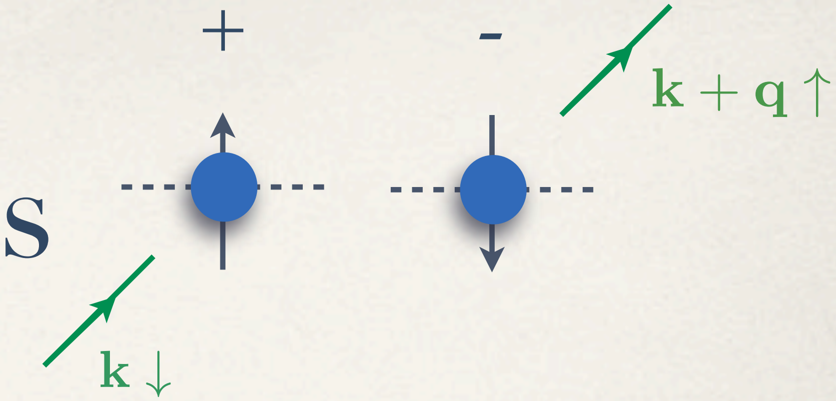

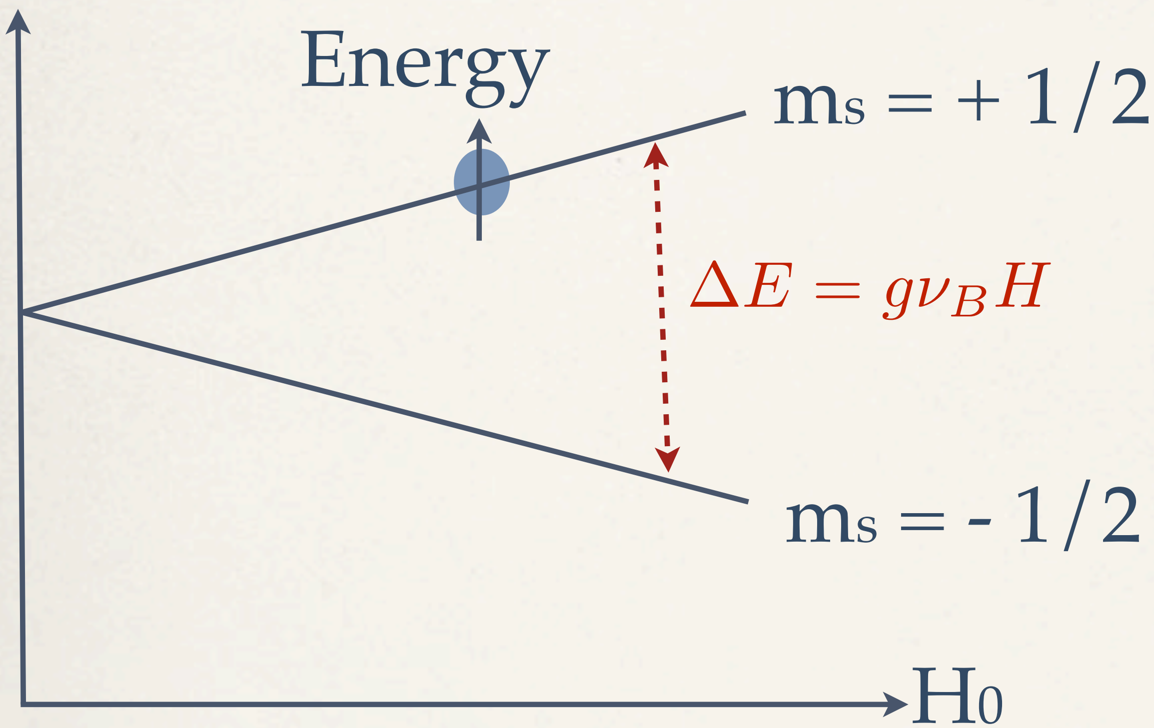

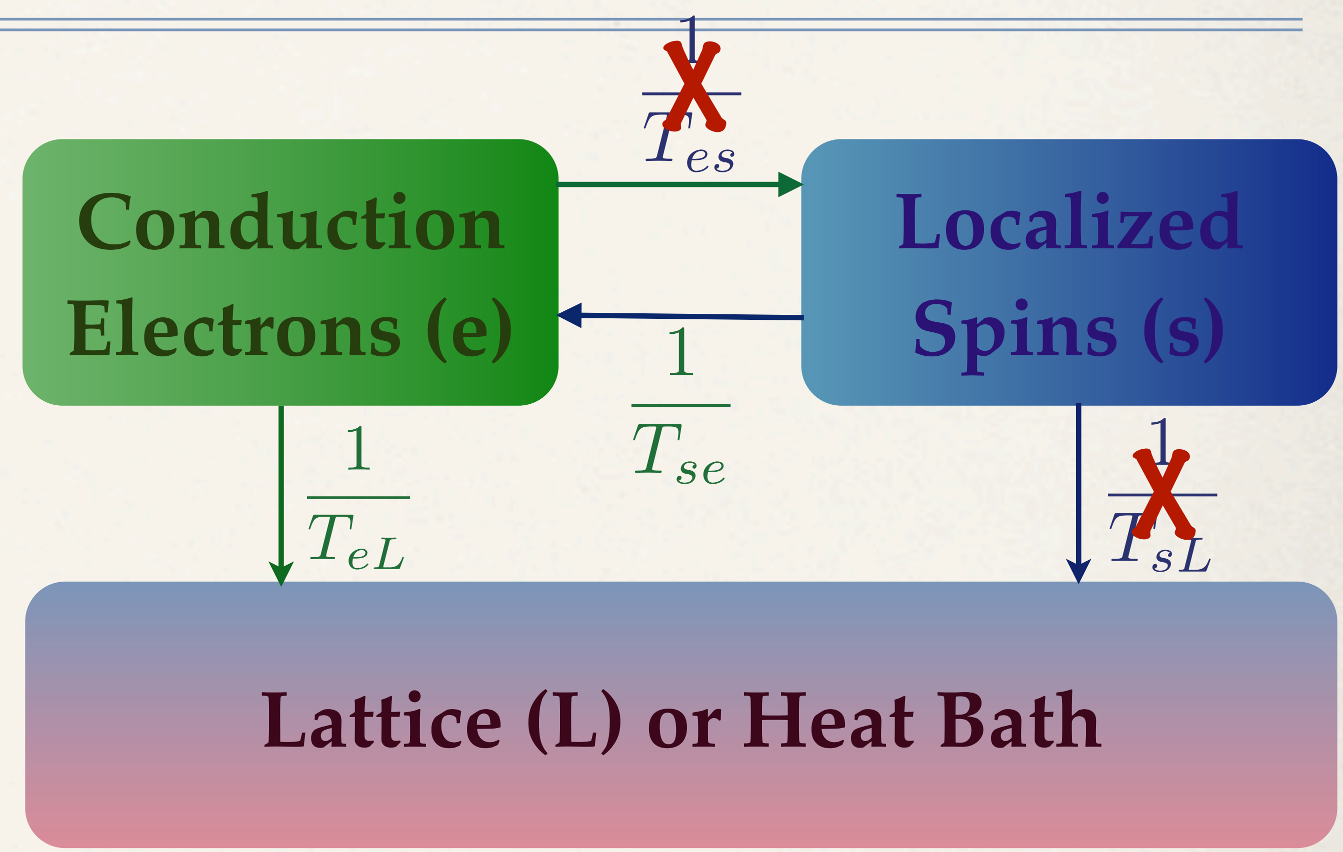

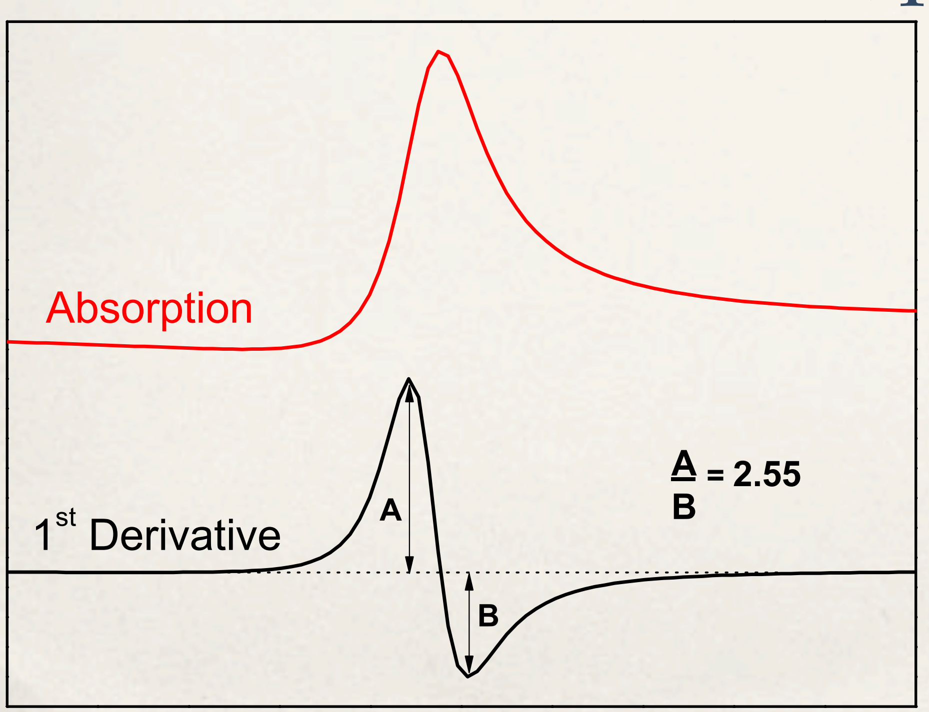

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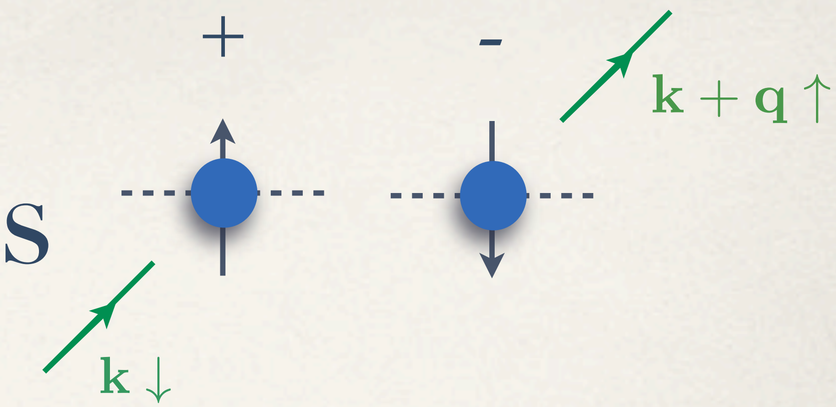
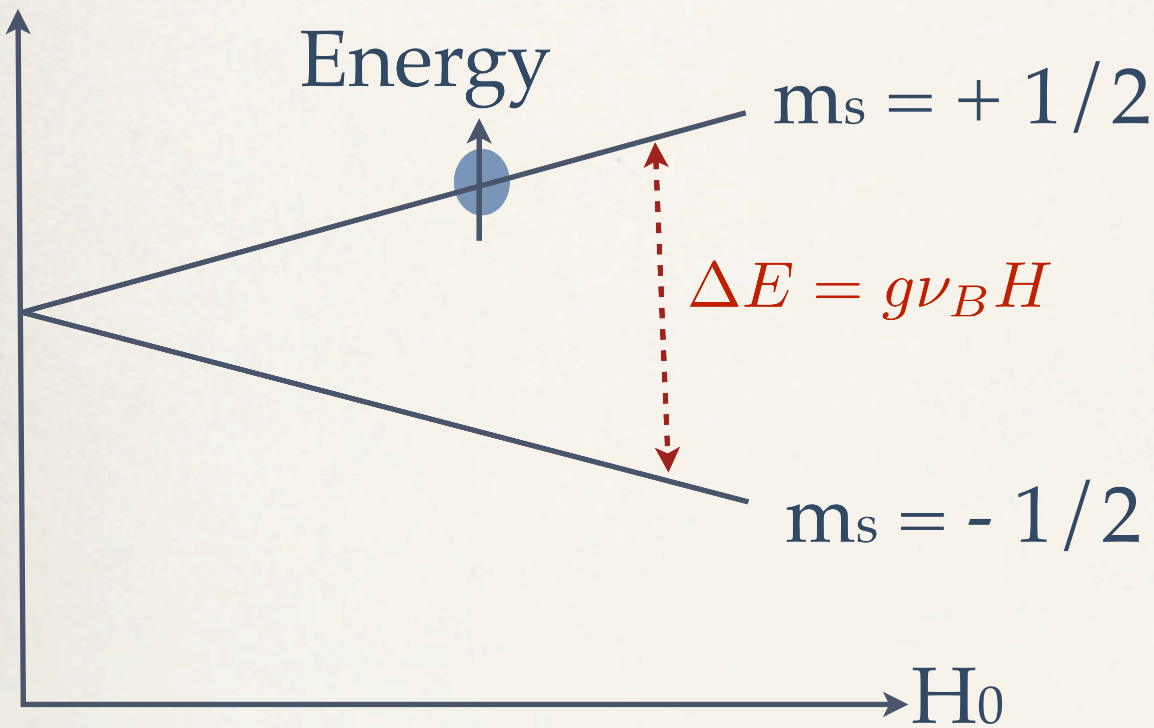
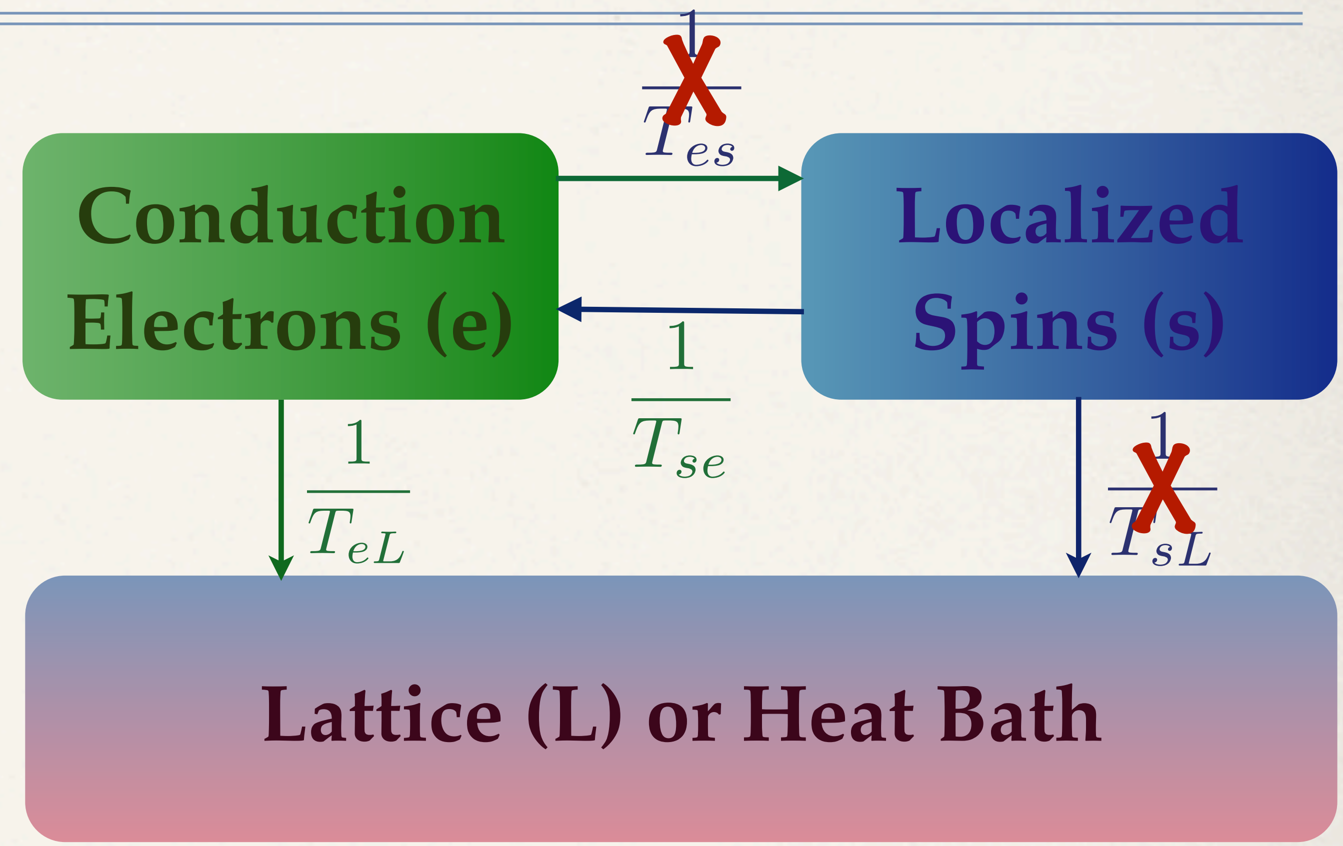
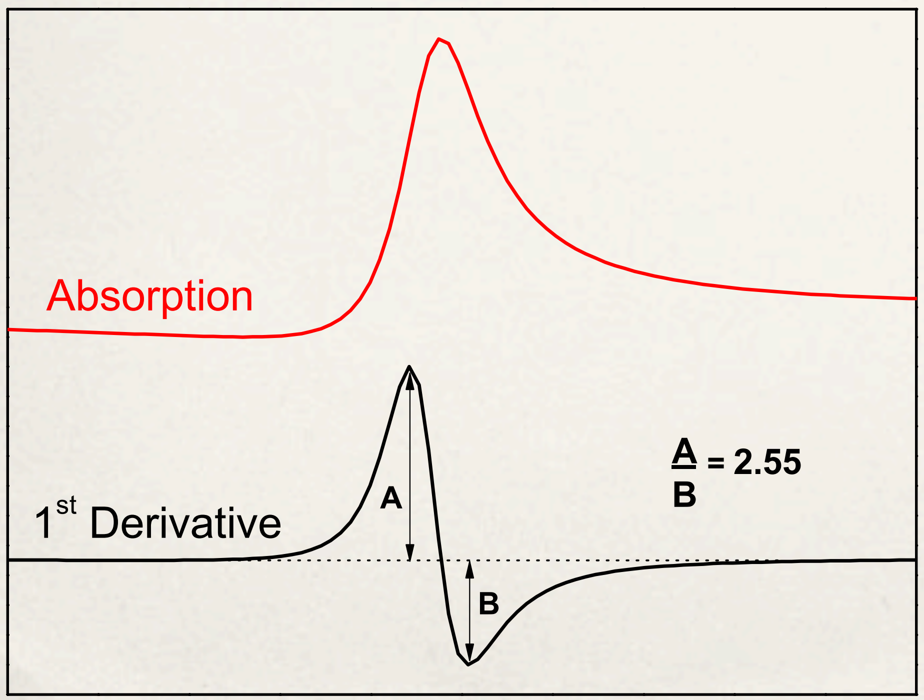








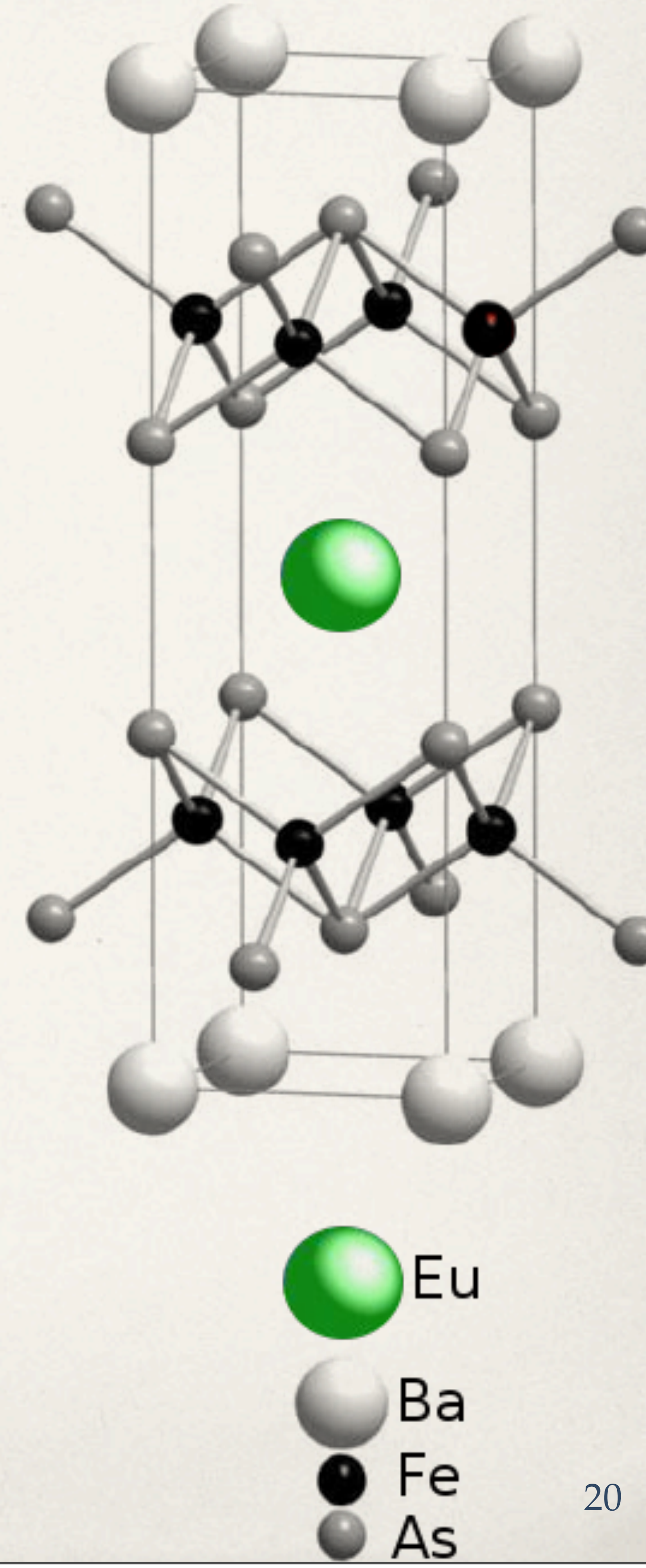
$$\frac{1}{T_{se}} = a + bT$$

$$b = \frac{d\,(\Delta H)}{dT} = \frac{\pi k_B}{g\mu_B} \langle J_{fs}^2(\mathbf{q}) \rangle \eta^2\,(E_F)\ \frac{K(\alpha)}{(1-\alpha)^2}$$

$$\Delta g \equiv g - g_{insulator} = J_{fs}(\mathbf{0})\ \frac{\eta\,(E_F)}{1-\alpha}\ .$$

J. Korringa. Physica 16, 601 (1950).

Magnetic Series $Ba_{1-x}Eu_xFe_2As_2$



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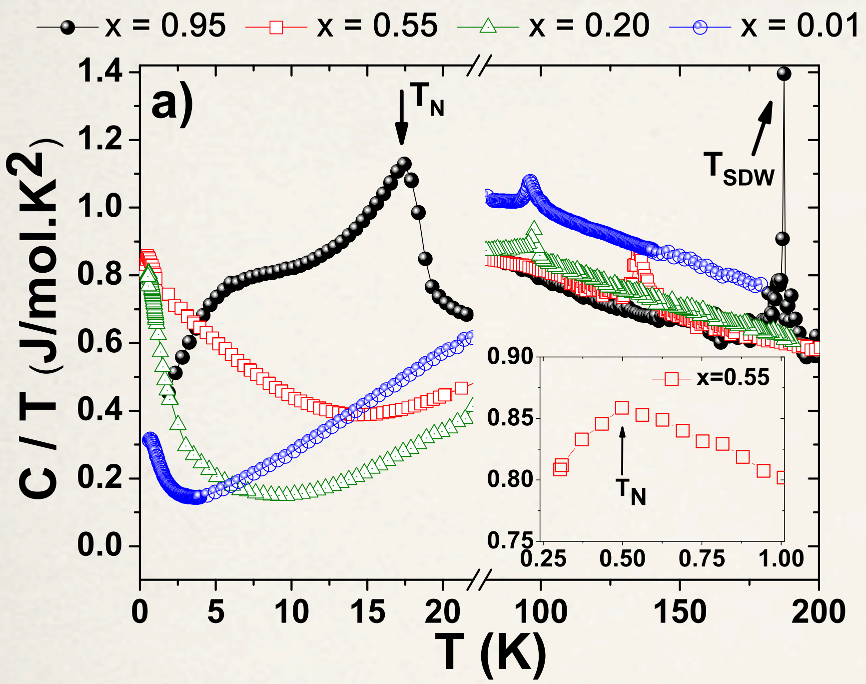

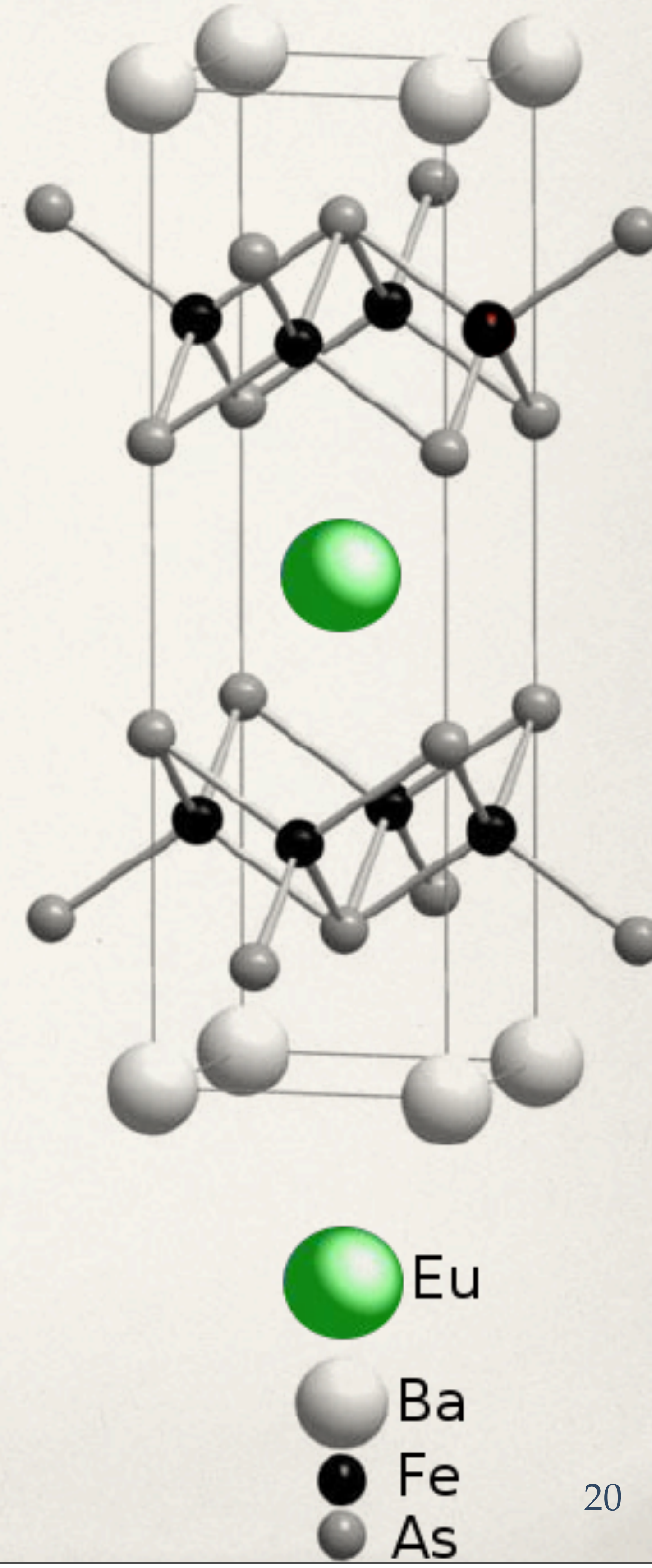

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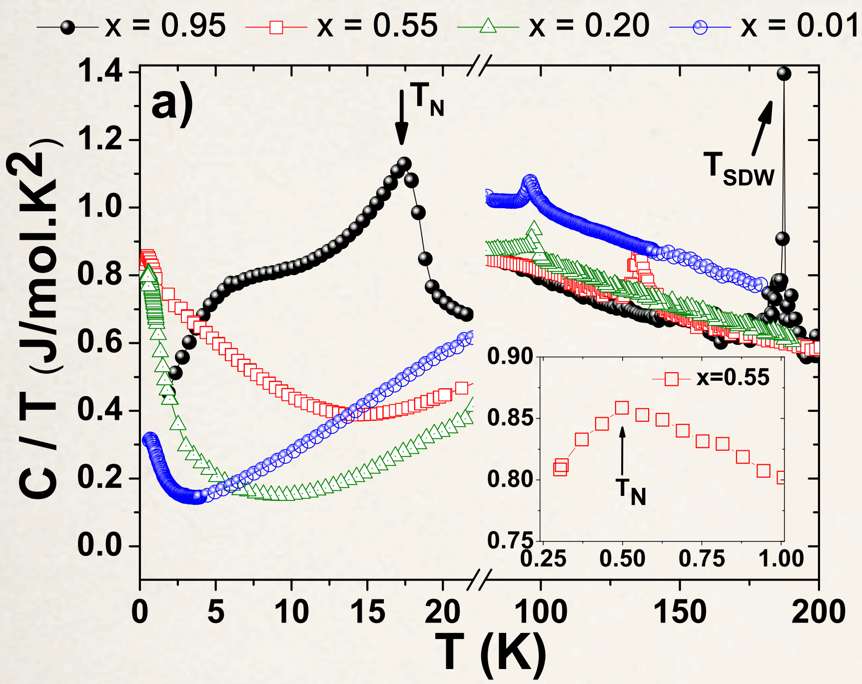
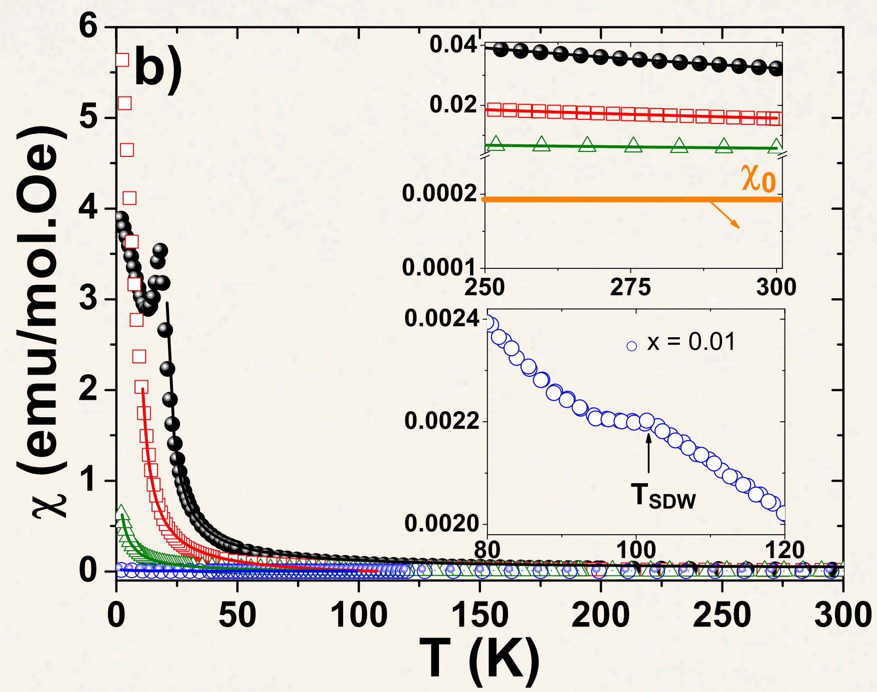
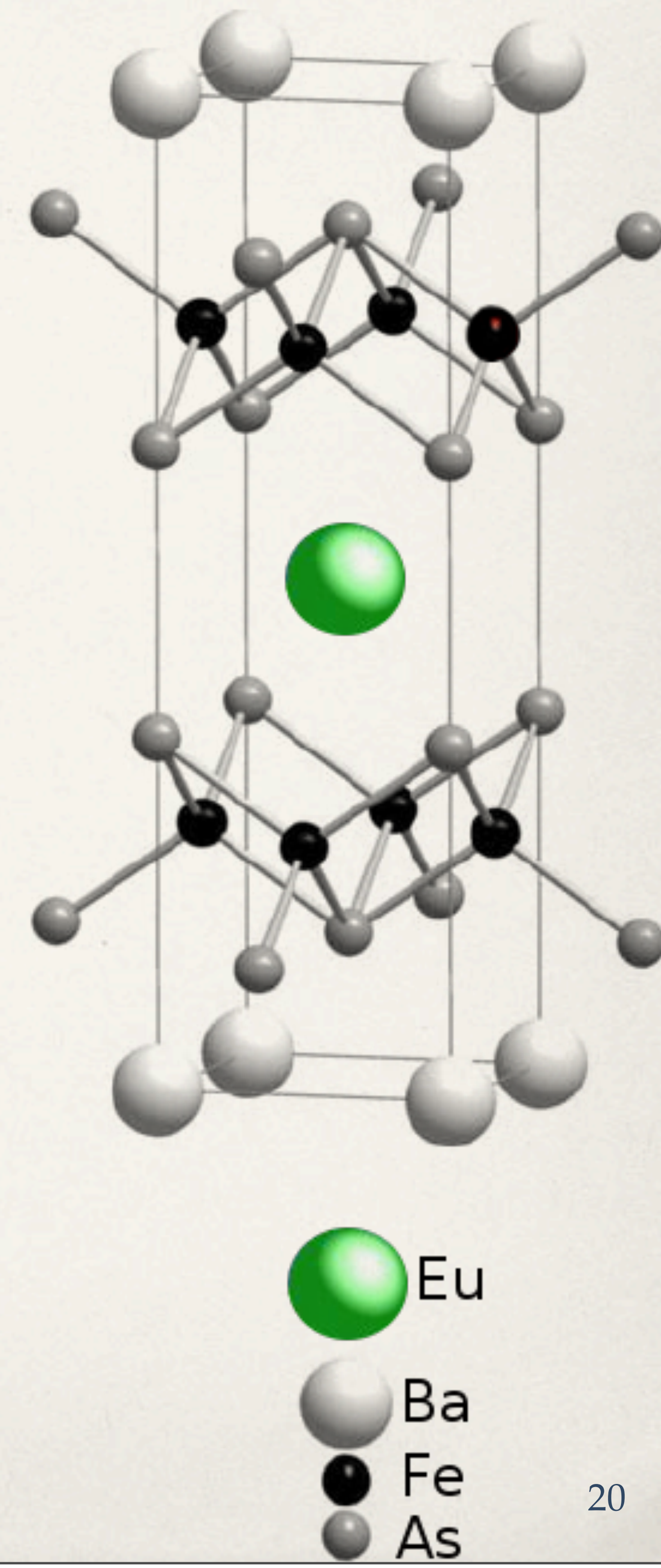
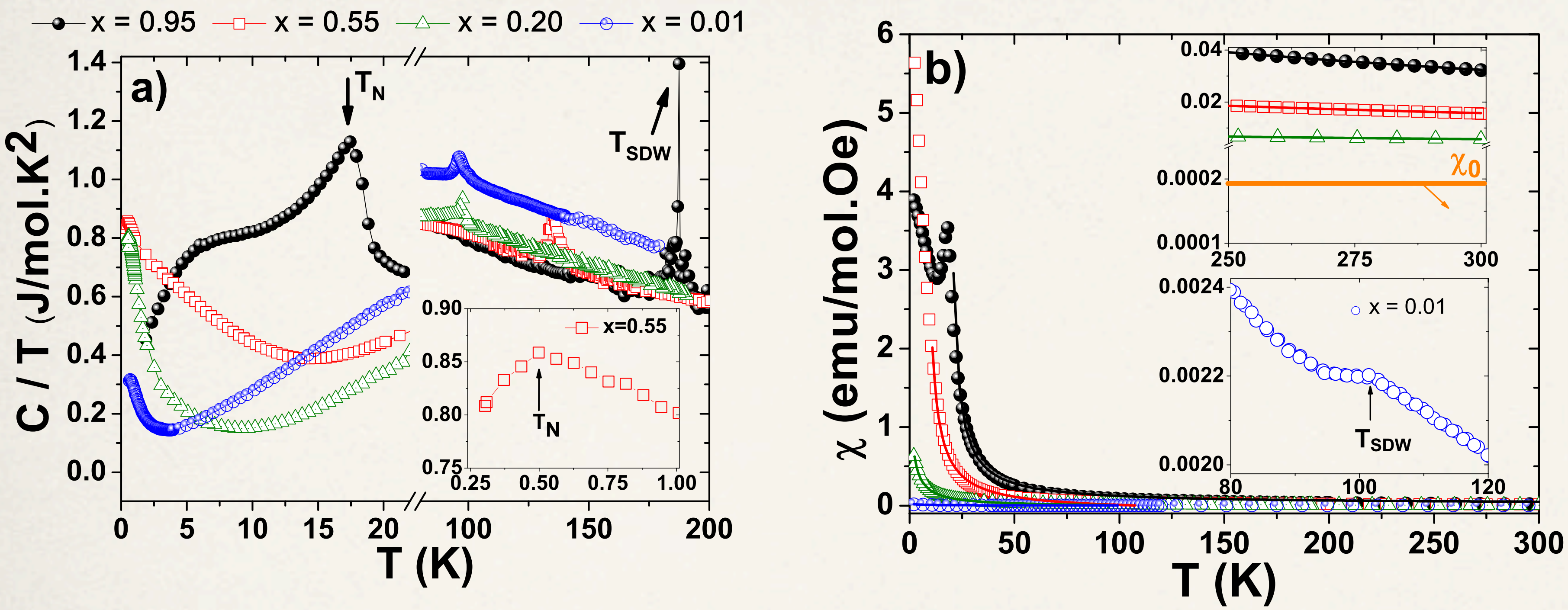
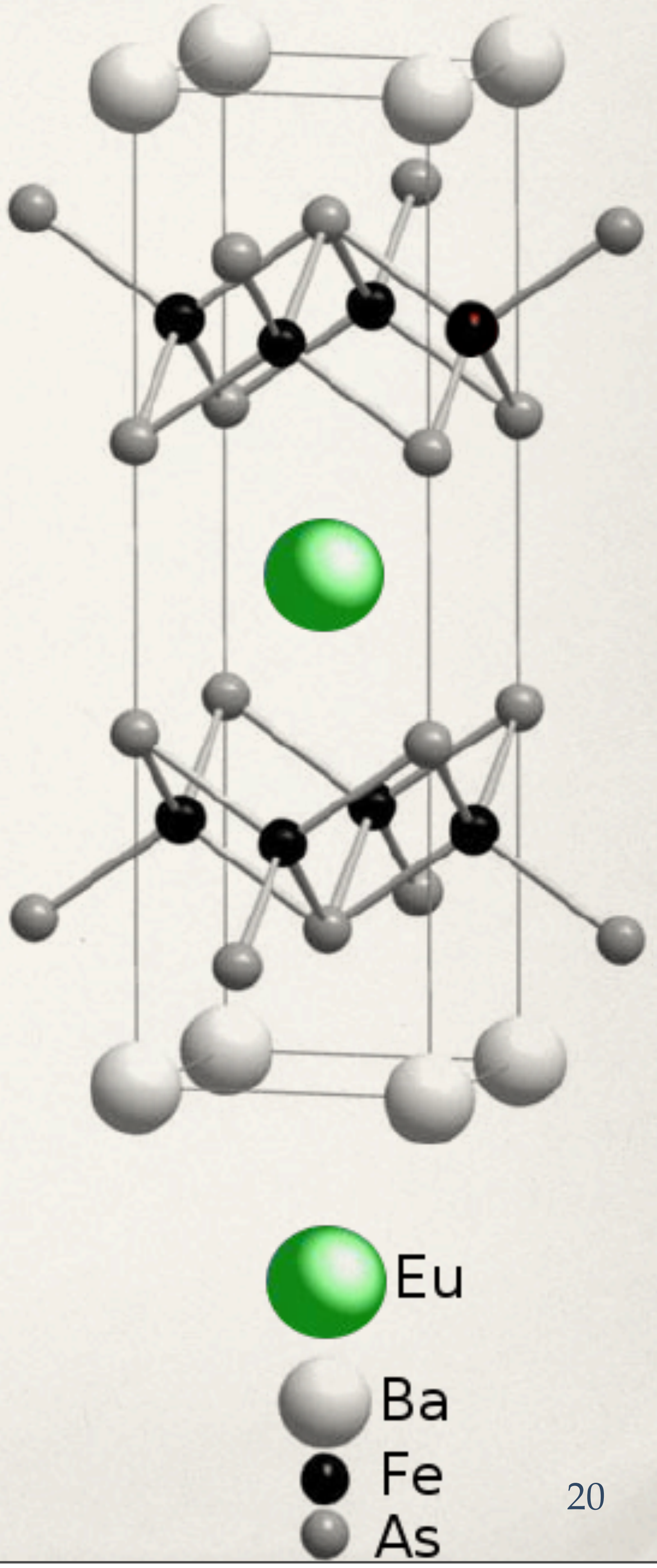






Magnetic Series $Ba_{1-x}Eu_xFe_2As_2$





$$\chi_0 = 2\mu_B^2 \frac{\eta(E_F)}{1-\alpha}$$

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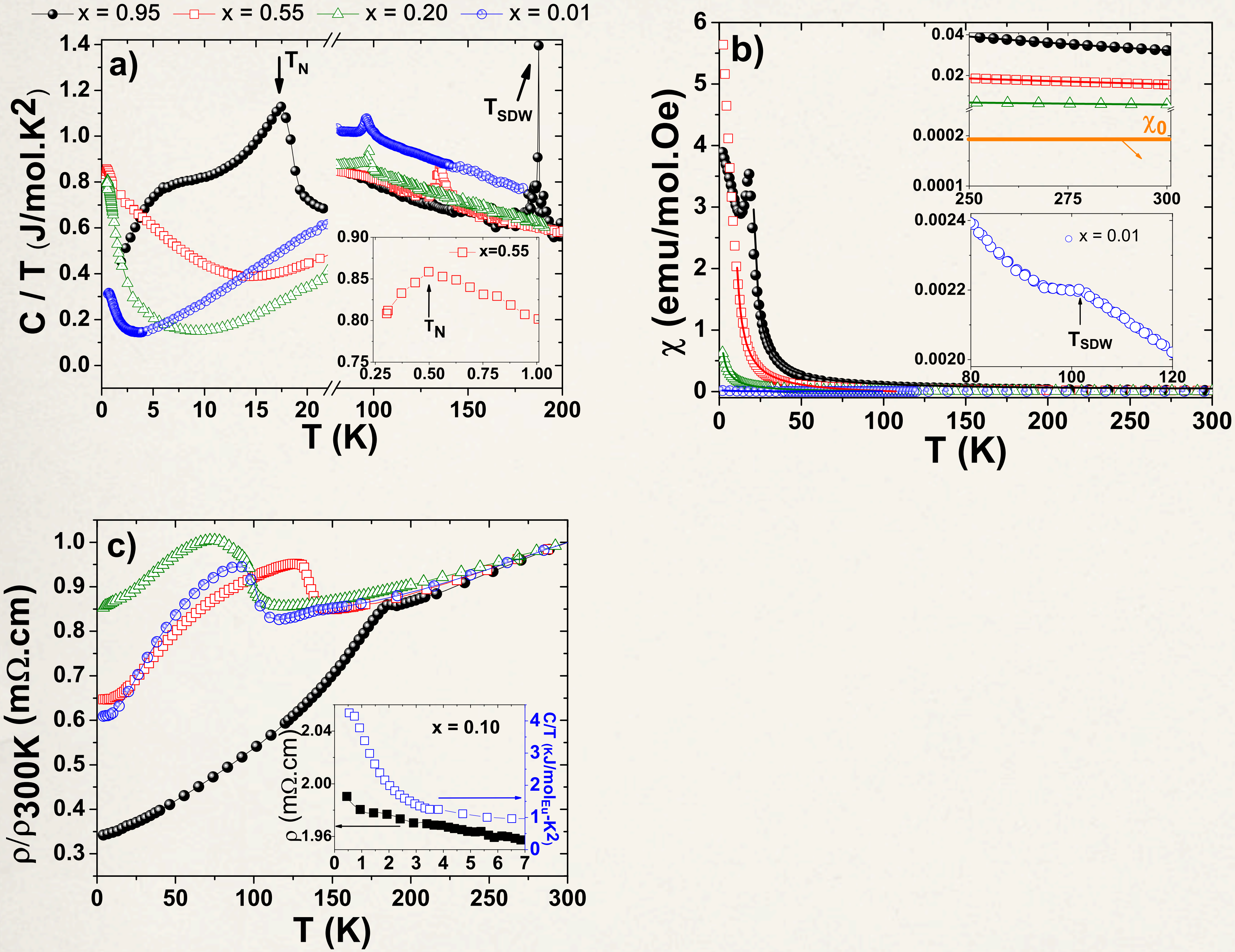

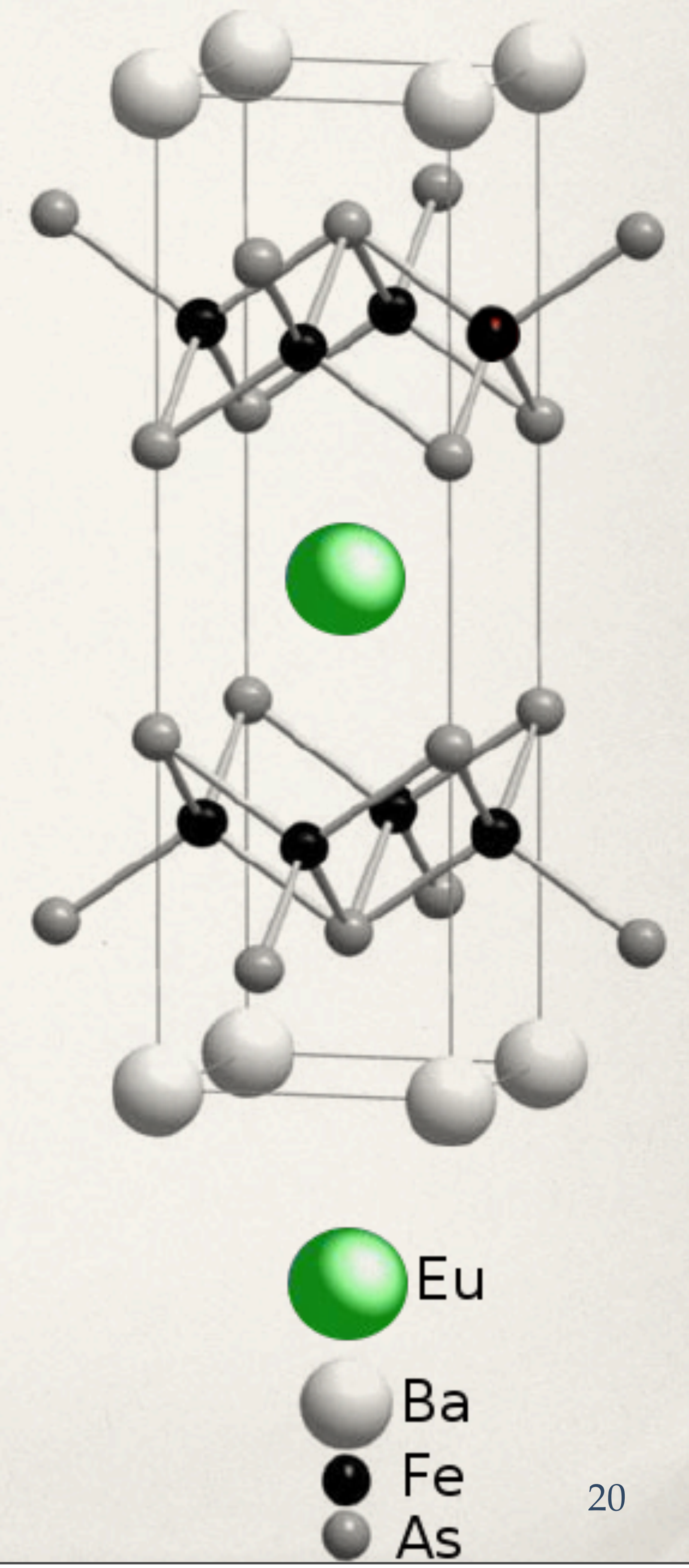

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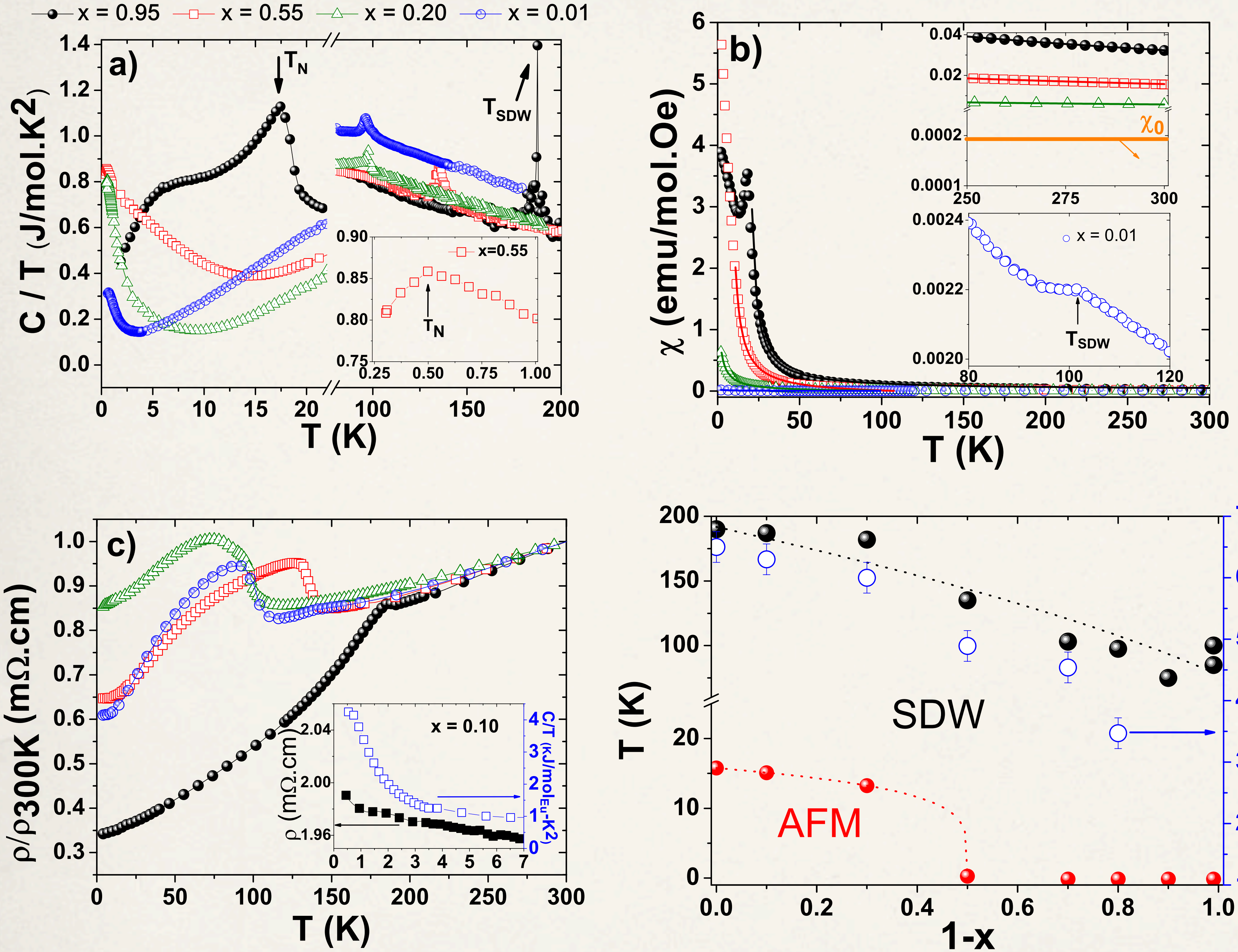

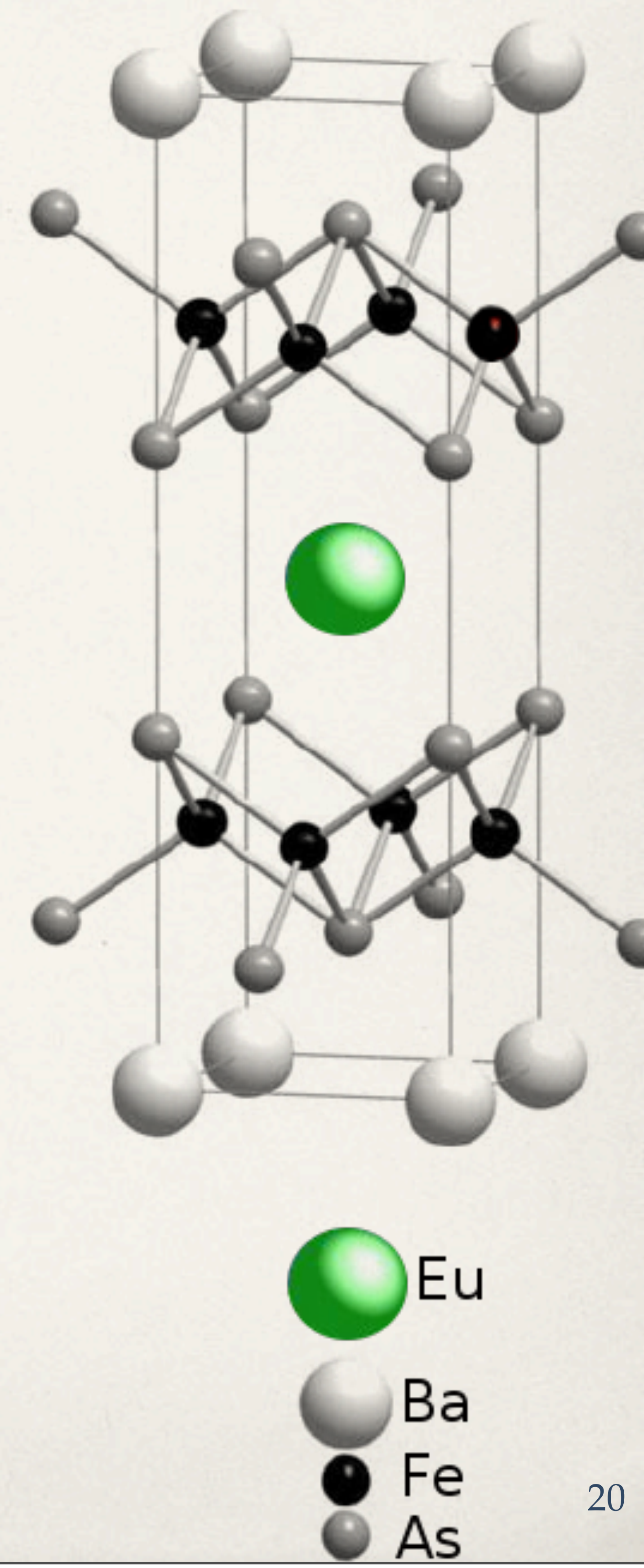

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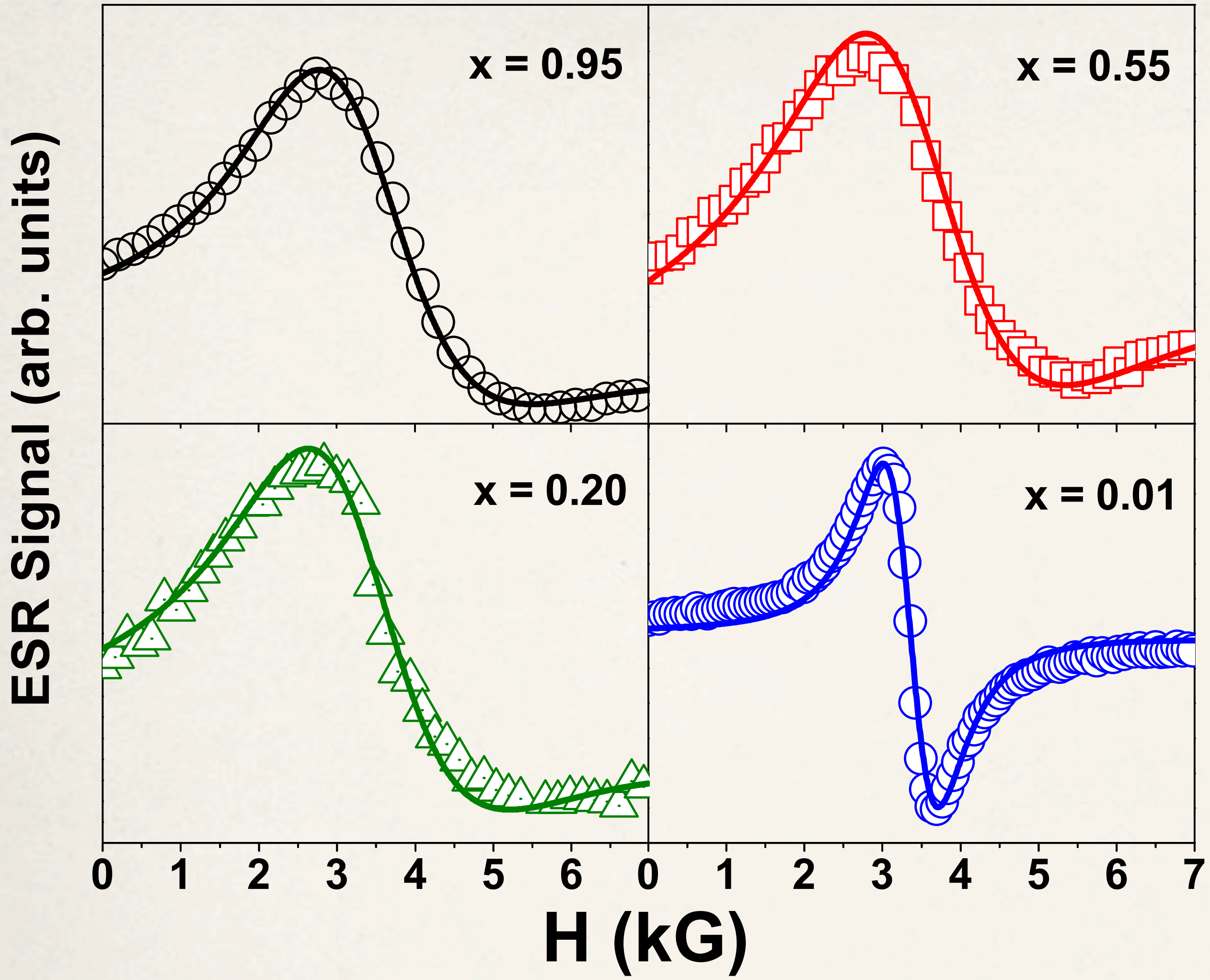
Eu^{2+} ESR Analysis



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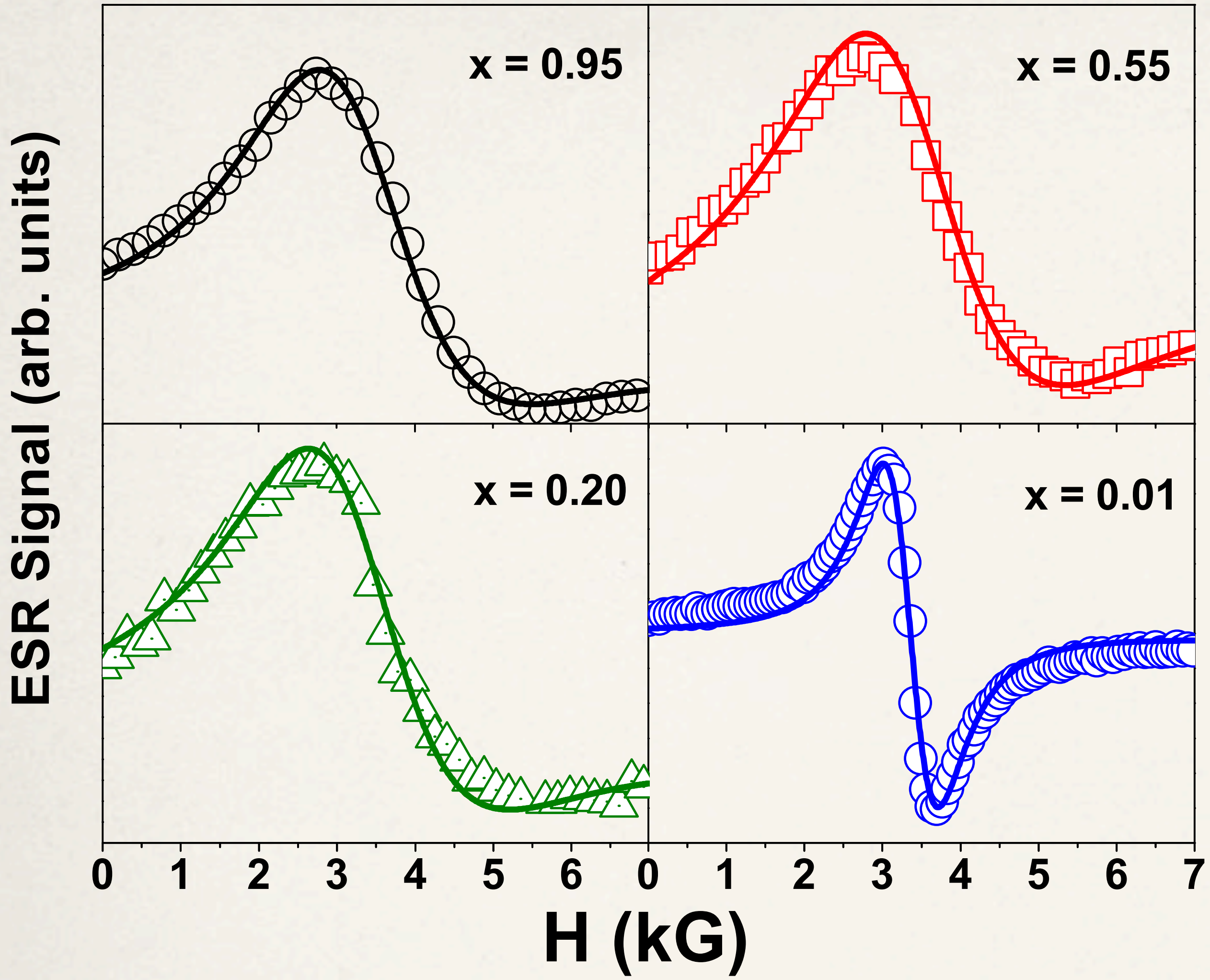

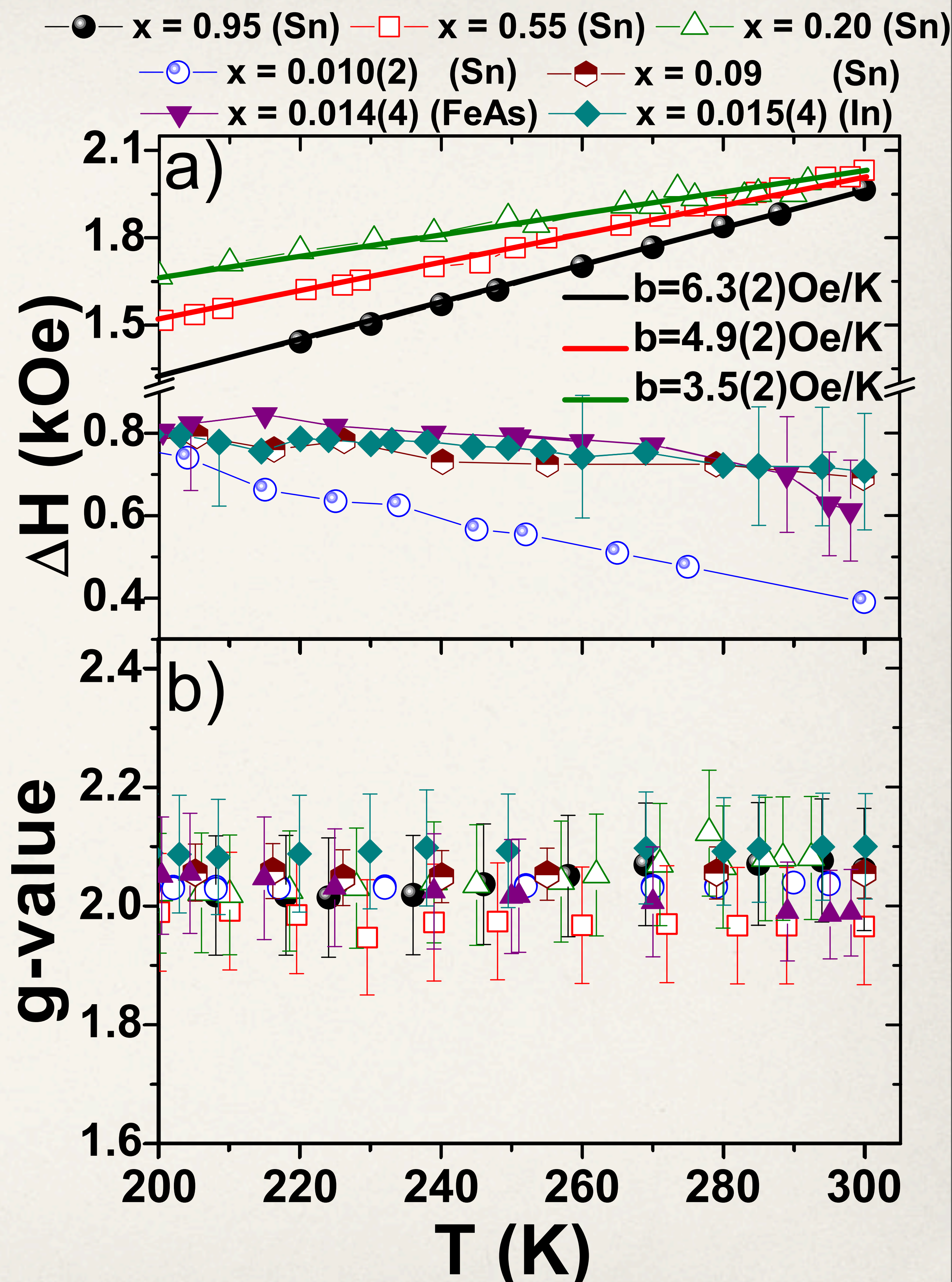

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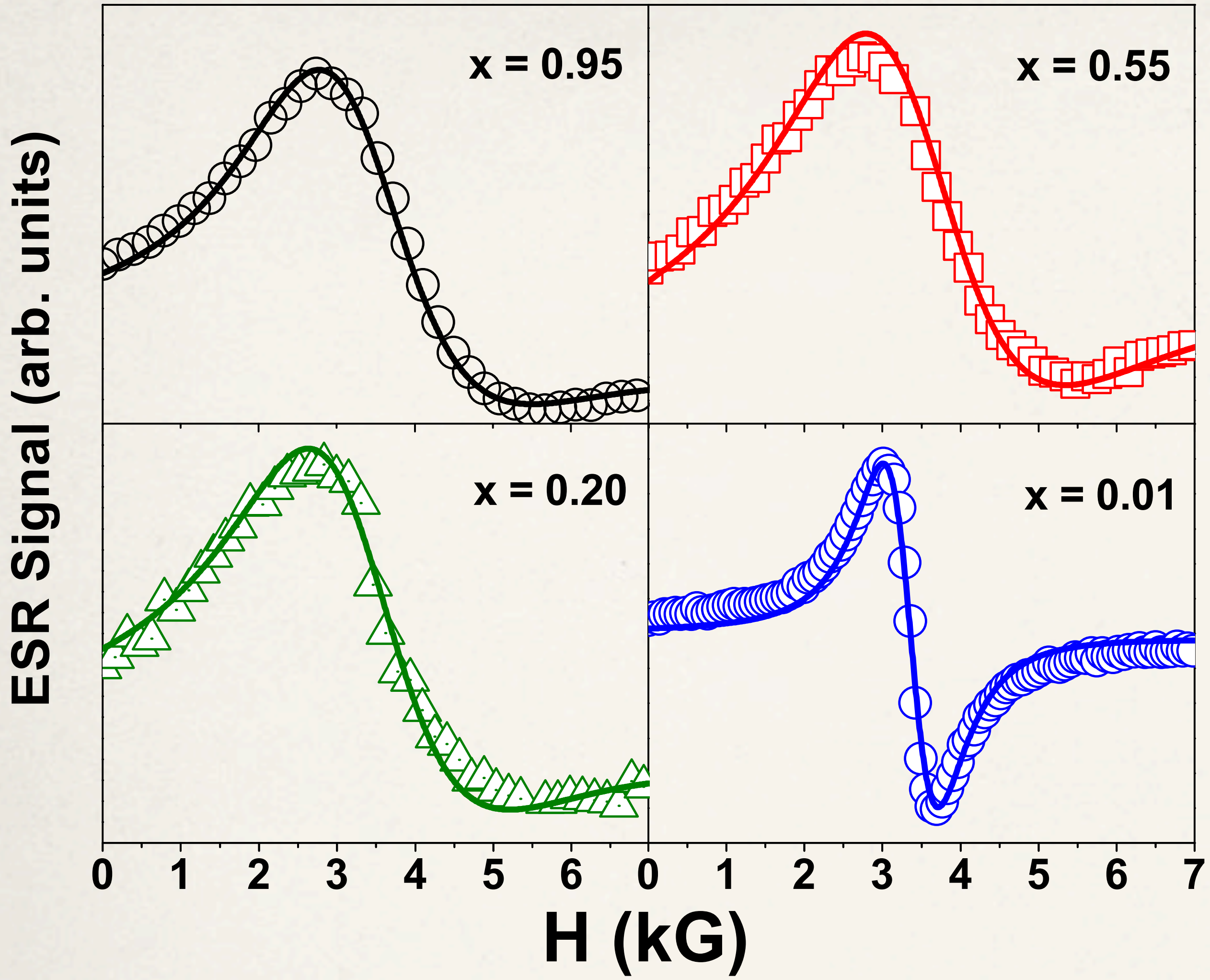

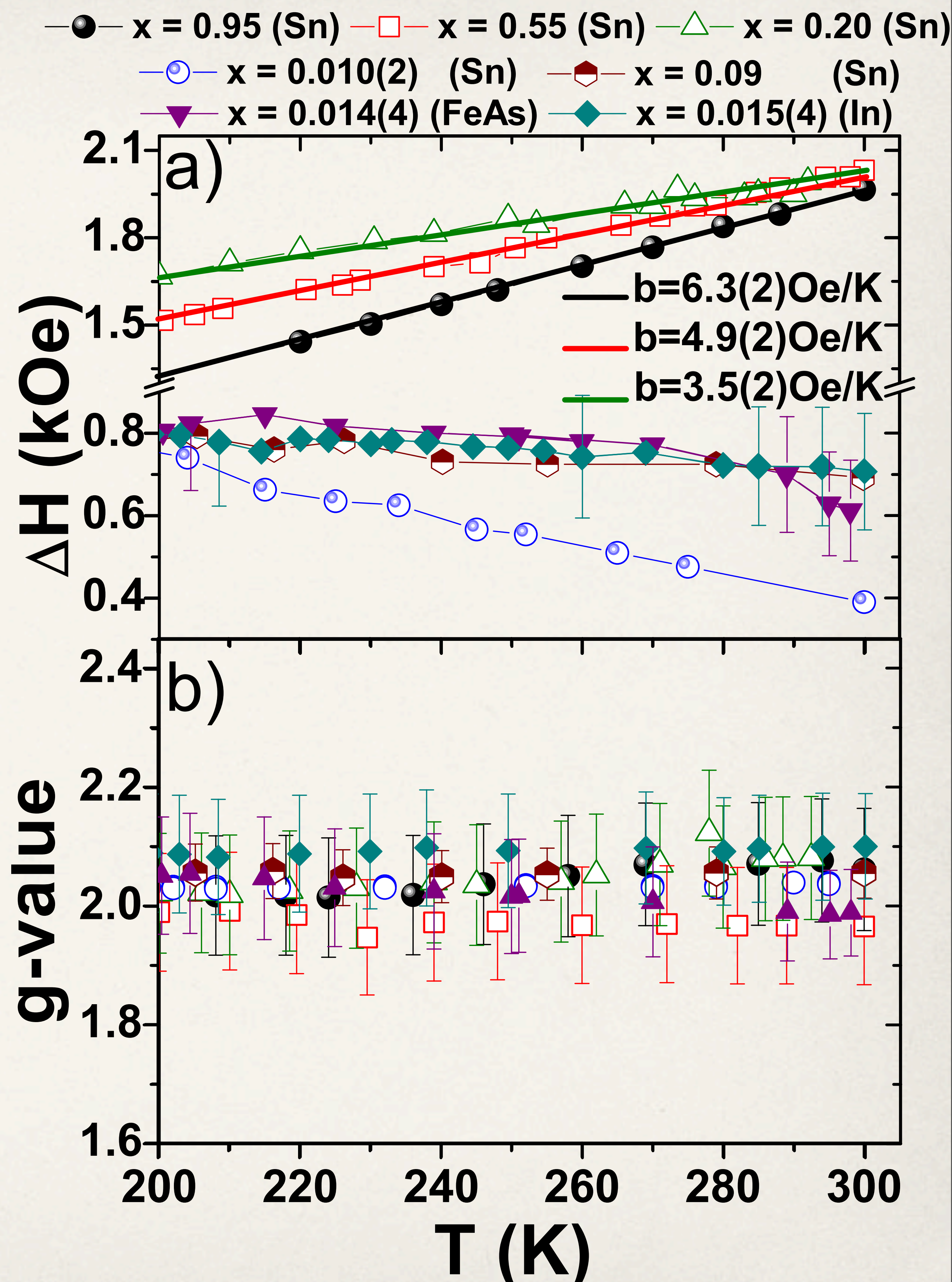

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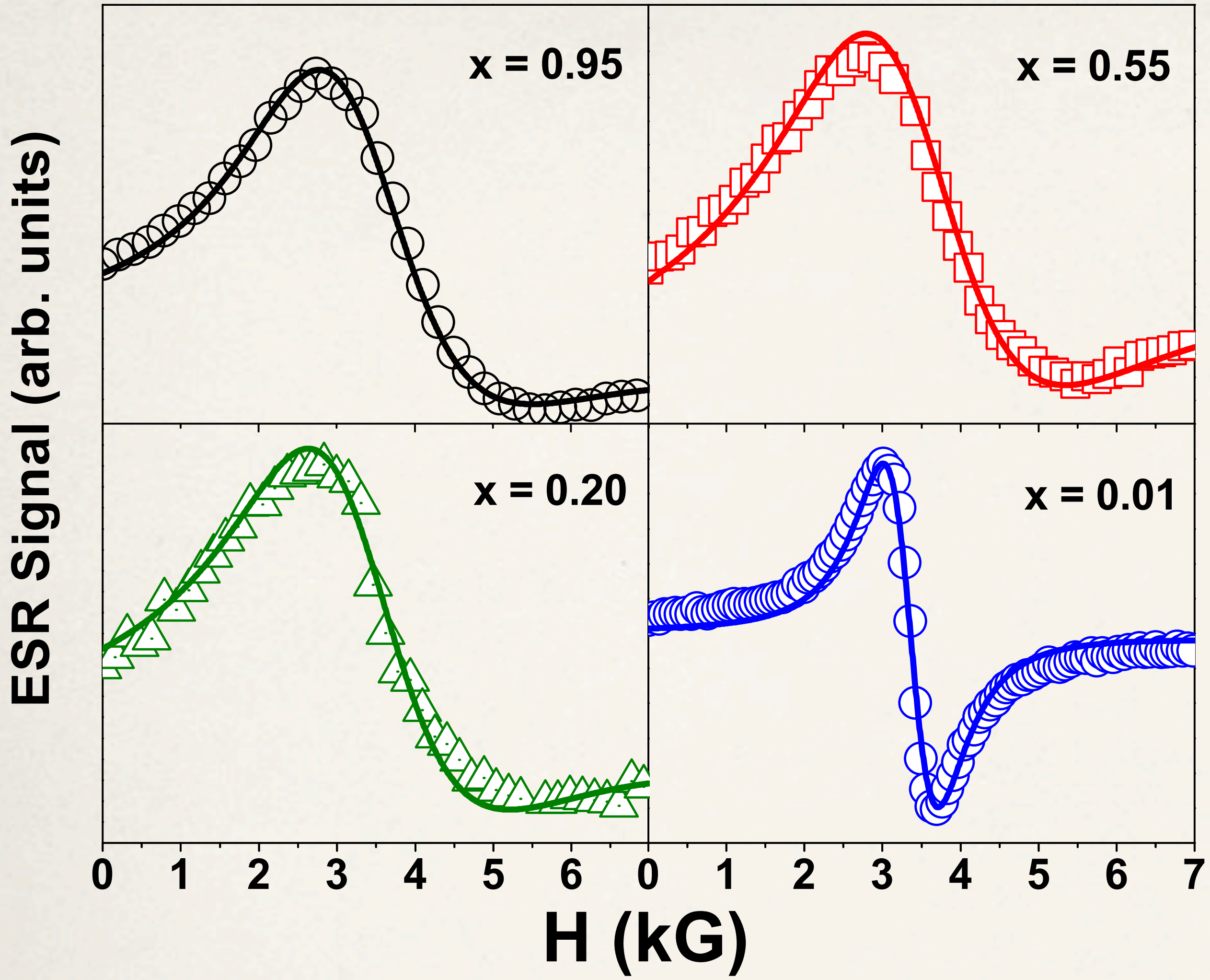

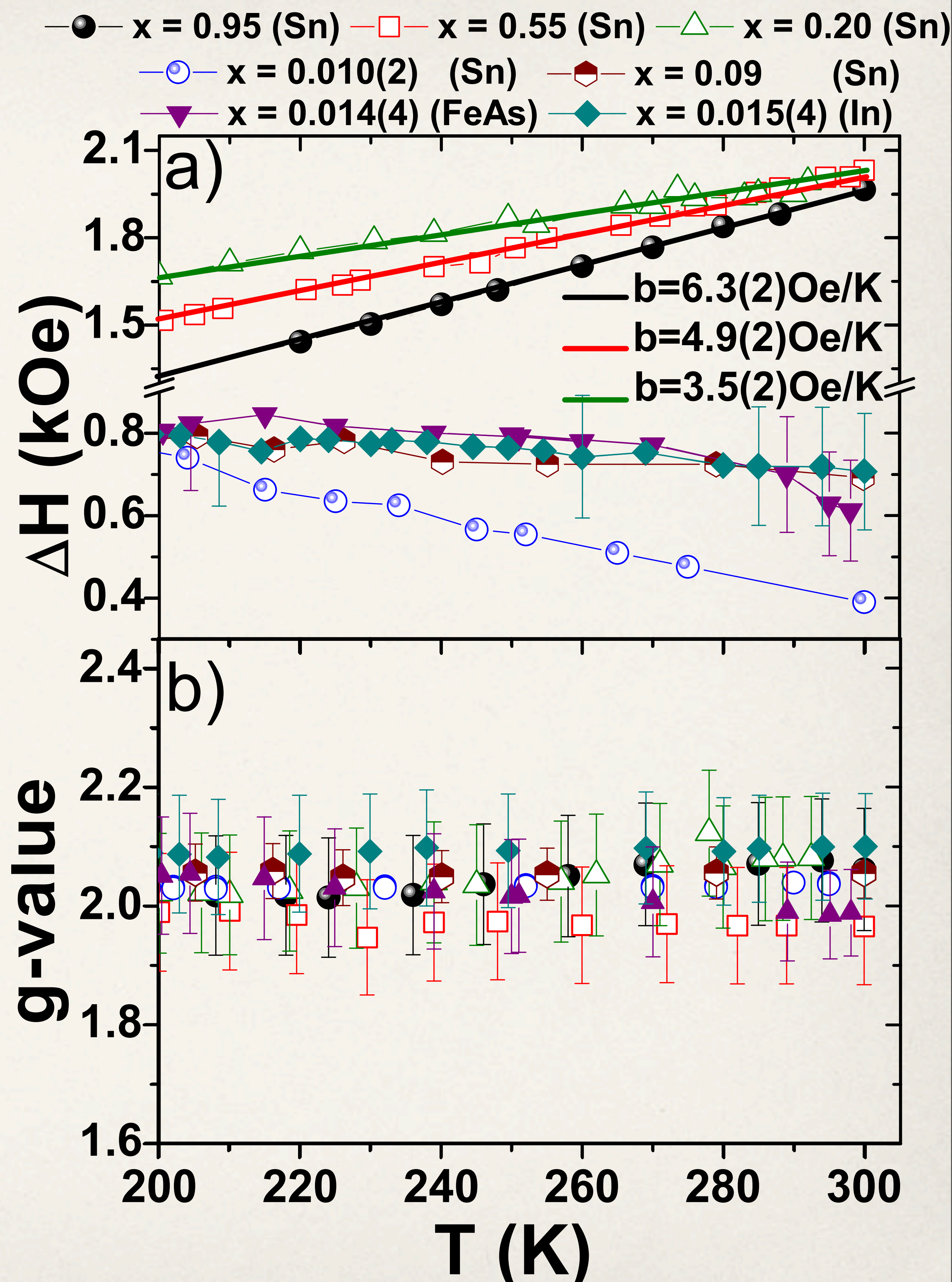

Constant!

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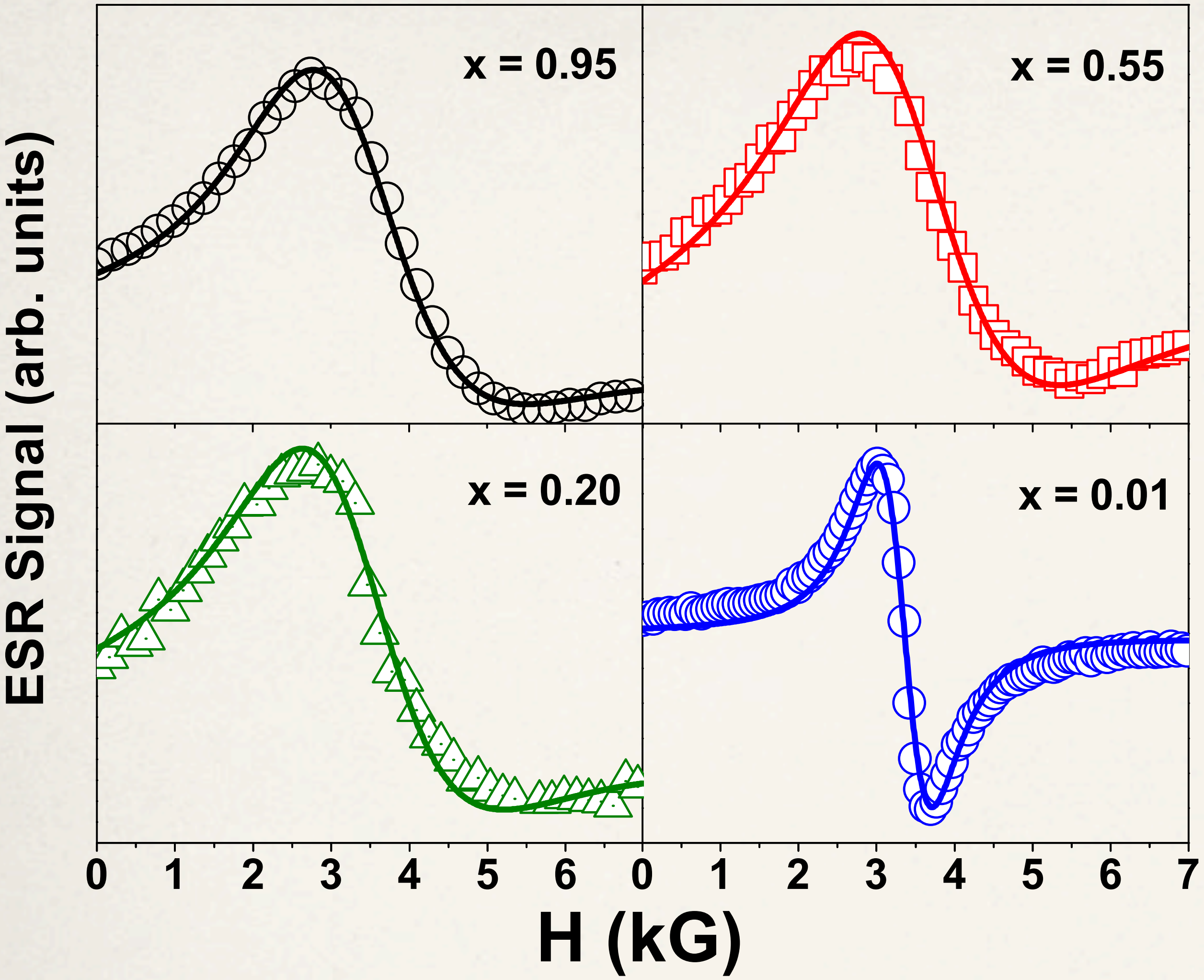

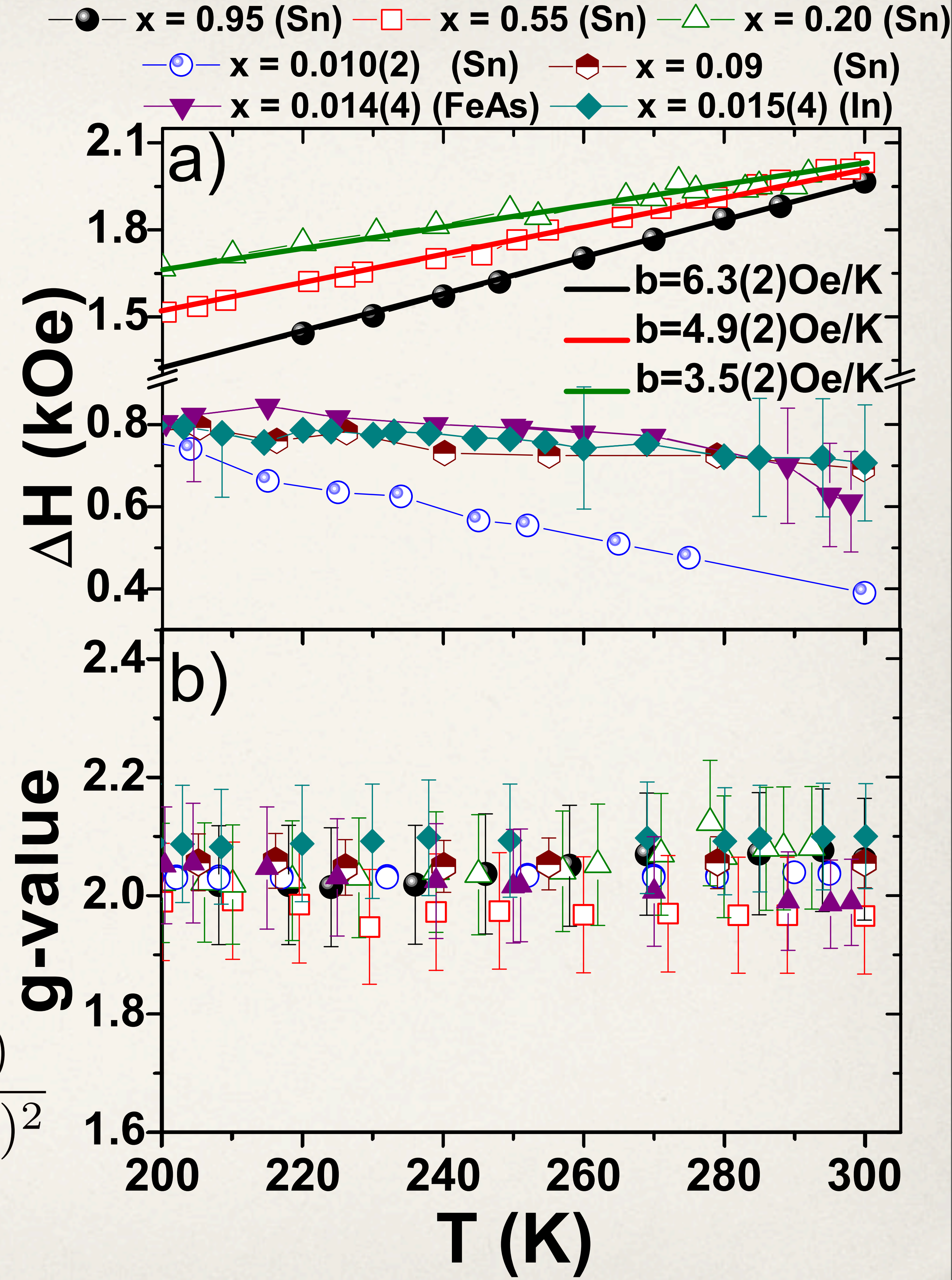

Constant!

$$\Delta g = J_{fs}(\mathbf{0}) \frac{N(E_F)}{1-\alpha}$$

$$\frac{d(\Delta H)}{dT} = \frac{\pi k}{g\mu_B} \langle J_{fs}^2(\mathbf{q}) \rangle N(E_F)^2 \frac{K(\alpha)}{(1-\alpha)^2}$$

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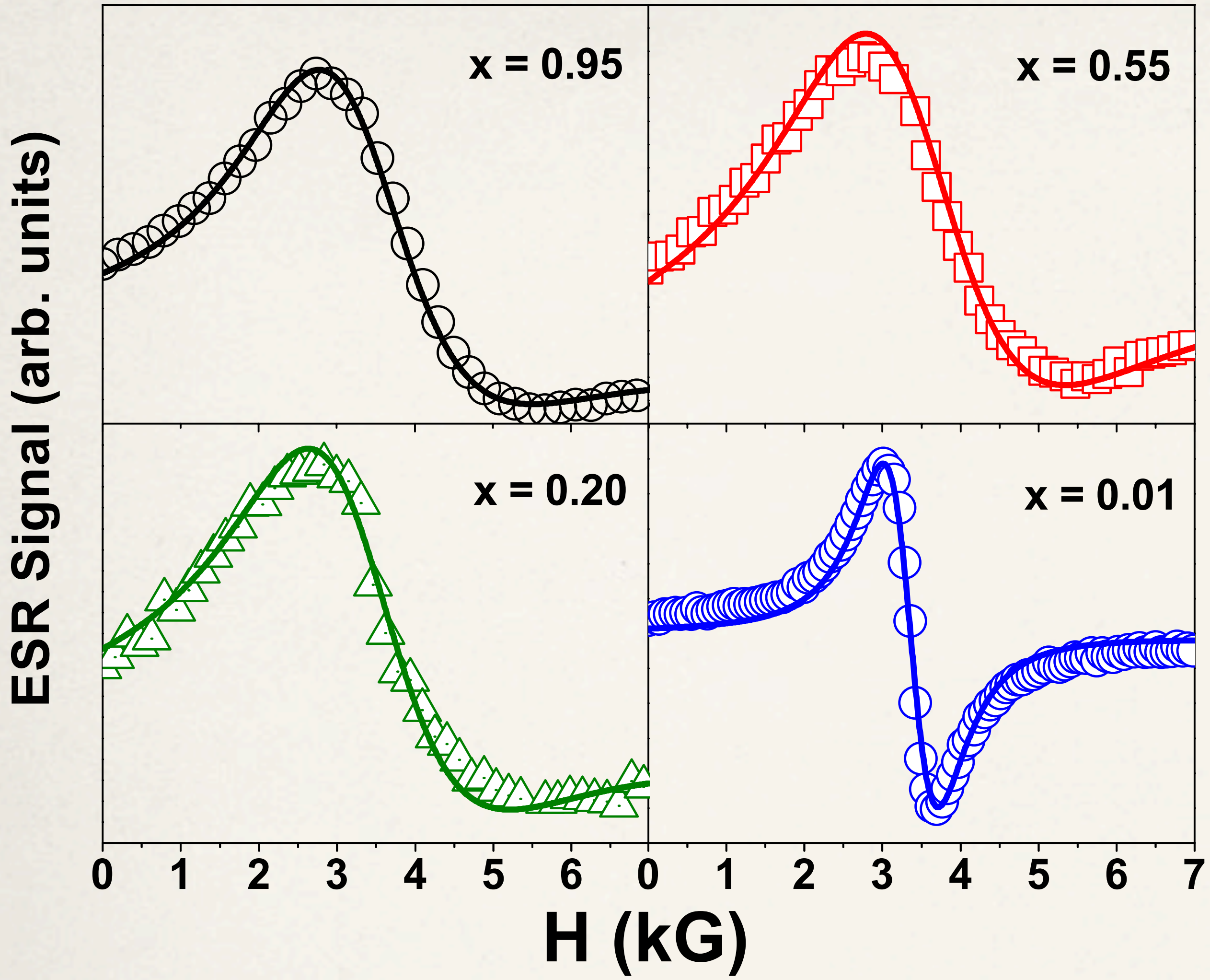

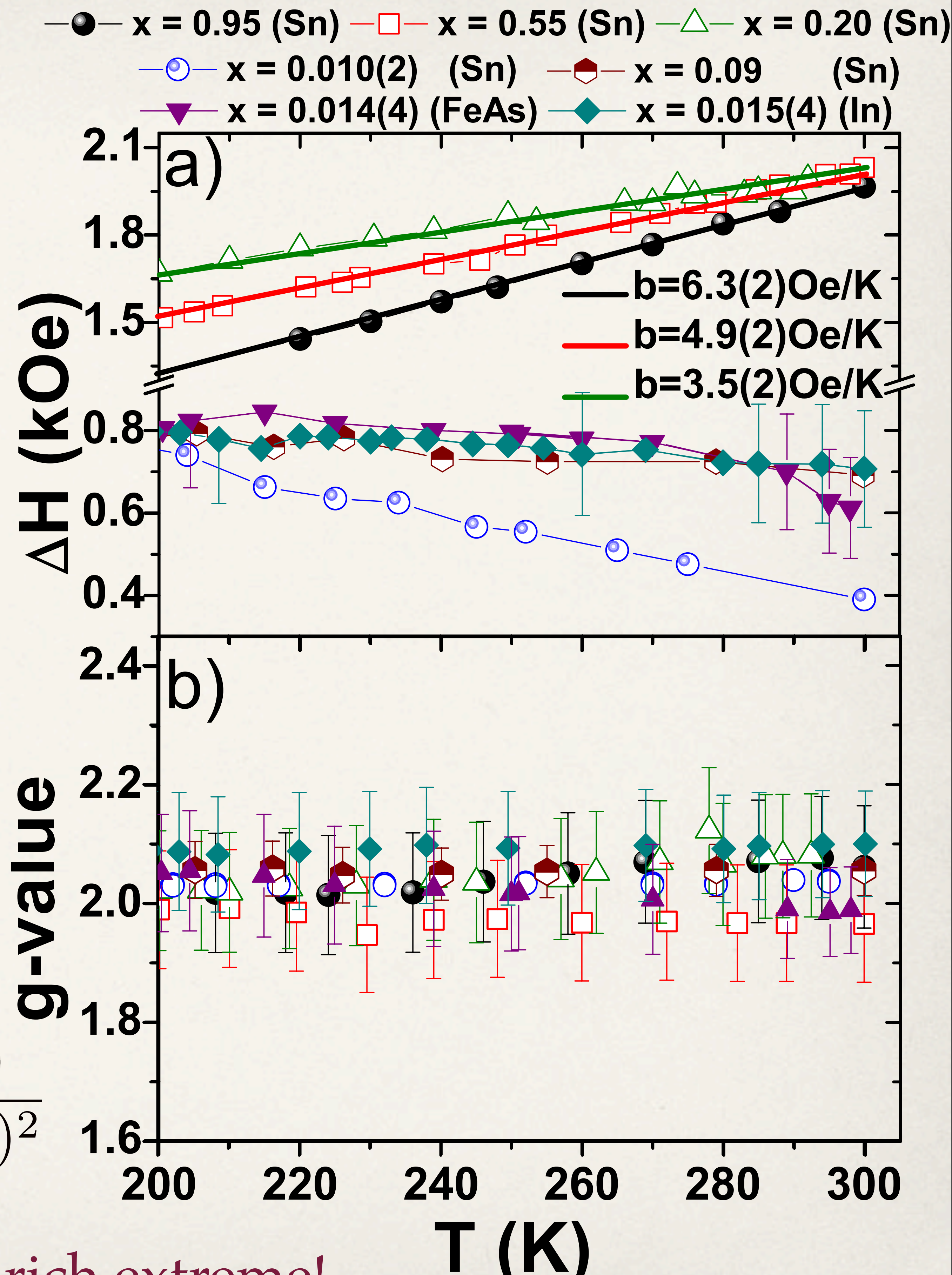

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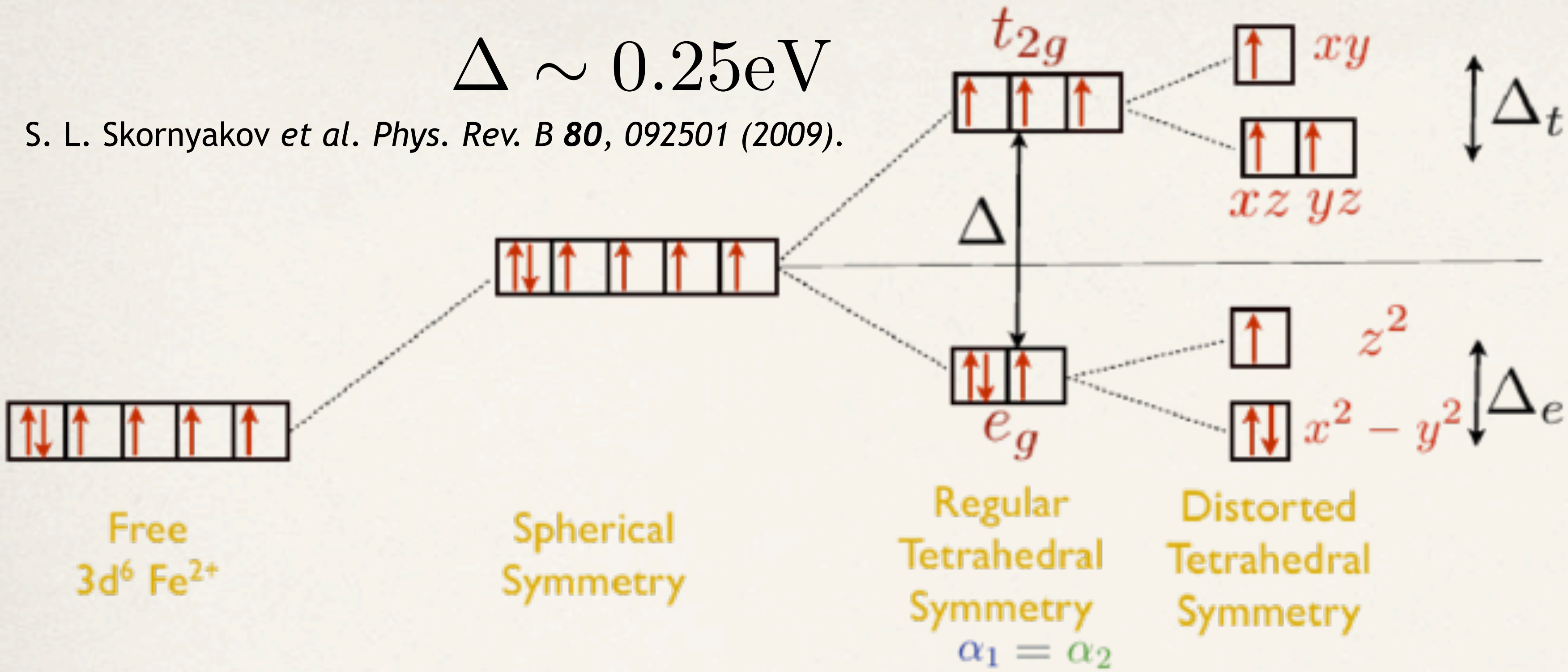
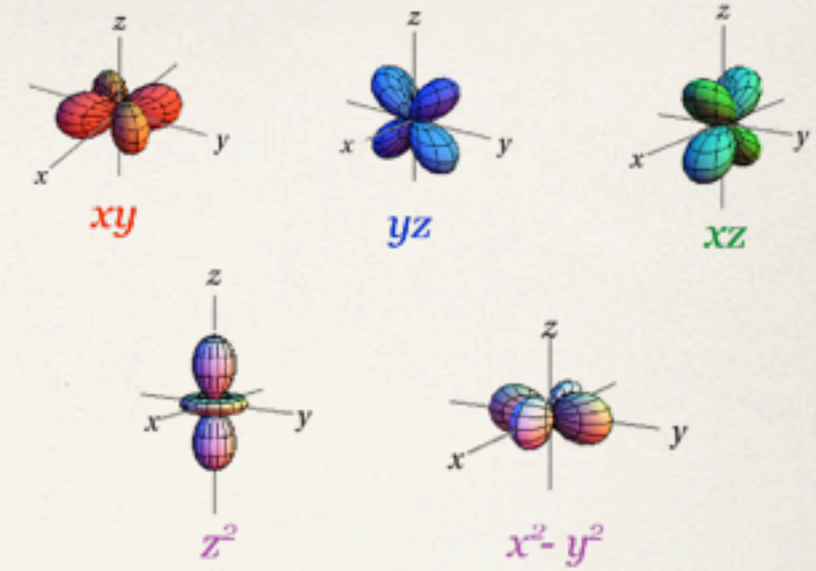
Decreases in the Ba-rich extreme!

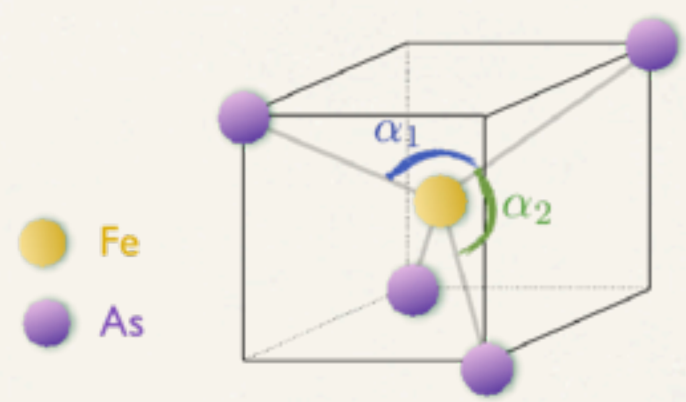
Importance of the Crystal Field

$\Delta \sim 0.25\text{eV}$

S. L. Skornyakov *et al. Phys. Rev. B* **80**, *092501 (2009).*







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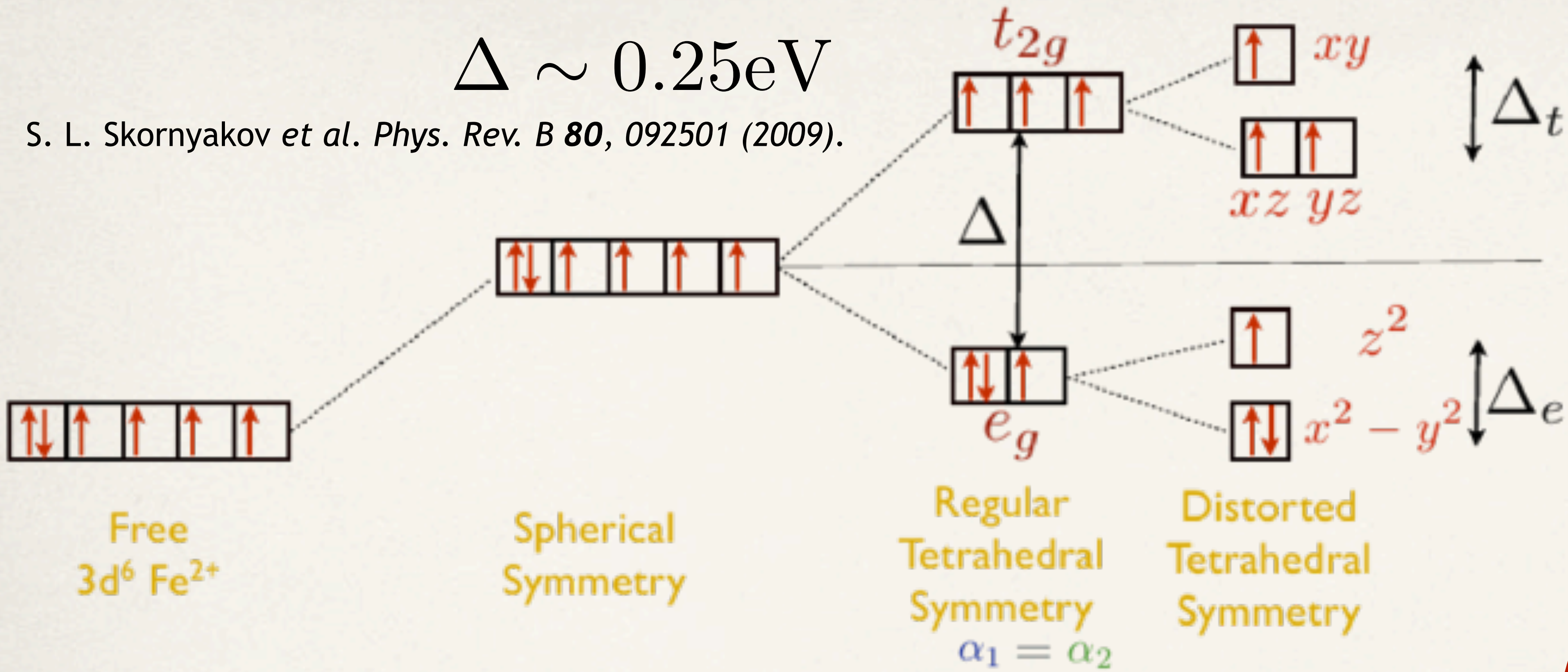

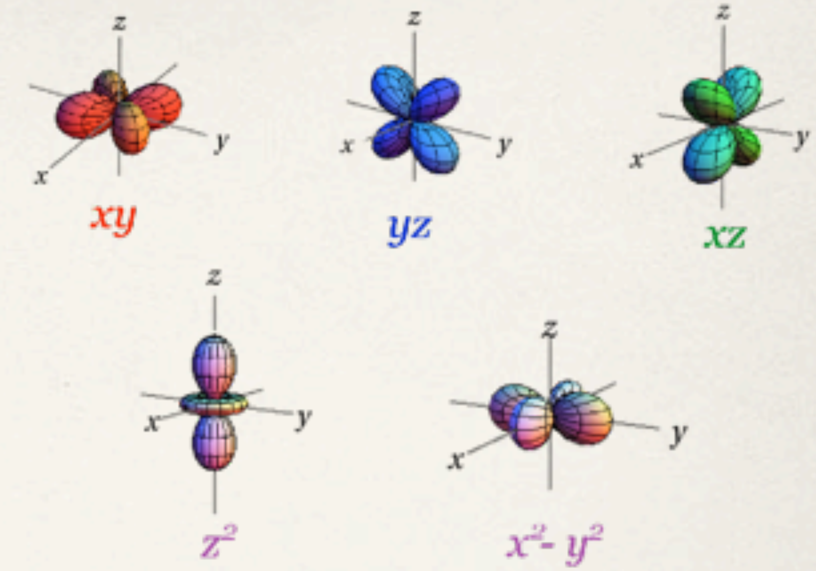

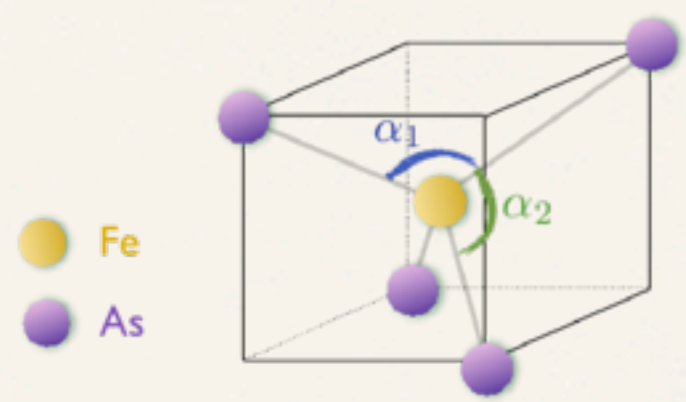

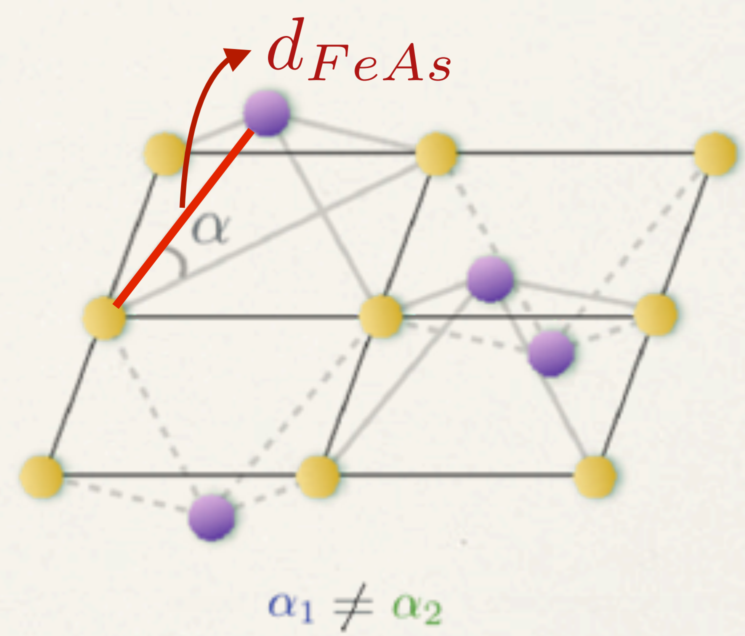

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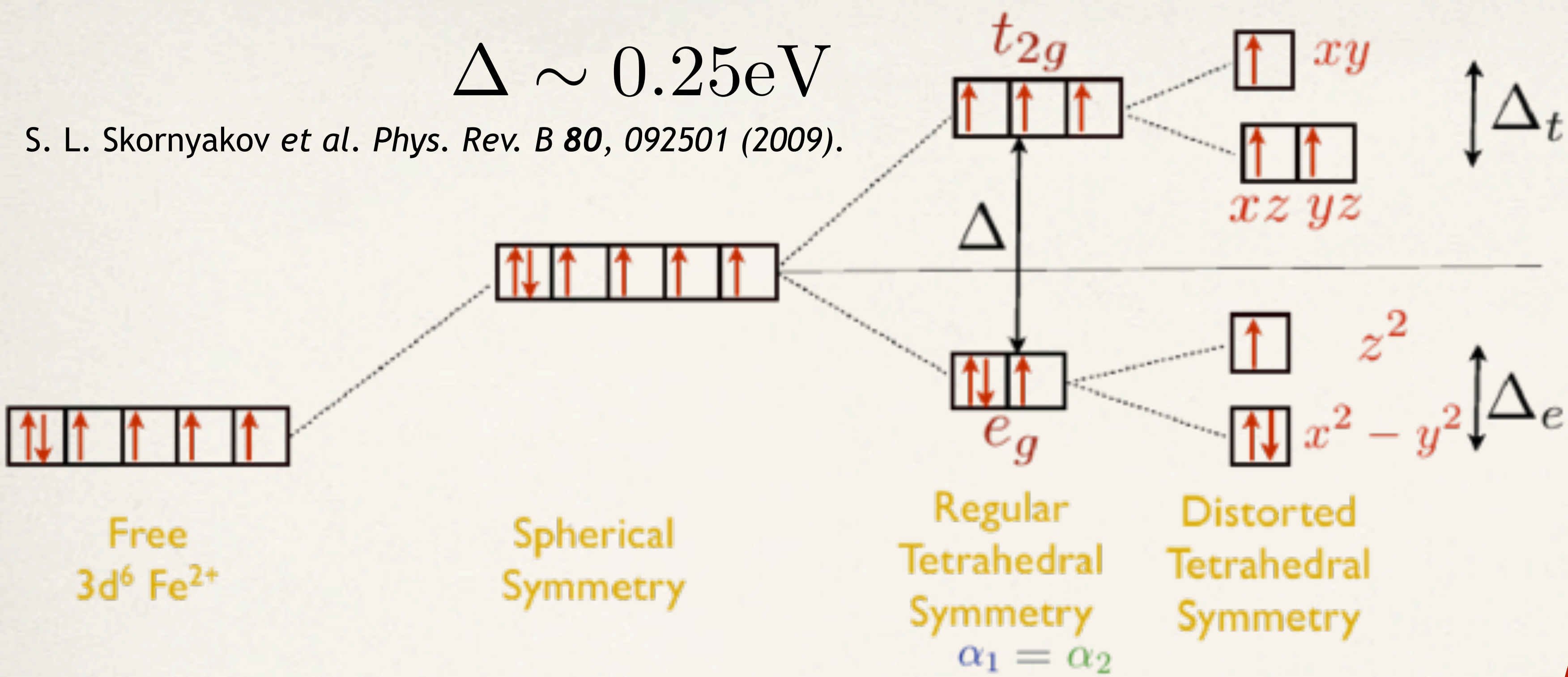
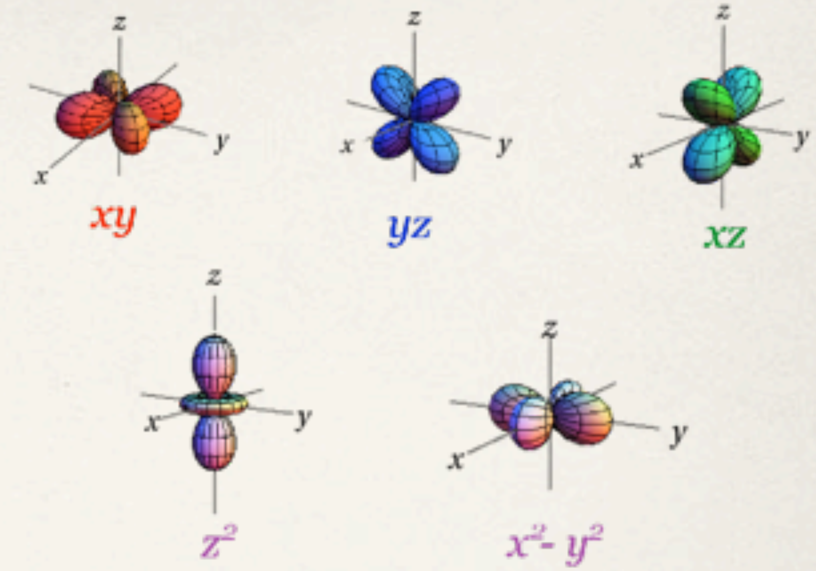
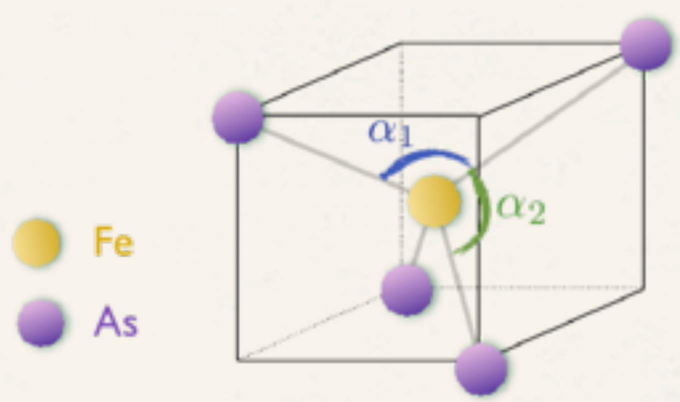
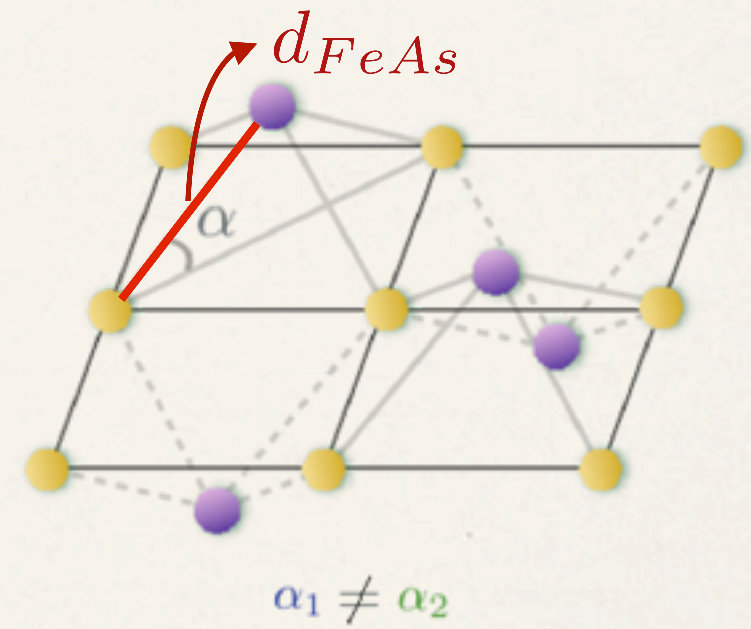
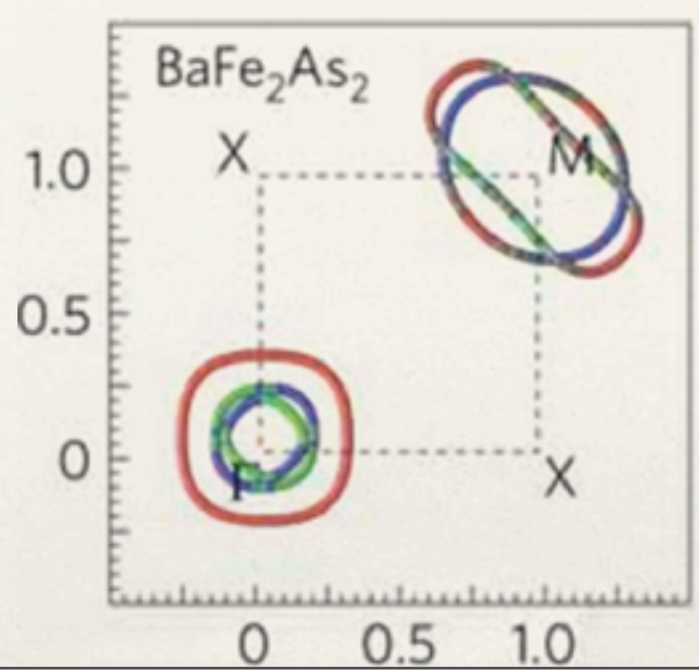


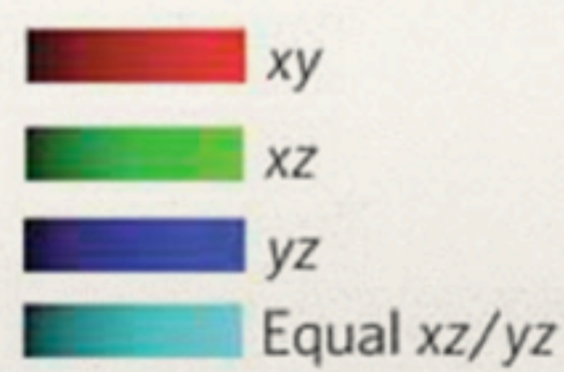




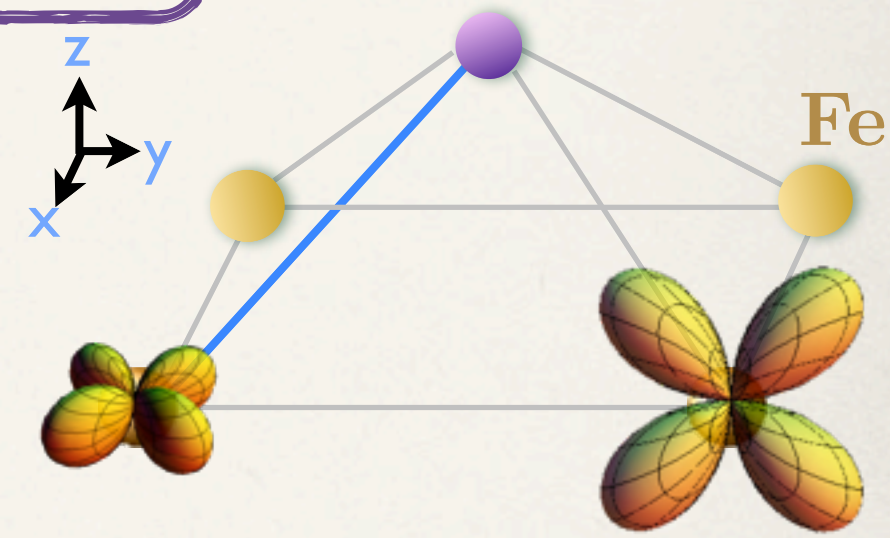




Z. P. Yin *et al. Nature Materials*, **10** 932-935 (2011).



Decreasing Korringa rate (b) ➡ Decreasing $\langle J_{fs}(\mathbf{q}) \rangle$



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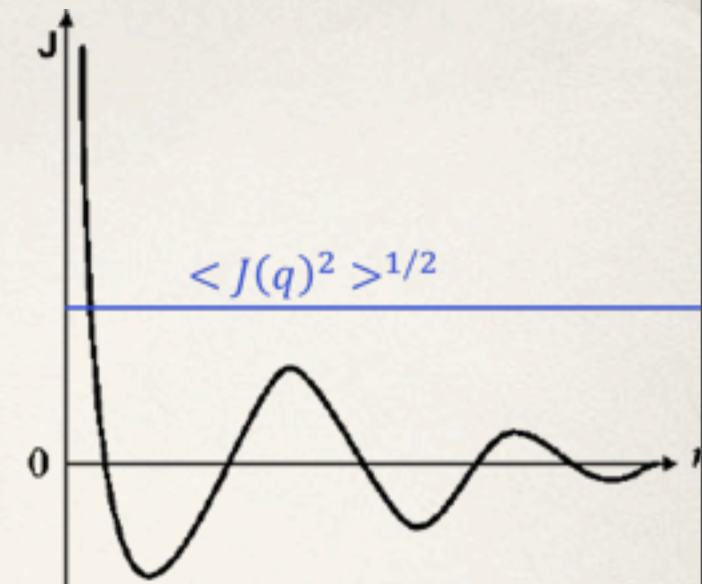

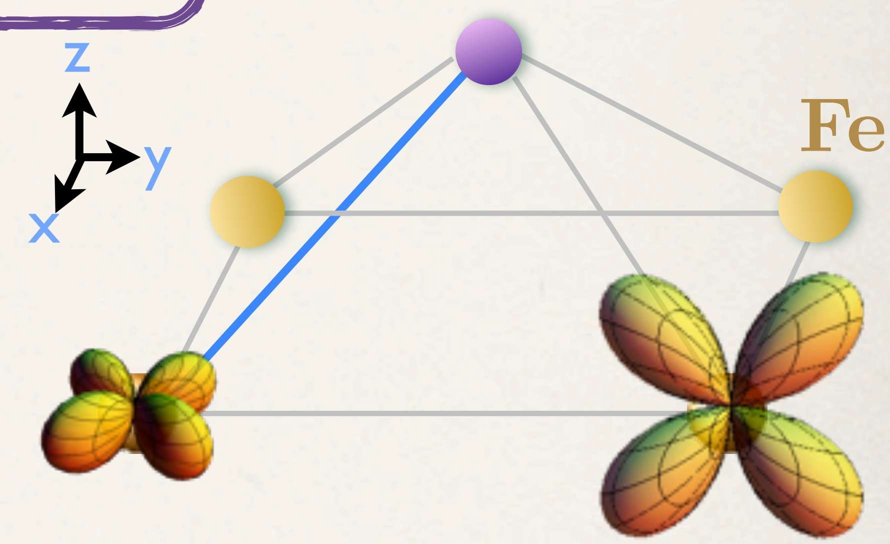

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- *3d* Fe bands are more anisotropic (less *s*-like) and are, in average, further away from the Eu site, i.e., the planar orbital character xy / x^2-y^2 increases!

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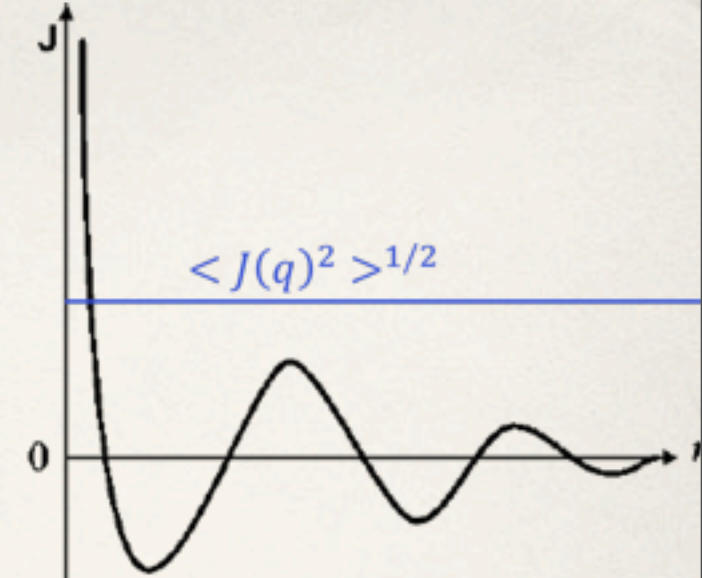

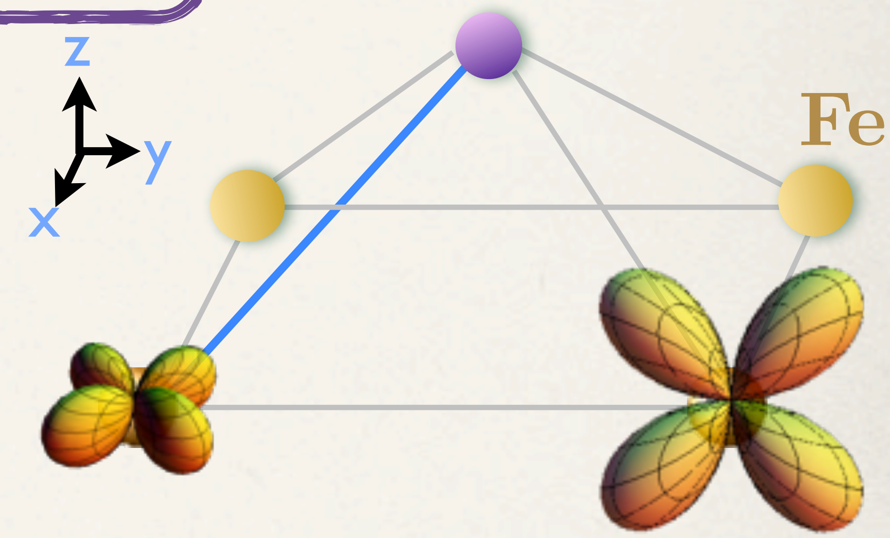

Thursday, October 9, 2014

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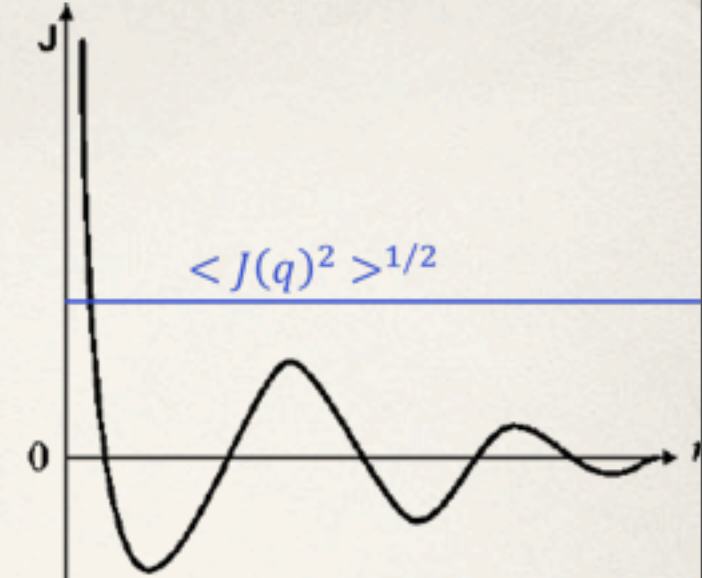

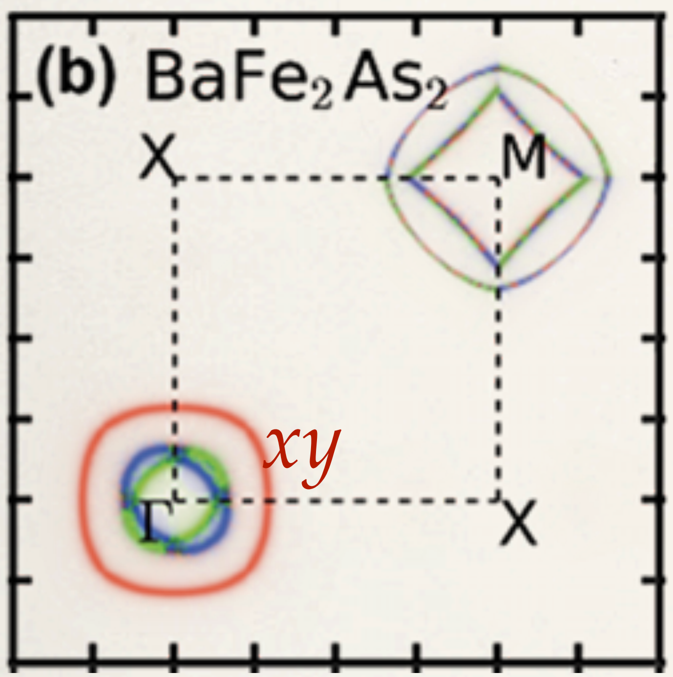

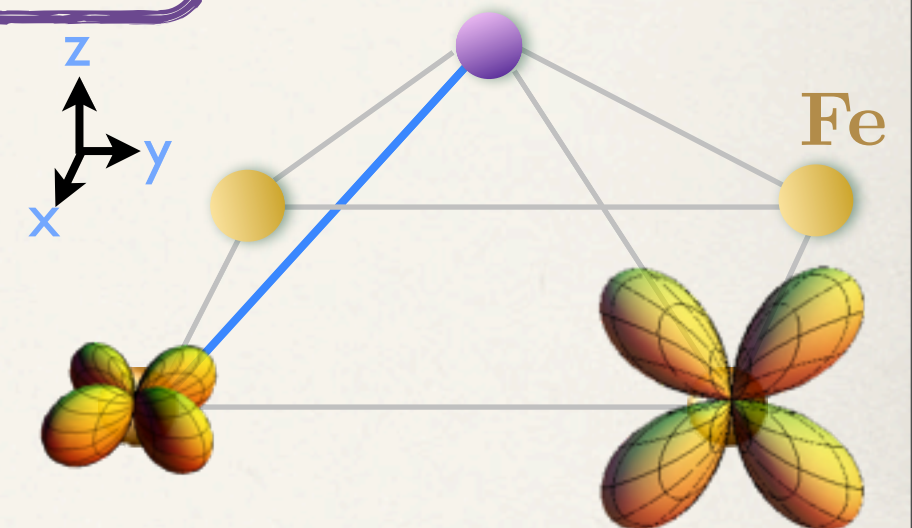

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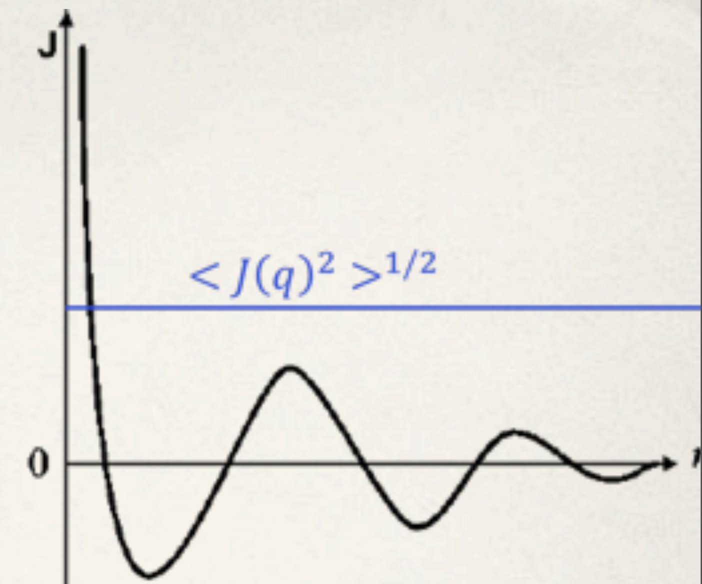

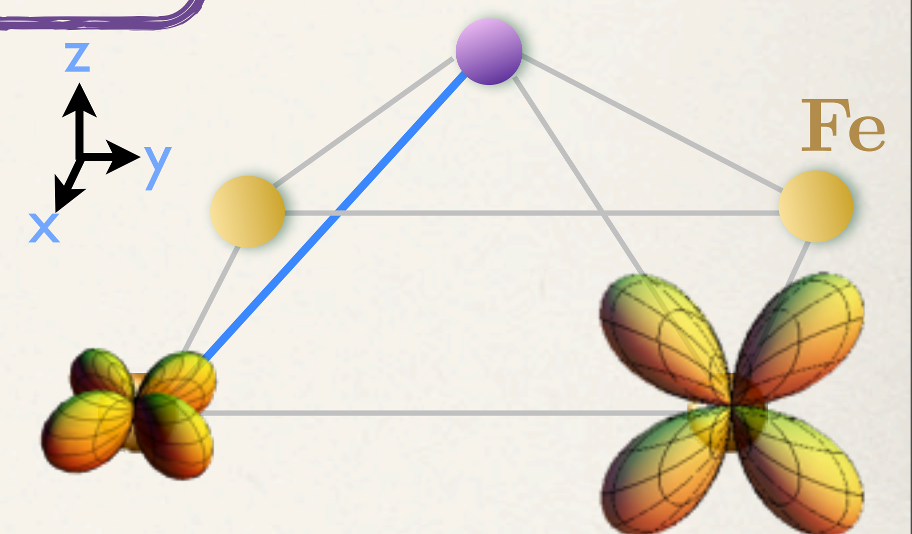

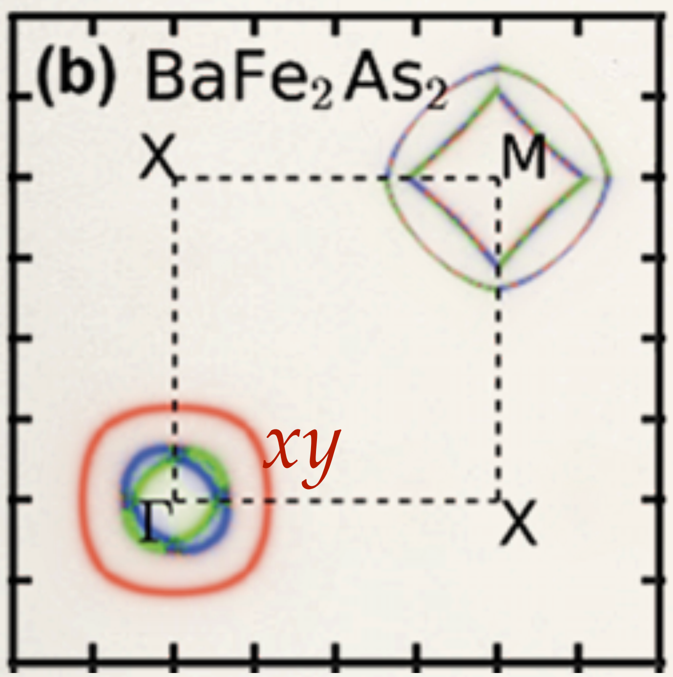

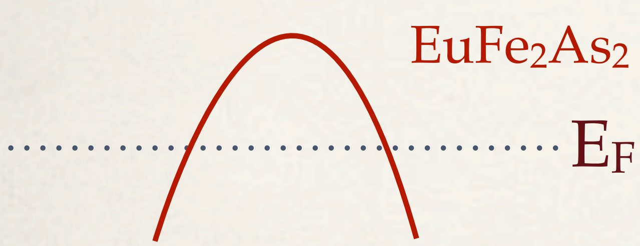

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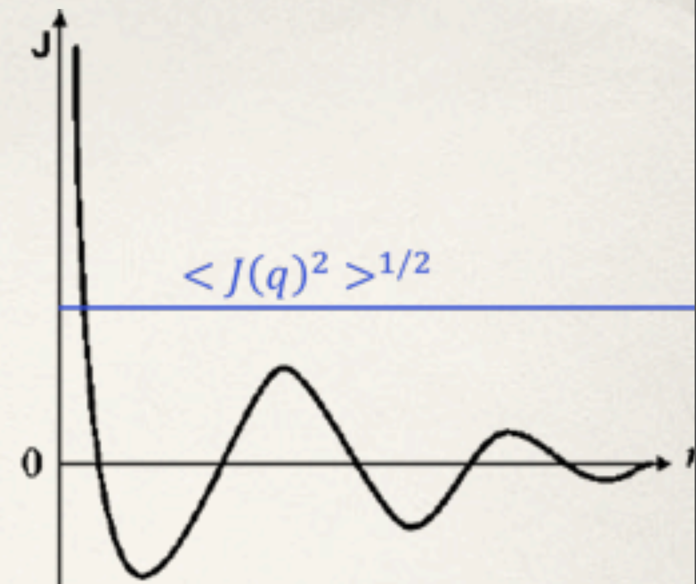

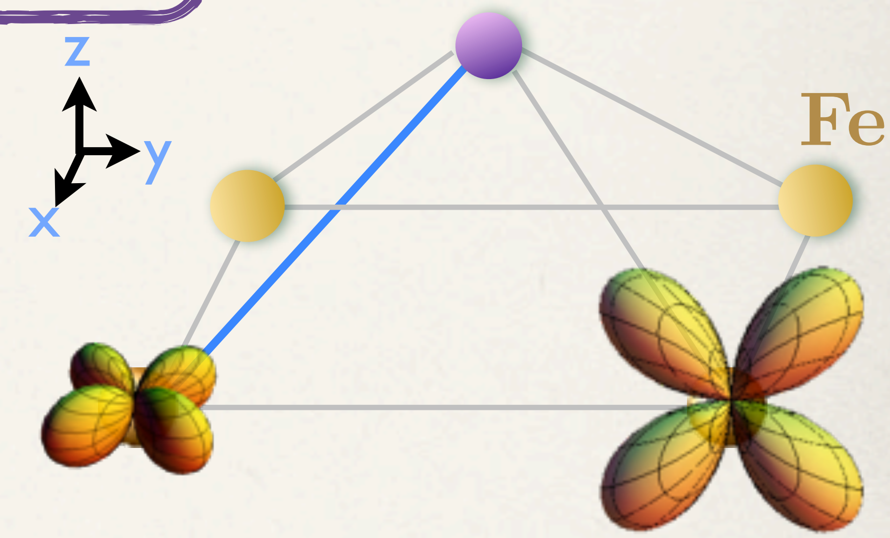

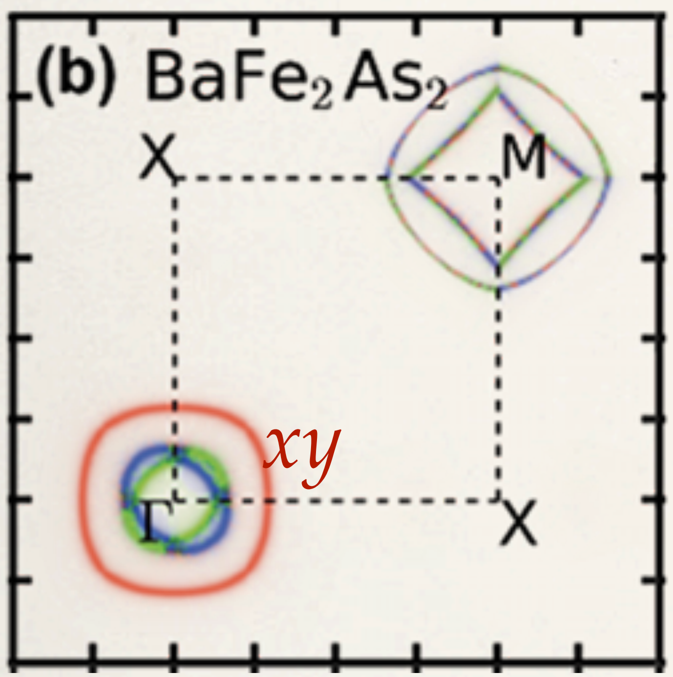

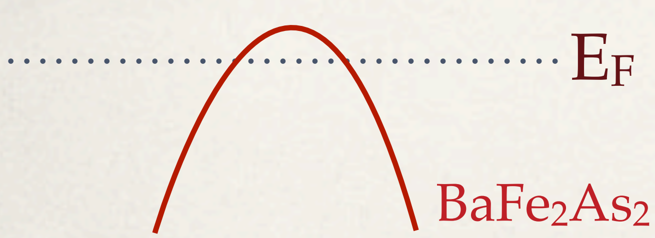

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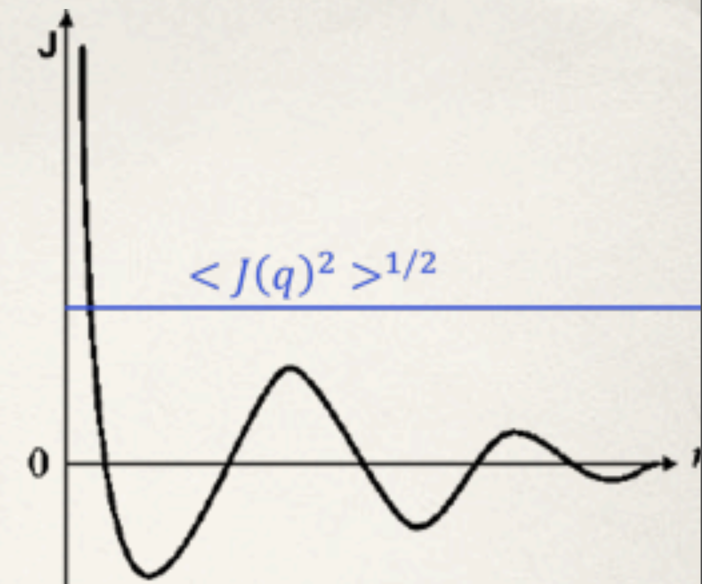

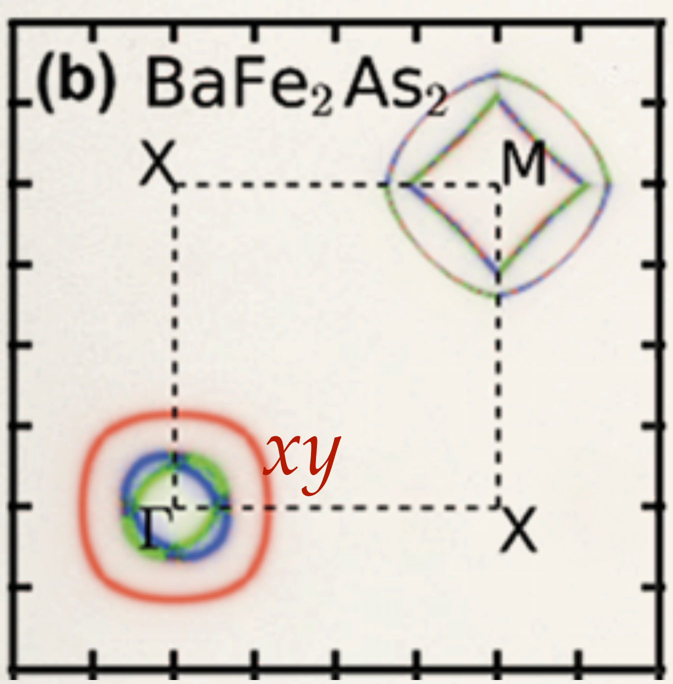

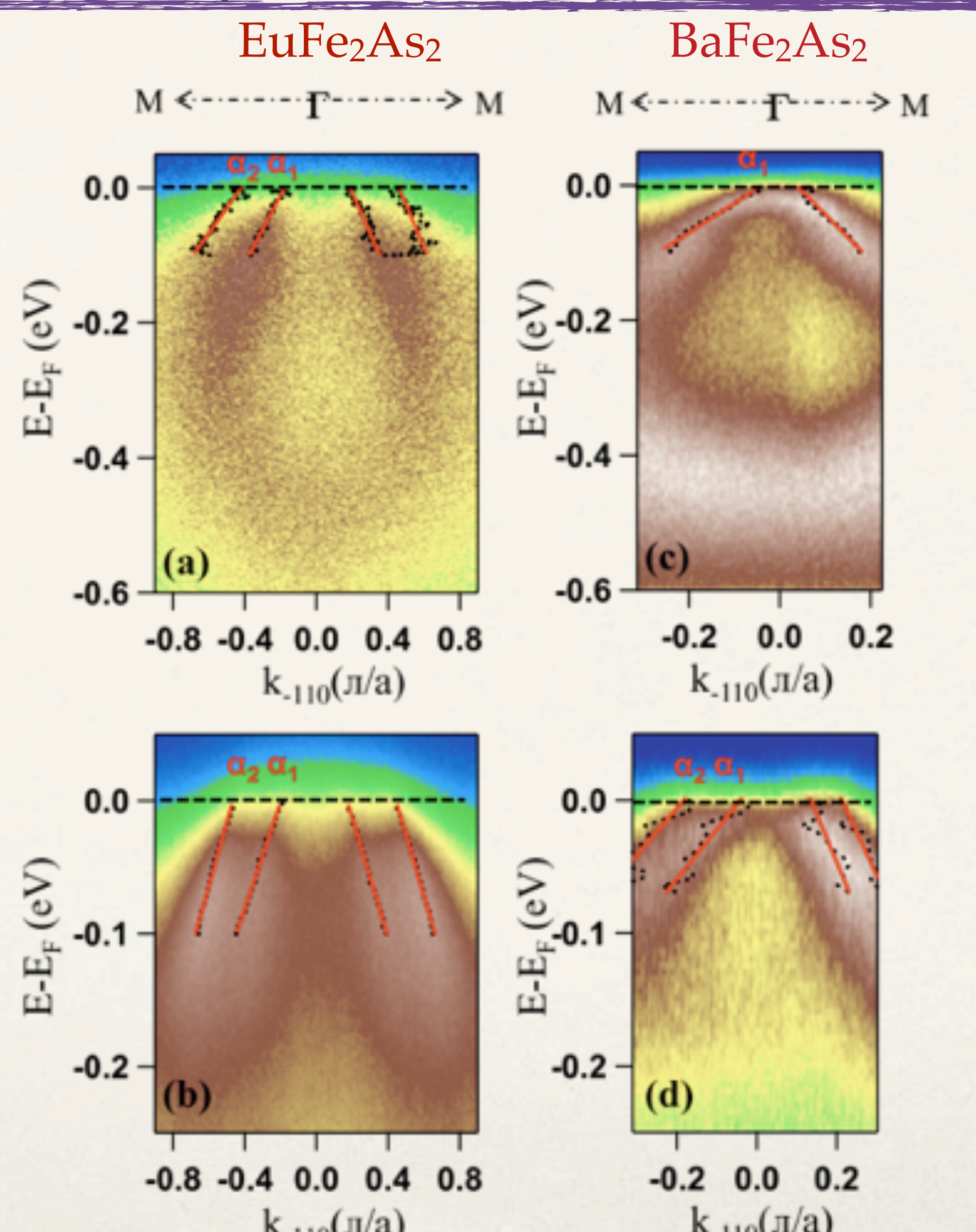

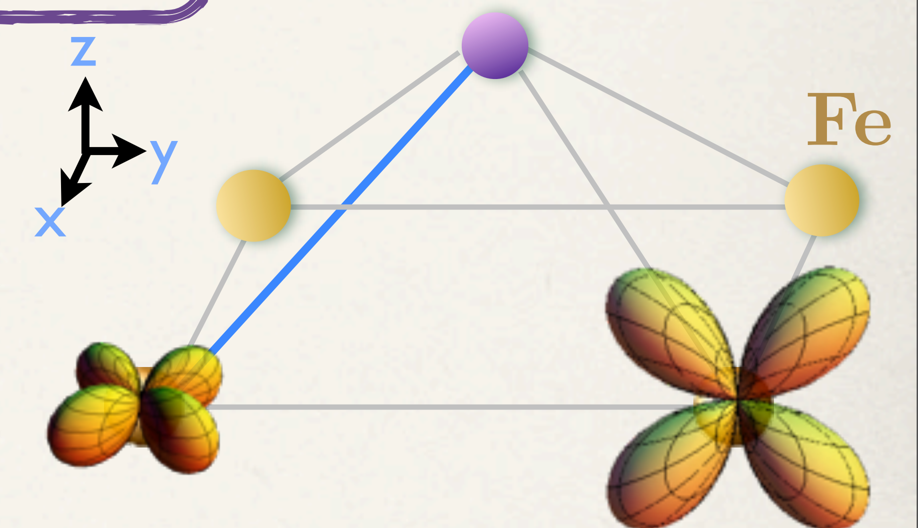

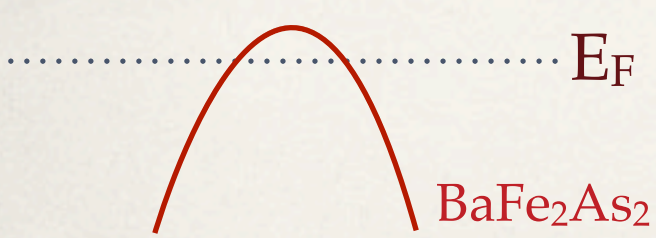

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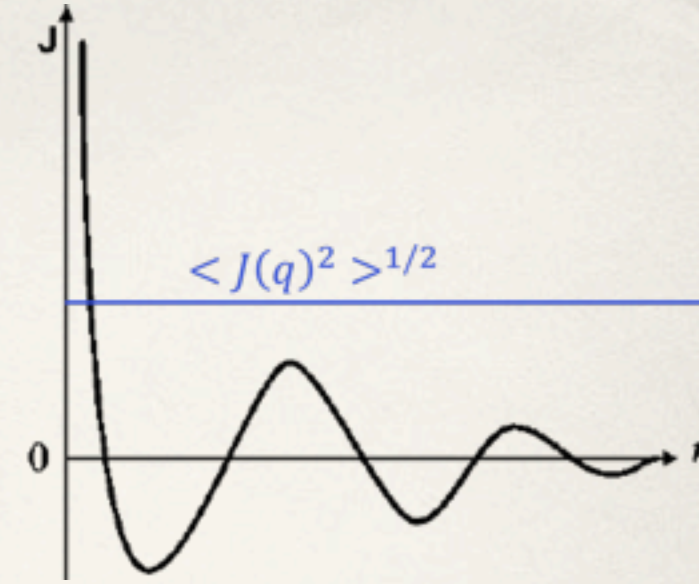

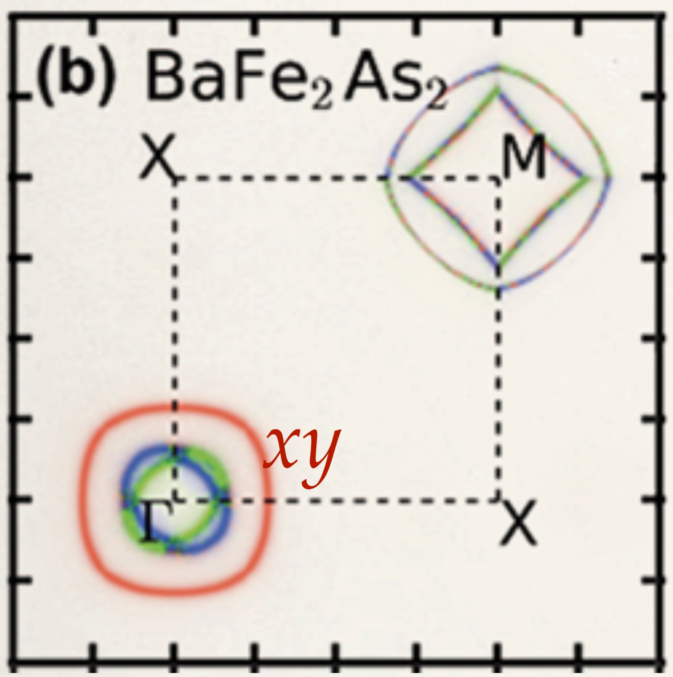

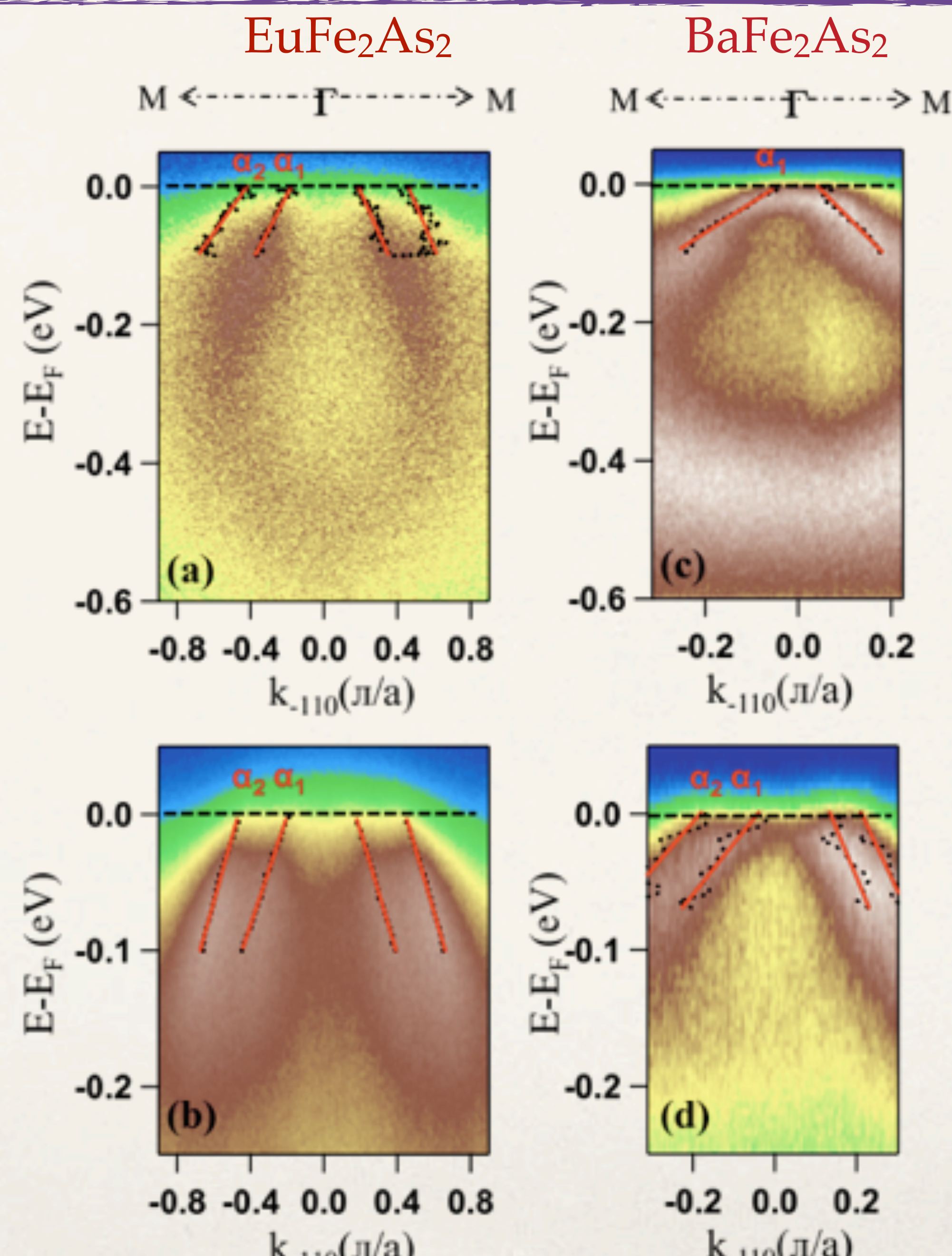

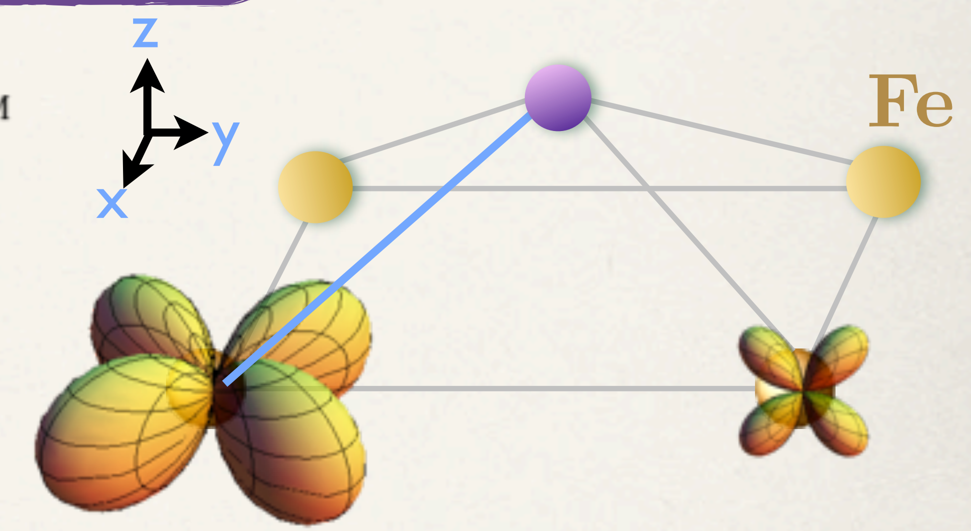

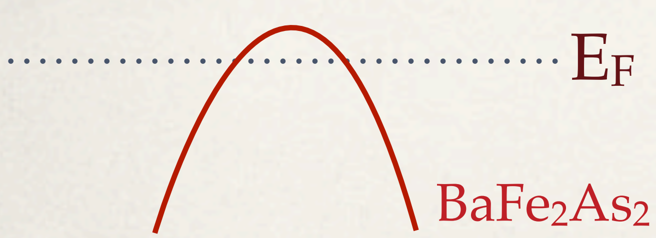

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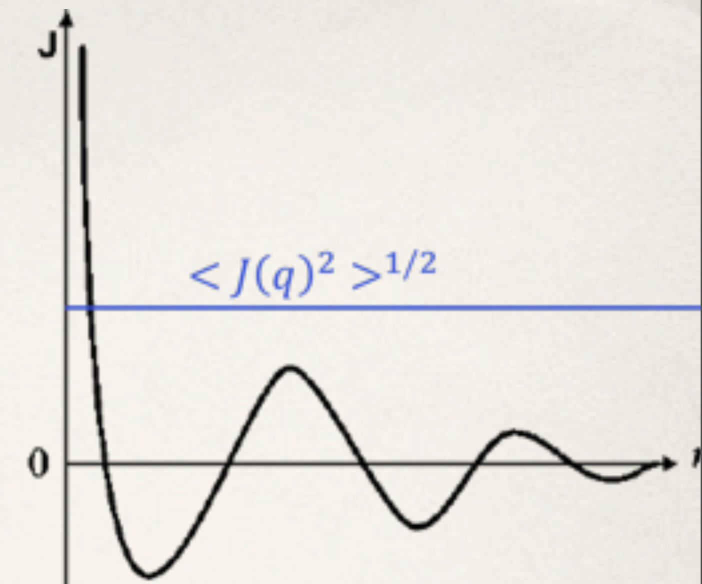

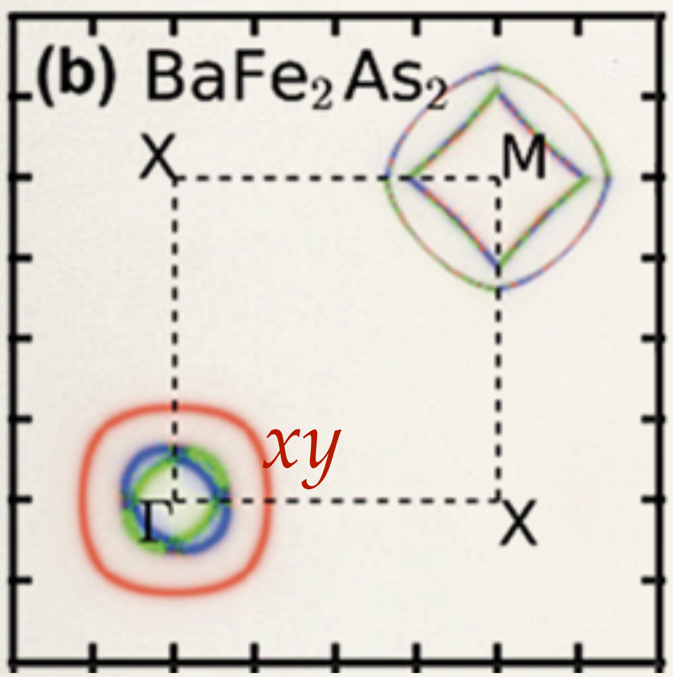

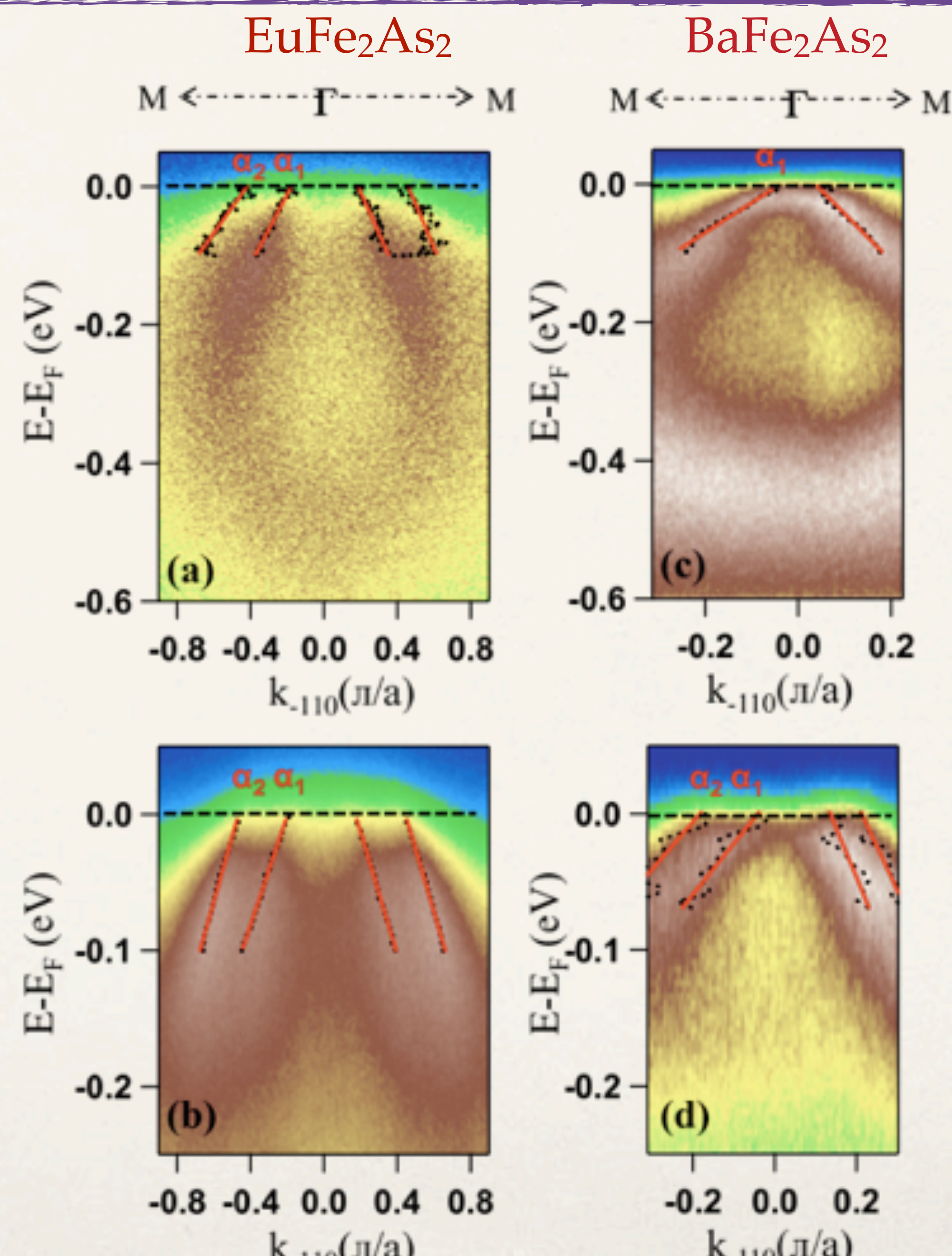

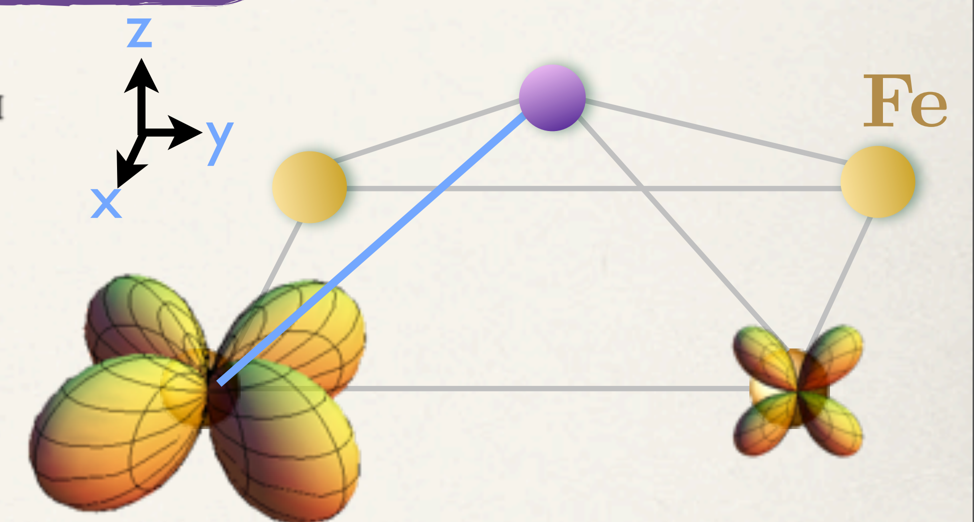

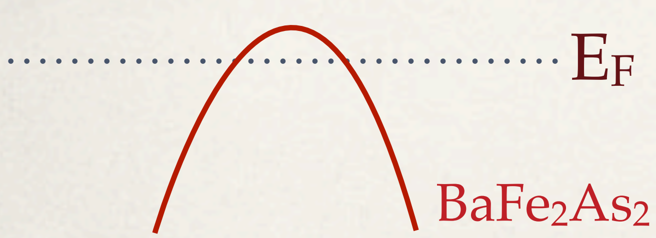

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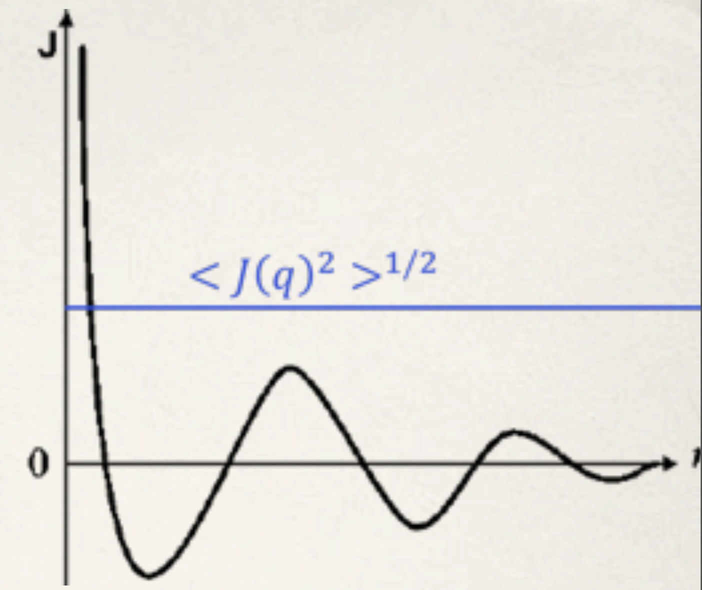
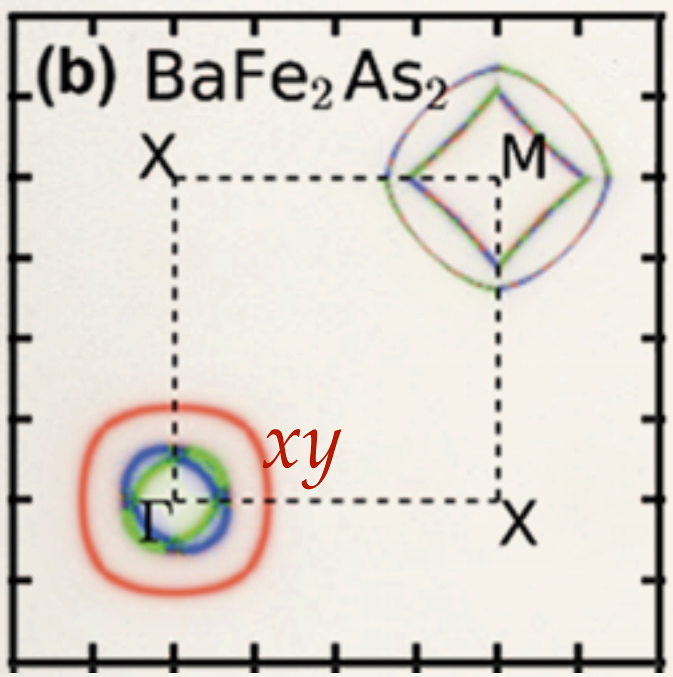
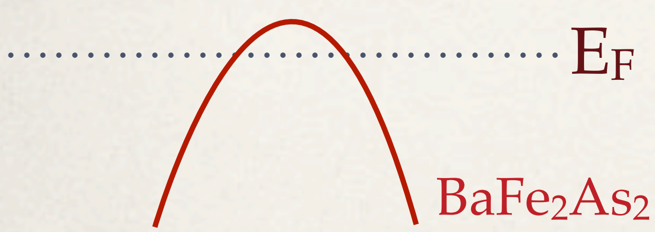
- *3d* Fe bands are more anisotropic (less *s*-like) and are, in average, further away from the Eu site, i.e., the planar orbital character xy / x^2-y^2 increases!

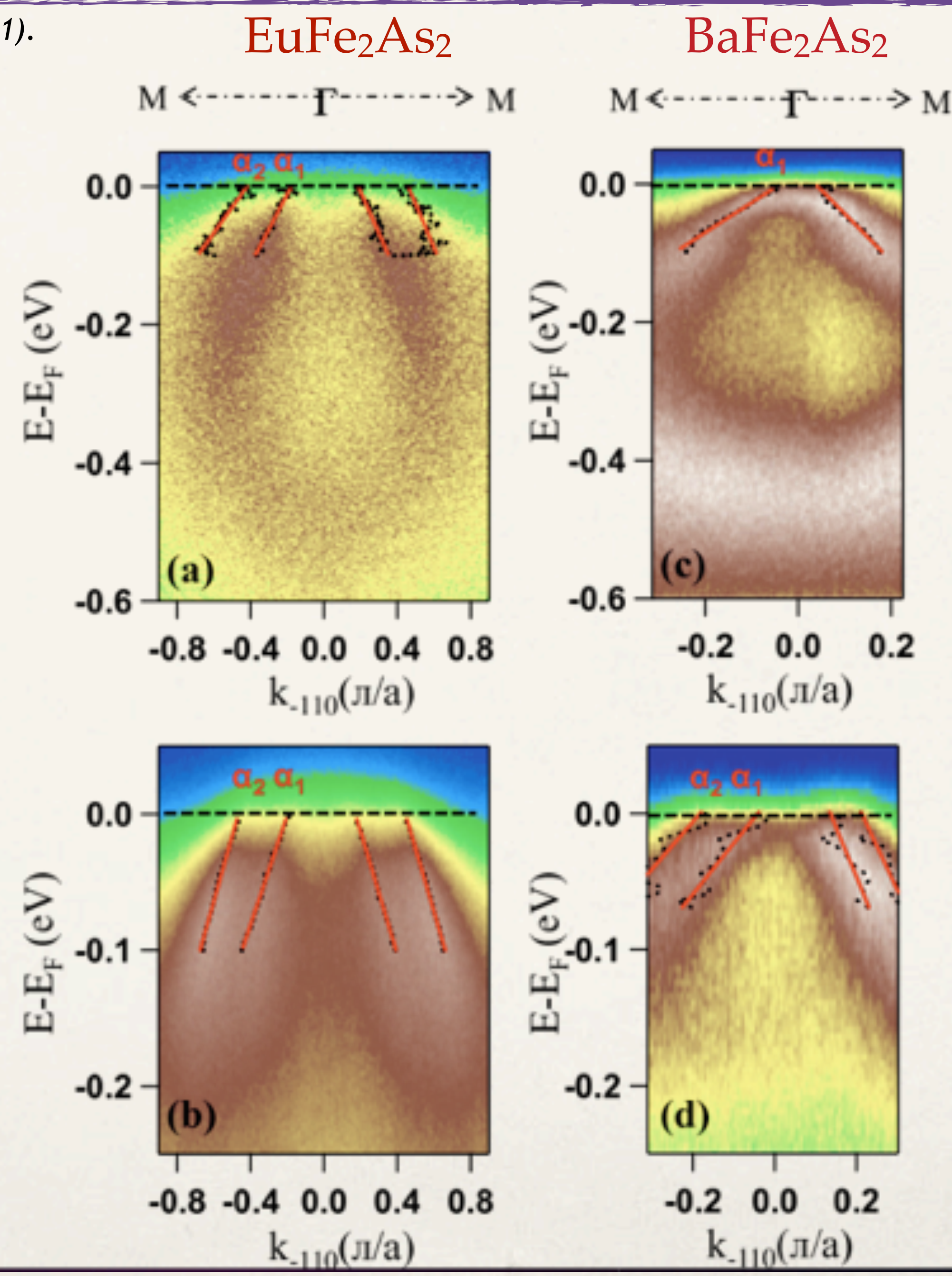
P. F. S. Rosa et al. Phys. Rev. B 86 165131 (2012).



Z. P. Yin *et al. Nature Materials*, ***10*** *932-935 (2011).*







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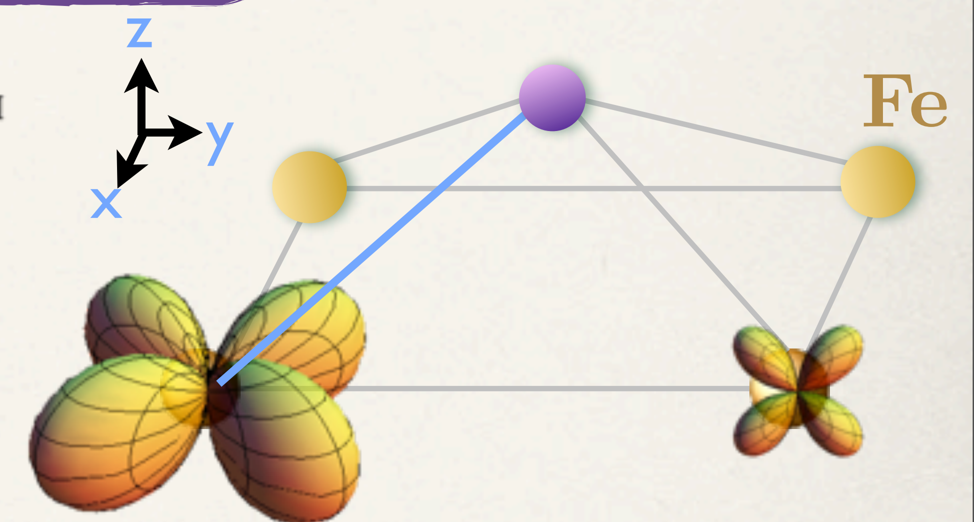
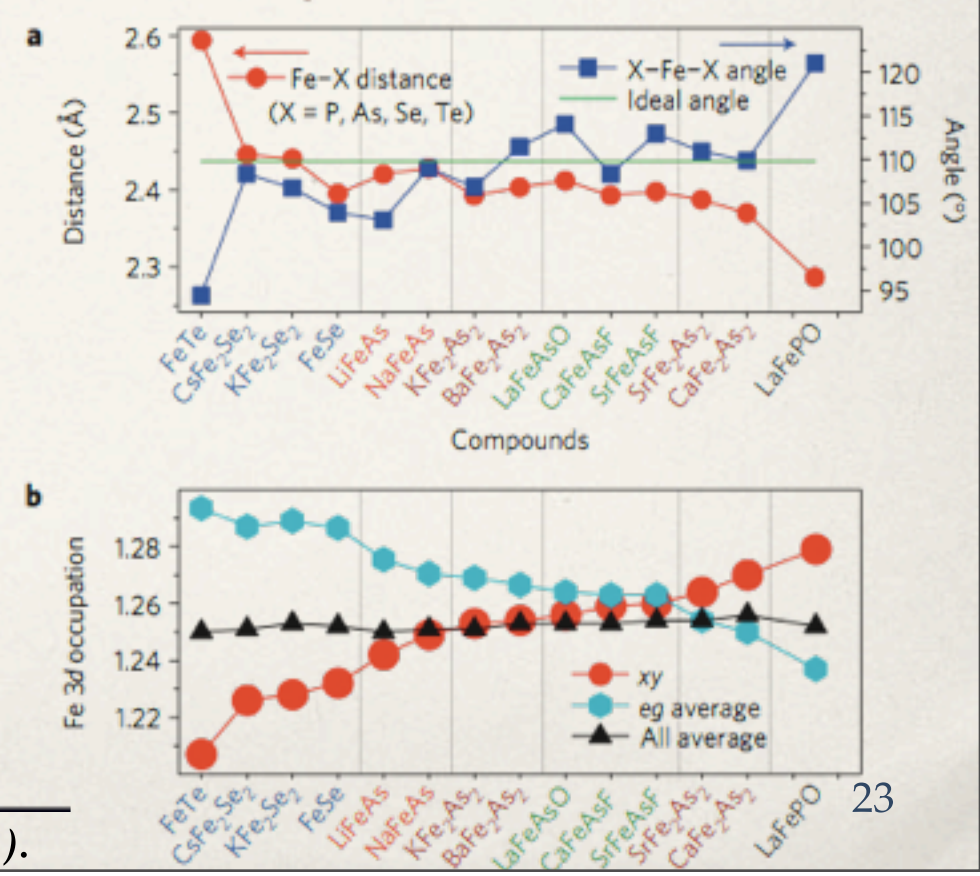
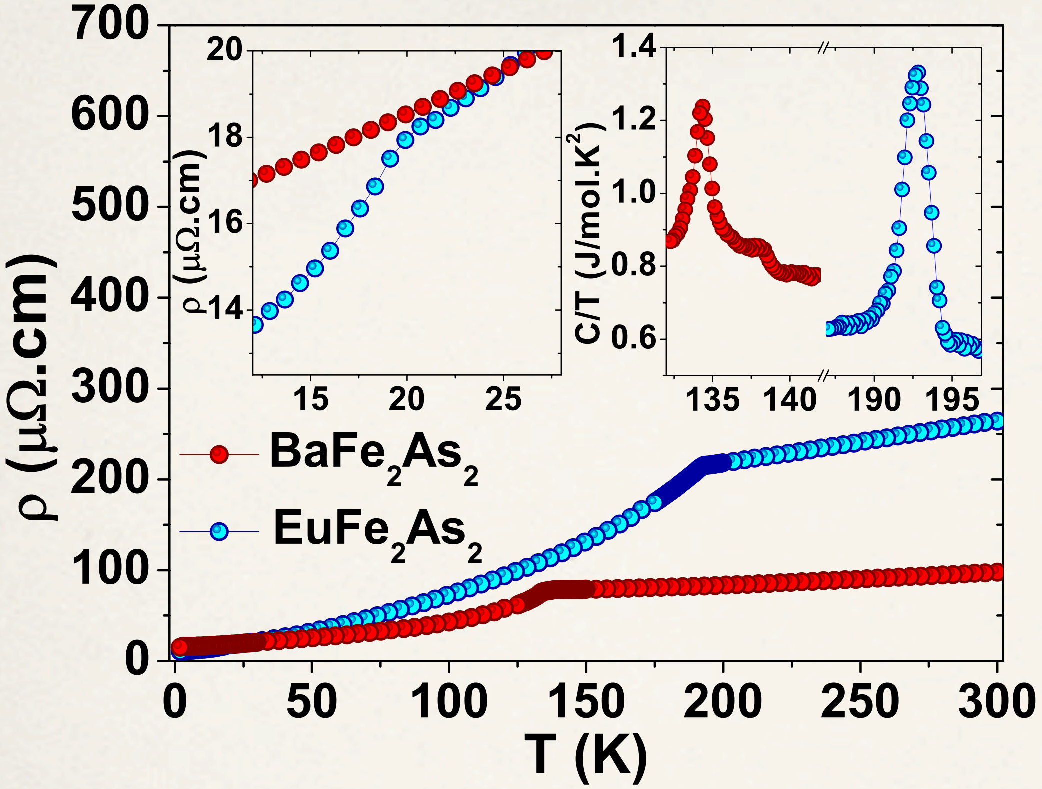




Quantum Oscillations in $EuFe_2As_2$



Thursday, October 9, 2014

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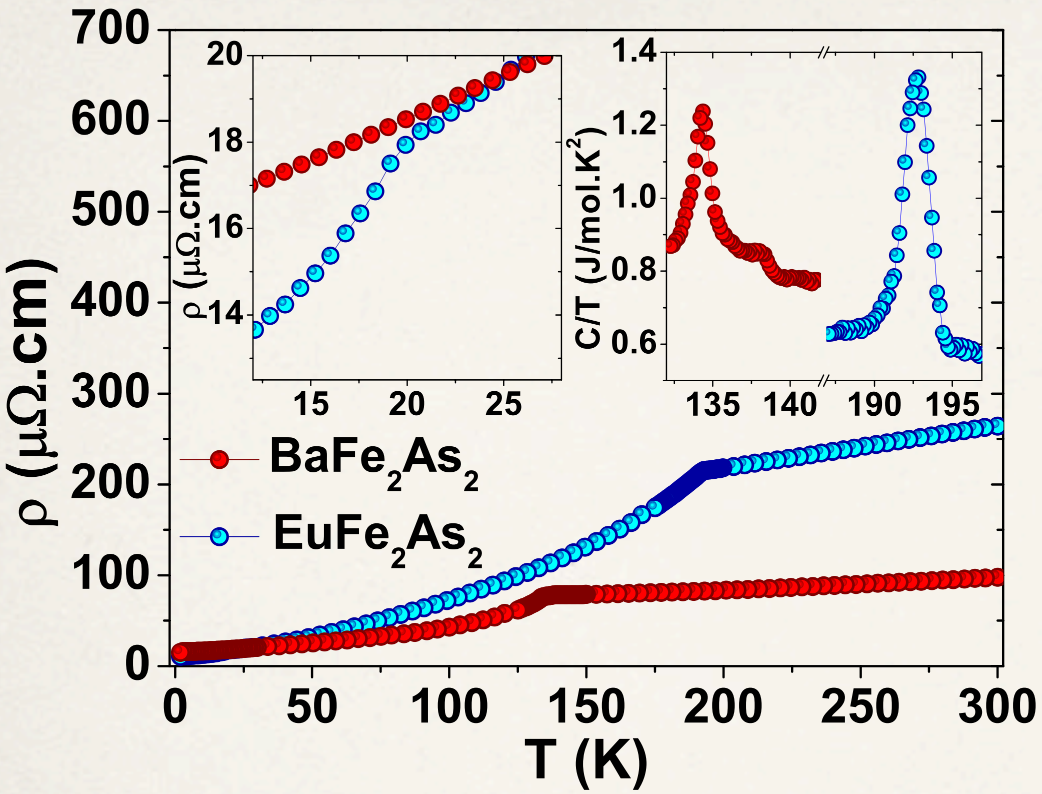

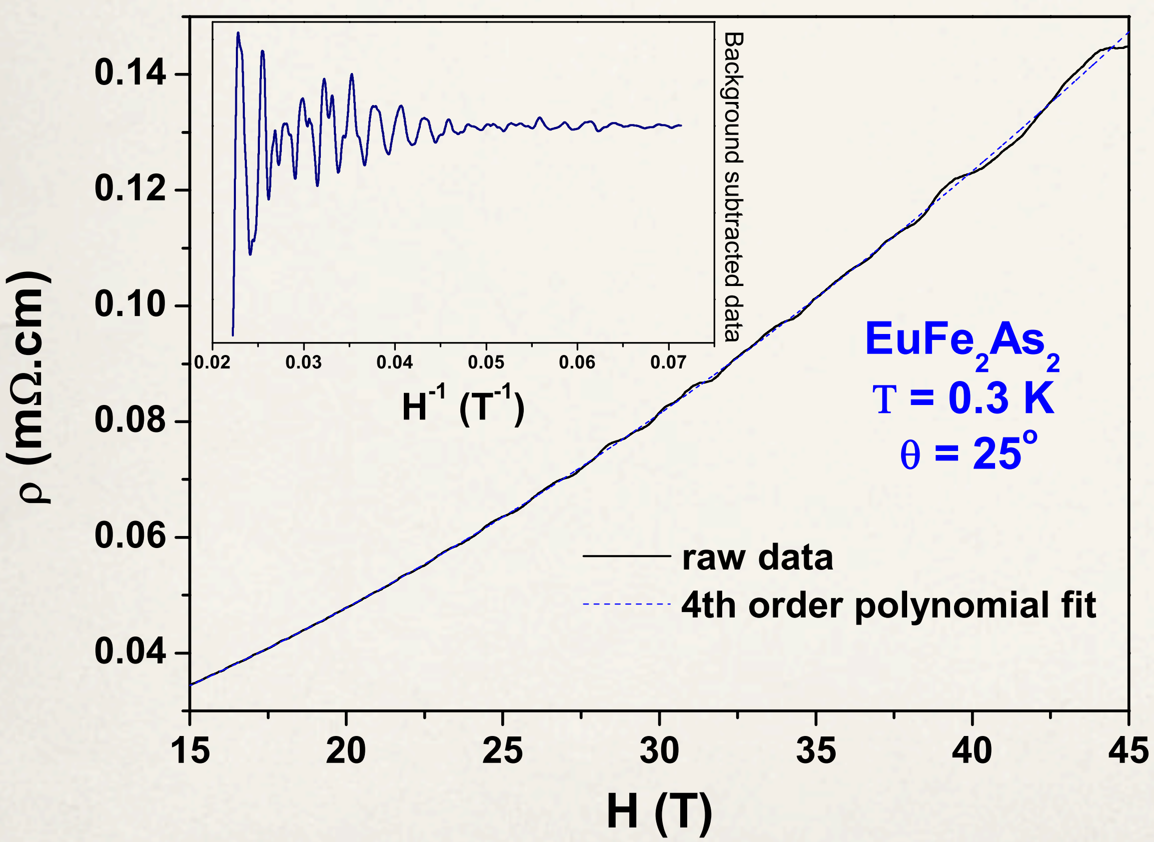

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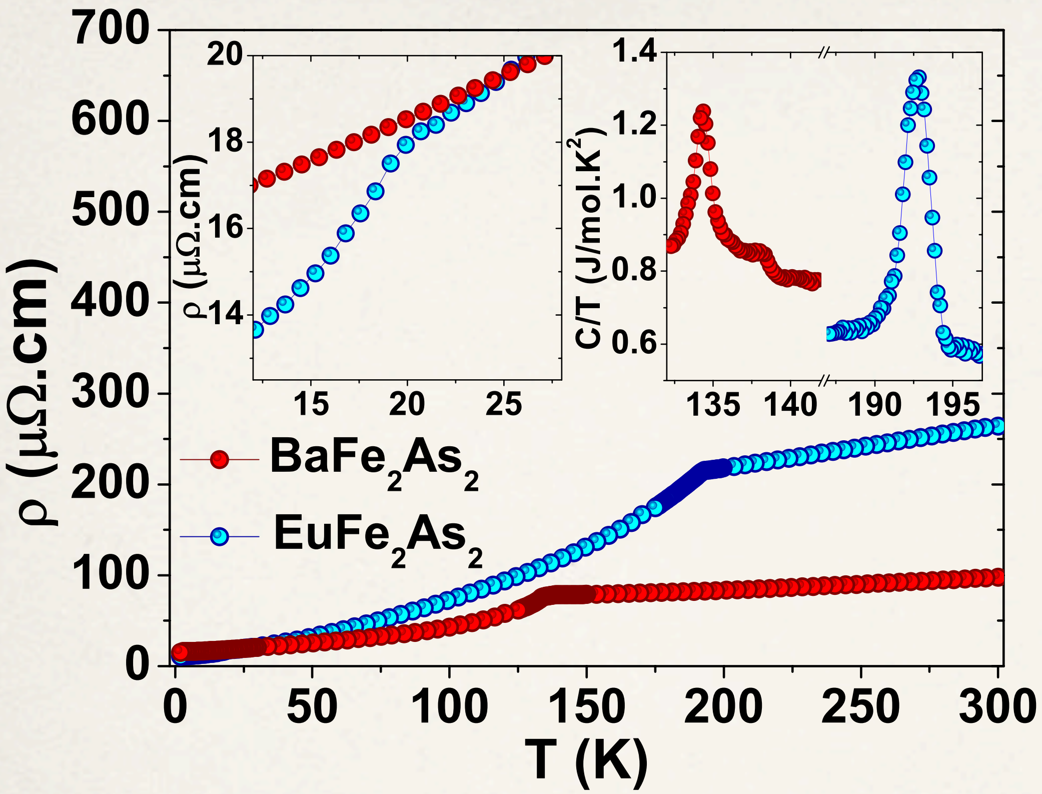

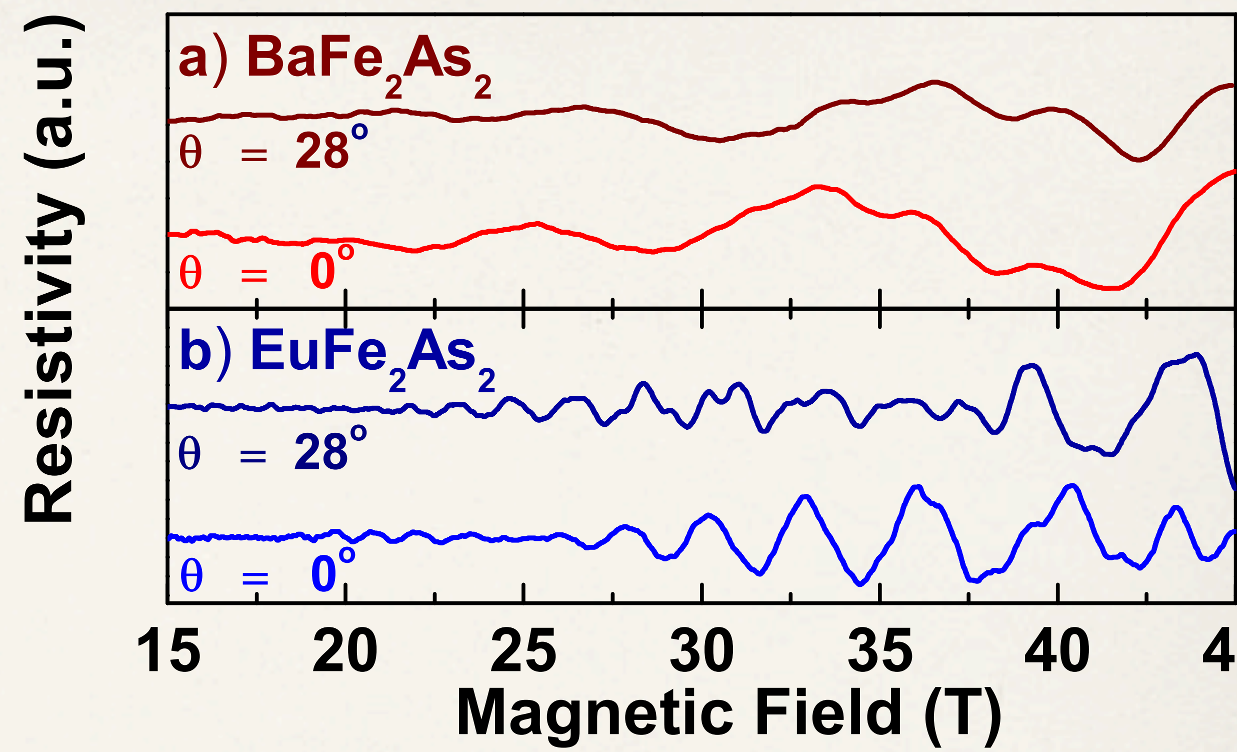

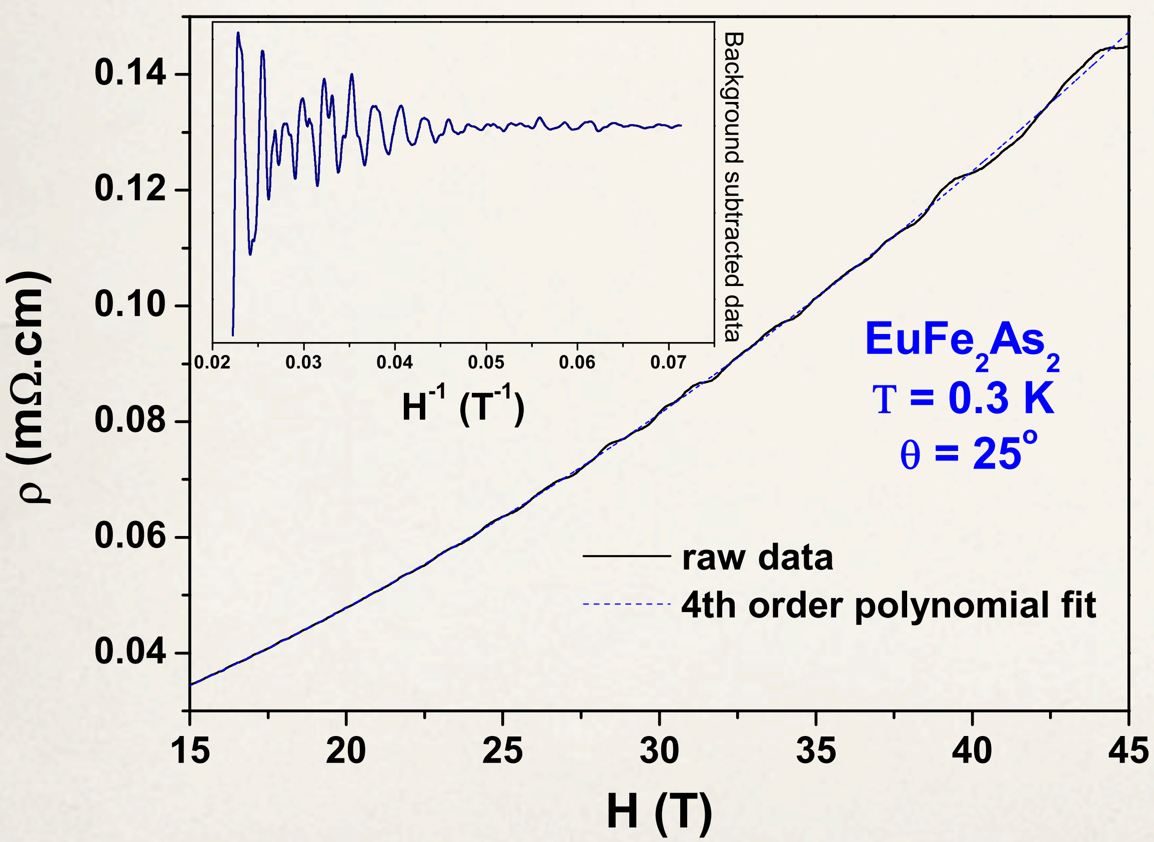

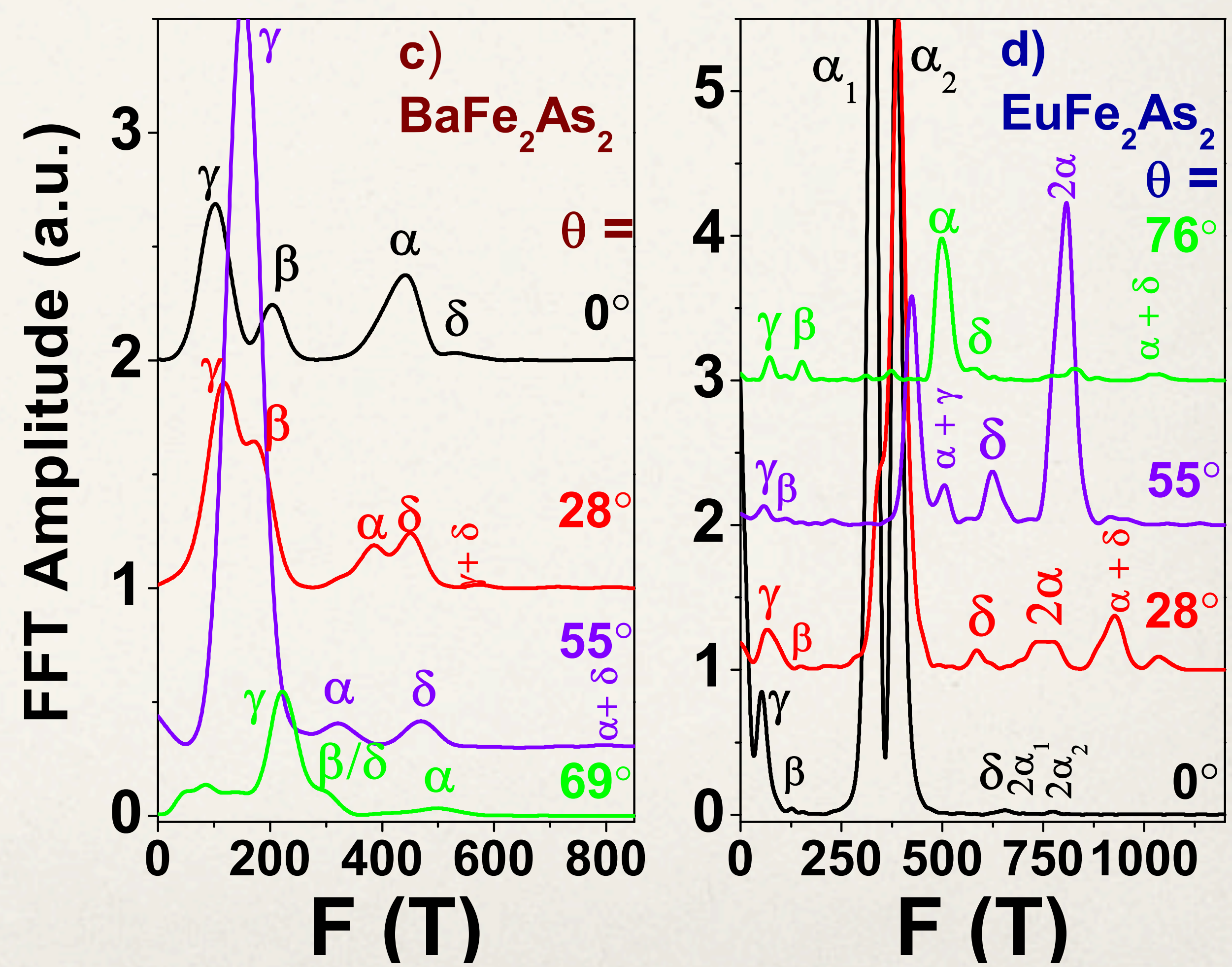

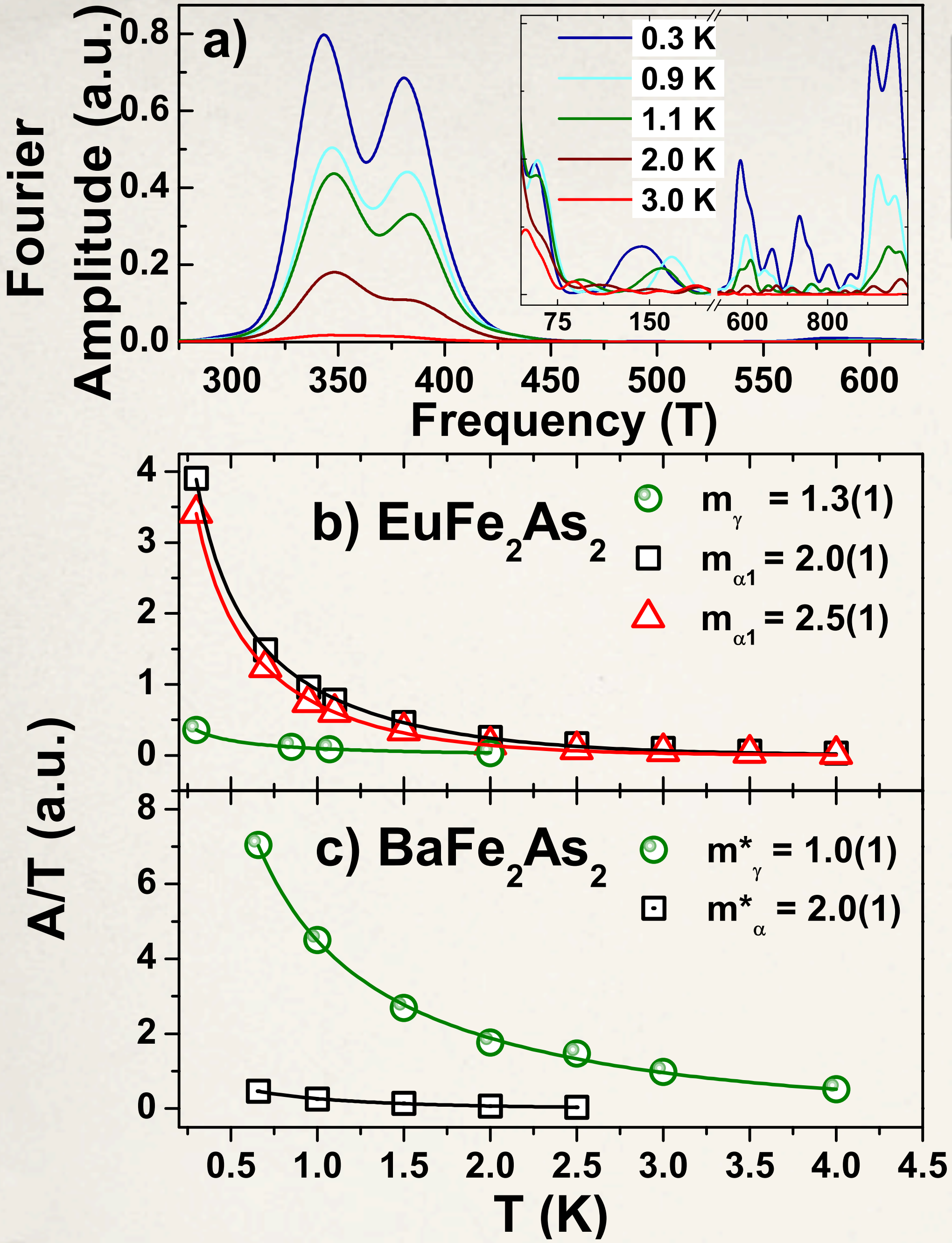

TABLE I: Comparison between the SdH frequencies of Ba122 and Eu122 obtained experimentally in this work.

	$BaFe_2As_2$						$EuFe_2As_2$					
Pocket	$F(T)$	A/A_{BZ} (%)	m^*/m_e^*	m^*_{DFT}/m_e^*	R	T_D (K)	F (T)	A/A_{BZ}	m^*/m_e^*	m^*_{DFT}/m_e^*	R	T_D
γ	90(10)	0.3	0.7(2)	0.4	2.1	5(2)	60(10)	0.2	1.0(2)	0.4	1.2	-
α	430(10)	1.4	1.5(2)	-0.8	2.1	4(1)	340(10)/380(10)	1.3	1.5(2)/1.9(2)	-0.8	1.4	4(1)
δ	510(10)	1.7	-	1.2	0.8	3(1)	580(10)	1.4	-	1.7	0.5	3(1)

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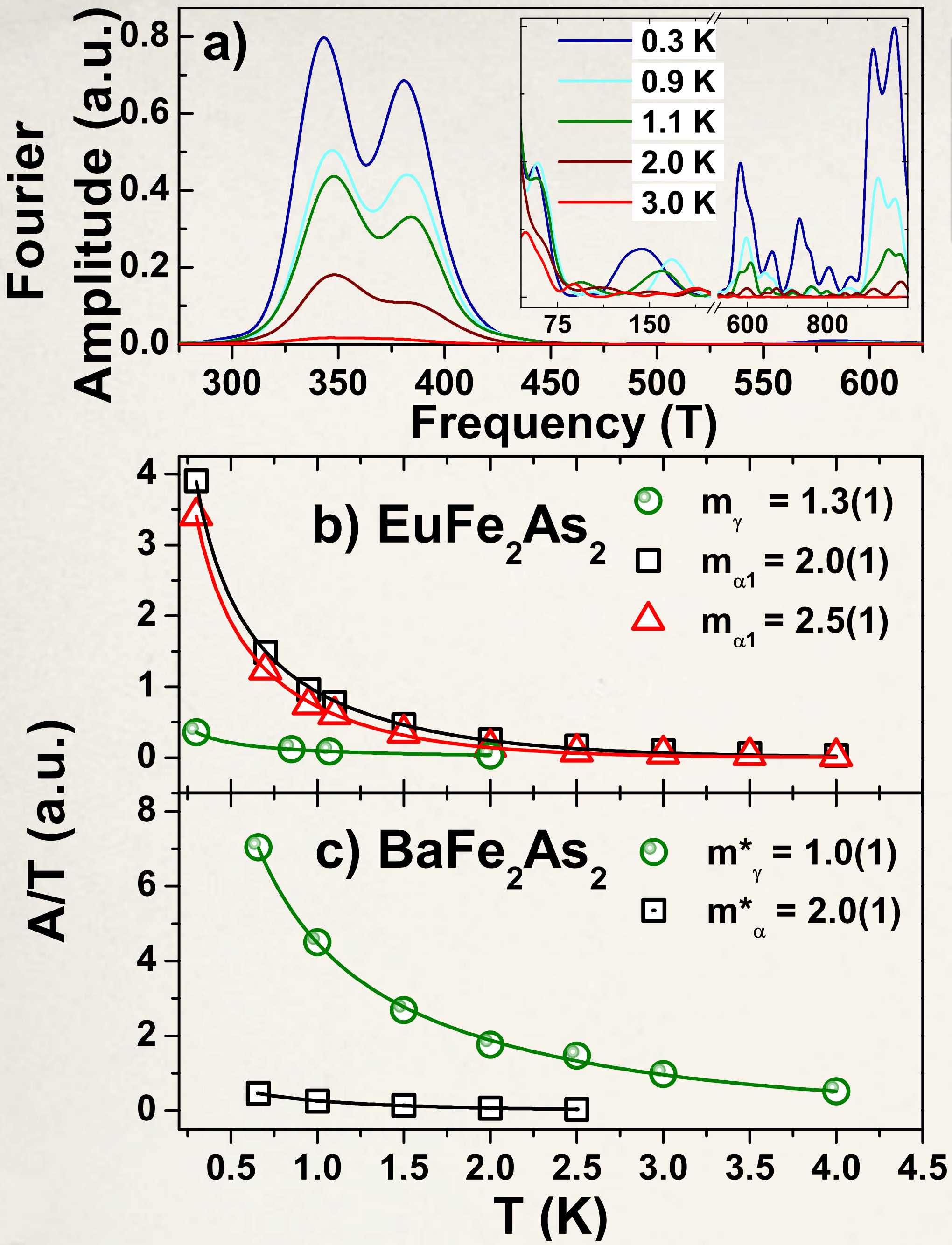

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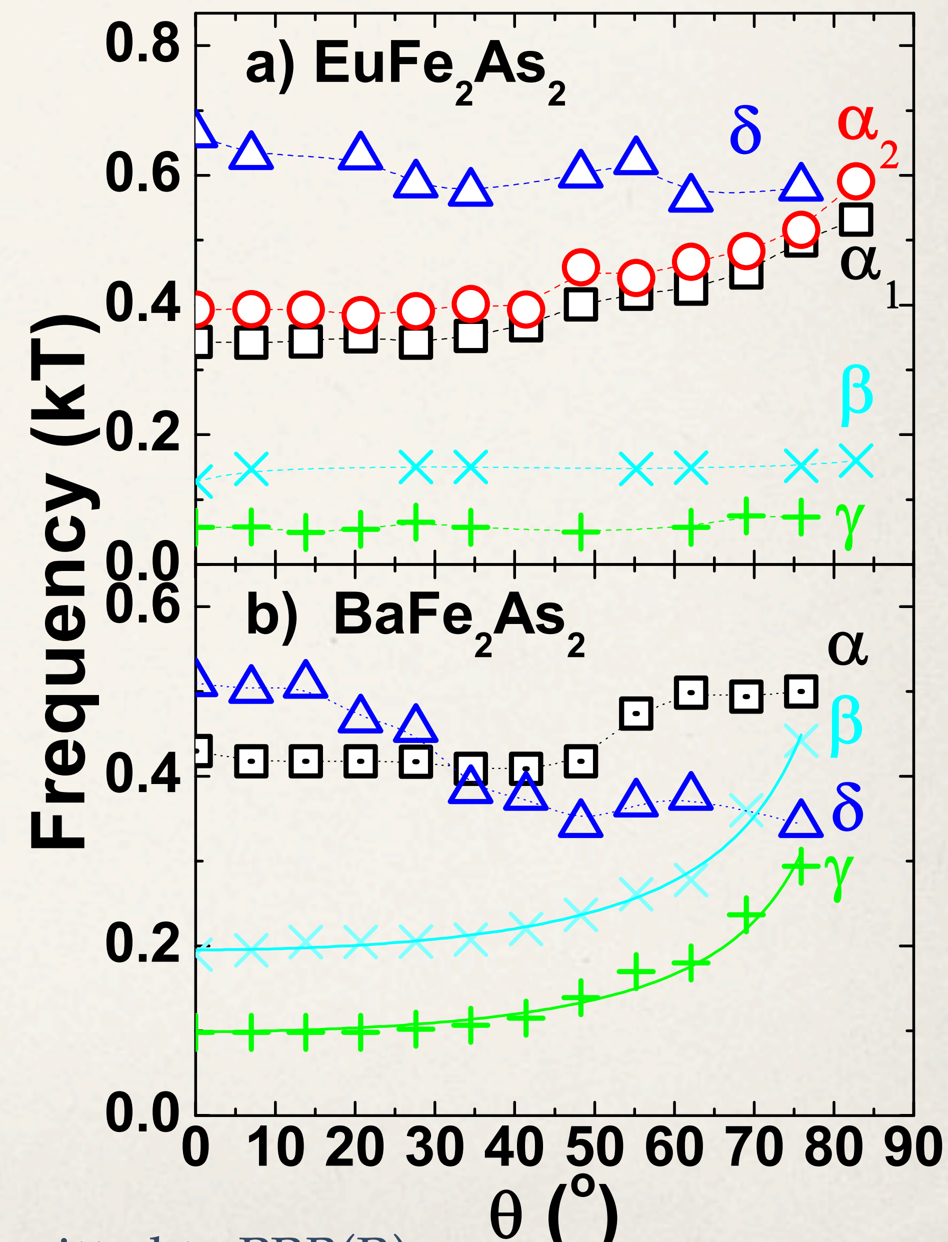

P. F. S. Rosa *et al*. Submitted to PRB(R).

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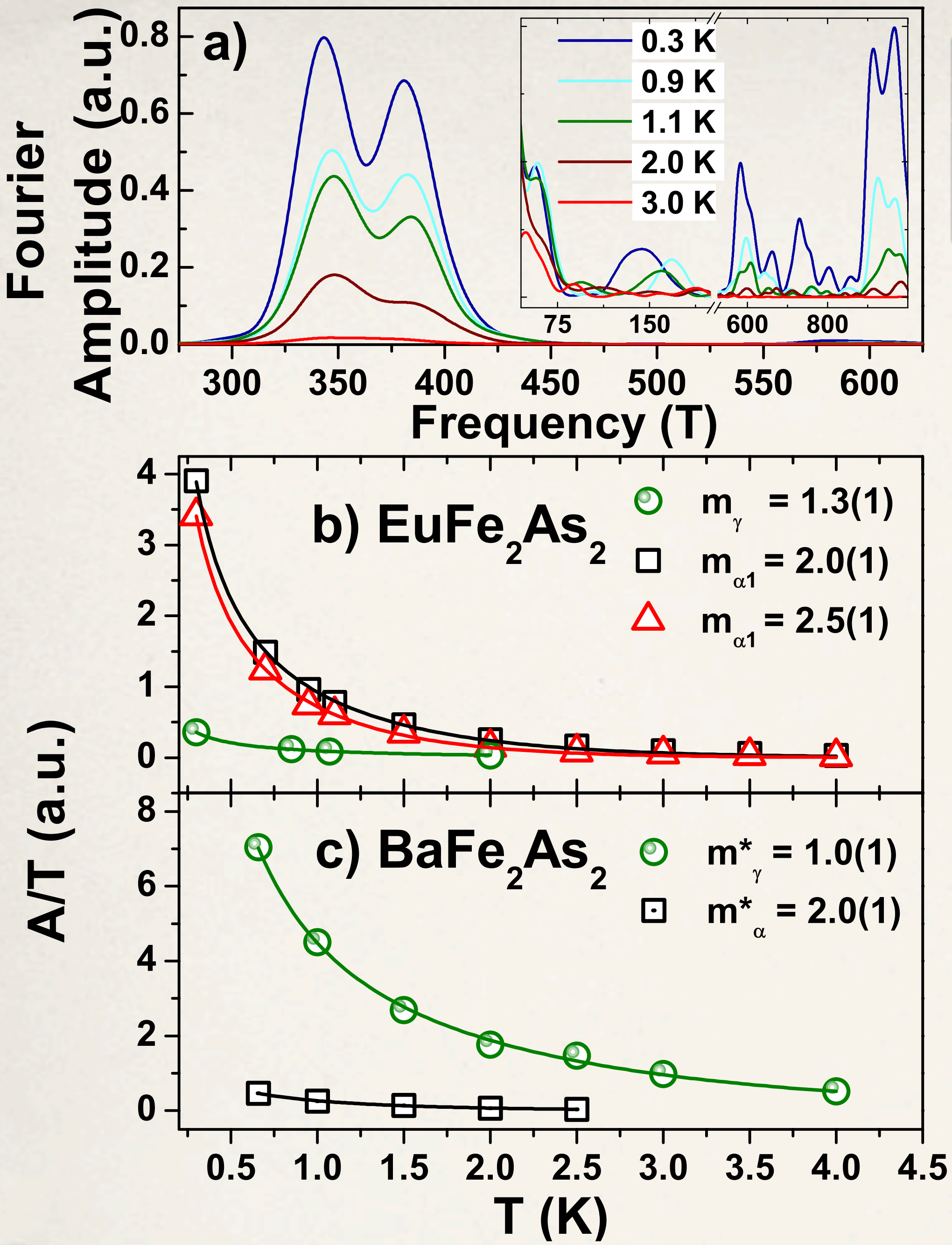

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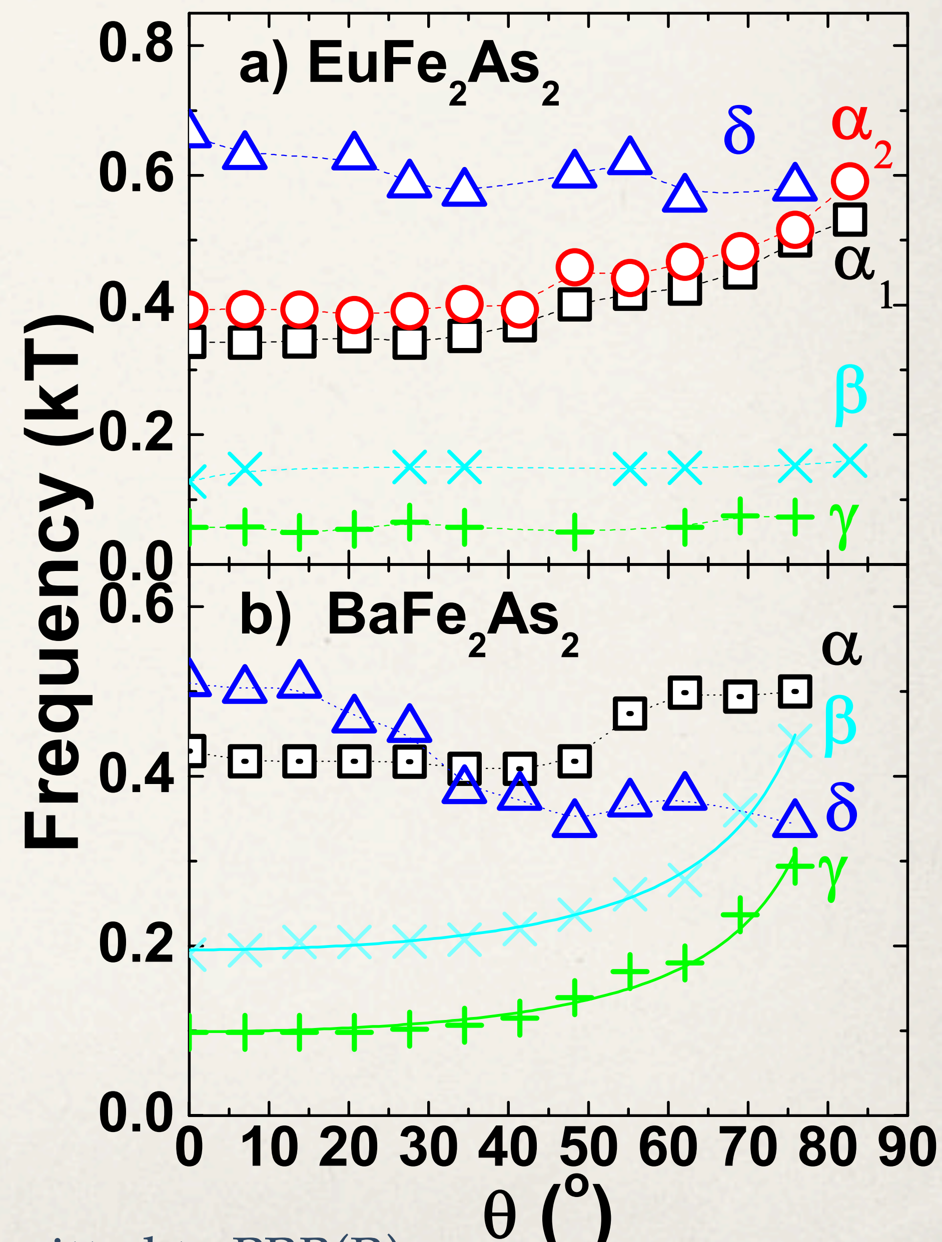
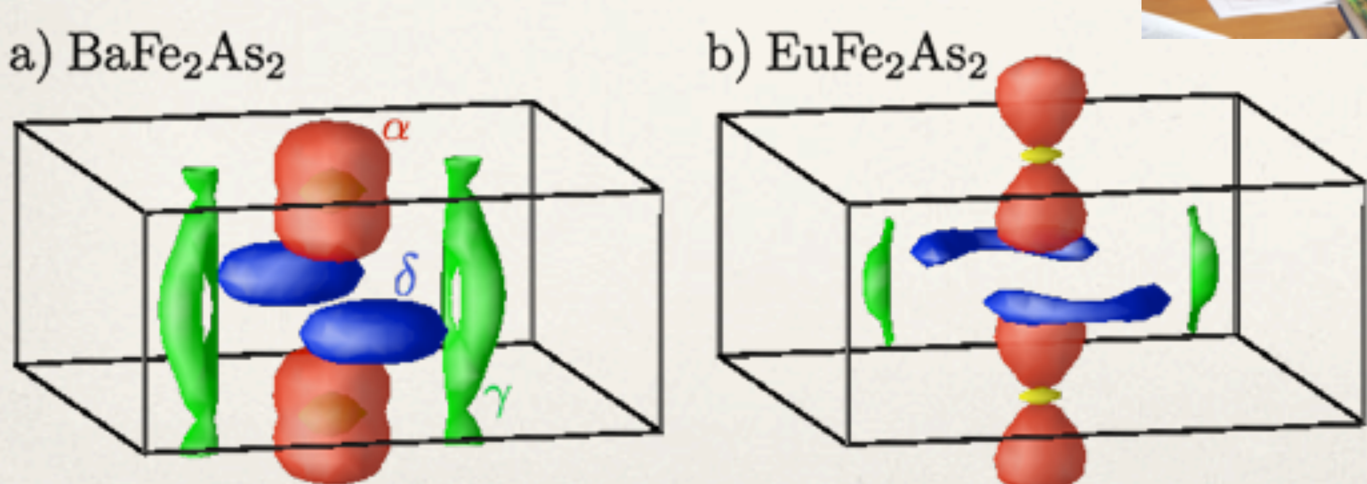
Michelle Johannes





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Evidence for the *3d* Fe band contribution to the FS

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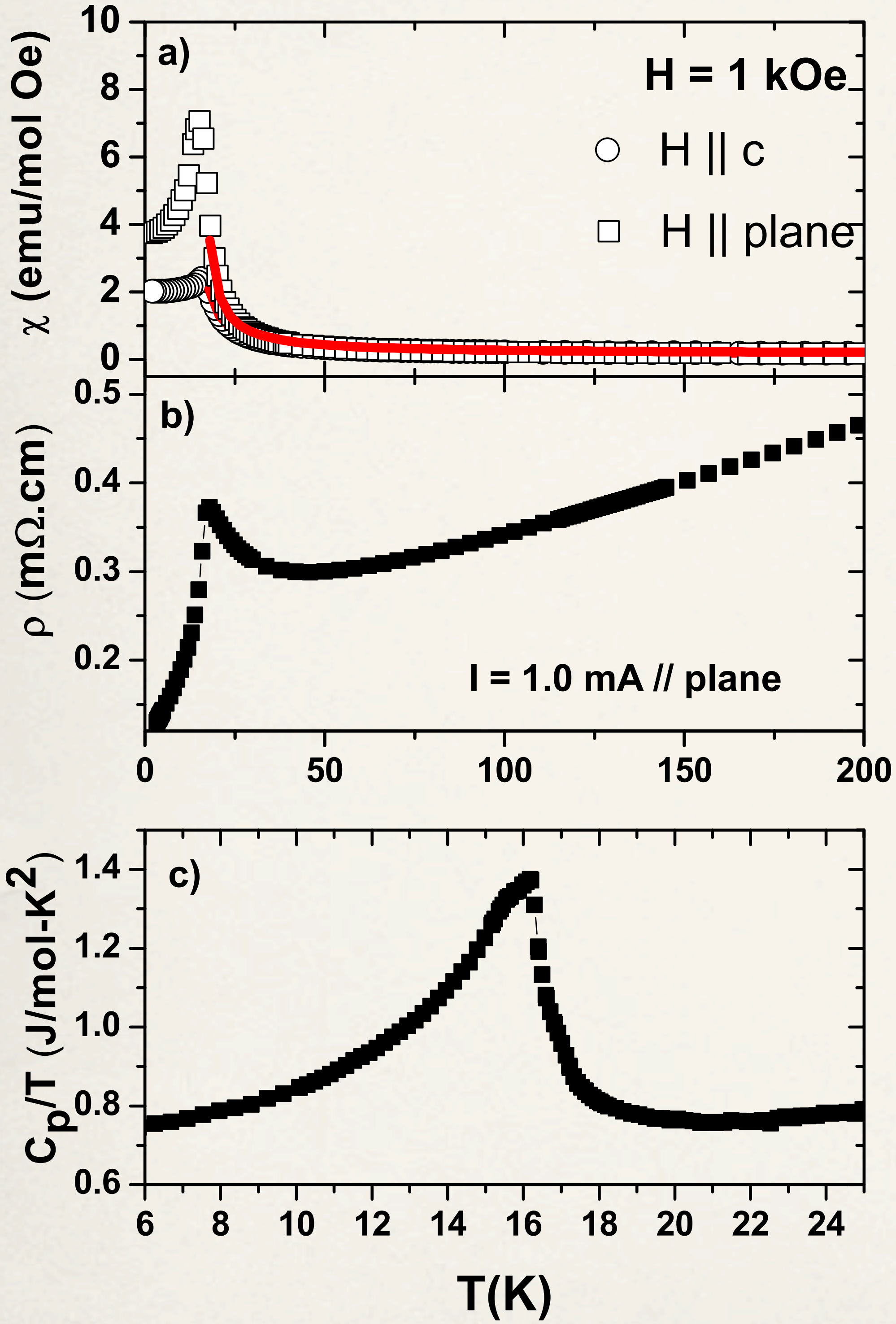

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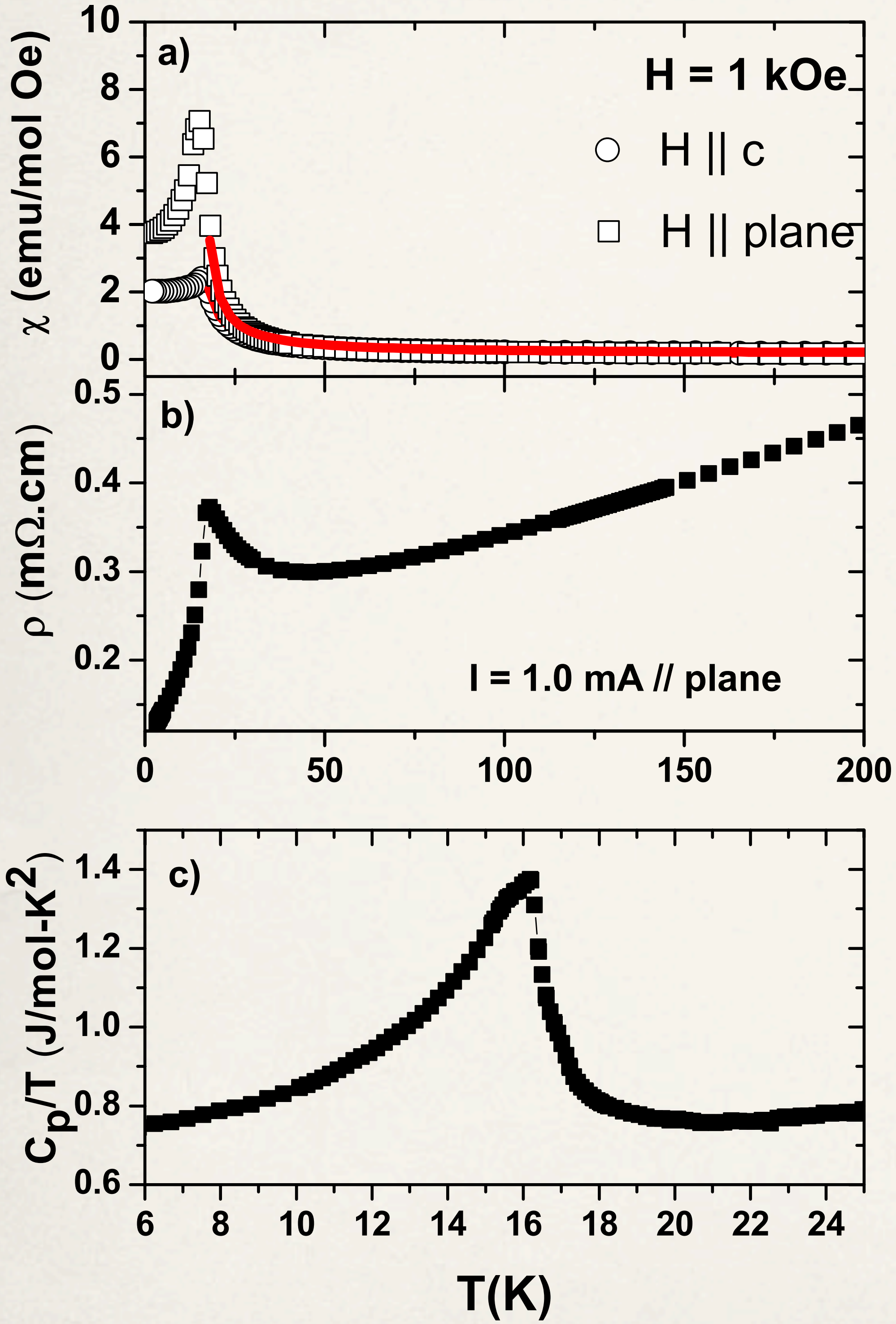

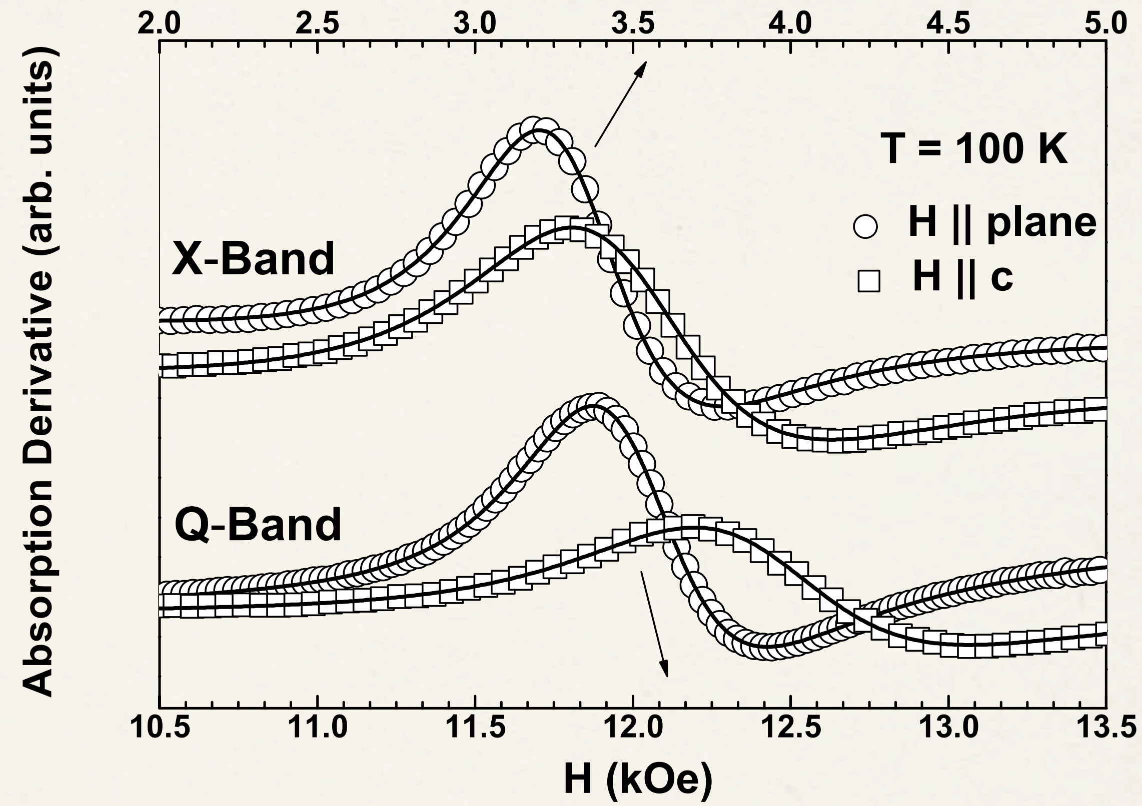

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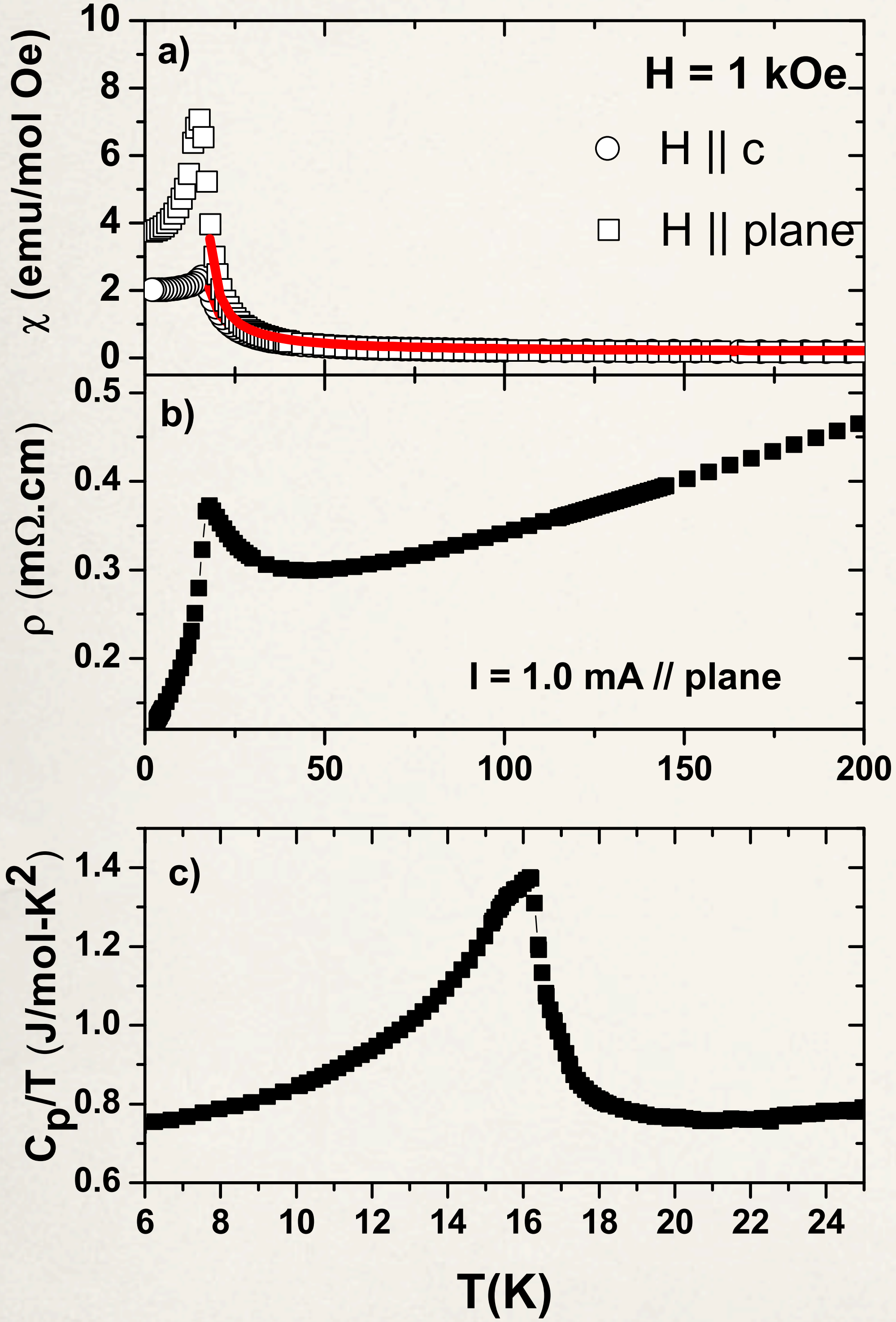

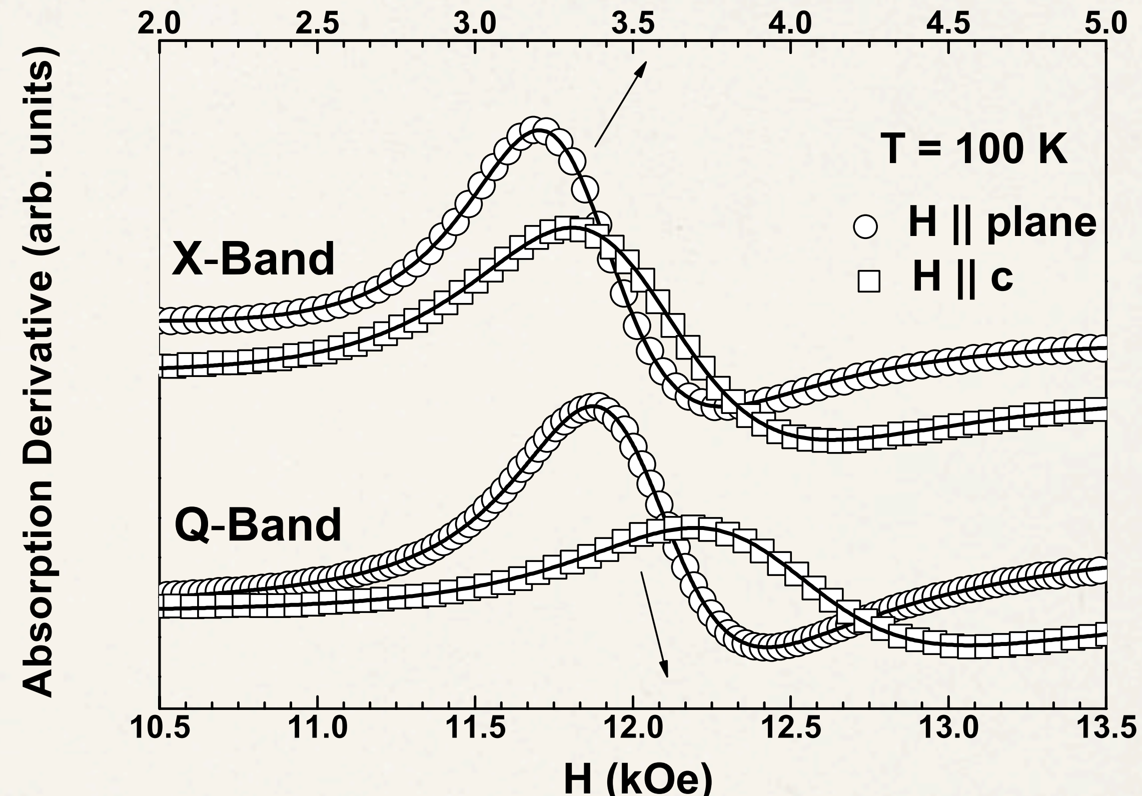

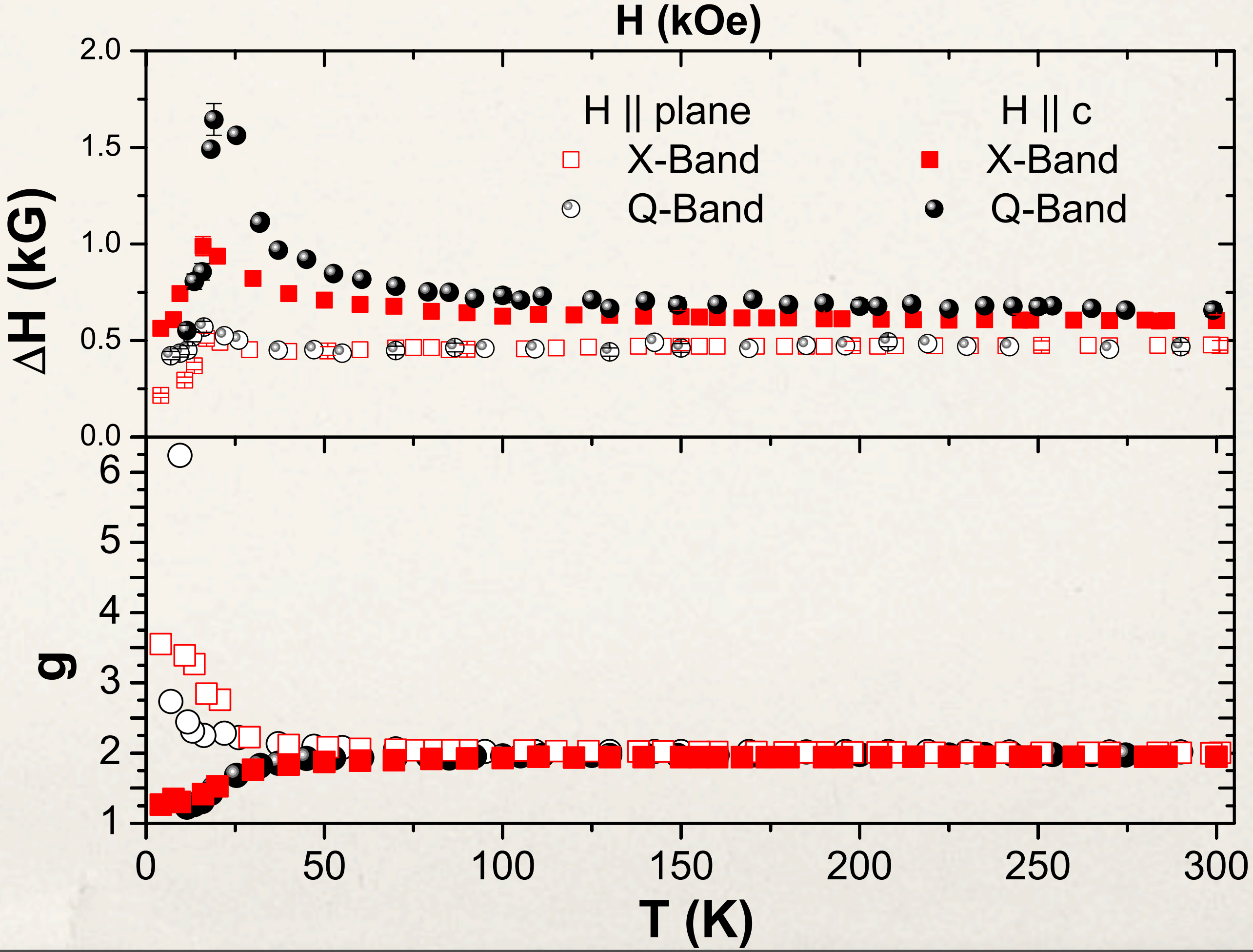

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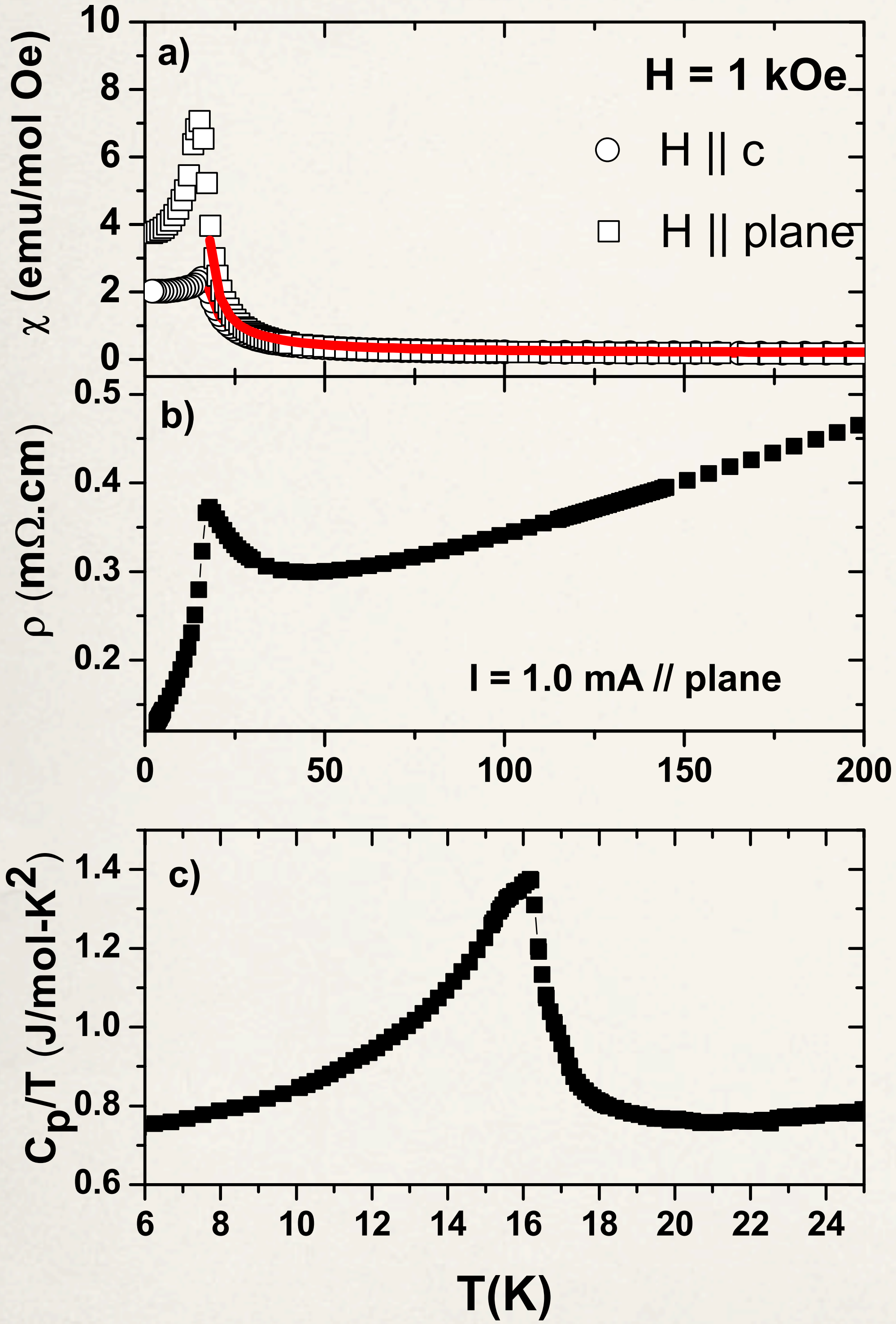
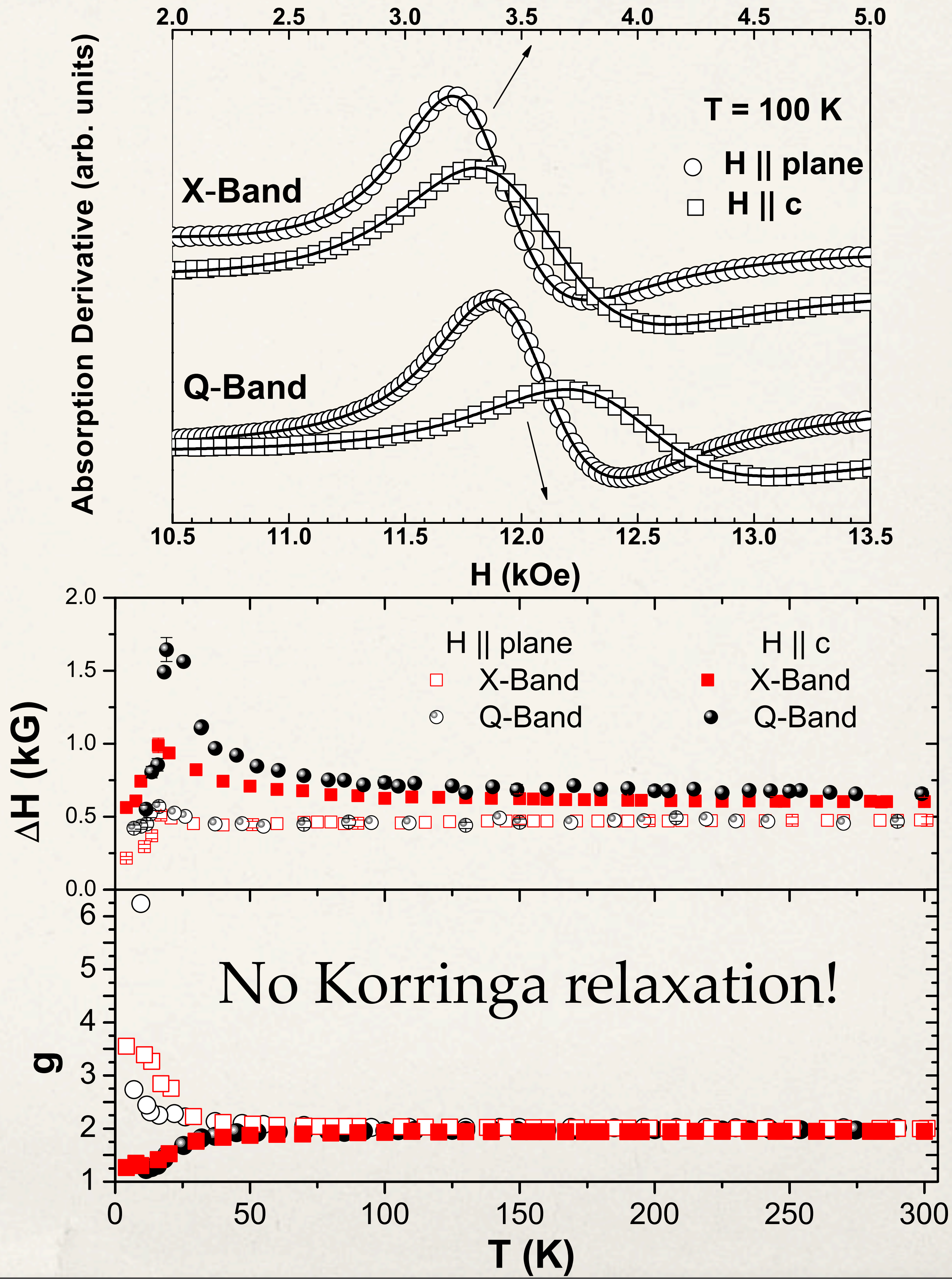
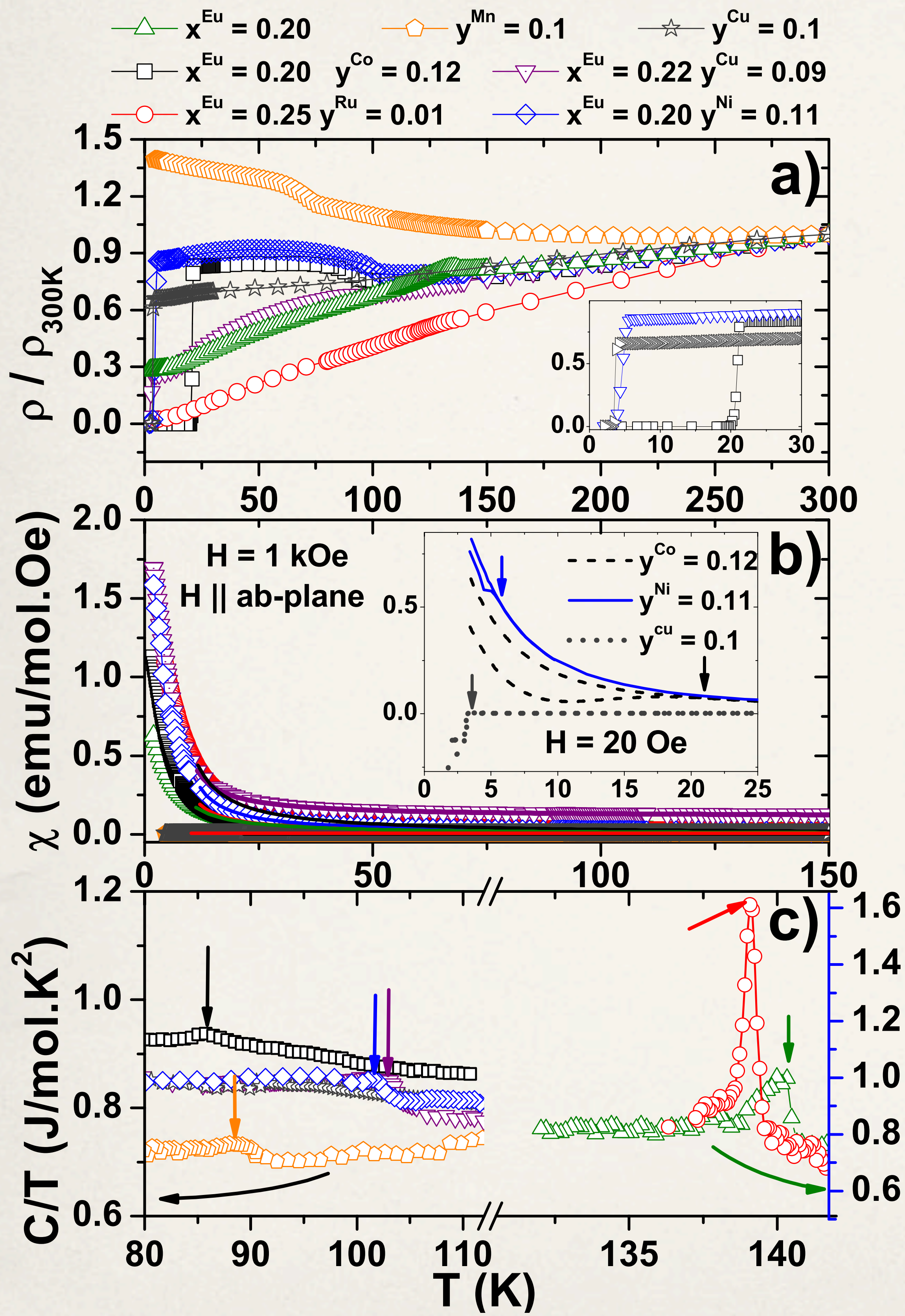




P. F. S. Rosa et al. Phys. Rev. B. **86,** 094408 (2012).

Site-specific ESR on $Ba_{1-x}Eu_xFe_{2-y}M_yAs_2$ (M = Co, Cu, Ni, and Ru)



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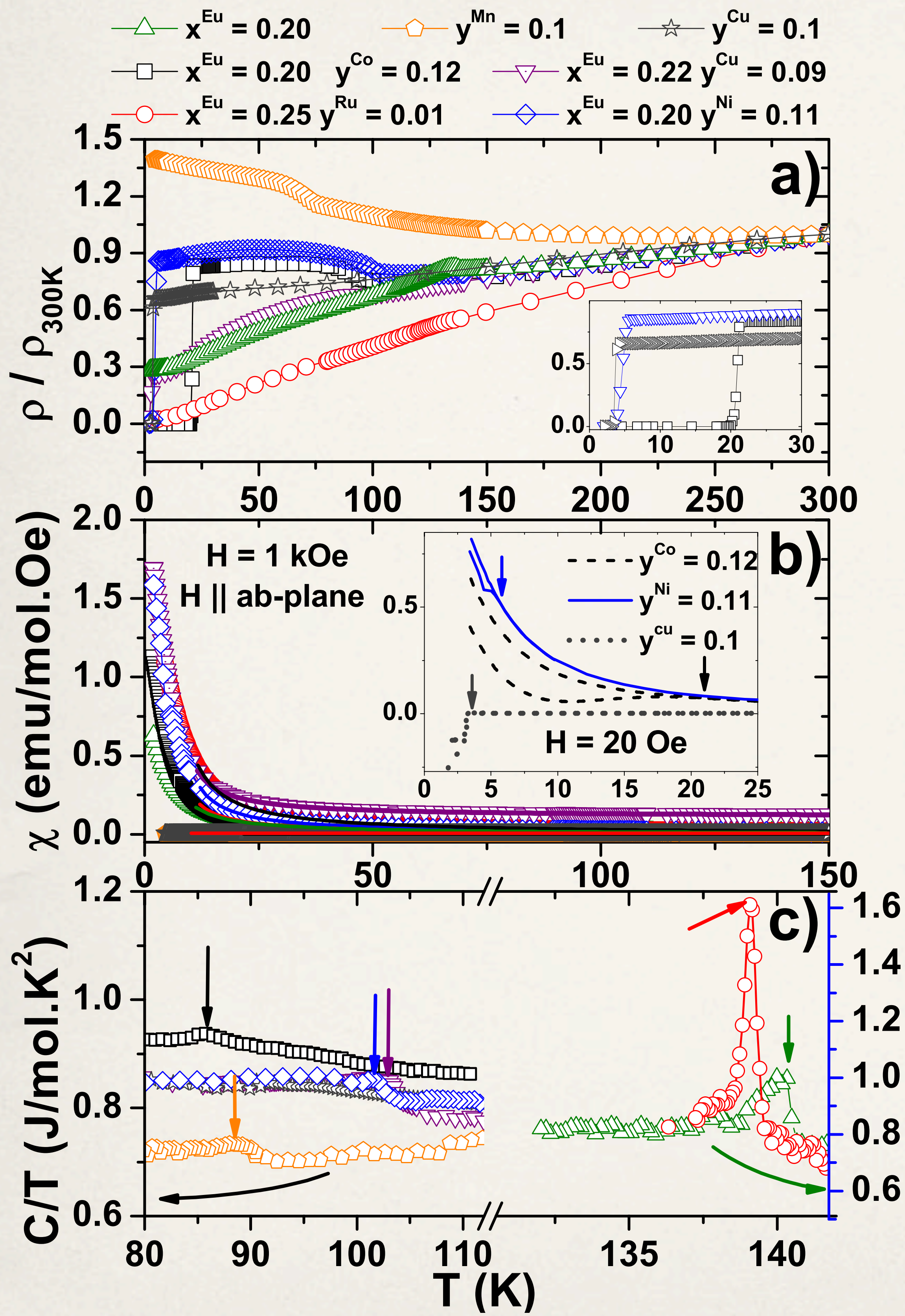
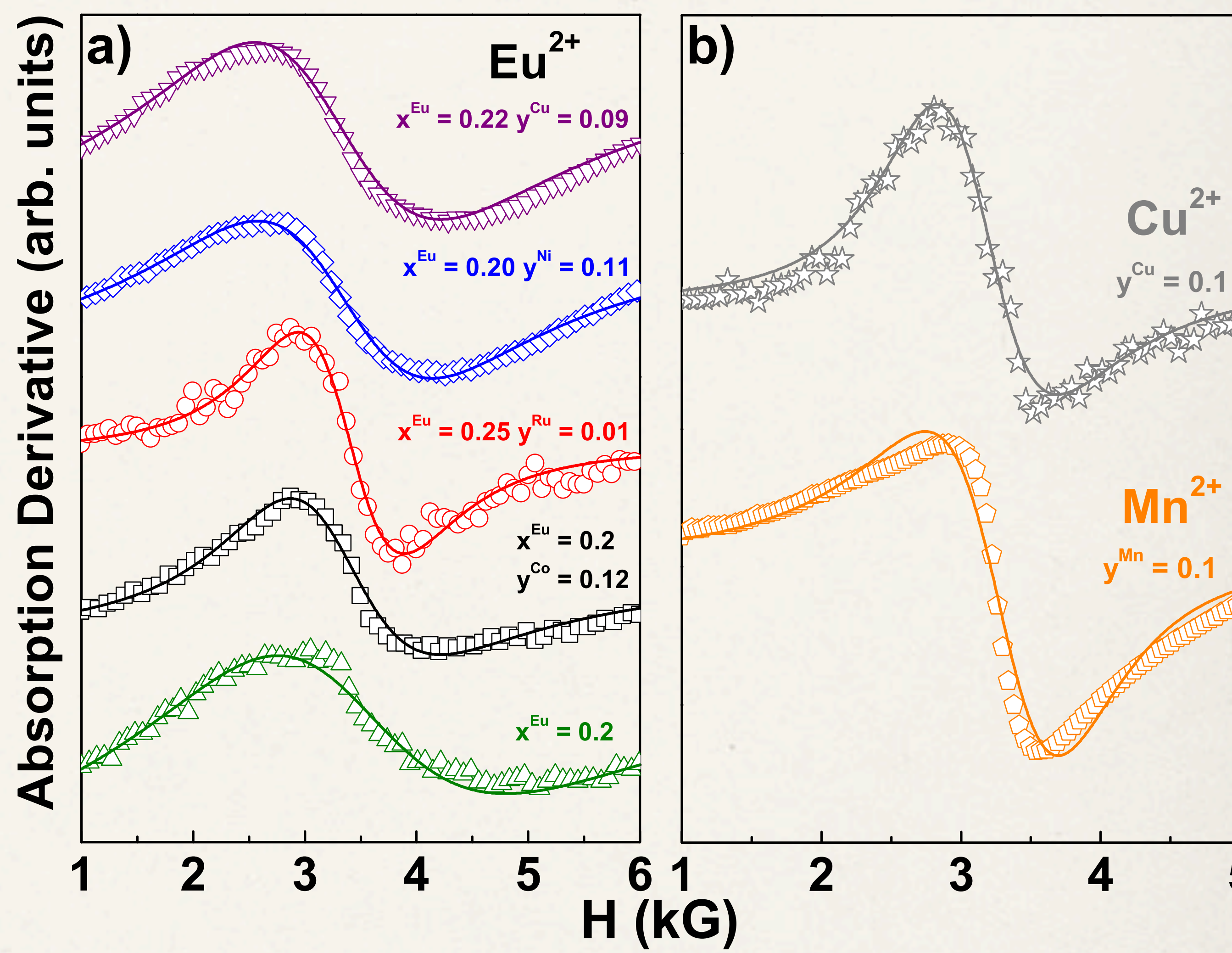
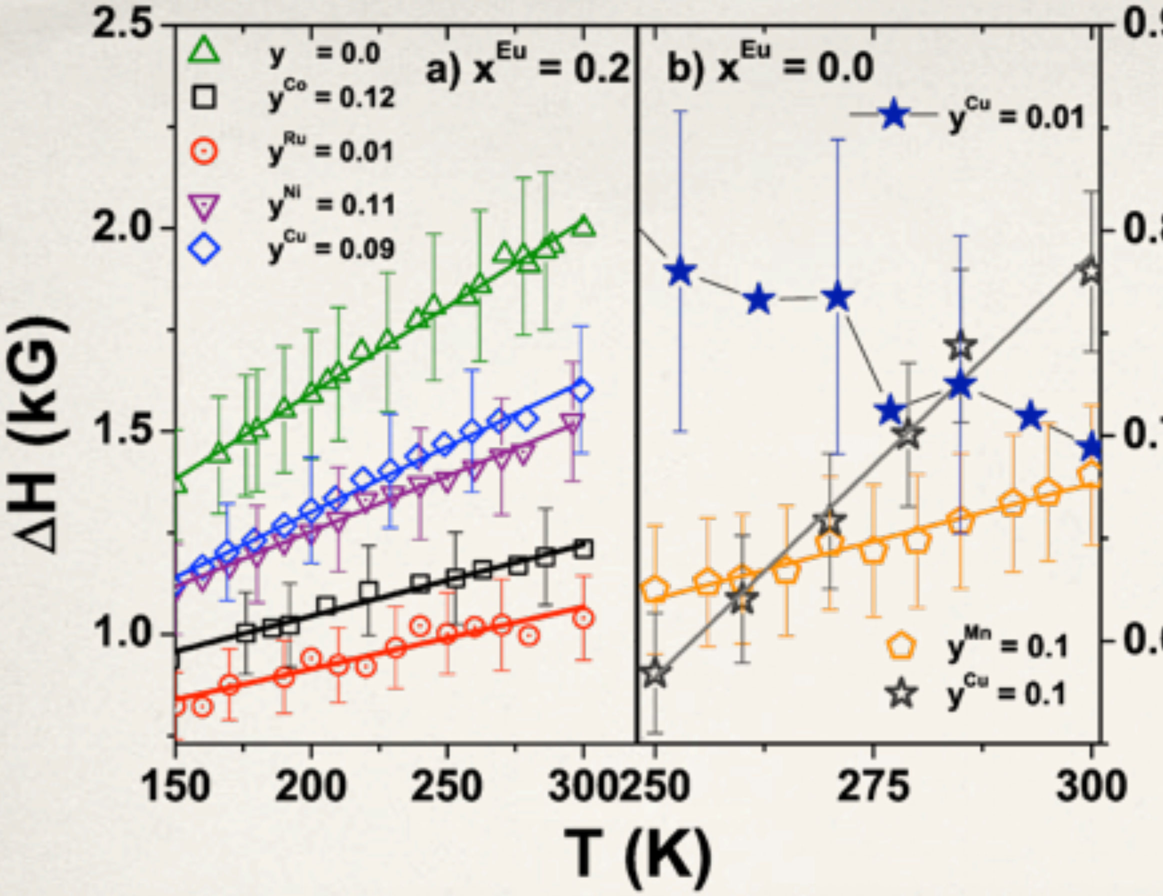
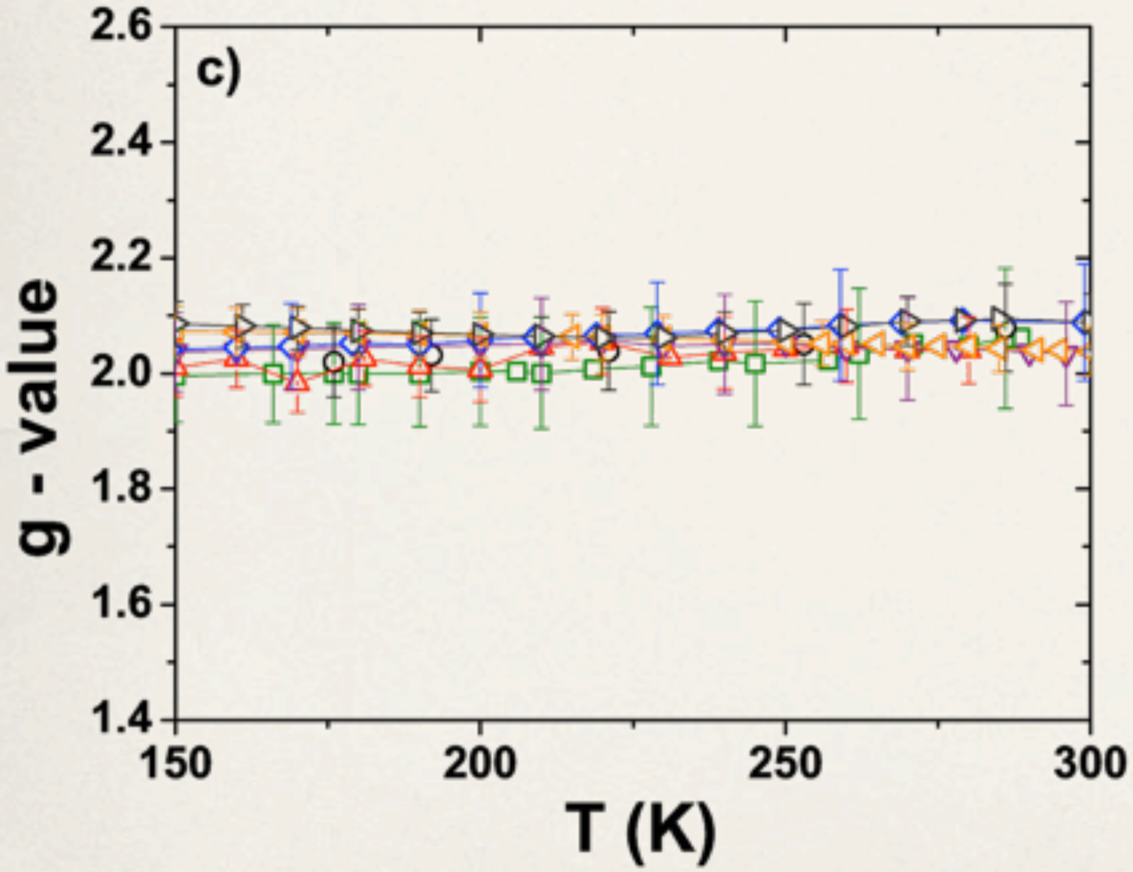
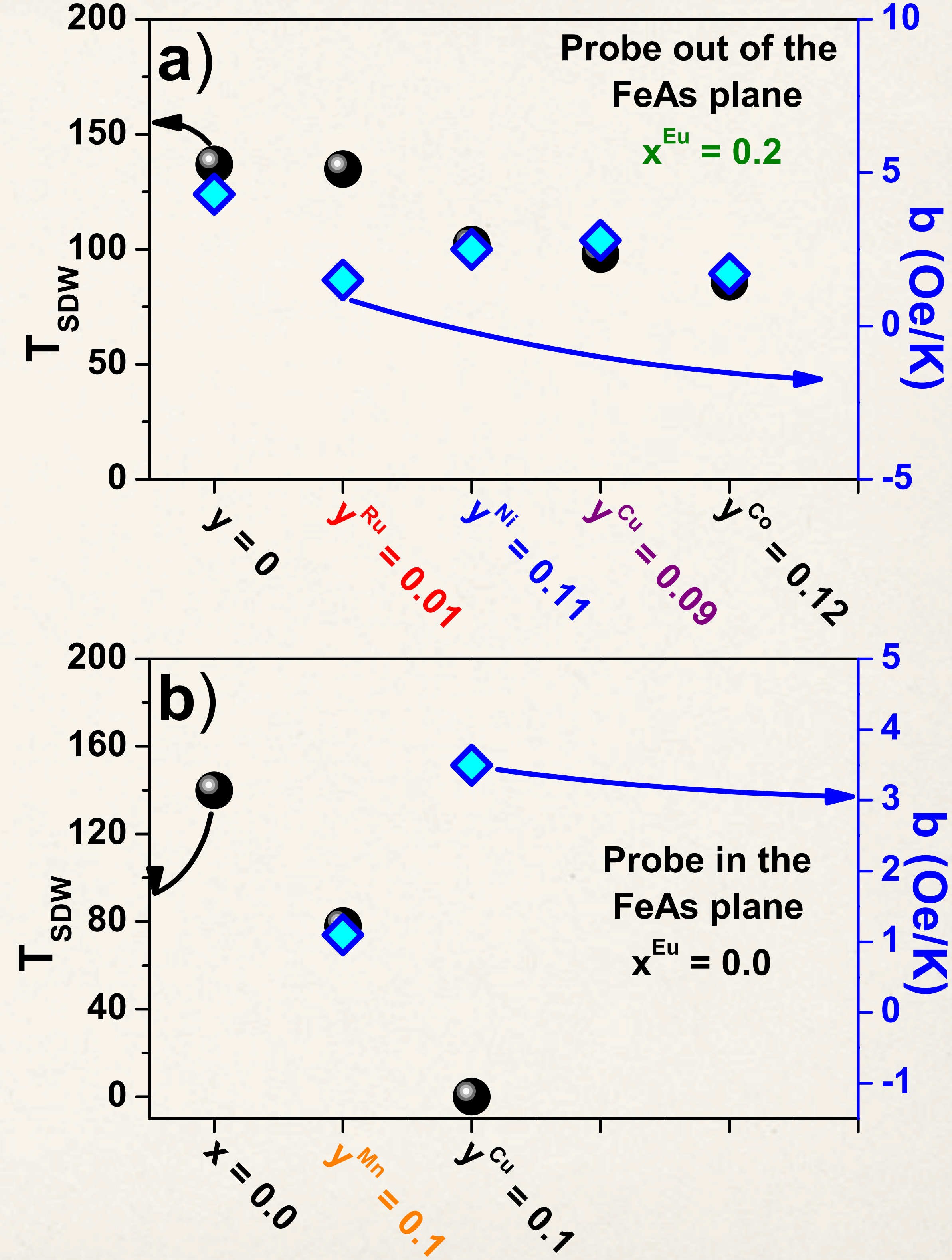





a) x^Eu = 0.2
b) x^Eu = 0.0
y = 0.0
y^Co = 0.12
y^Ru = 0.01
y^Ni = 0.11
y^Cu = 0.09
y^Cu = 0.01
y^Mn = 0.1
y^Cu = 0.1
ΔH (kG)
T (K)


c)
g - value
T (K)


a)
Probe out of the
FeAs plane
x^Eu = 0.2
T_SDW
b (Oe/K)
y = 0
y^Ru = 0.01
y^Ni = 0.11
y^Cu = 0.09
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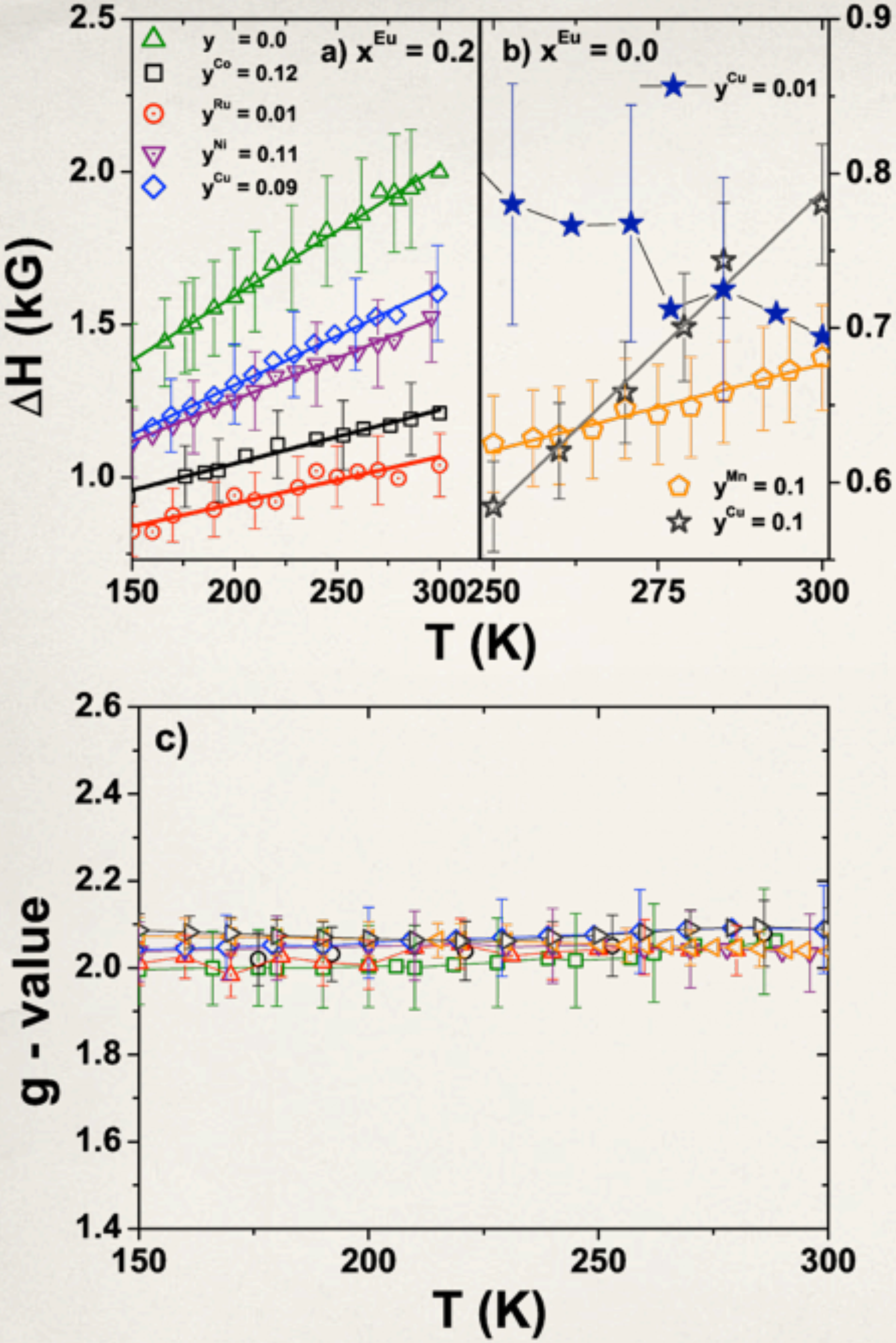
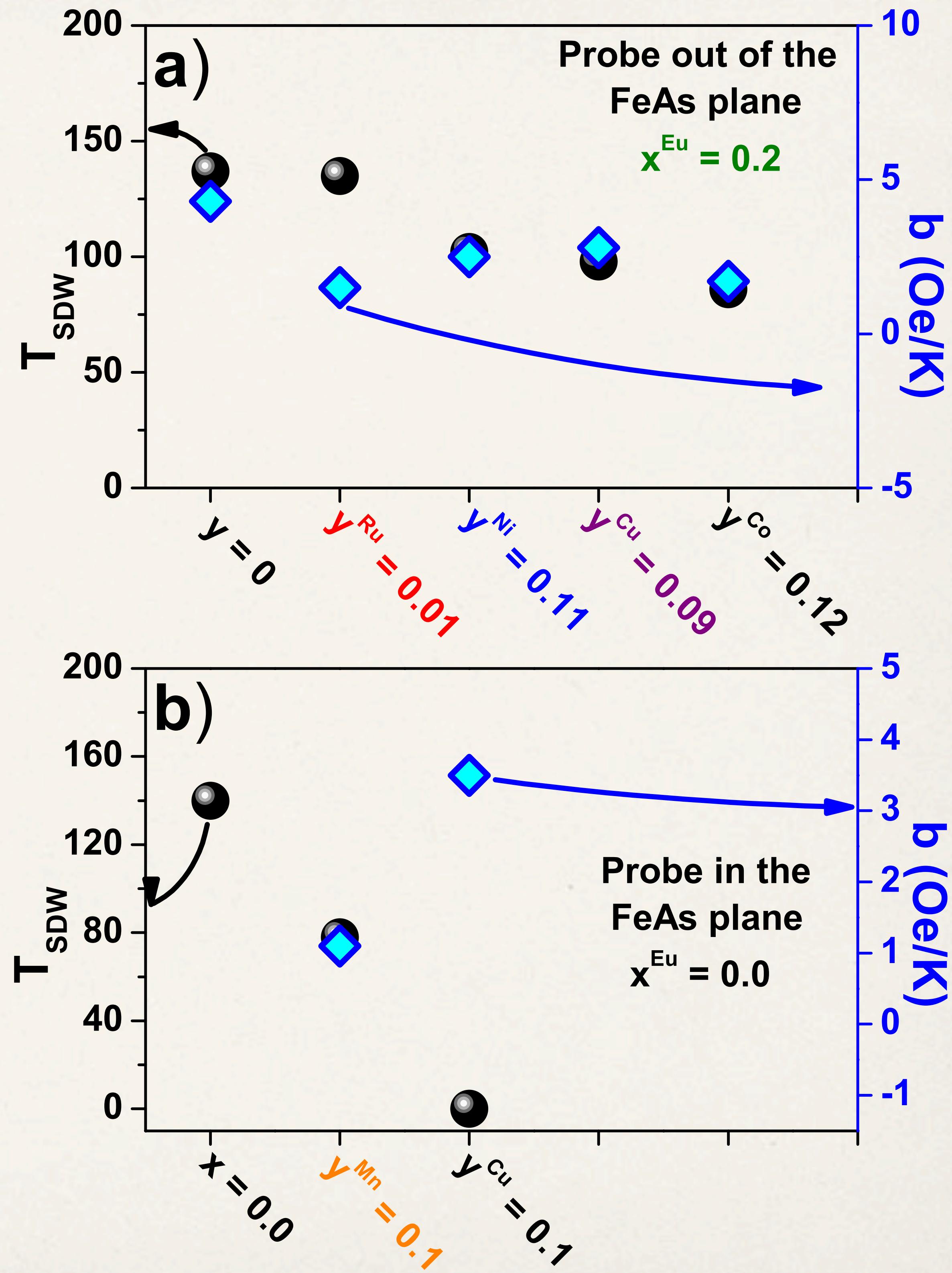
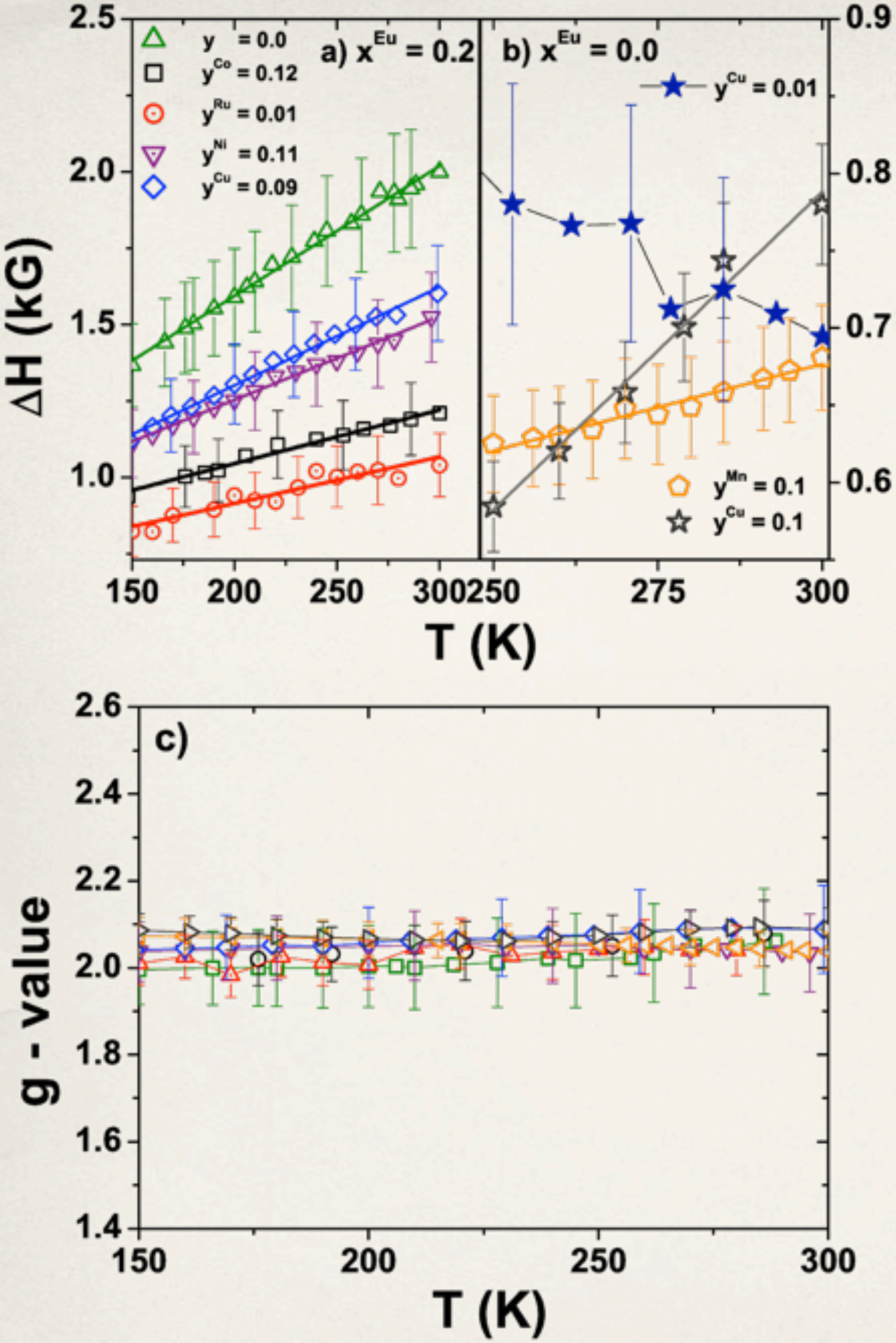
b)
Probe in the
FeAs plane
x^Eu = 0.0
x = 0.0
y^Mn = 0.1
y^Cu = 0.1



Eu^{2+} Korringa rate decreases for any substitution!





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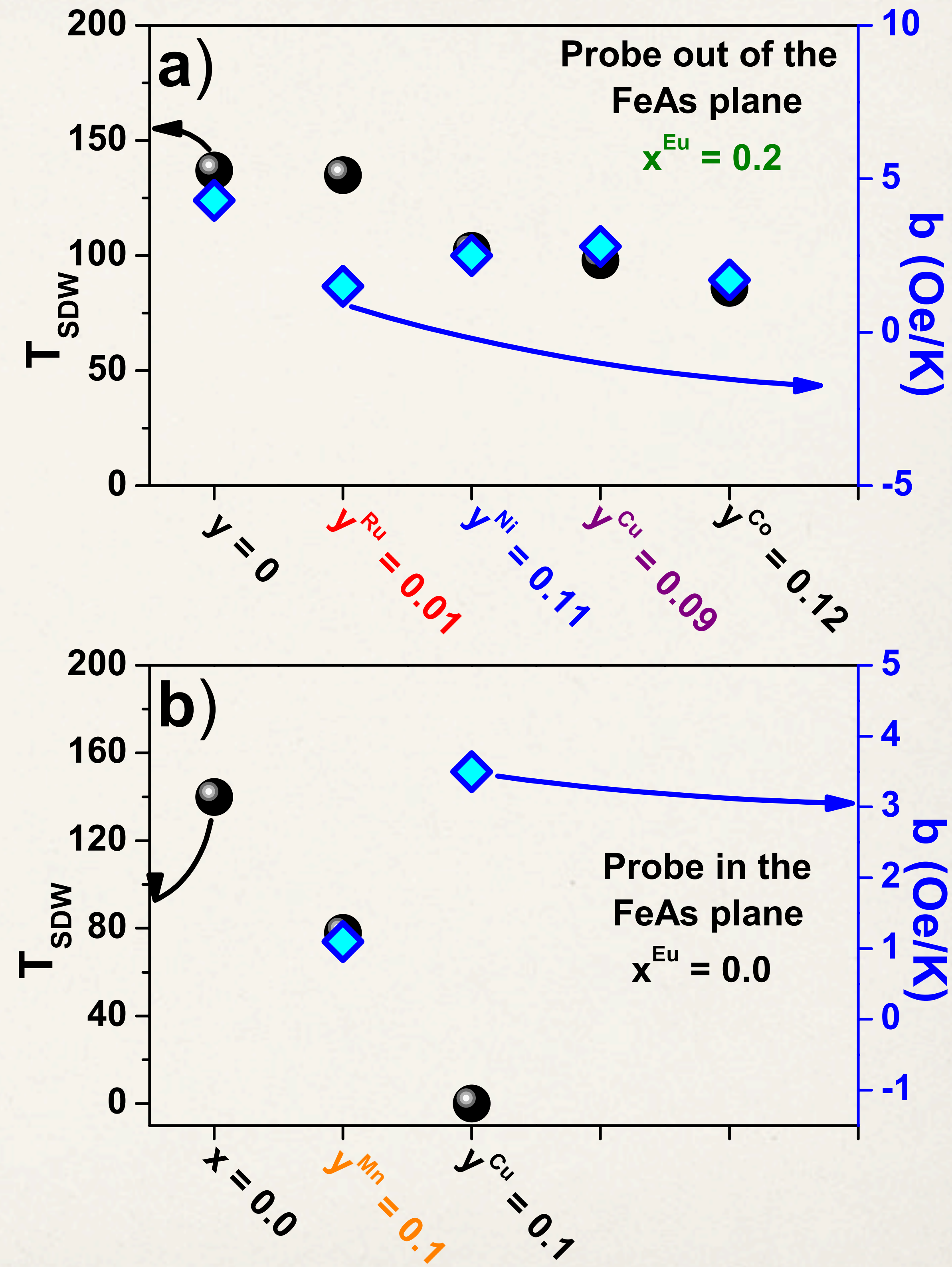

Mn^{2+} and Cu^{2+} Korringa rate increases as the SDW phase is suppressed!

Rosa, P.F.S. et al. Site specific spin dynamics in BaFe2As2: tuning the ground state by orbital differentiation. Sci. Rep. 4, 6543; DOI:10.1038/srep06543 (2014).

Outline

- Introduction and Motivation: Fe-based Superconductors
- Crystal Synthesis and Characterization
- Microscopic Techniques: X-Ray Absorption Spectroscopy (XANES and EXAFS) and Electron Spin Resonance (ESR)
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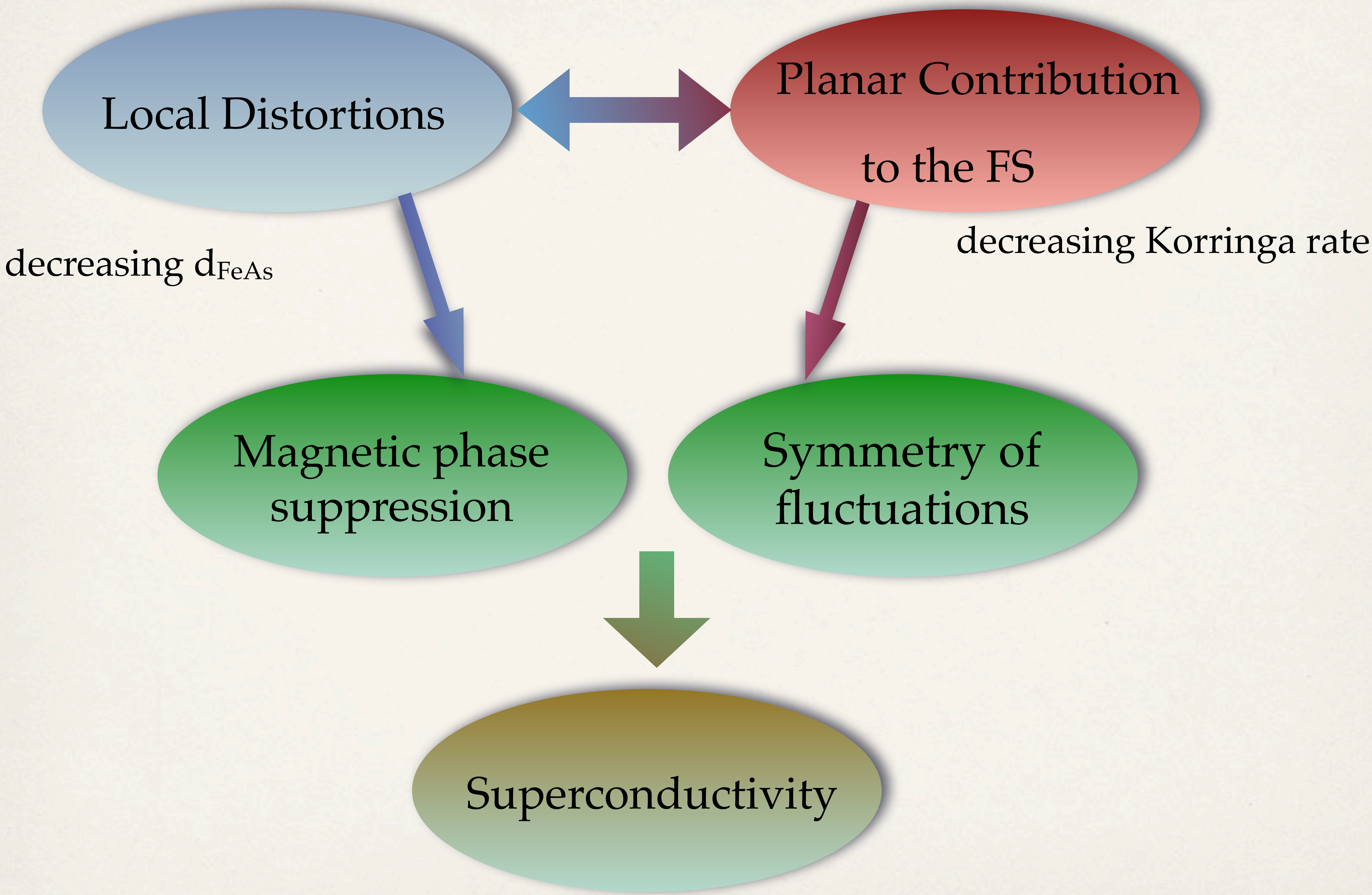
Local Distortions
Planar Contribution to the FS
decreasing d_{FeAs}
decreasing Korringa rate
Magnetic phase suppression
Symmetry of fluctuations
Superconductivity

Thank you for your attention!