Superconducting Fe-pnictides: lessons from the normal state

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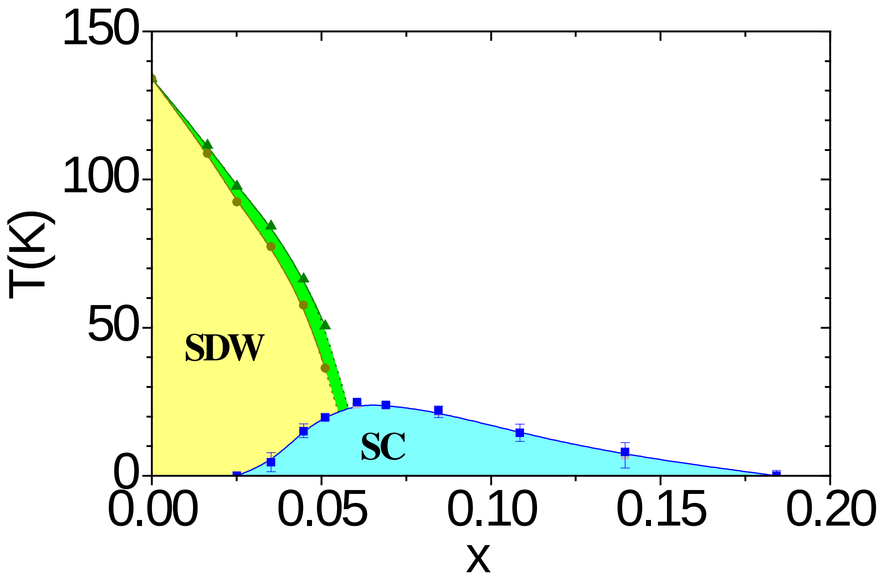


Acknowledgments

Stanford:
J. G. Analytis, J.-H. Chu,
F. Corredor, H.-H Kuo, C. Kucharzyk, H. M. Lewis
David Press, Kristiaan De Greve, Thaddeus D. Ladd, Yoshihisa Yamamoto

NHMFL:
R. McDonald, S. Riggs

Bristol:
A. Carrington, A. Coldea, C. Andrew, A. Bangura
S. Hayden

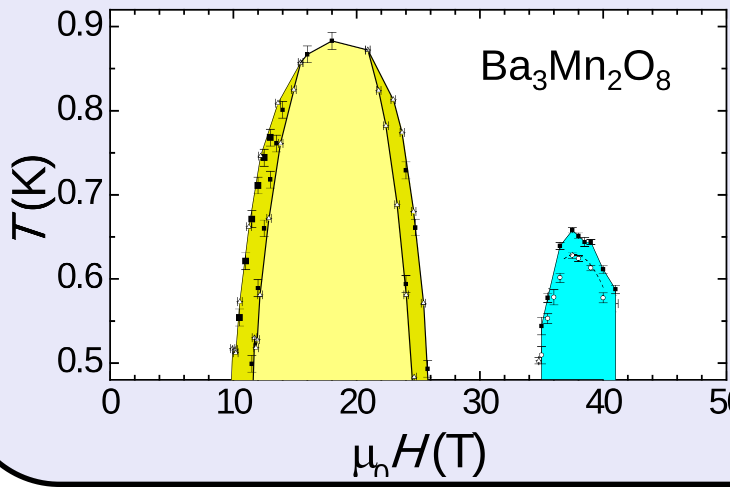
APS:
Z. Islam

NRL:
M. Johannes

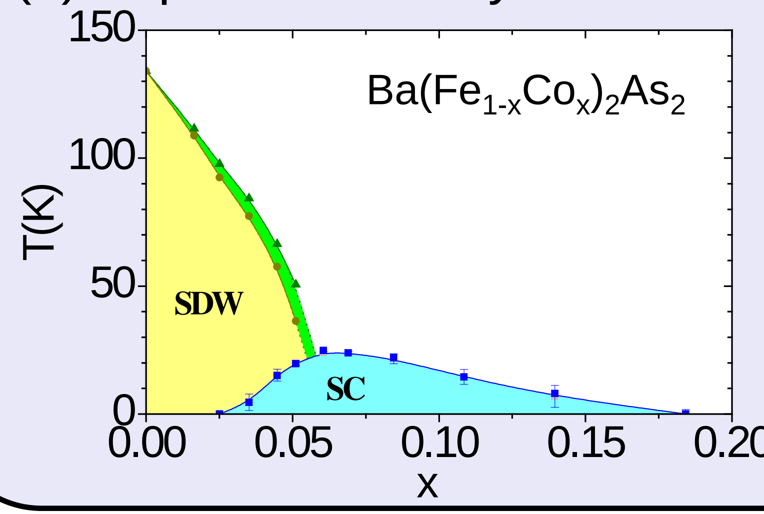
This work is supported by the Department of Energy, Office of Basic Energy Sciences under contract DE-AC02-76SF00515

Research program: New materials – unconventional magnetic & electronic ground states & phase transitions

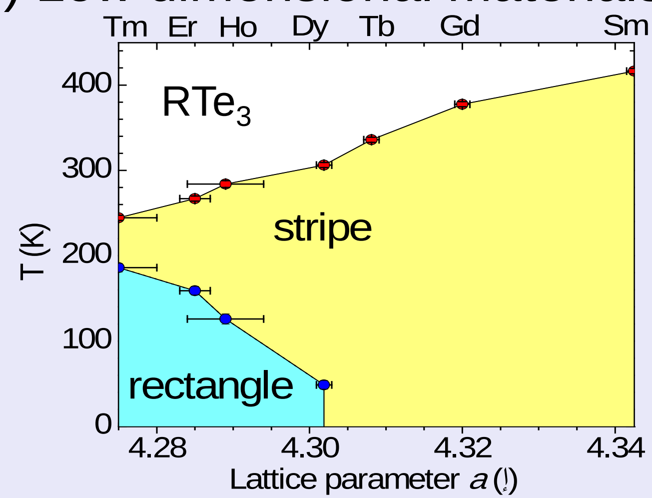
(1) Quantum magnetism:



(2) Superconductivity:

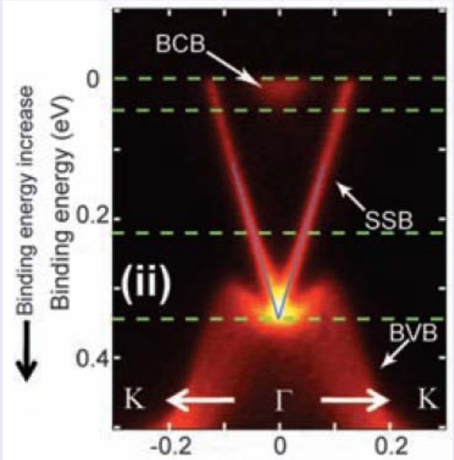


(3) Low dimensional materials:



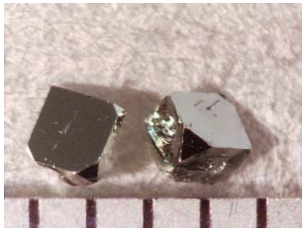
(4) Topological insulators:

Bi2Te3

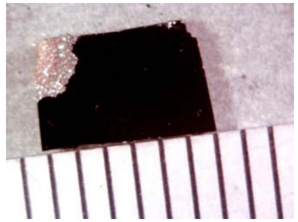


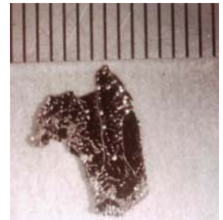
http://www.stanford.edu/group/Fisher

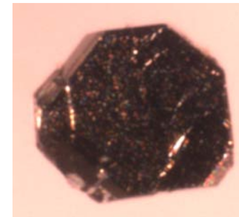
Crystal growth

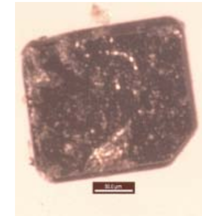

$Pb_{1-x}Tl_xTe$

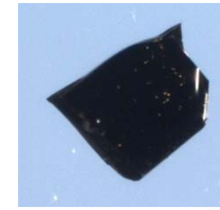

$Sn_{1-x}In_xTe$

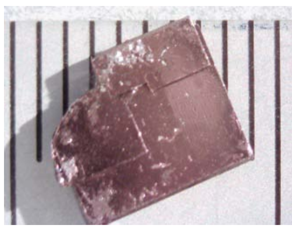

$BaPb_{1-x}Bi_xO_3$

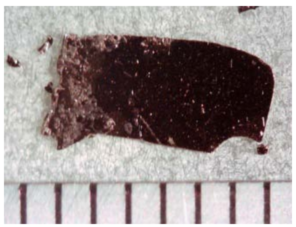

$BaFe_2As_2$

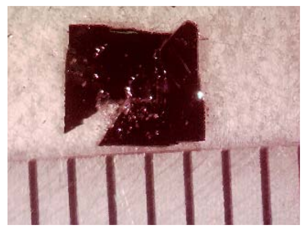

$CaFe_2P_2$


LaFePO


$CsAuI_3$

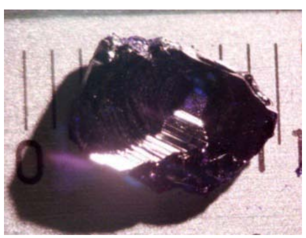

RTe_3

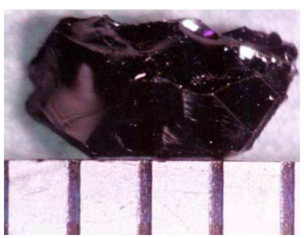

RTe_2


R_2Te_5

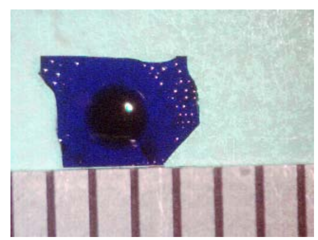

Bi_2Se_3


Bi_2Te_3

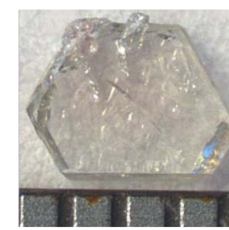

$BaCuSi_2O_6$

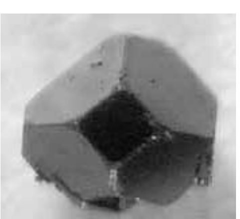

$Sr_2Cu(BO_3)_2$

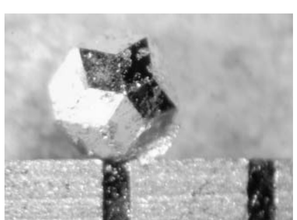
$Ba_2Cu(BO_3)_2$

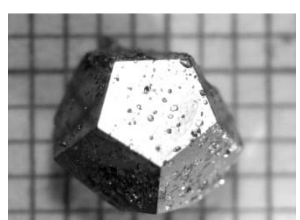

$BaCu_2Si_2O_7$

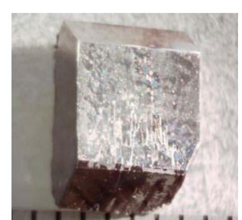
$Ba_3Mn_2O_8$


$Ba_3V_2O_8$


Ba_2NaOsO_6

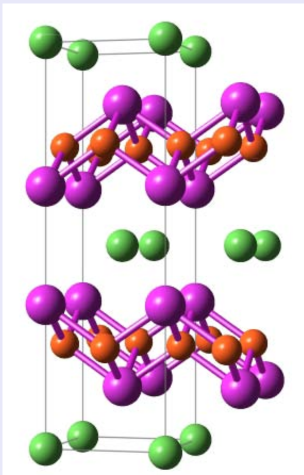

R-Mg-Cd


Al-Pd-Re


$R_6Mo_4Al_{43}$

Fe-arsenides

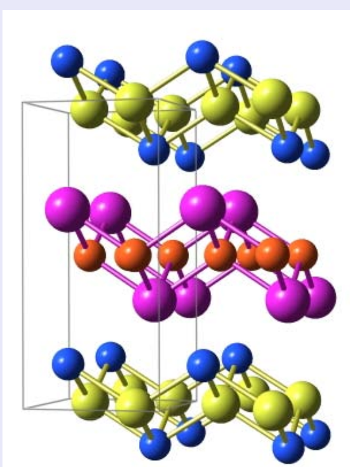
"122":



$Ba_{0.5}$

FeAs

"1111":

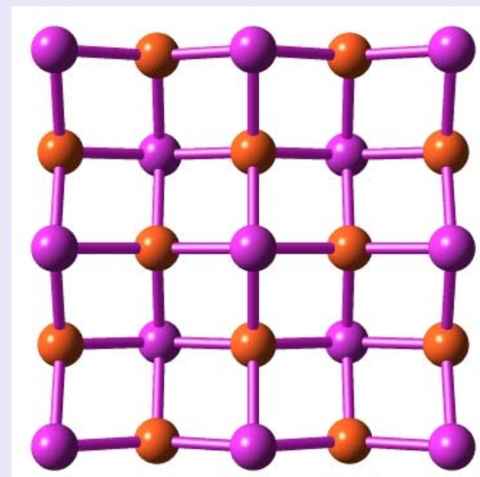


LaO

FeAs

e^-

$Ba_{0.5}(FeAs)$

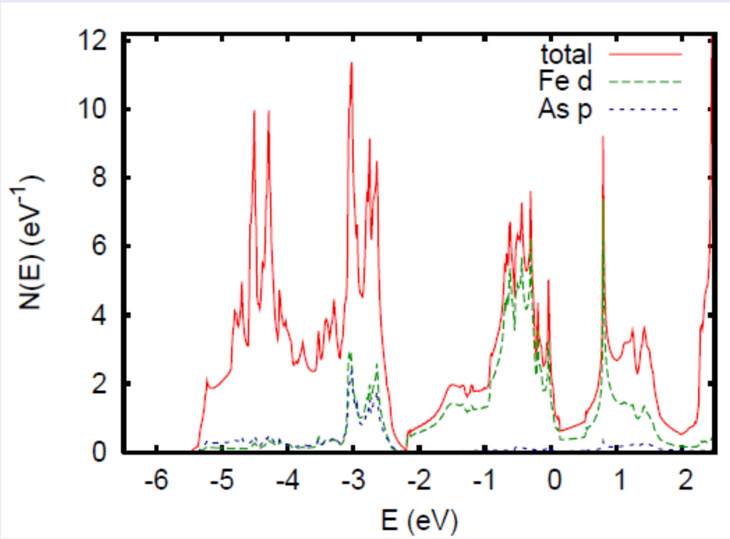


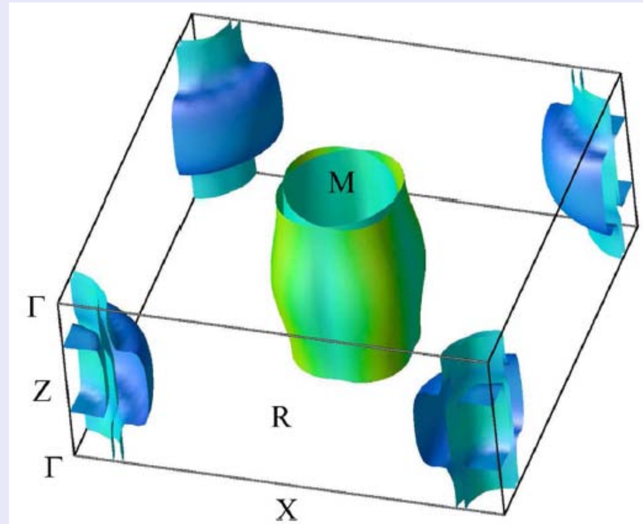
e^-

(LaO)(FeAs)

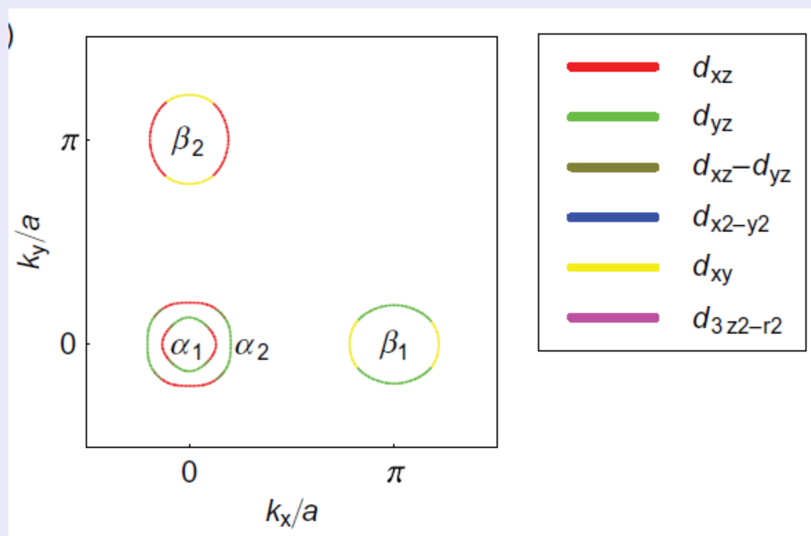
Electronic structure

eg: LaFeAsO





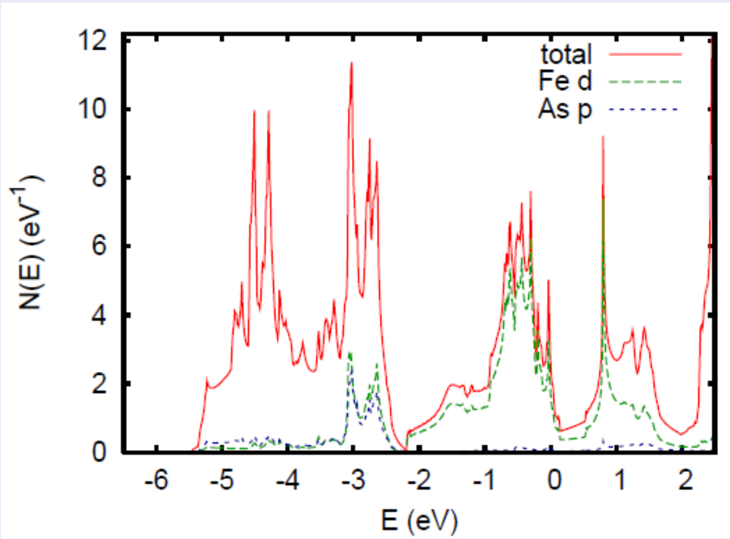
Singh & Du, PRL **100** 237003 (2008).
Singh Physica C **469**, 418 (2009).

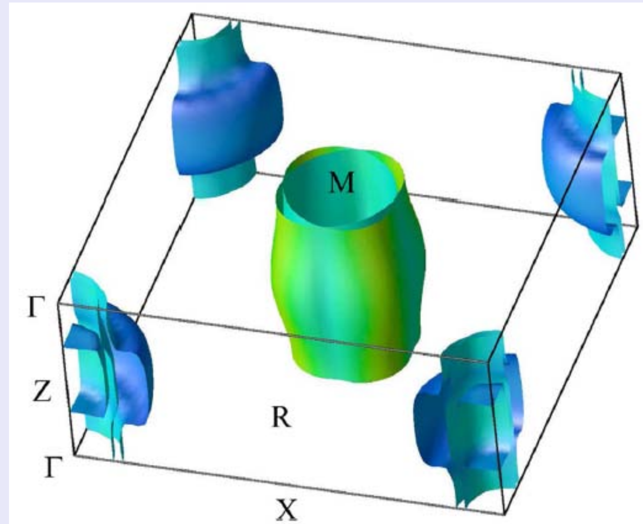


Graser et al, NJP **9**, 025016 (2009).

Electronic structure

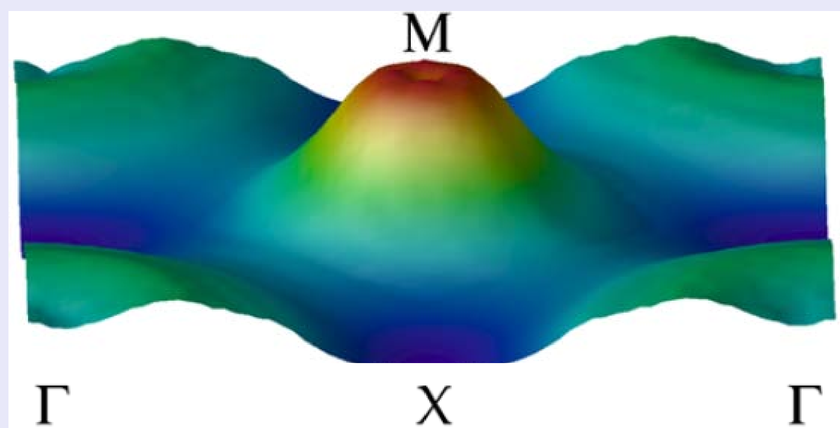
eg: LaFeAsO





Singh & Du, PRL **100** 237003 (2008).
Singh Physica C **469**, 418 (2009).

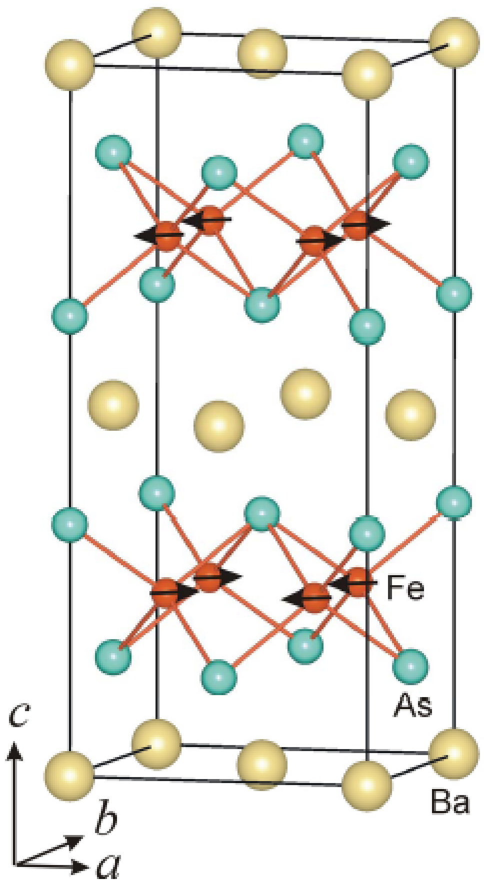
$$\chi(q) \propto \int \frac{f_k - f_{k+q}}{E_k - E_{k+q}} d^3k$$



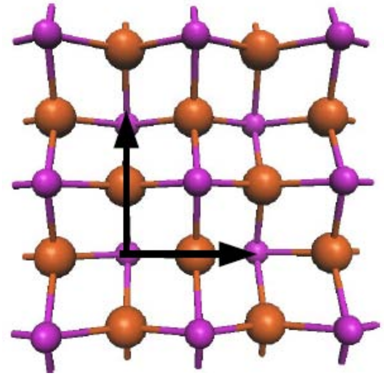
Mazin, et al, PRL **101**, 057003 (2008).

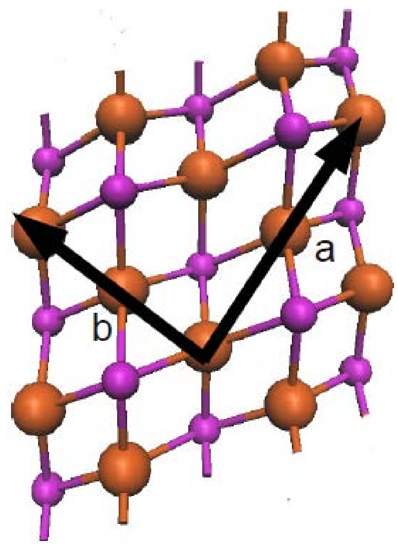
Antiferromagnetism & superconductivity

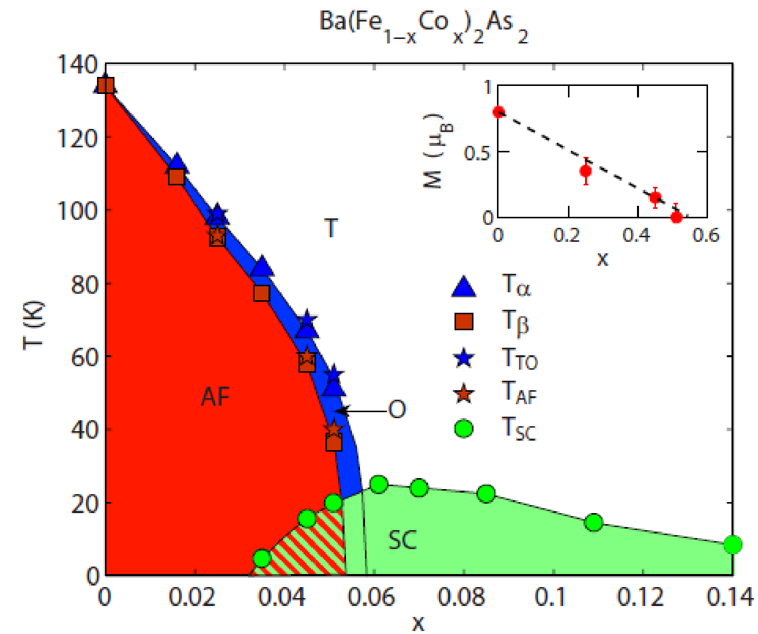
eg: $Ba(Fe_{1-x}Co_x)_2As_2$



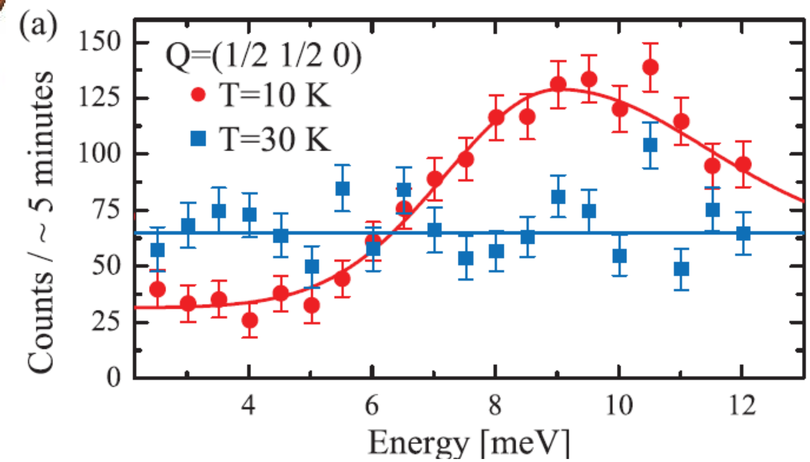
Huang, Lynn et al, PRL **101**, 257003 (2008).







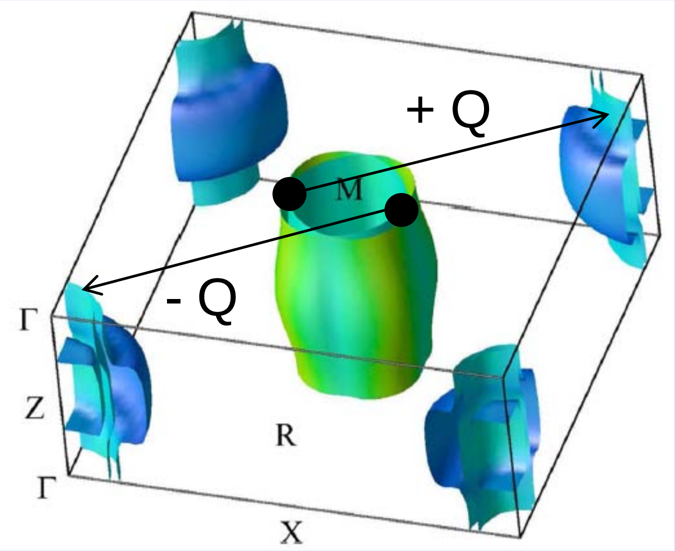
Hayden et al, PRB **79**, 144523 (2009).



Lumsden et al, PRL **102**, 107005 (2009).

The pairing mechanism?

Spin-fluctuation scattering?



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

$$\Delta_k = -\sum_{k'} \frac{V_{k,k'}\Delta_{k'}}{2E_{k'}}$$

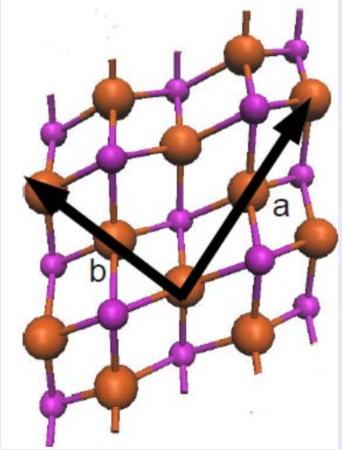
Key point:
If we are to determine whether this is a realistic scenario, we must know more about the actual electronic structure and Fermi surface of the doped material

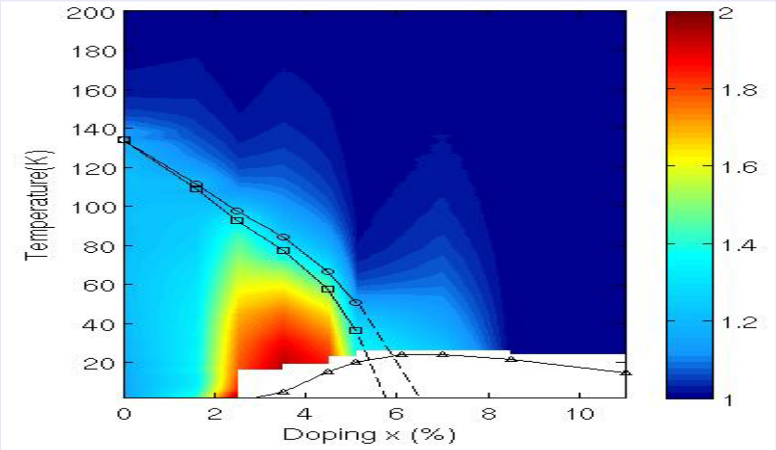
Two questions

(1) What drives the ortho transition, and is it significant?

Is the electronic structure altered in any profound way?

In plane electronic anisotropy in $Ba(Fe_{1-x}Co_x)_2As_2$:



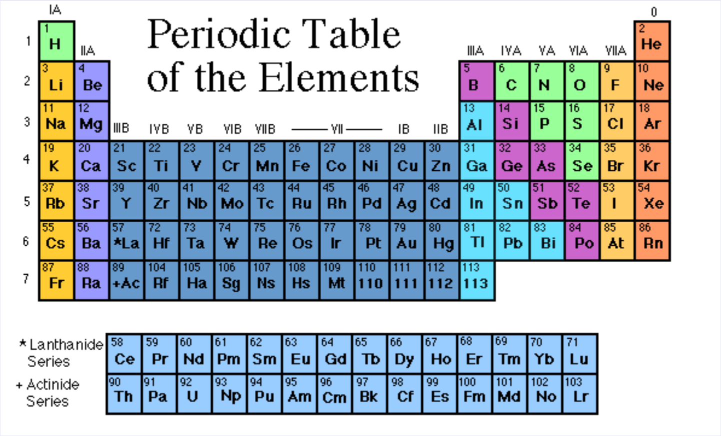


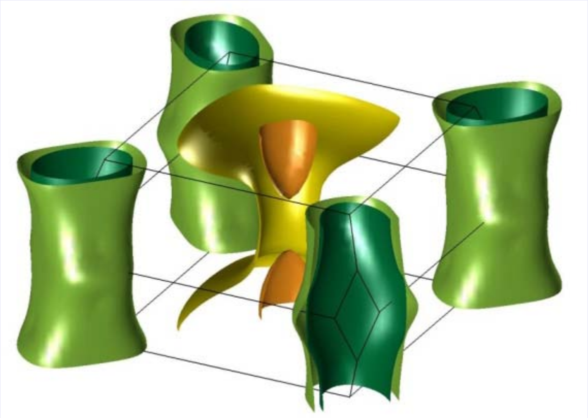
Two questions

(2) What role does Fermi surface nesting really play?

Does the phase diagram correlate with changes in the FS morphology?

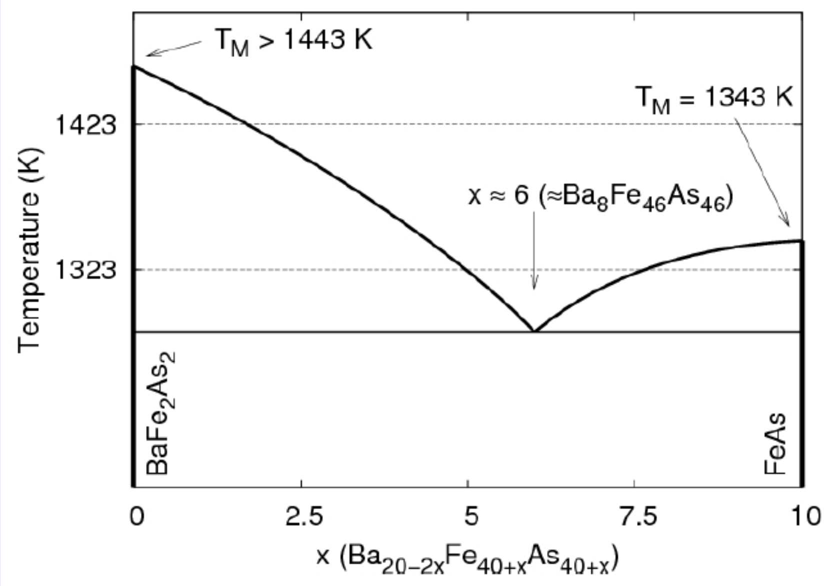
Fermiology of $BaFe_2(As_{1-x}P_x)_2$:





A bit about synthesis

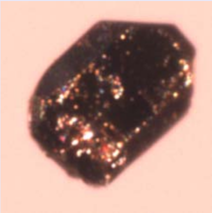
Self flux:

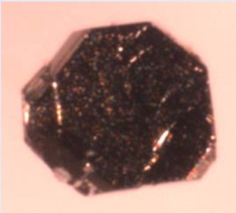


T. Sato J. Appl. Phys. **48** 013004 (2009).

- AFe_2As_2 (A = Ca, Sr, Ba)
- $Ba(Fe_{1-x}Co_x)_2As_2$
- $BaFe_2(As_{1-x}P_x)_2$
- *etc*

Sn flux:



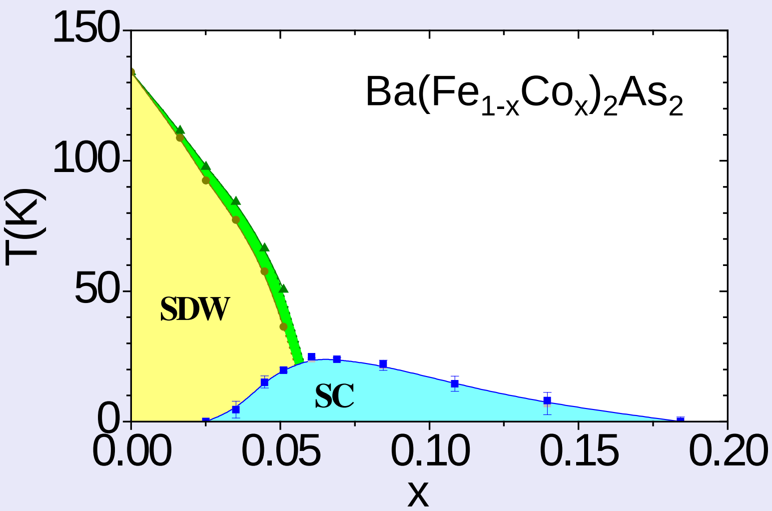


- LaFePO
- LaFeAsO
- AFe_2P_2 (A = Ca, Sr, Ba)
- *etc*

Principle hazards:

- high vapor pressure (P, As)
- reactive (Ba, K)
- toxic (As)

Part 1: The orthorhombic transition

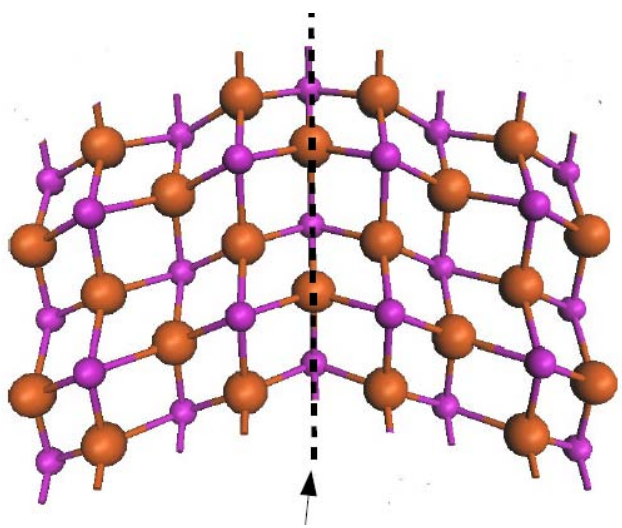


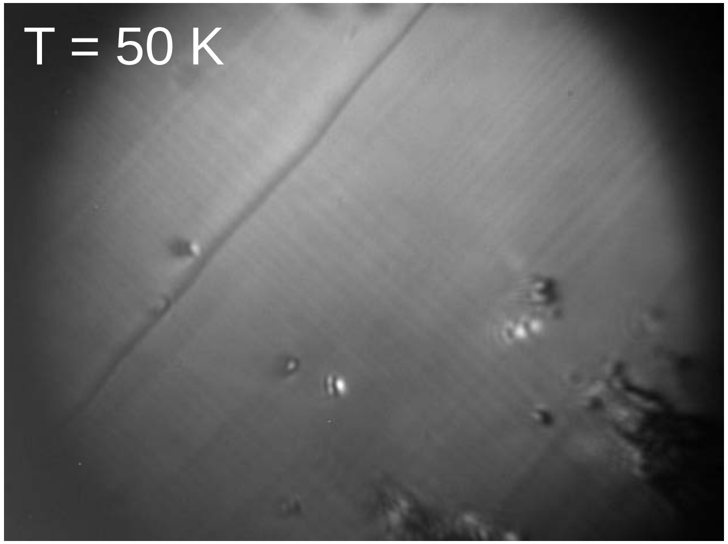
What drives the orthorhombic transition?

Why should we care?

(1) SDW & SC born out of it!

(2) Are fluctuations associated with the additional QCP important?





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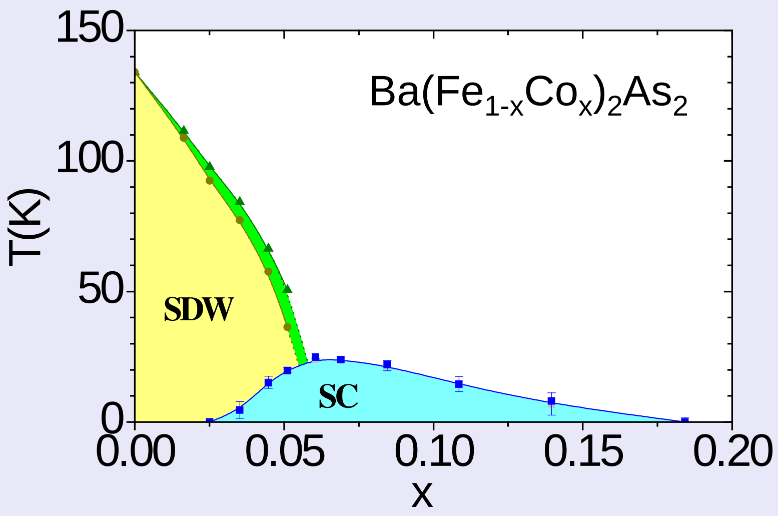

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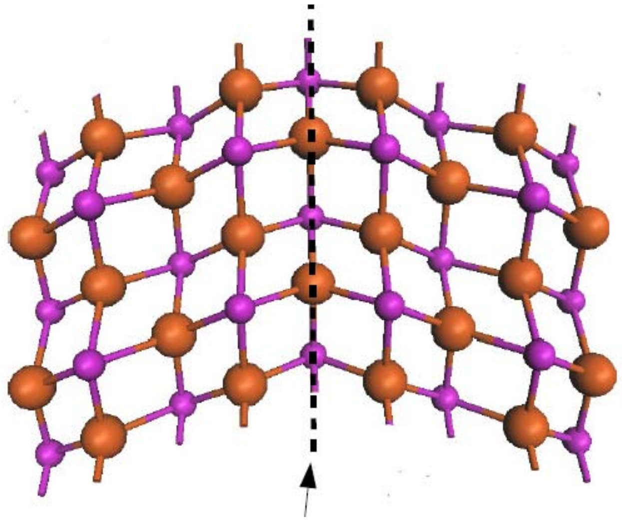
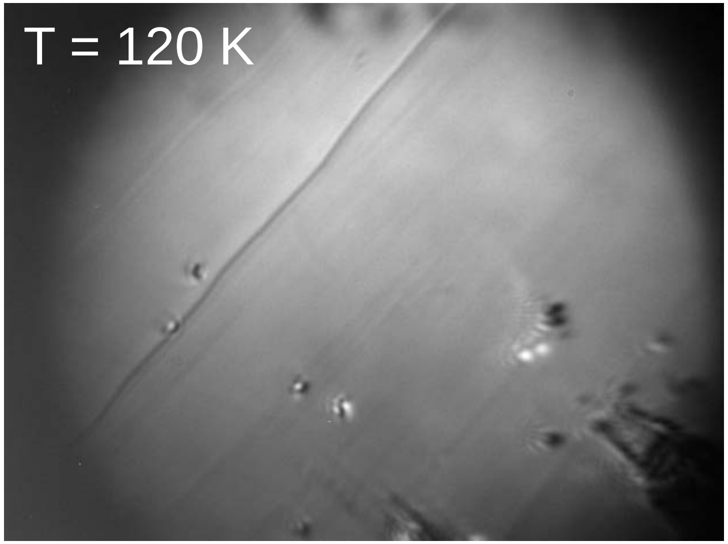
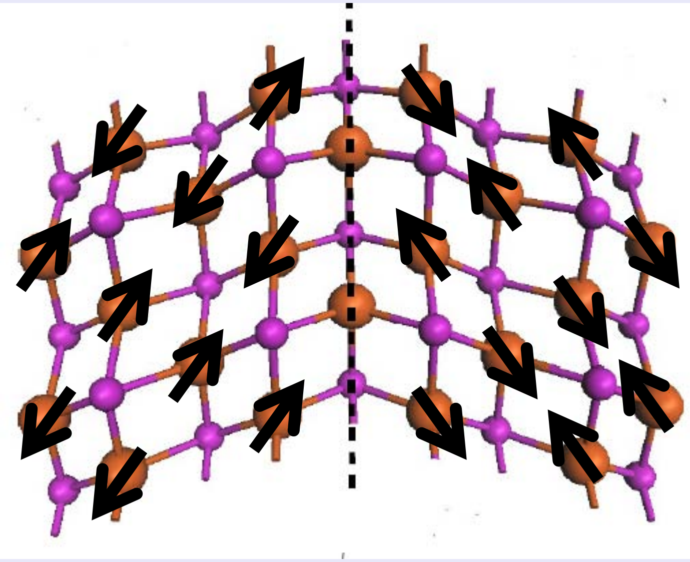


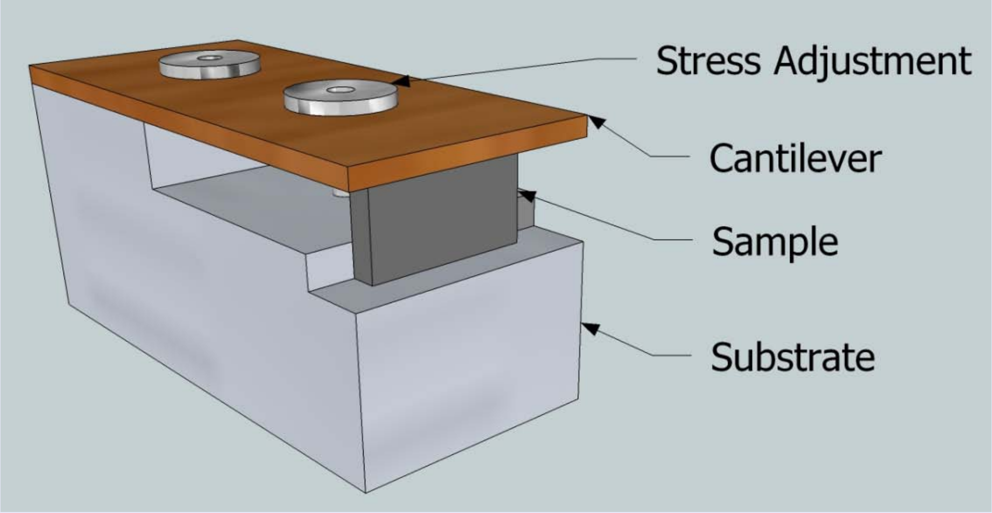


Two avenues to detwin underdoped samples in situ

In-plane magnetic field:



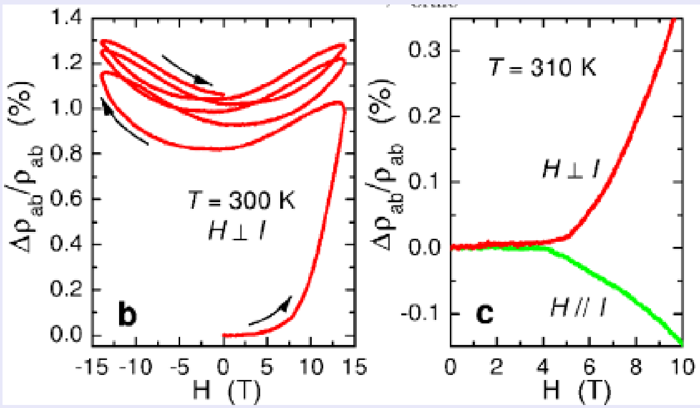
Isostatic pressure:

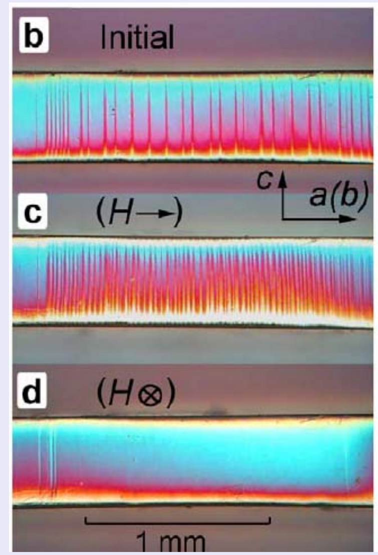


Two avenues to detwin underdoped samples in situ

In-plane magnetic field:

eg. $La_{2-x}Sr_xCuO_4$

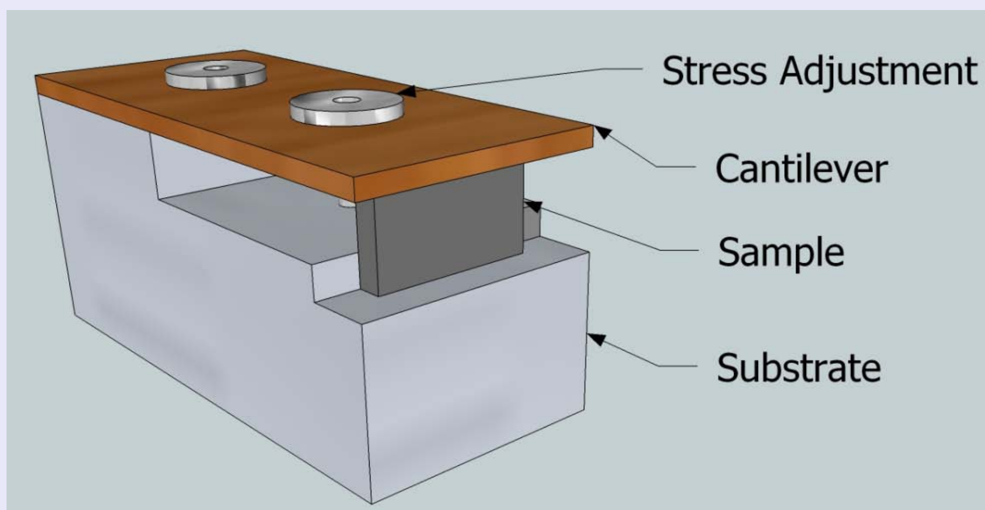




Ando et al, Nature **418**, 385 (2002).

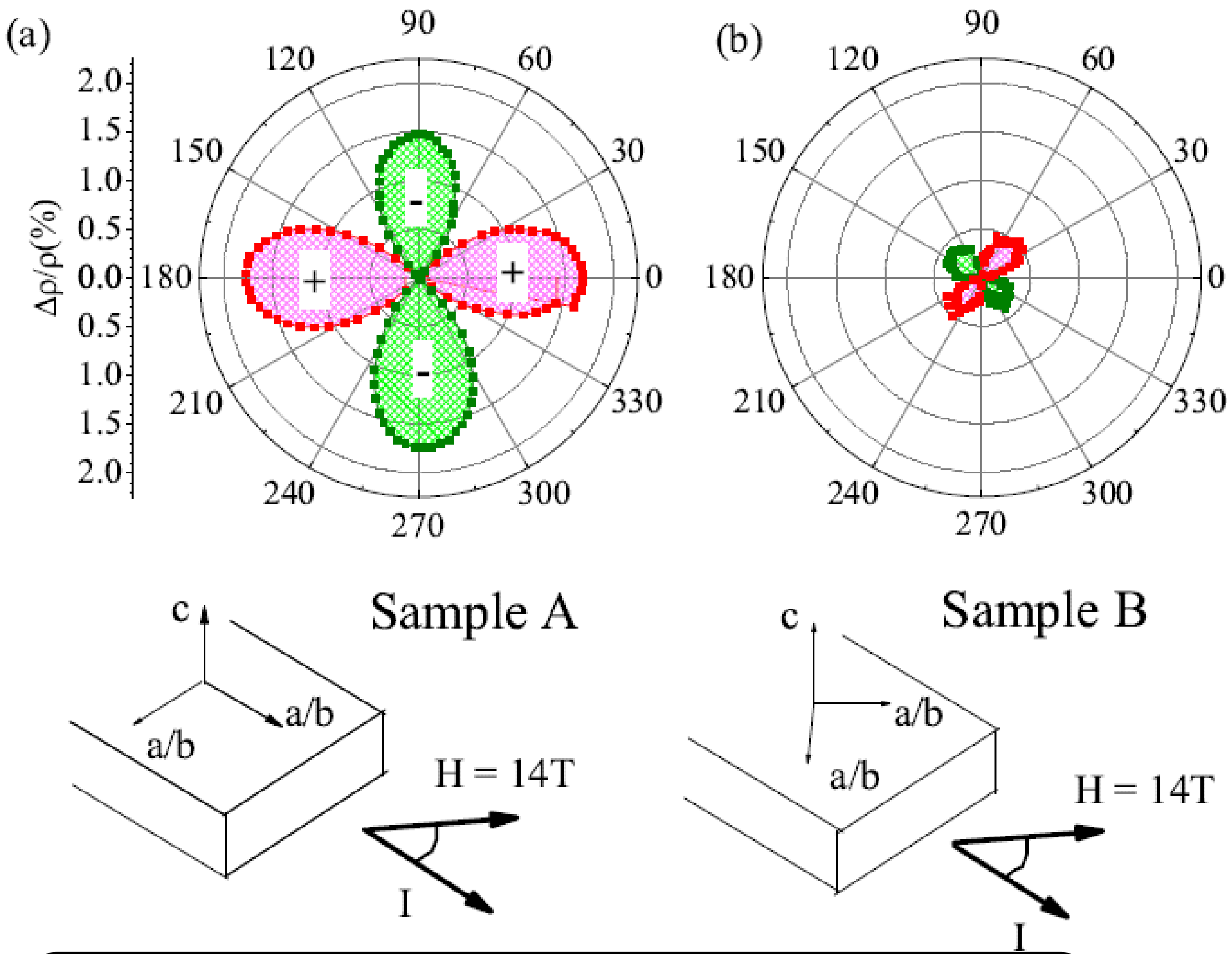
- Is a similar effect operative in the pnictides?

Isostatic pressure:



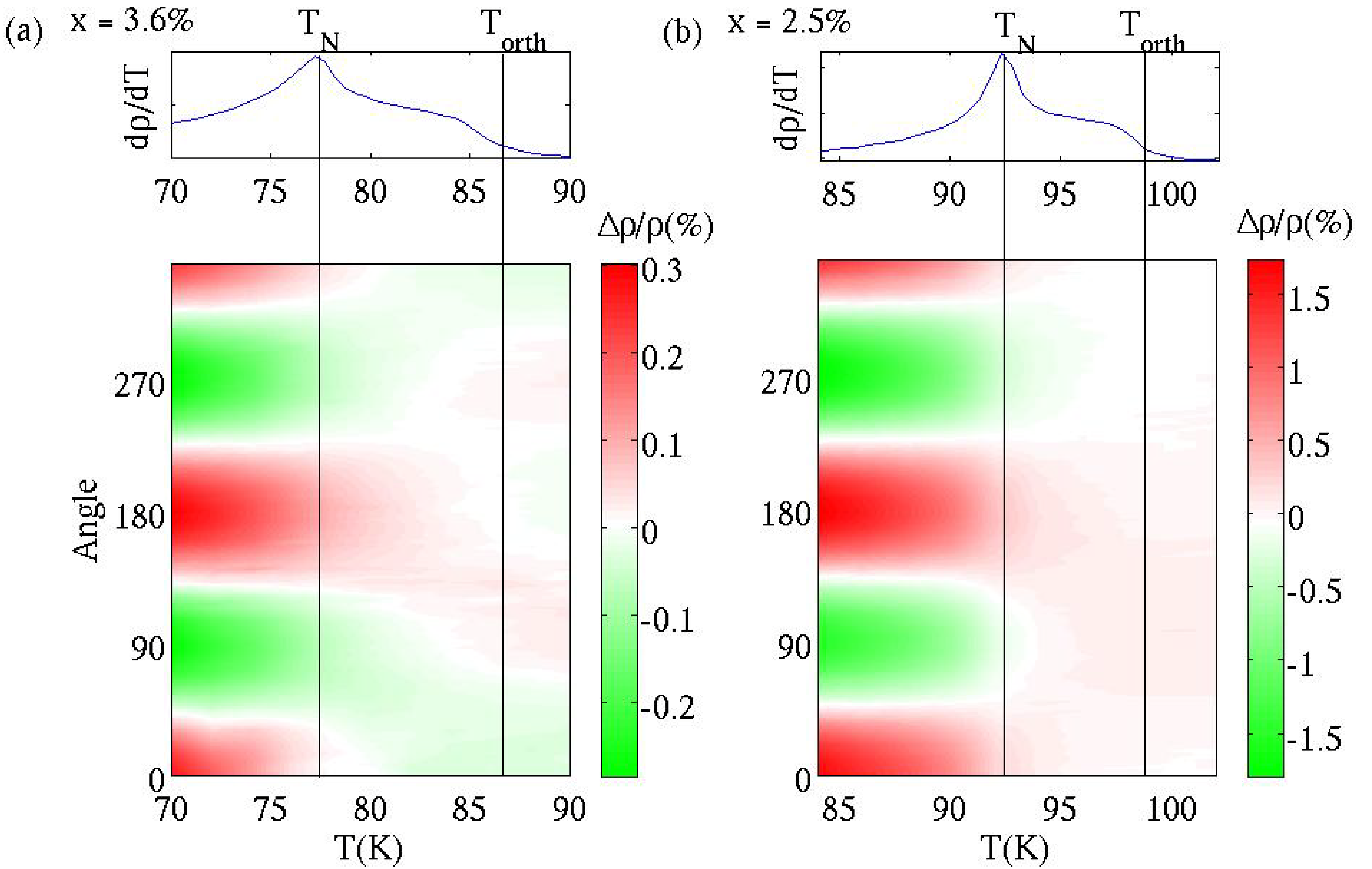
In-plane magnetoresistance

e.g. x = 2.5% at 84 K
T_{ortho} = 98. 5 K
T_N = 92.5 K



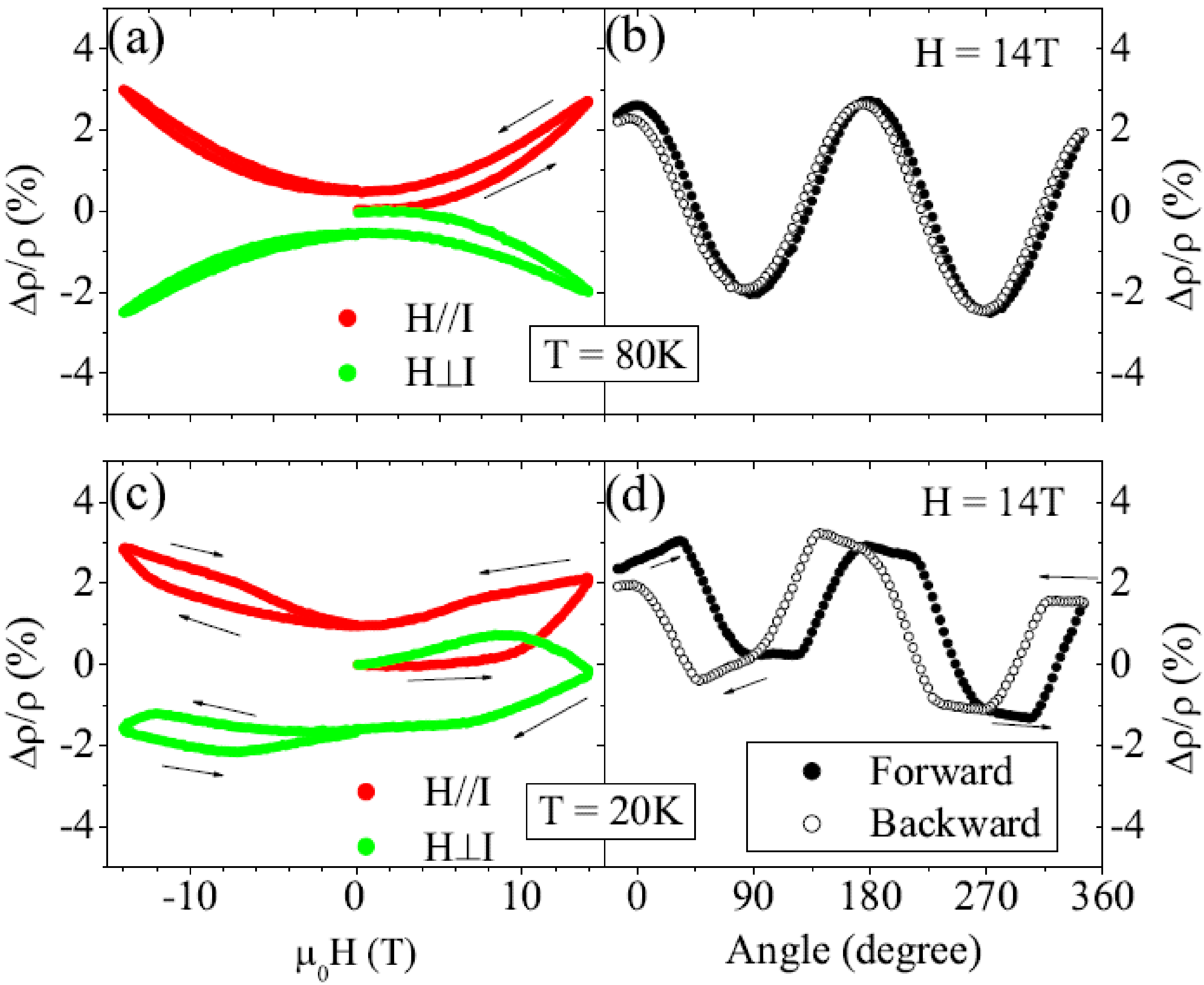
- Substantial in-plane magnetoresistance
- Tied to crystal axes (largest for H || a,b)

T-dependence



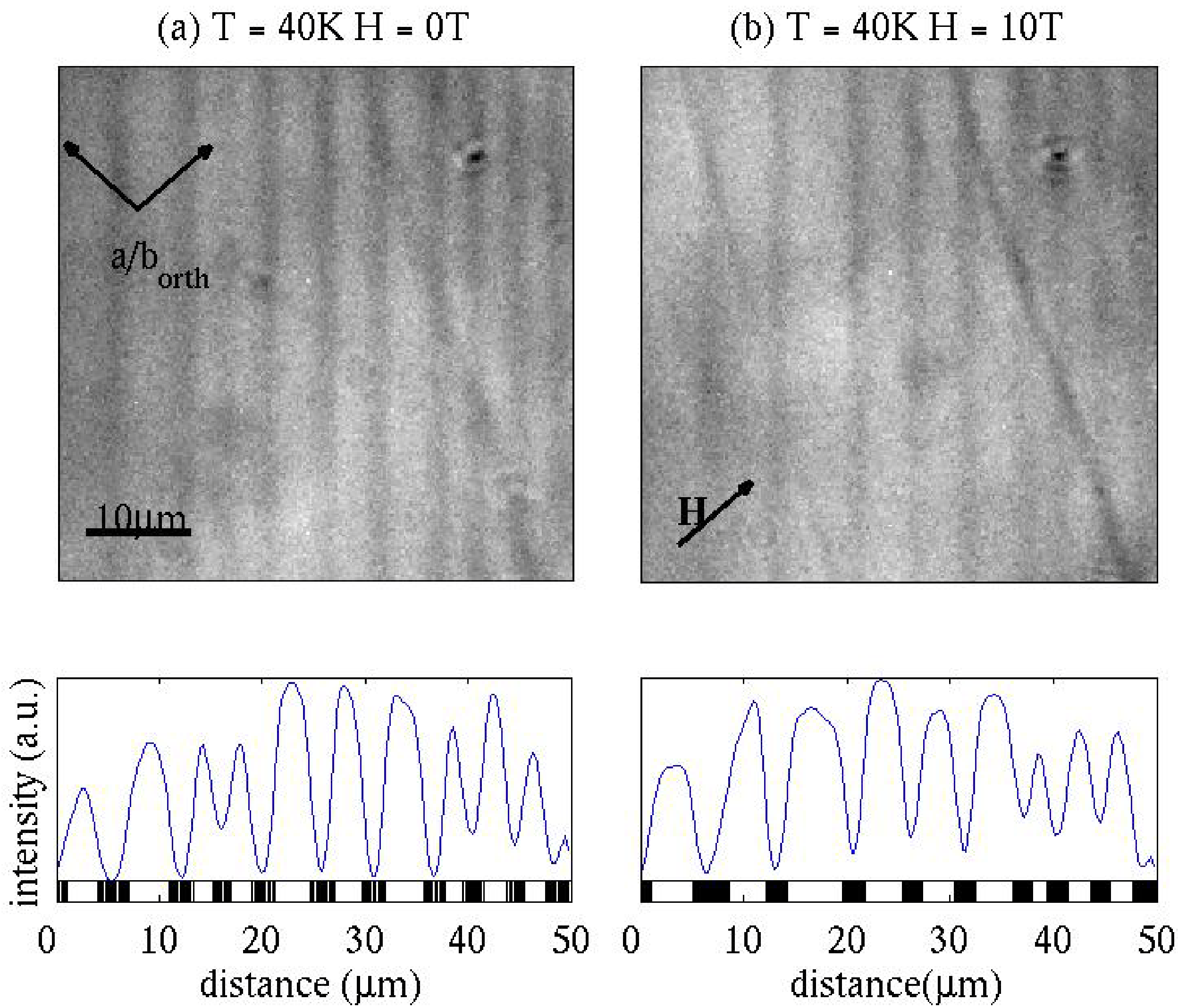
Chu *et al*, arXiv 0911.3878

Hysteresis



Chu *et al*, arXiv 0911.3878

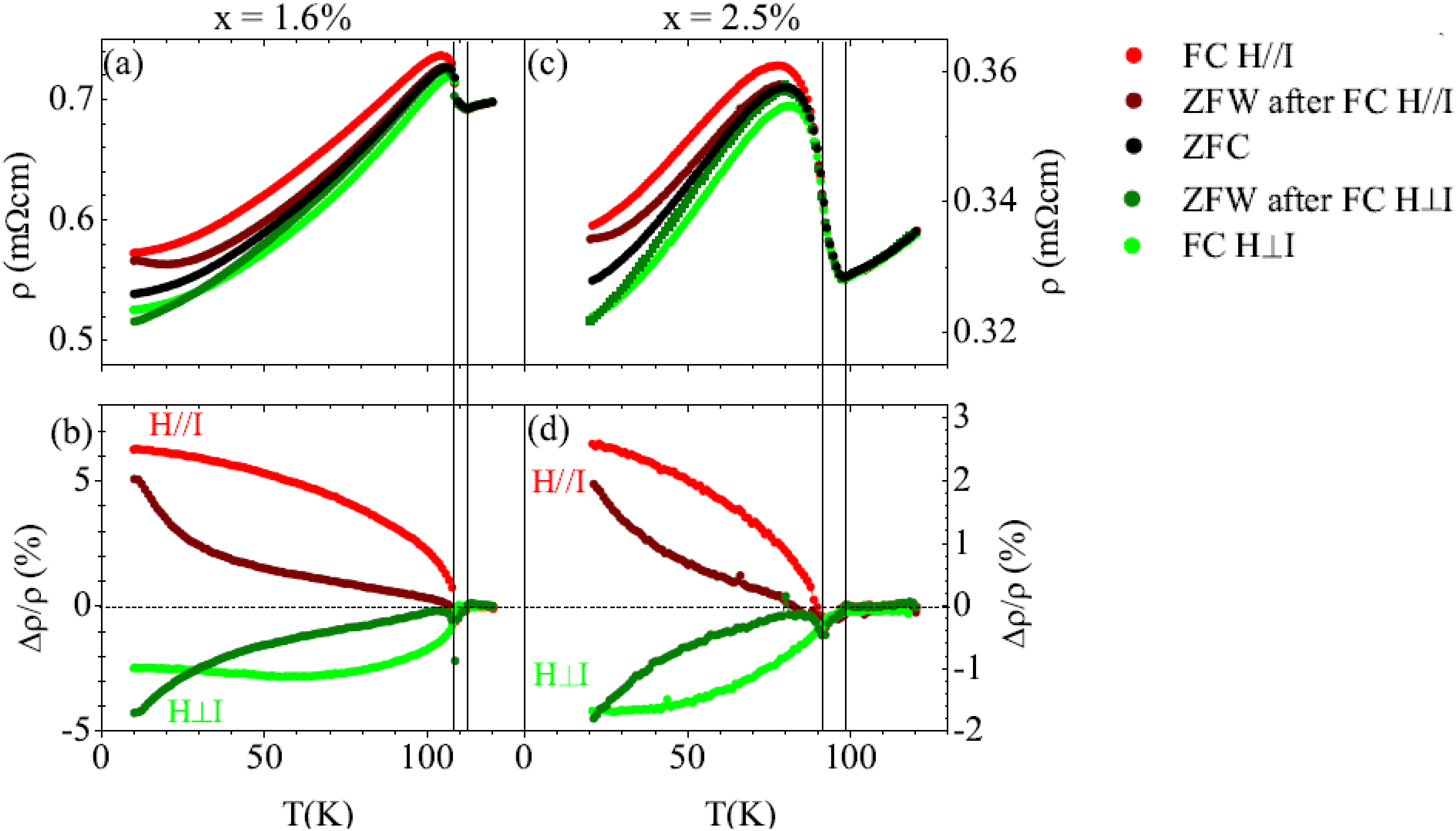
Optical evidence for detwinning



$$f = \frac{V_b}{V_a + V_b} \approx 54\,\%$$

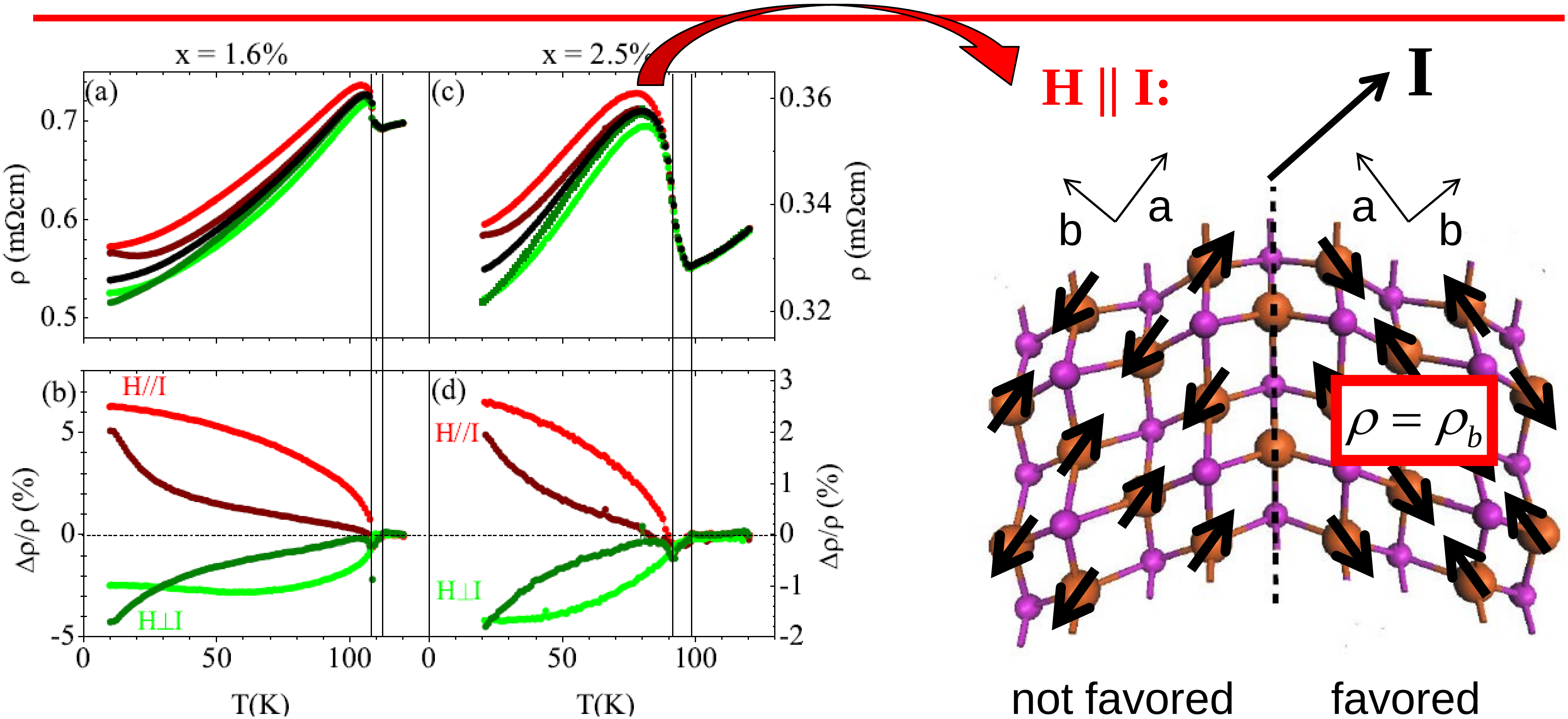
$$\approx 61\,\%$$

Field cooling



Chu *et al*, arXiv 0911.3878

Resistivity anisotropy



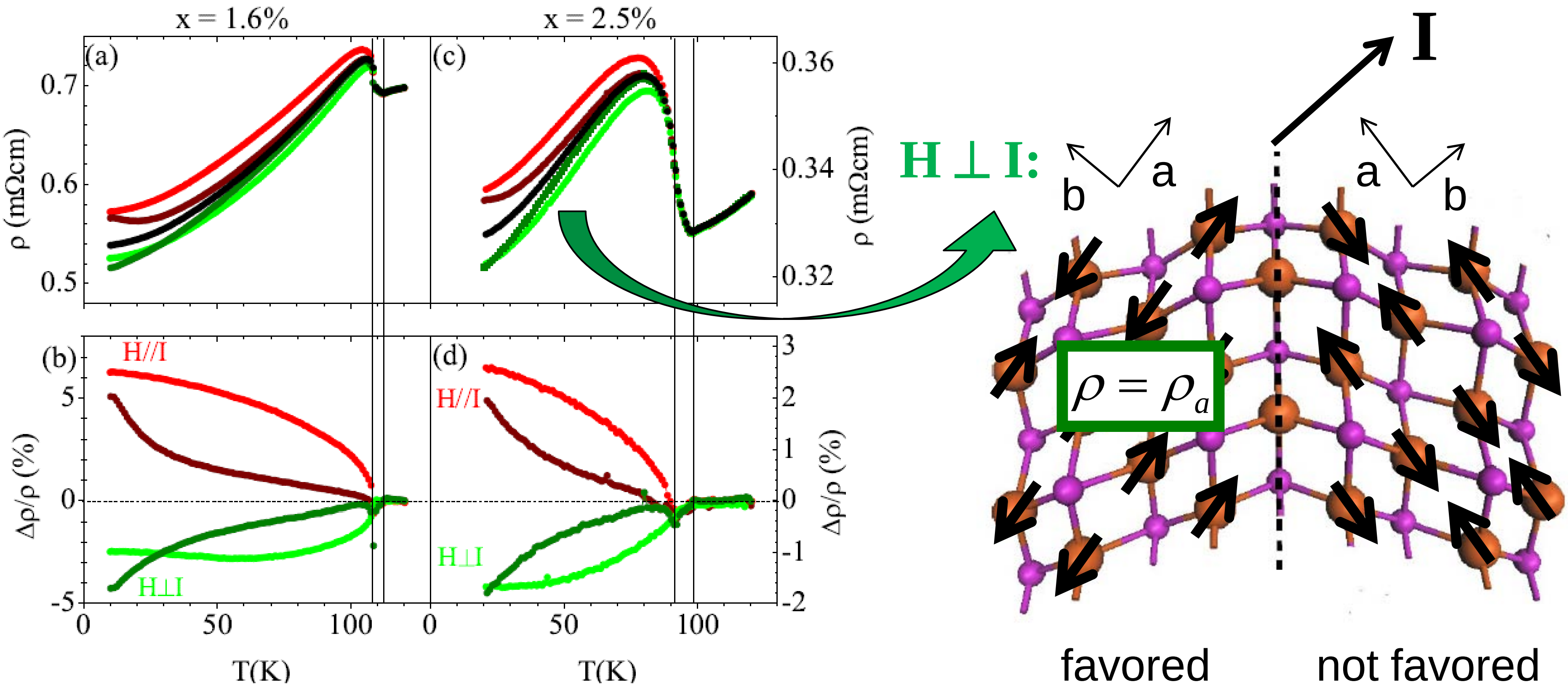
(1) $\rho_b > \rho_a$ --- counterintuitive!

(2) Significant anisotropy for Δf ~ 5 – 15 %

Excited but dissatisfied…

- wish to completely detwin samples
- wish to explore in-plane anisotropy above T_N

Resistivity anisotropy



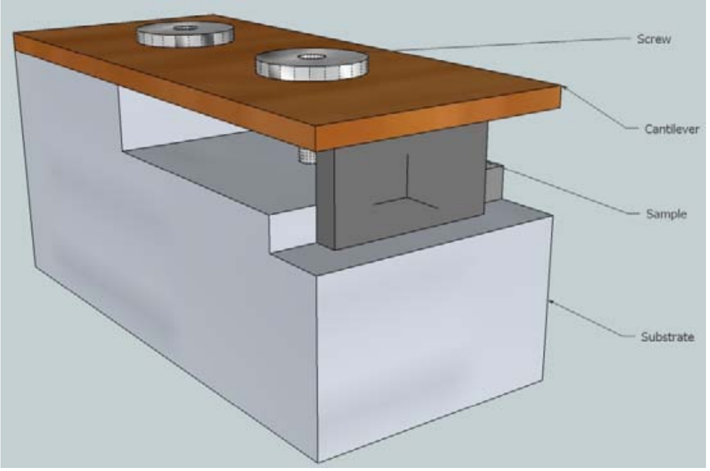
(1) $\rho_b > \rho_a$ --- counterintuitive!

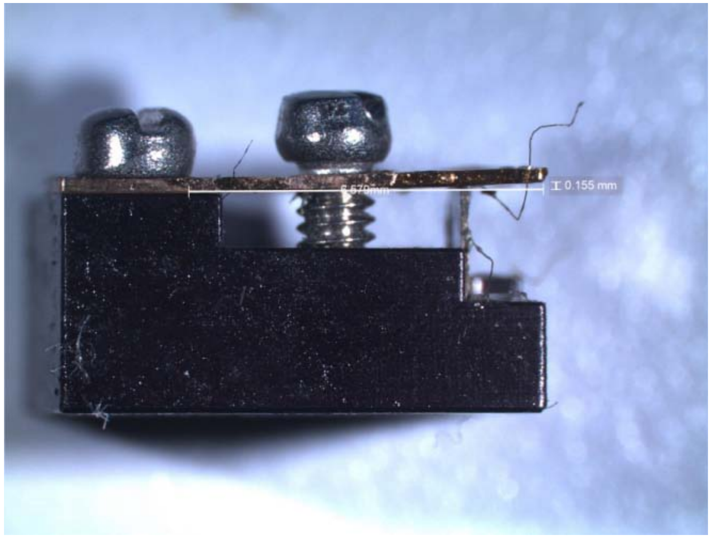
(2) Significant anisotropy for Δf ~ 5 – 15 %

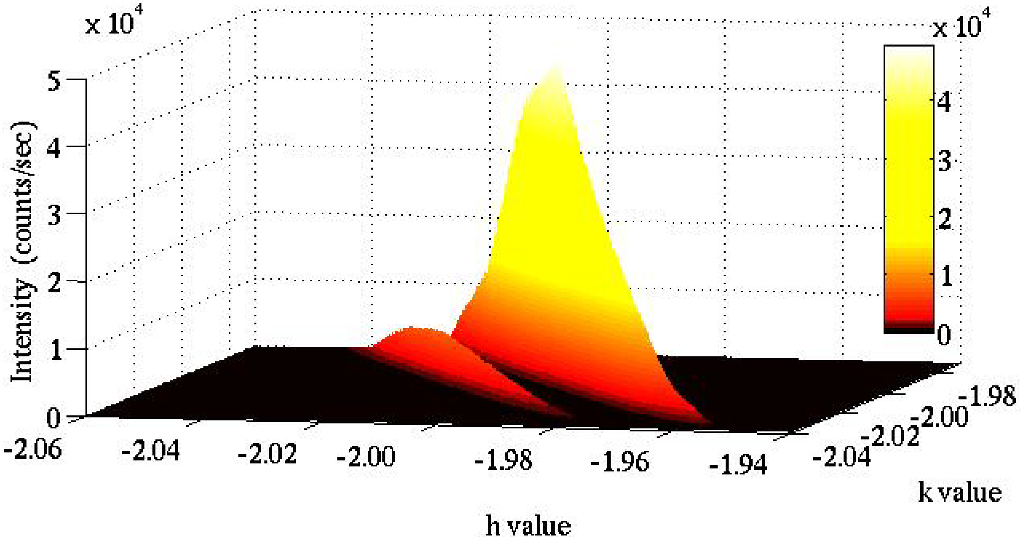
Excited but dissatisfied…

- wish to completely detwin samples
- wish to explore in-plane anisotropy above T_N

Mechanical detwinning *in situ*



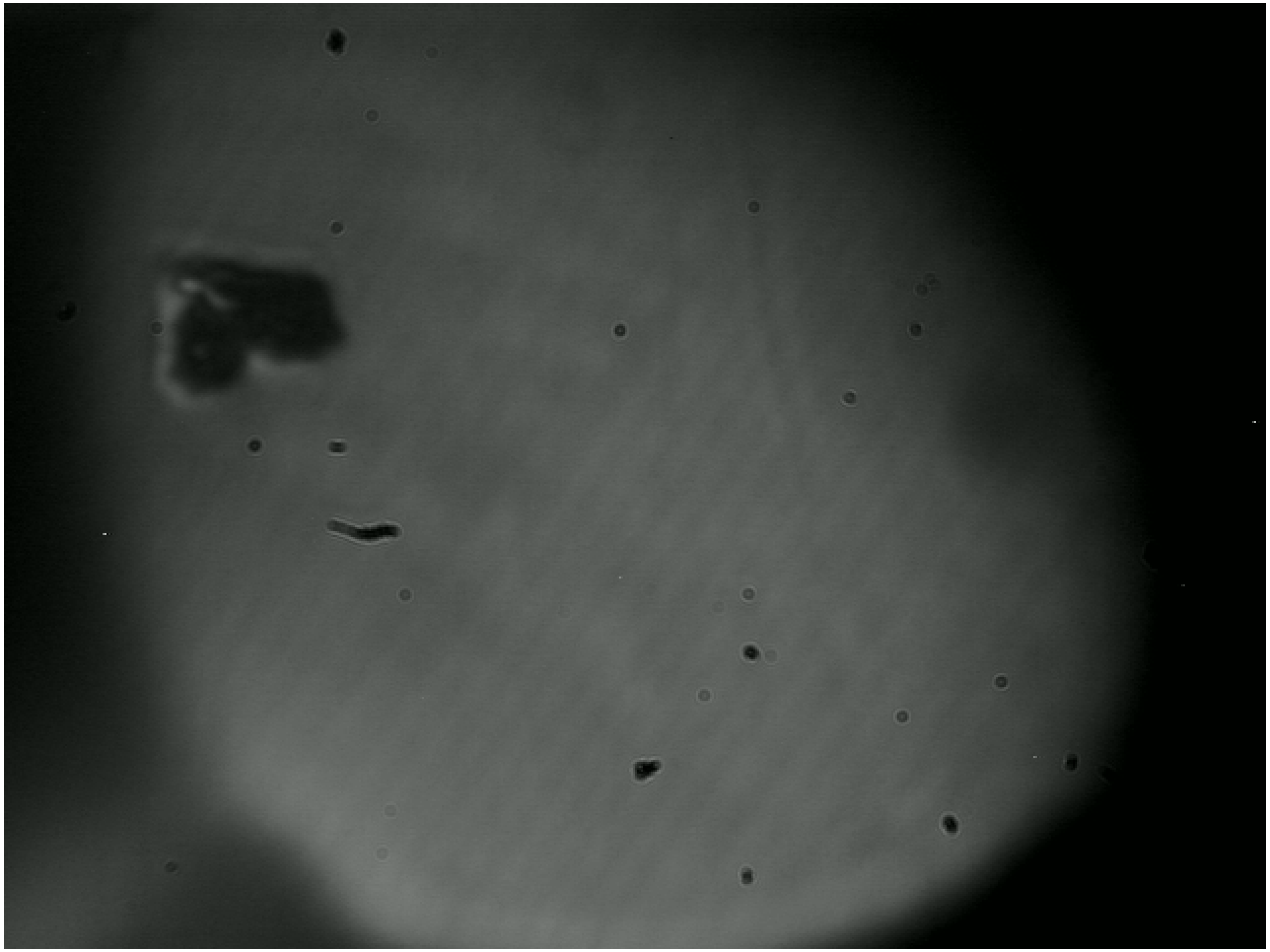




x = 2.5 %
T = 20 K
86% of a single twin orientation!

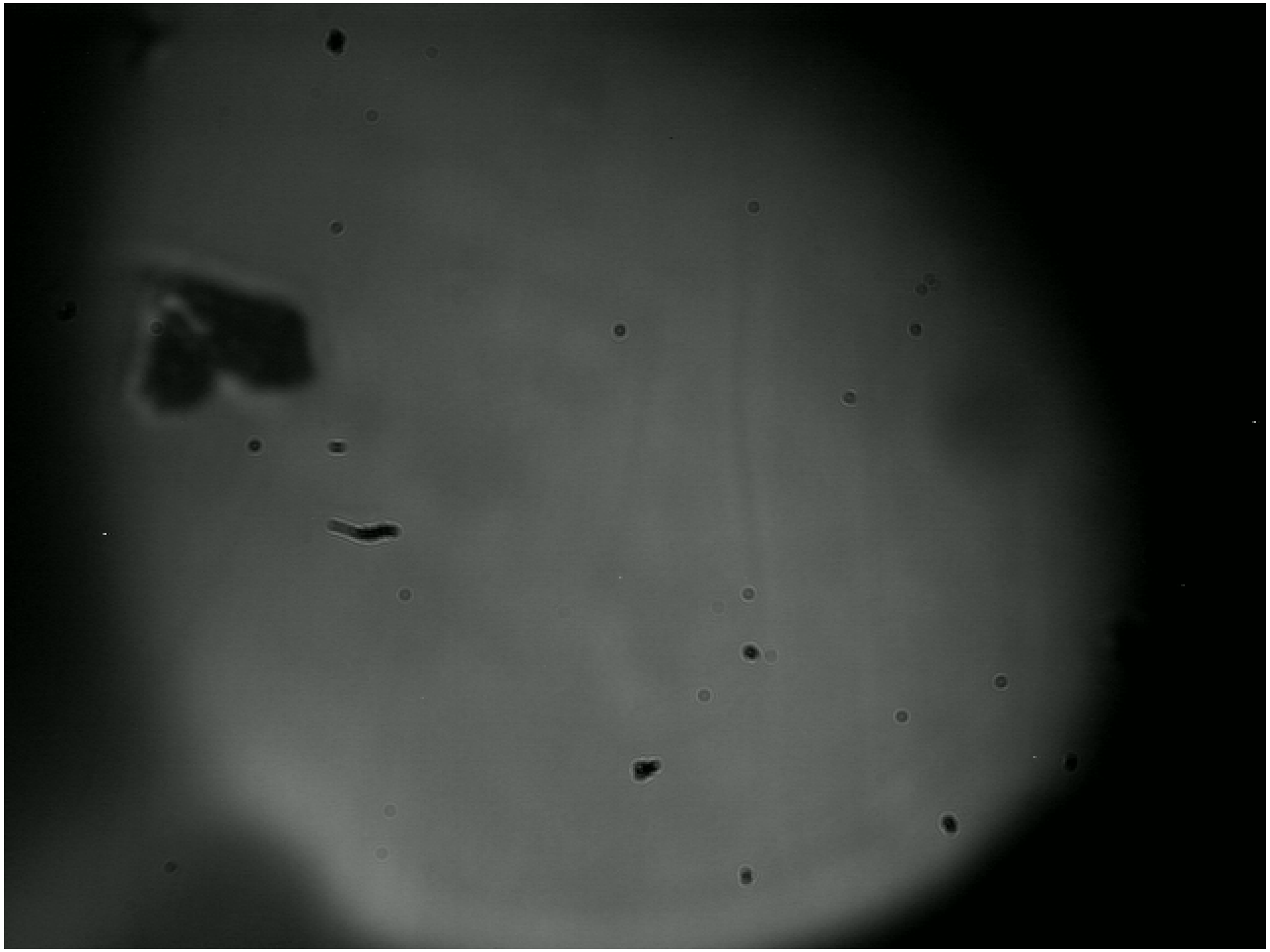
Mechanical detwinning *in situ*

x = 0 %
T = 5 K

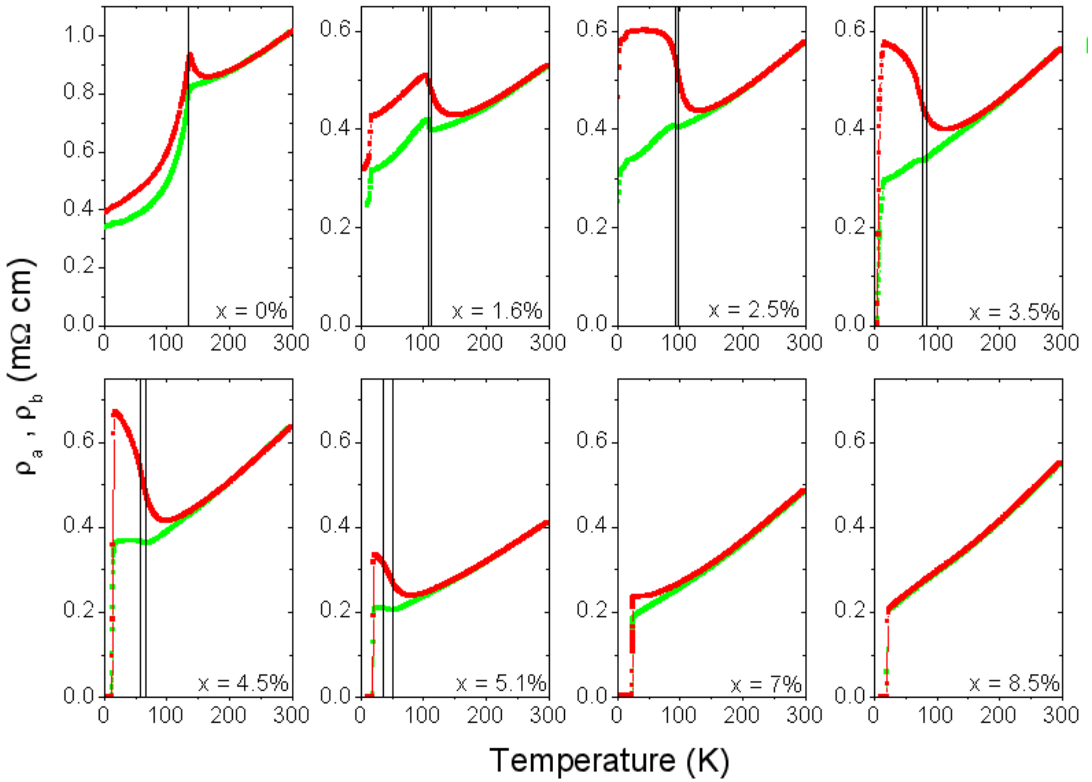


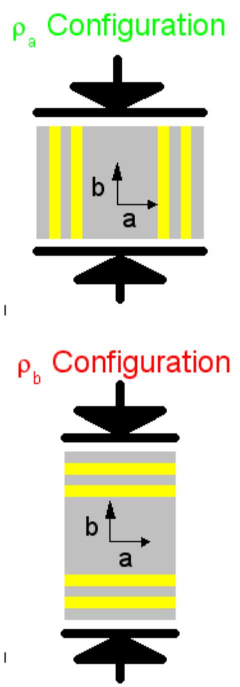
Mechanical detwinning *in situ*

x = 0 %
T = 5 K



In-plane resistivity anisotropy

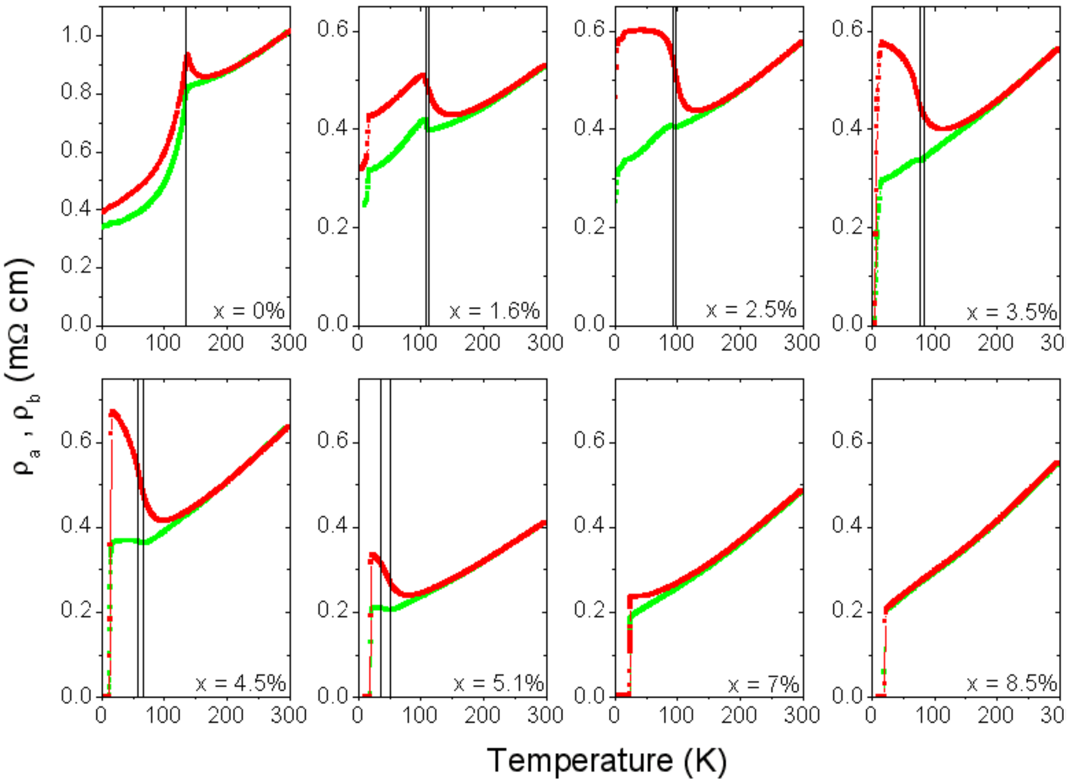


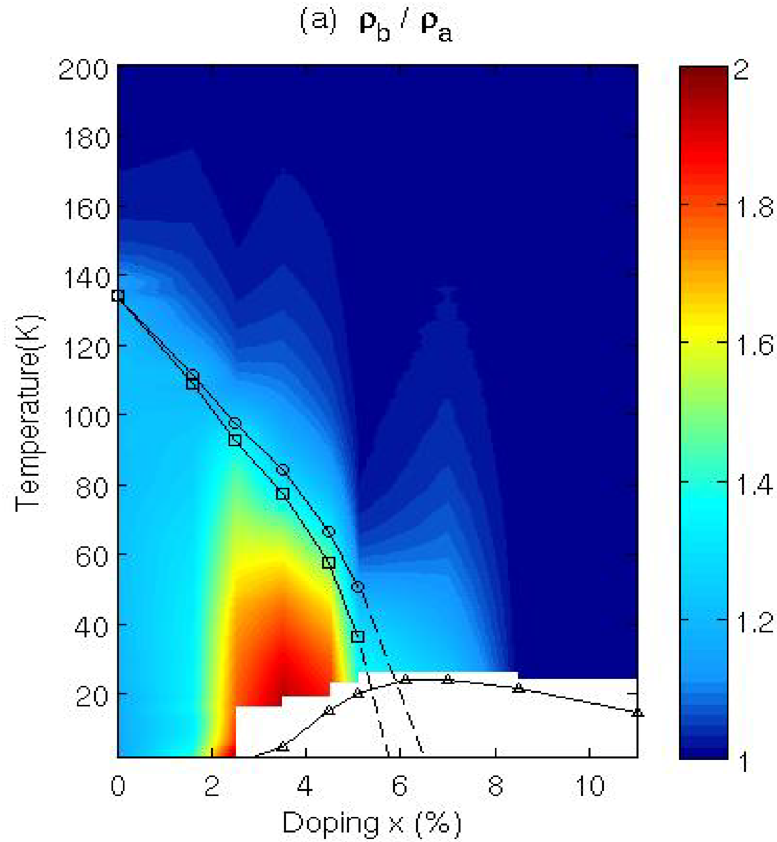


- Substantial in-plane electronic anisotropy ($\rho_b > \rho_a$)
- Insulating vs metallic T-dependence!
- Incipient anisotropy visible up to ~$2T_{ortho}$

Chu *et al*, arXiv:1002.3364

In-plane resistivity anisotropy



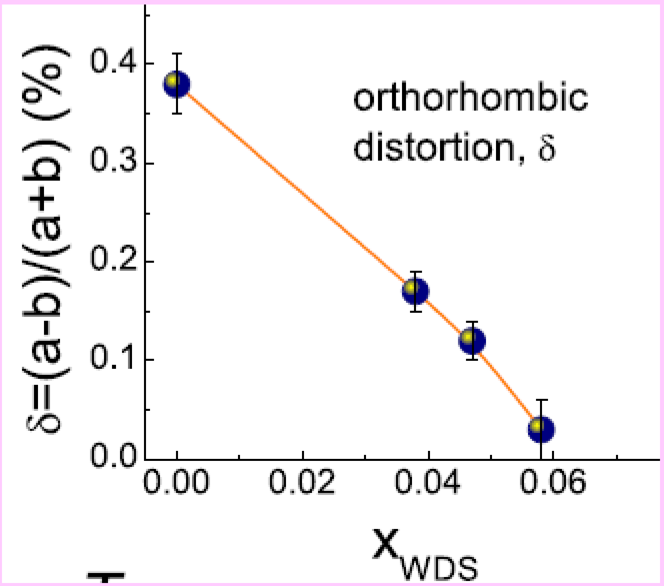


- Substantial in-plane electronic anisotropy ($\rho_b > \rho_a$)
- Insulating vs metallic T-dependence!
- Incipient anisotropy visible up to ~$2T_{ortho}$

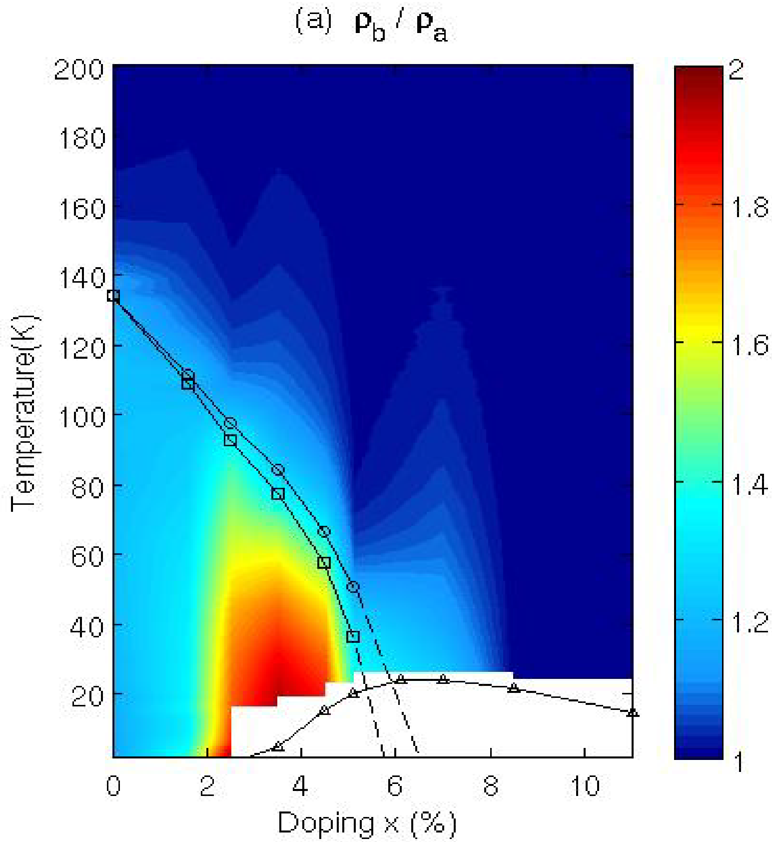
Chu *et al*, arXiv:1002.3364

In-plane resistivity anisotropy

Comparison with orthorhombic distortion:



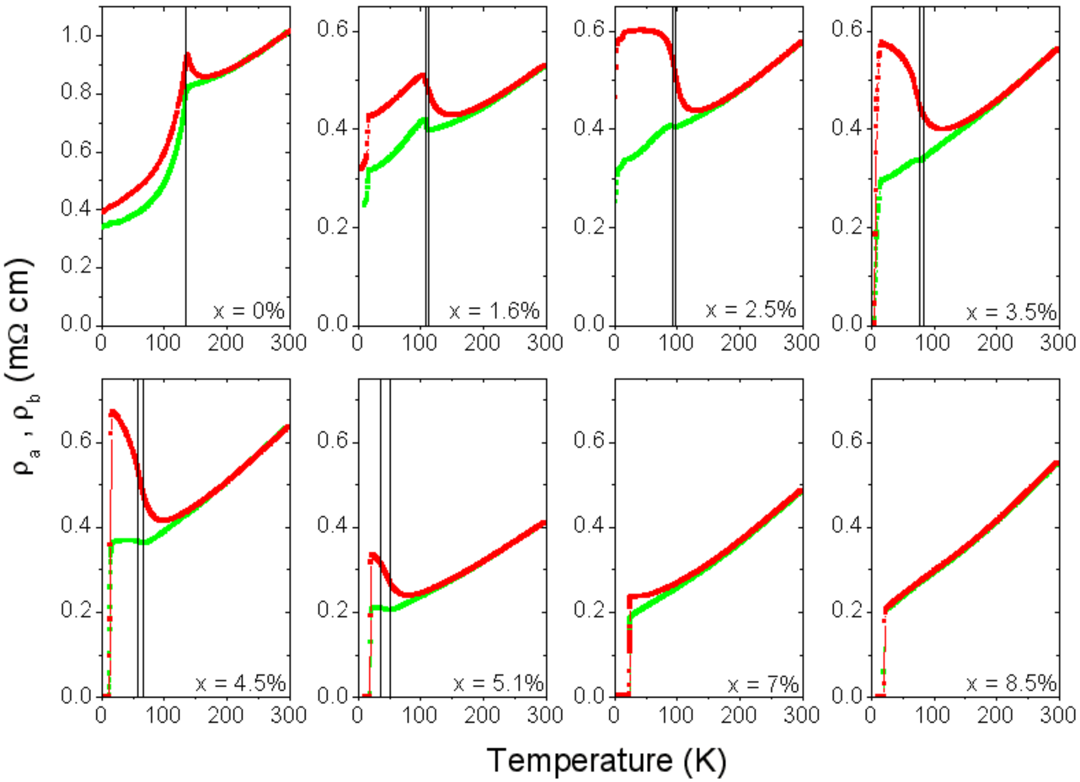
Prozorov et al, PRB **80**, 174517 (2009)

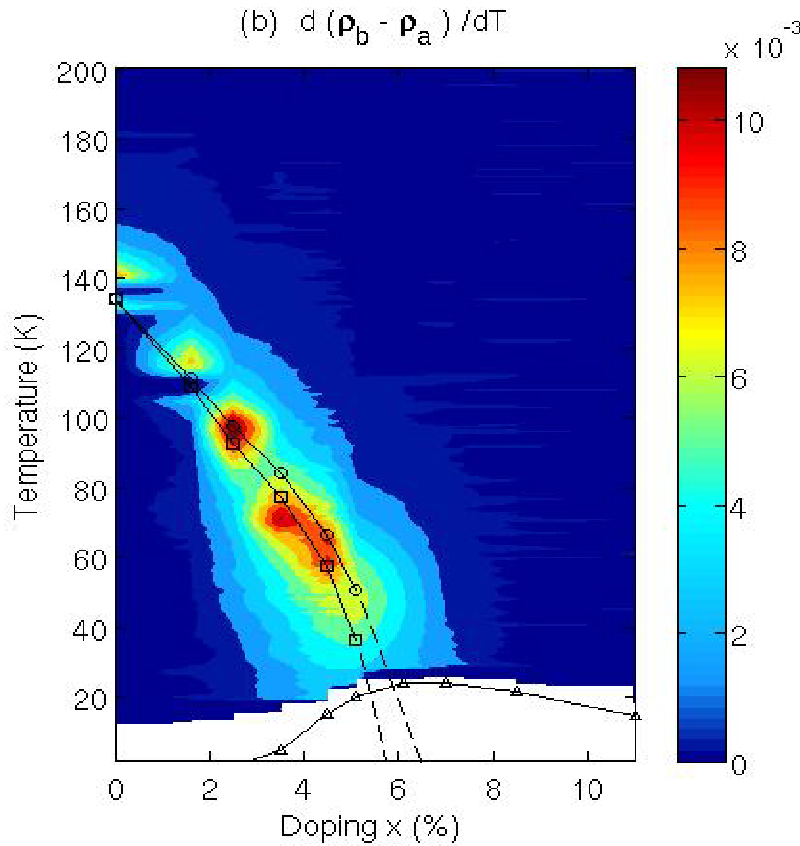


- S… a)
- Insulating vs metallic T-dependence!
- Incipient anisotropy visible up to ~2T_{ortho}

Chu *et al*, arXiv:1002.3364

In-plane resistivity anisotropy



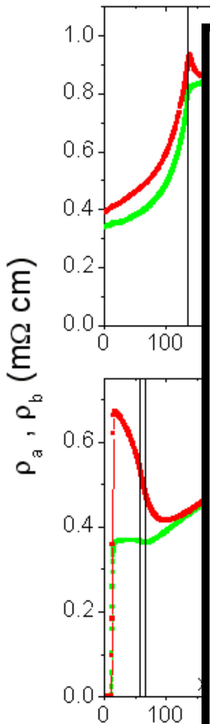


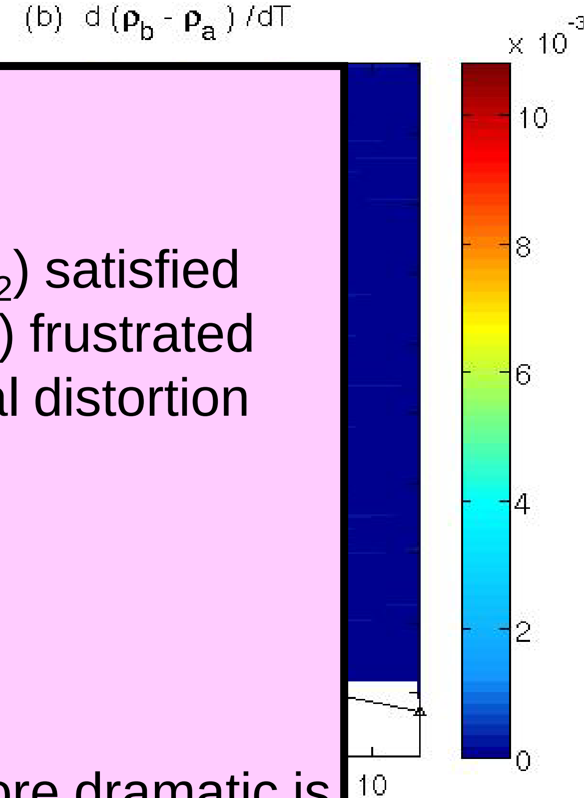
- Substantial in-plane electronic anisotropy ($\rho_b > \rho_a$)
- Insulating vs metallic T-dependence!
- Incipient anisotropy visible up to ~2T_{ortho}

- Unanticipated for a simple structural distortion
- "Electron nematic order"
- Origin unclear from these measurements alone…

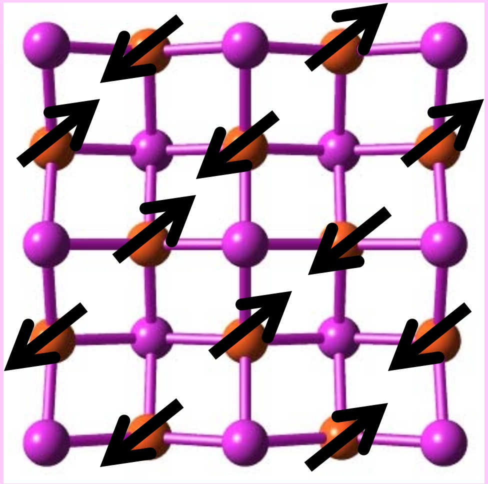
Chu *et al*, arXiv:1002.3364

In-plane resistivity anisotropy





Geometric frustration:



nnn interaction (J_2) satisfied
nn interaction (J_1) frustrated
Lifted by structural distortion

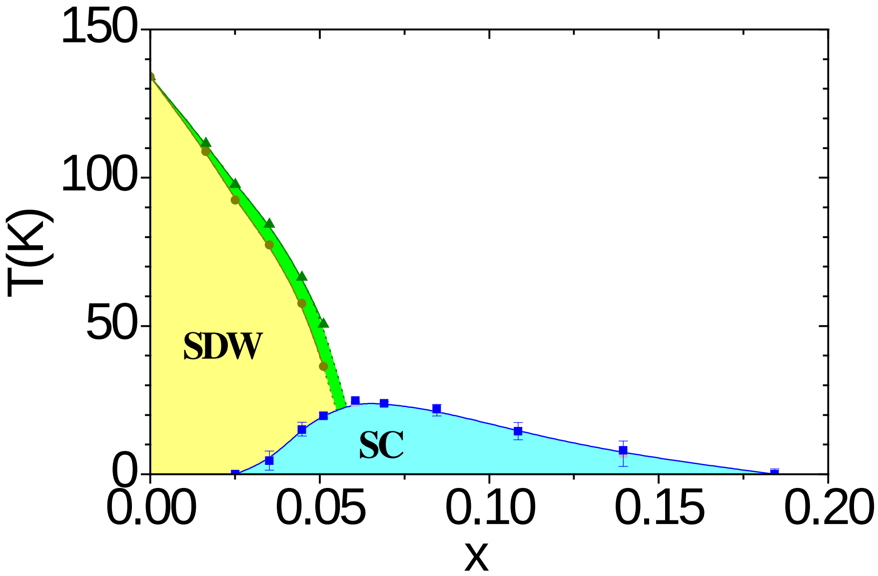
- Resistivity anisotropy implies something more dramatic is going on

- Substantial in-plane electronic anisotropy ($\rho_b > \rho_a$)
- Insulating vs metallic T-dependence!
- Incipient anisotropy visible up to ~$2T_{ortho}$

- …imple structural distortion
- "Electron nematic order"
- Origin unclear from these measurements alone…

Chu *et al*, arXiv:1002.3364

Does any of this matter?



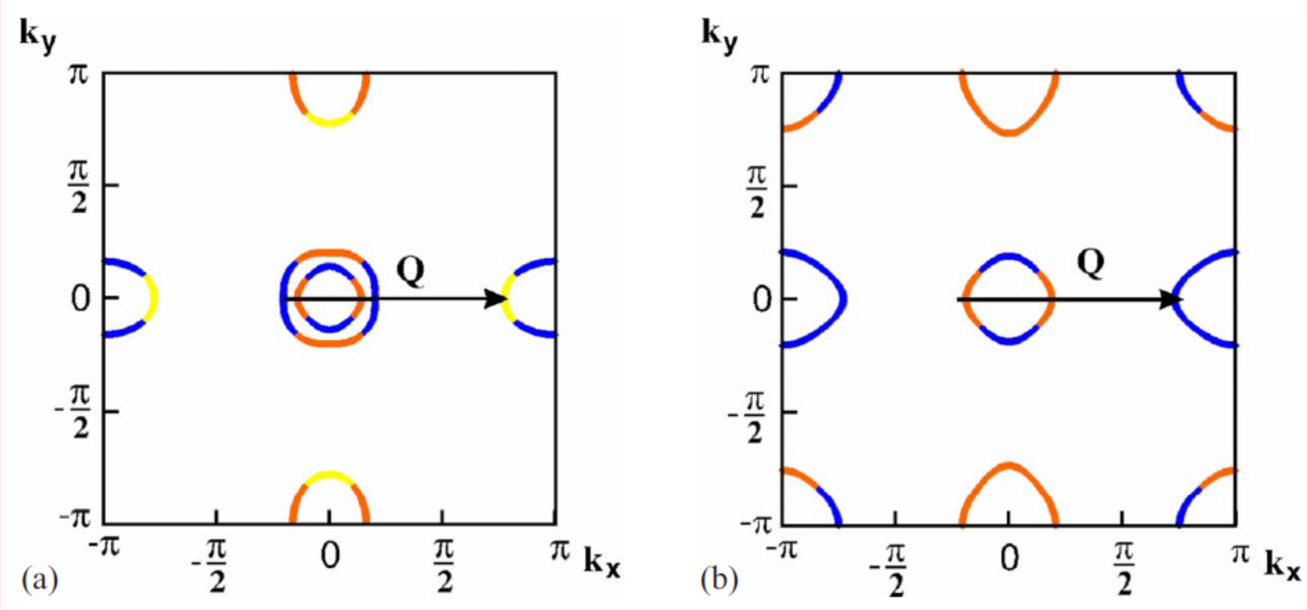
- Implication for our understanding of the FS for underdoped compositions?
- Buried under the SC dome are *two* QCPs, each of which is associated with the itinerant electrons from which the superconductivity draws

Bottom line: Origin of this dramatic electronic anisotropy must be determined if we are to have any hope of a comprehensive theory of superconductivity in this family of compounds.

Does any of this matter?

150

A possible role for orbital fluctuations:



Zhang, Schmalian et al, PRB **79**, 220502(R) (2009).

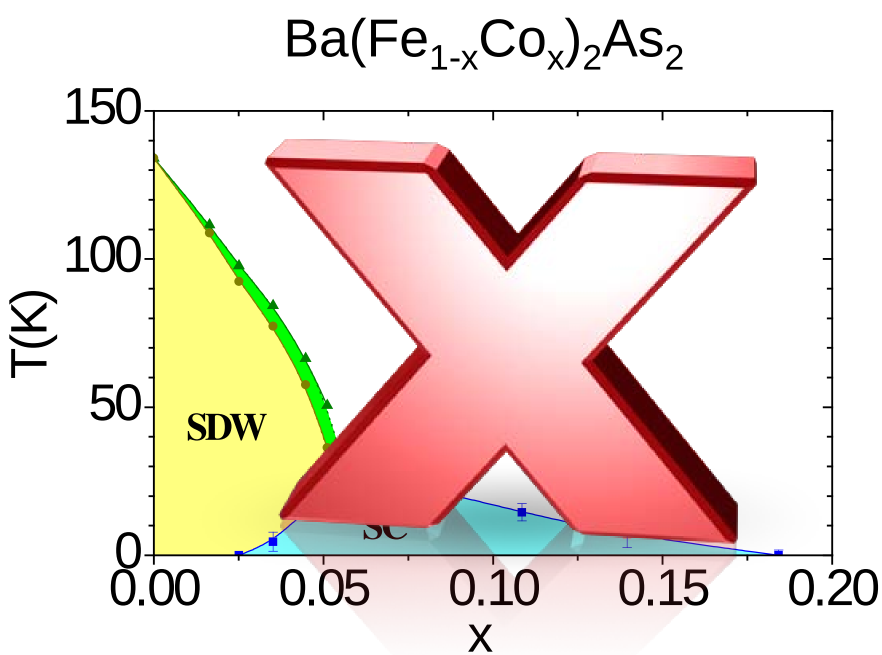
- Implic … itions?
- Buriec … ted with the itii …

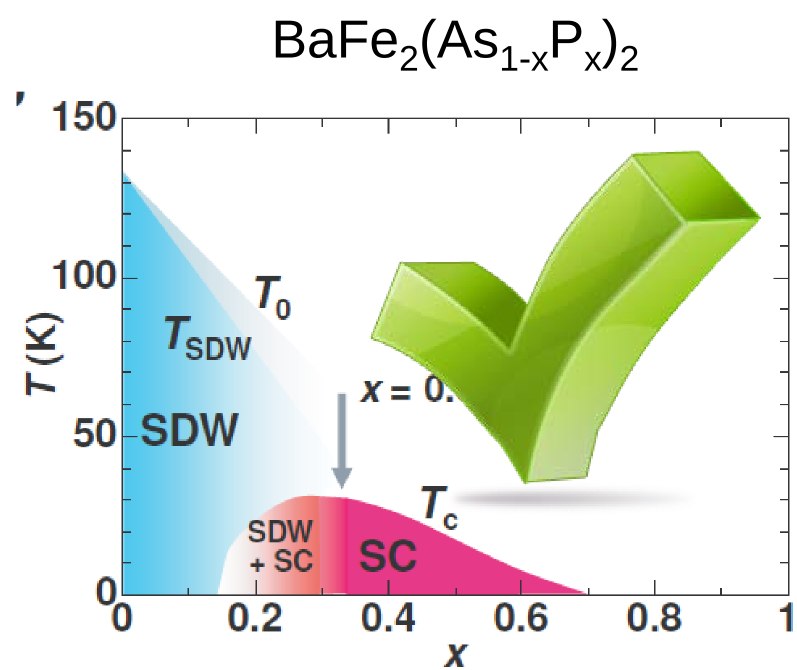
Botto… determined if we are to have any hope of a comprehensive theory of superconductivity in this family of compounds.

Part 2: Fermi surface nesting

(2) What role does Fermi surface nesting really play?

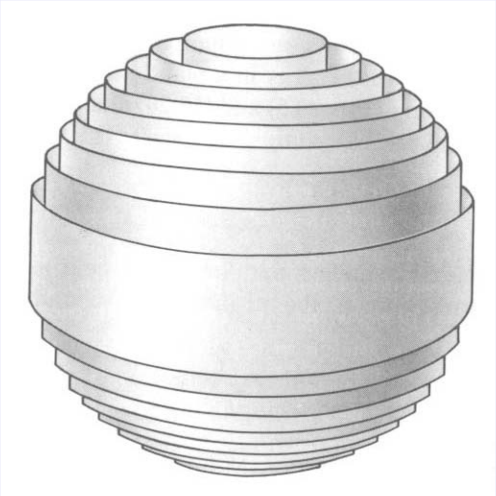
- Is there a correlation between phase diagram and changes in band parameters (FS morphology & effective mass)?
- Fermiology via quantum oscillations…





Matsuda et al, arXiv 0907.4399

Quantum oscillations



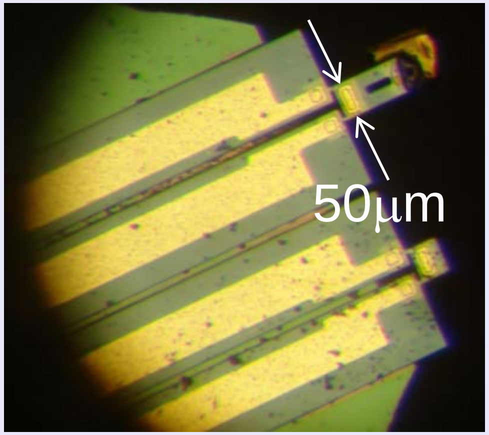
$$F = \frac{\hbar}{2\pi e} A_k$$

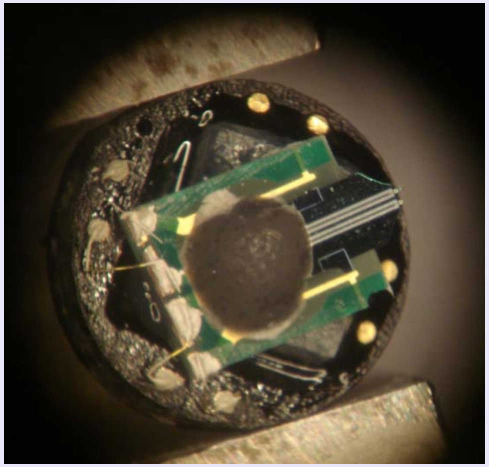
- Bulk measurement
- Precise determination of shape of FS
- Sensitive to subtle reconstruction
- Measurement of renormalized mass
- Measurement of mfp band-by-band

But…

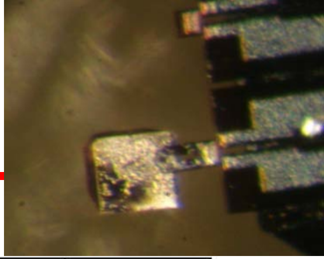
- Requires $\omega_c \tau > 1$
- No information about k-space

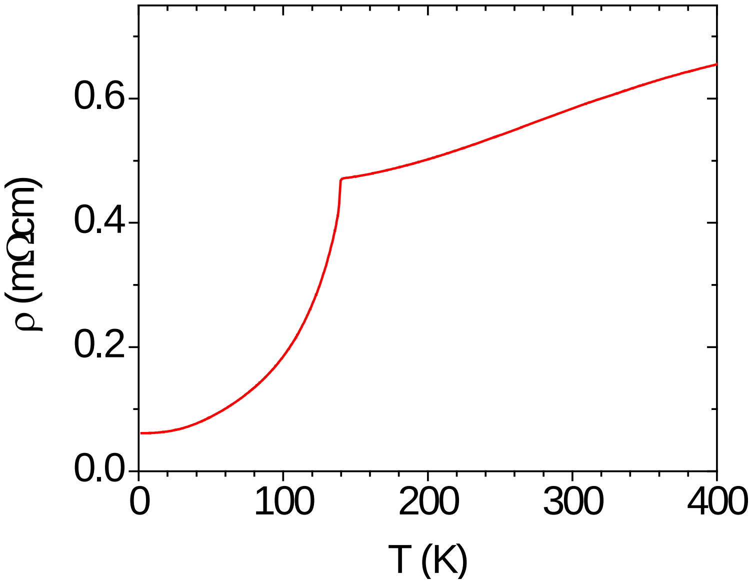
Torque:

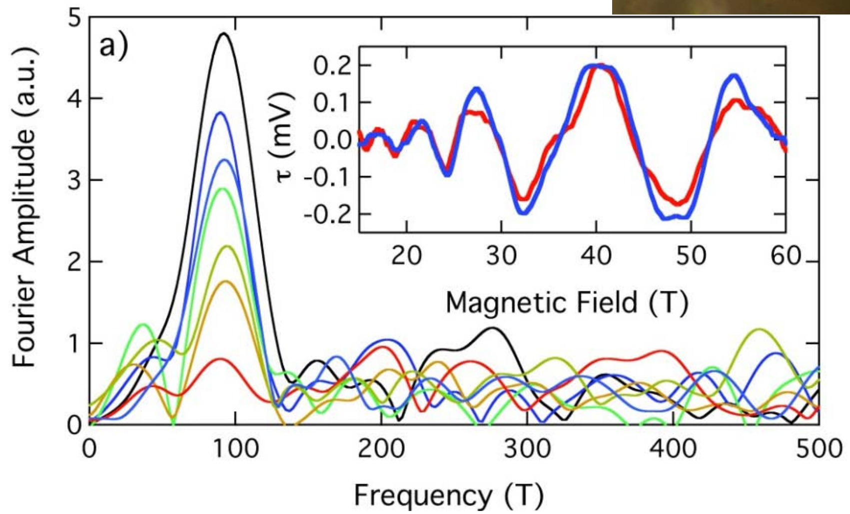


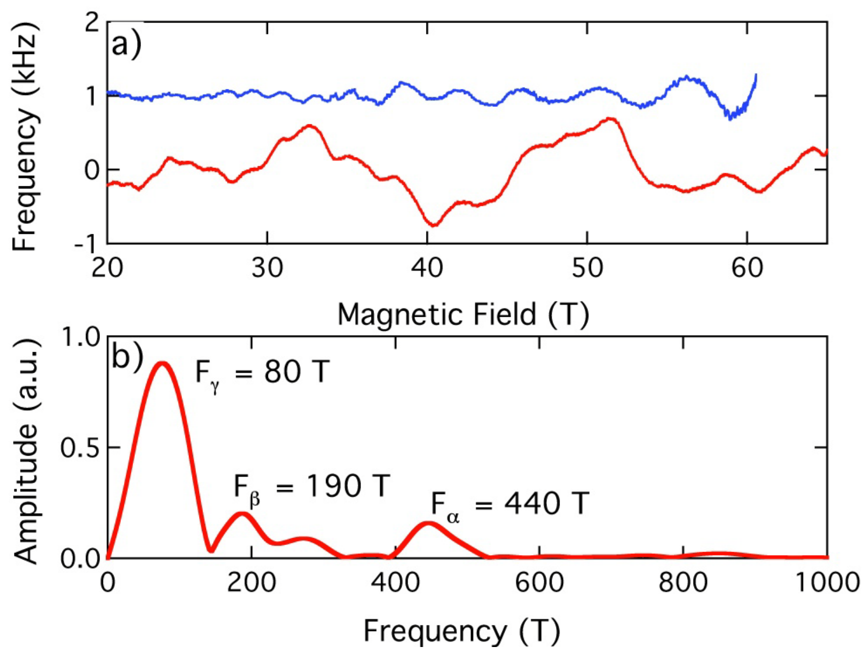


(a) $BaFe_2As_2$





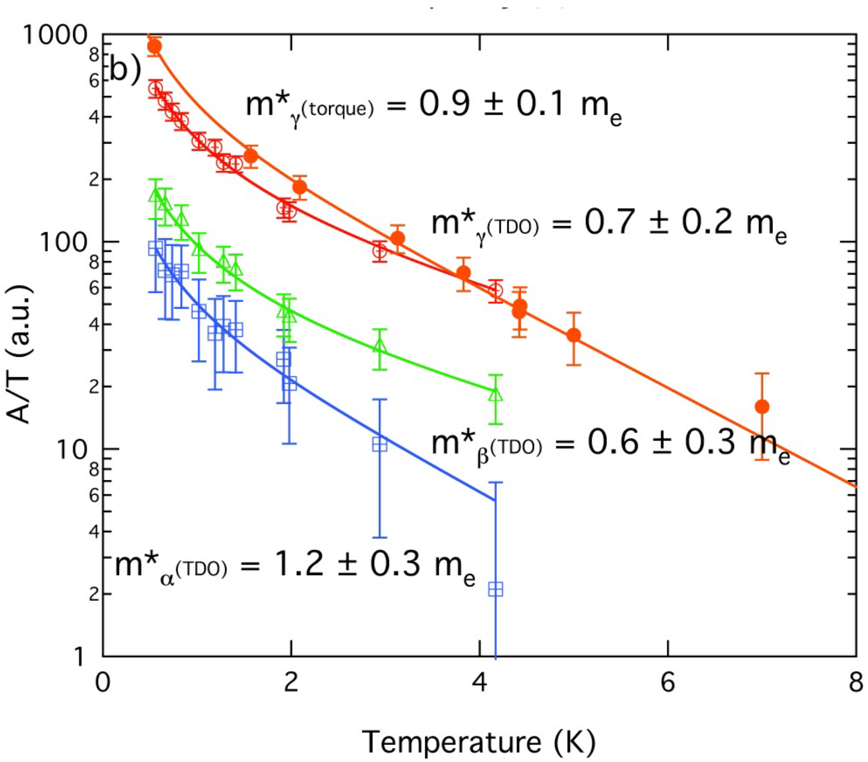


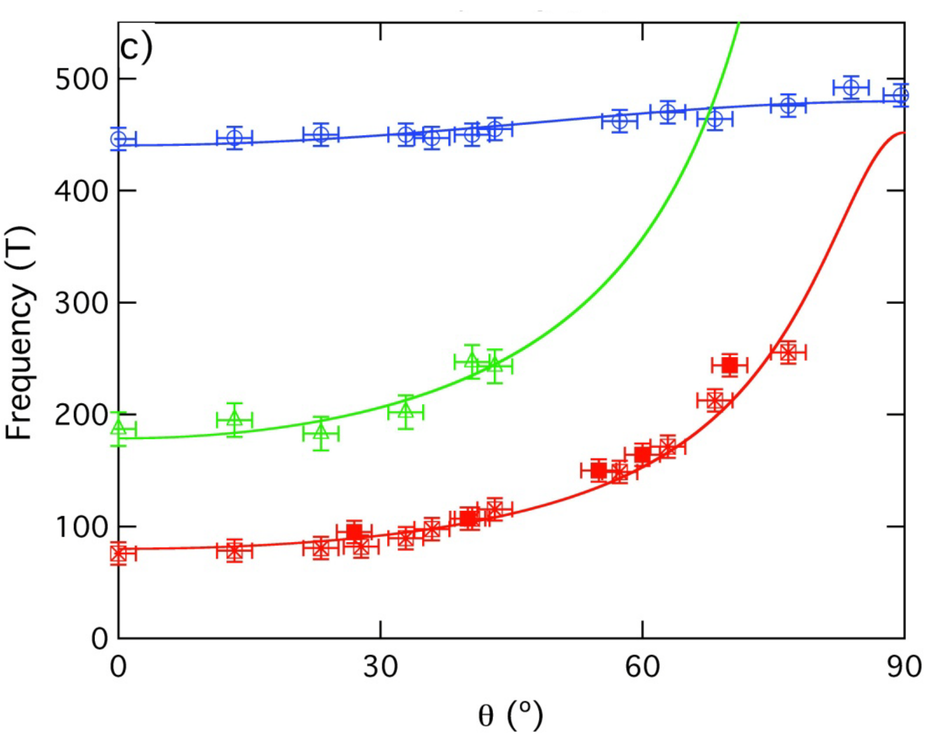


- Well-defined quasiparticles in the SDW state
- 1.7%, 0.7% and 0.3% of the paramagnetic BZ

Analytis et al, PRB **80**, 064507 (2009).

(a) $BaFe_2As_2$

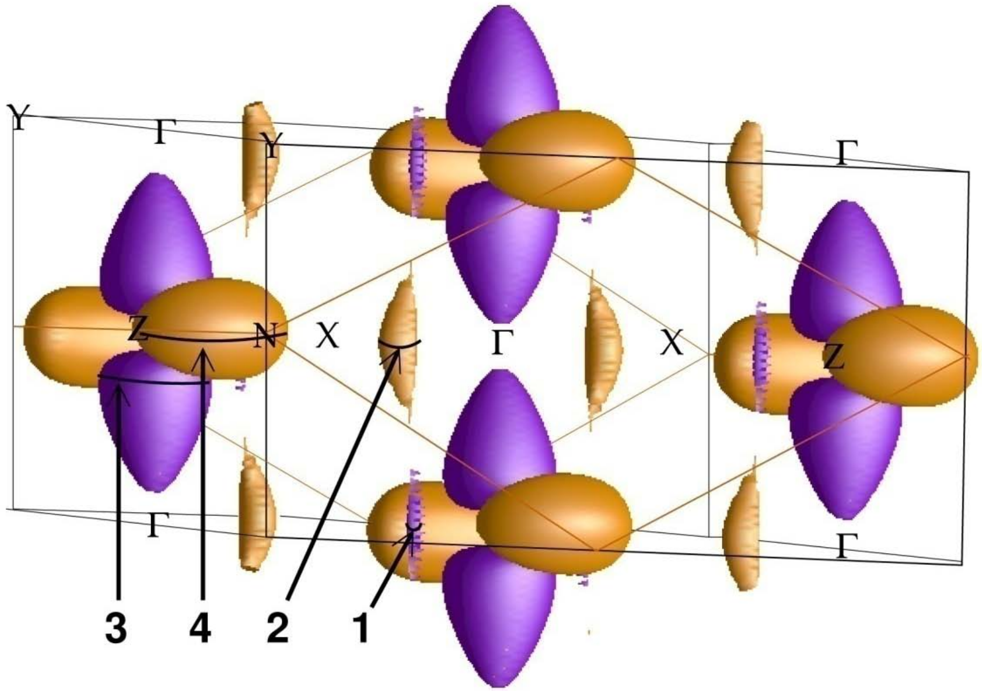




- $v_\alpha = 1.9\times10^5$ ms^{-1}, $v_\beta = 1.3\times10^5$ ms^{-1}, $v_\gamma = 0.8\times10^5$ ms^{-1}
- mfp ~ 100 Å
- ellipticity e_α ~ 1.1, e_β ~ 5, e_γ ~ 6

Analytis et al, PRB **80**, 064507 (2009).

(a) $BaFe_2As_2$



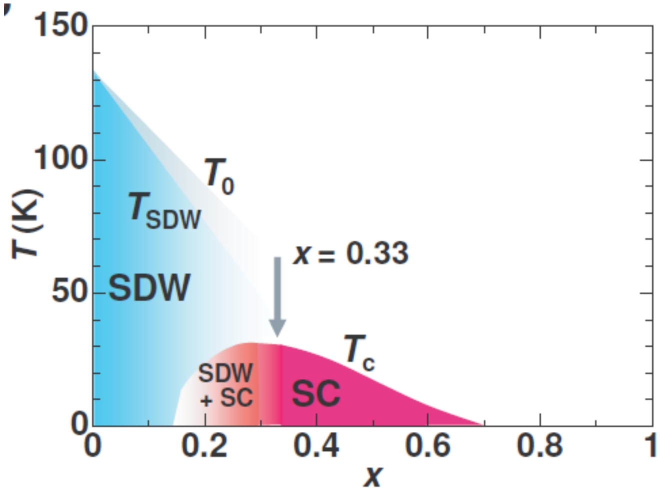
Orbit	Freq.	m^*/m_b
1 (hole)	γ	2
2 (electron)	β	1.1
3 (hole)	α	1.7
4 (electron)	-	-

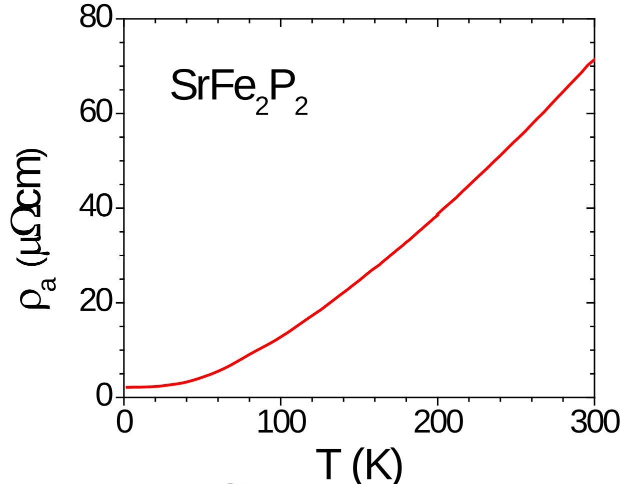
- The reconstructed state doesn't tell us too much about the original FS
- One would ideally like to study the unreconstructed FS…

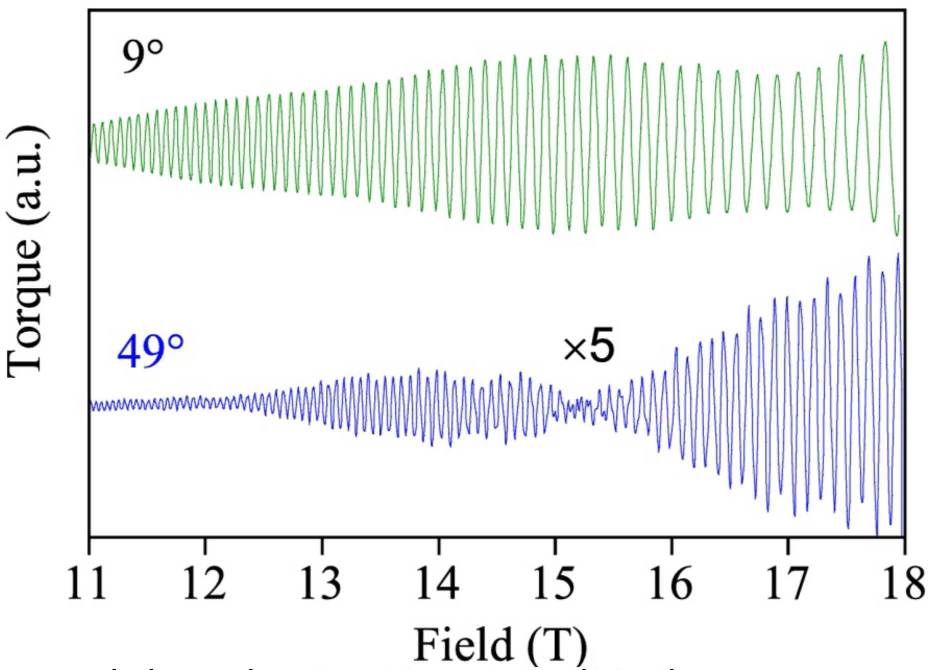
Analytis et al, PRB **80**, 064507 (2009).

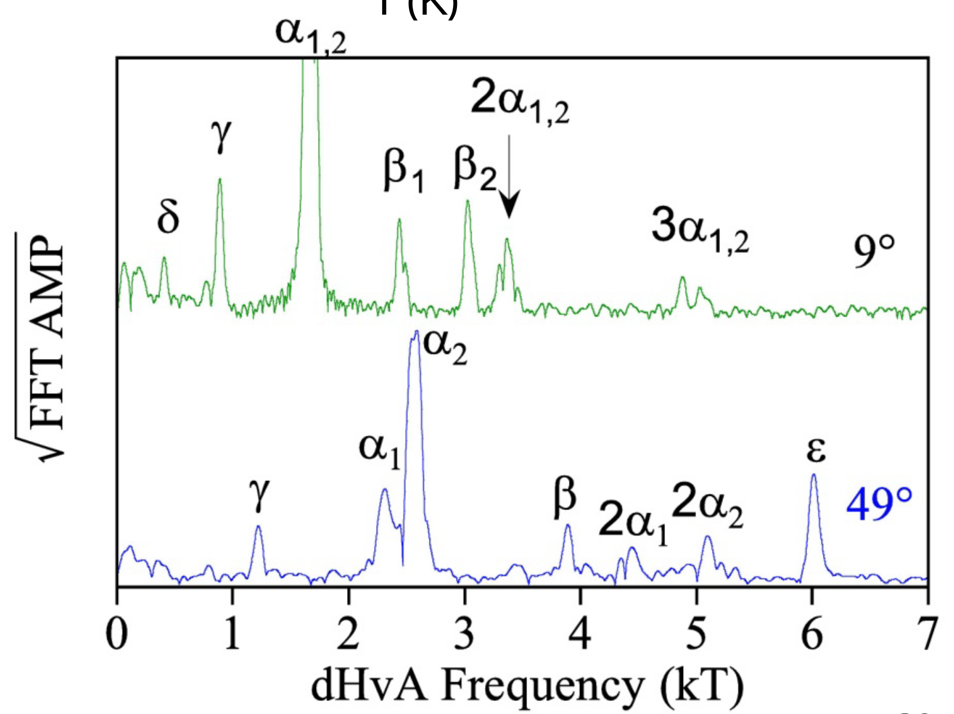
(b) $SrFe_2P_2$

Matsuda et al, arXiv 0907.4399



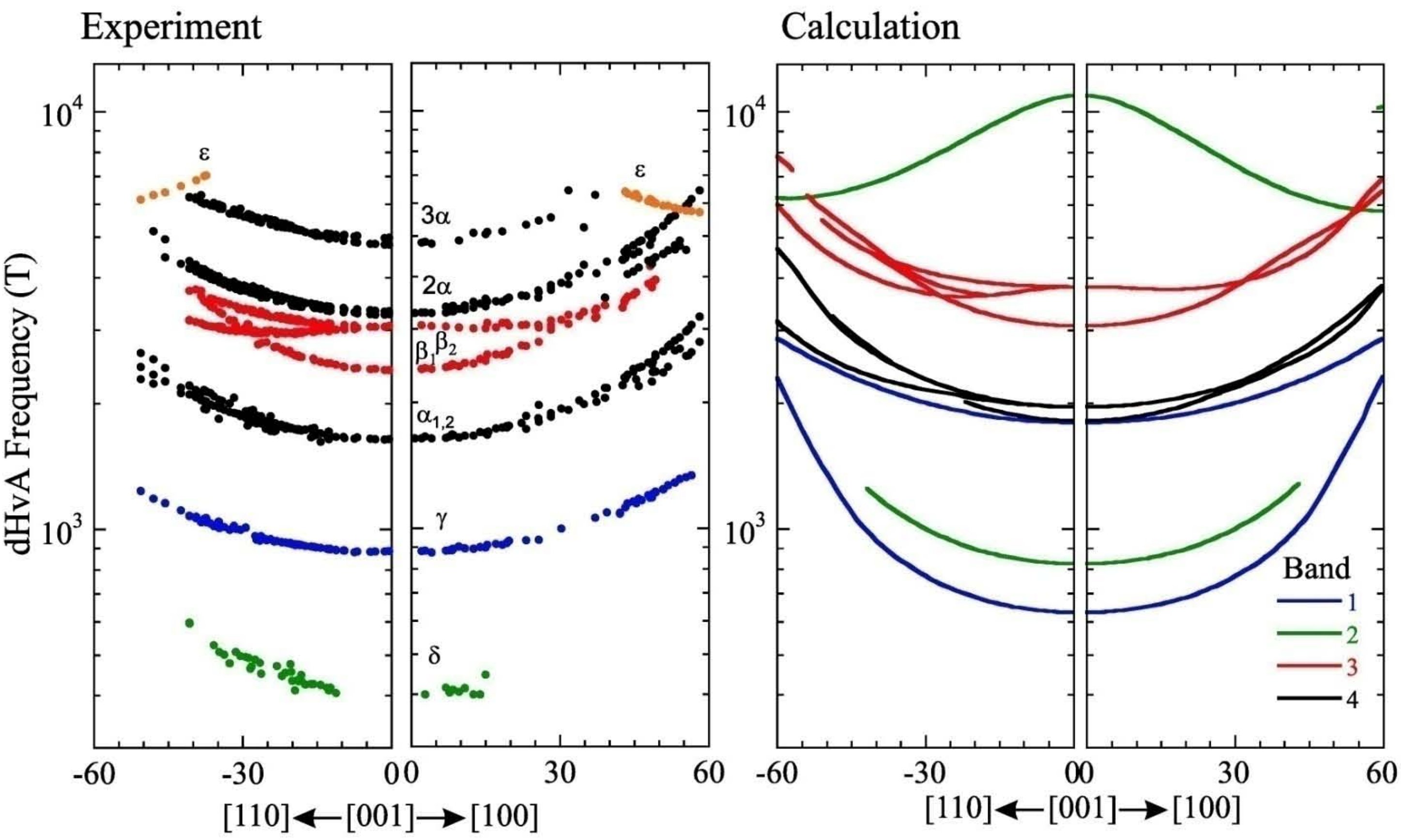


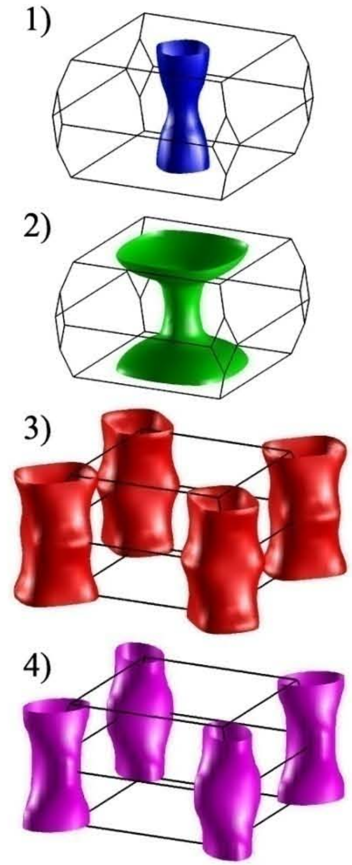


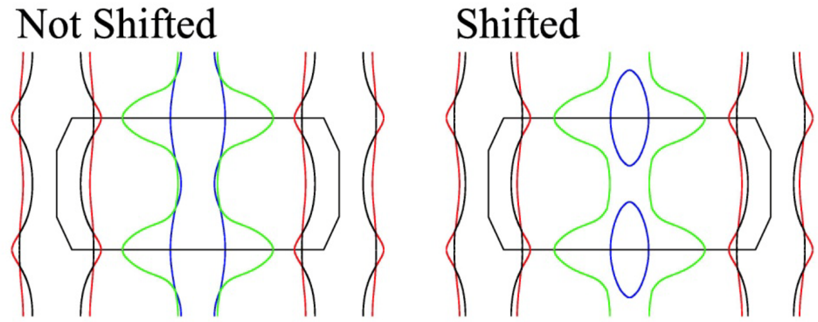


Analytis et al, PRL **103**, 076401 (2009).

(b) $SrFe_2P_2$







- LDA broadly correct
- Shift bands 3 & 4 up, and bands 1 & 2 down

Analytis et al, PRL **103**, 076401 (2009).

(b) $SrFe_2P_2$

	Experiment			Calculations			
	F(kT)	$\frac{m^*}{m_e}$	ℓ(nm)	Orbit	F(kT)	$\frac{m_b}{m_e}$	$\frac{m^*}{m_b}$
				1_{min}	0.632	0.97	
γ	0.89	1.49(2)	58	1_{max}	1.804	1.07	1.4
δ	0.41	1.6(1)	21	2_{min}	0.828	1.24	1.3
ϵ	6.02^*	$3.41(5)^*$	90	2_{max}	10.95	2.30	1.7
β_1	2.41	1.92(2)	63	3_{min}	3.077	1.25	1.6
β_2	3.06	2.41(3)	70	3_{max}	3.824	1.70	1.6
α_1	1.637	1.13(1)	100	4_{min}	1.823	0.55	2.1
α_2	1.671	1.13(1)	100	4_{max}	1.966	0.60	2.1

hole (1_{min} – 2_{max})

electron (3_{min} – 4_{max})

(1) Renormalised mass $m^* \sim (1+\lambda)m_b$

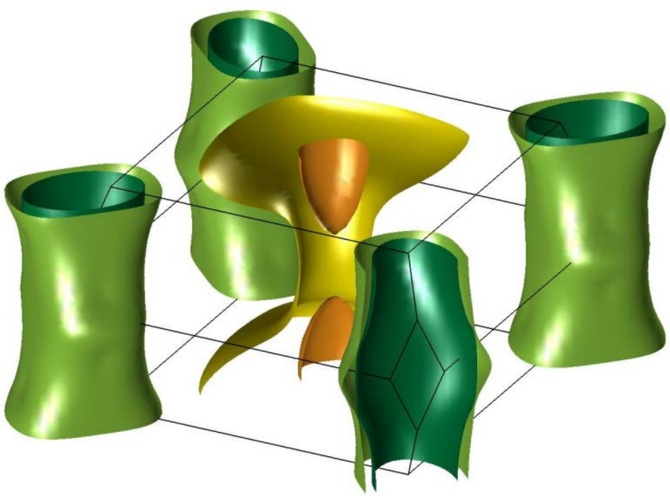
$\lambda = m^*/m_b - 1 \sim 0.3 – 1.1$ ($> \lambda_{e\text{-}ph}$)

(2) Mean free path longer on electron than hole pockets

Analytis et al, PRL **103**, 076401 (2009).

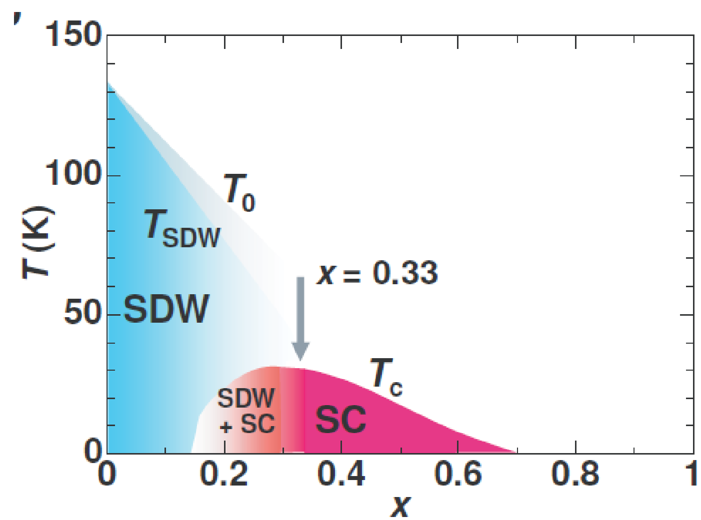
(b) $SrFe_2P_2$

Main point:
The experimentally determined FS of $SrFe_2P_2$ is very poorly nested



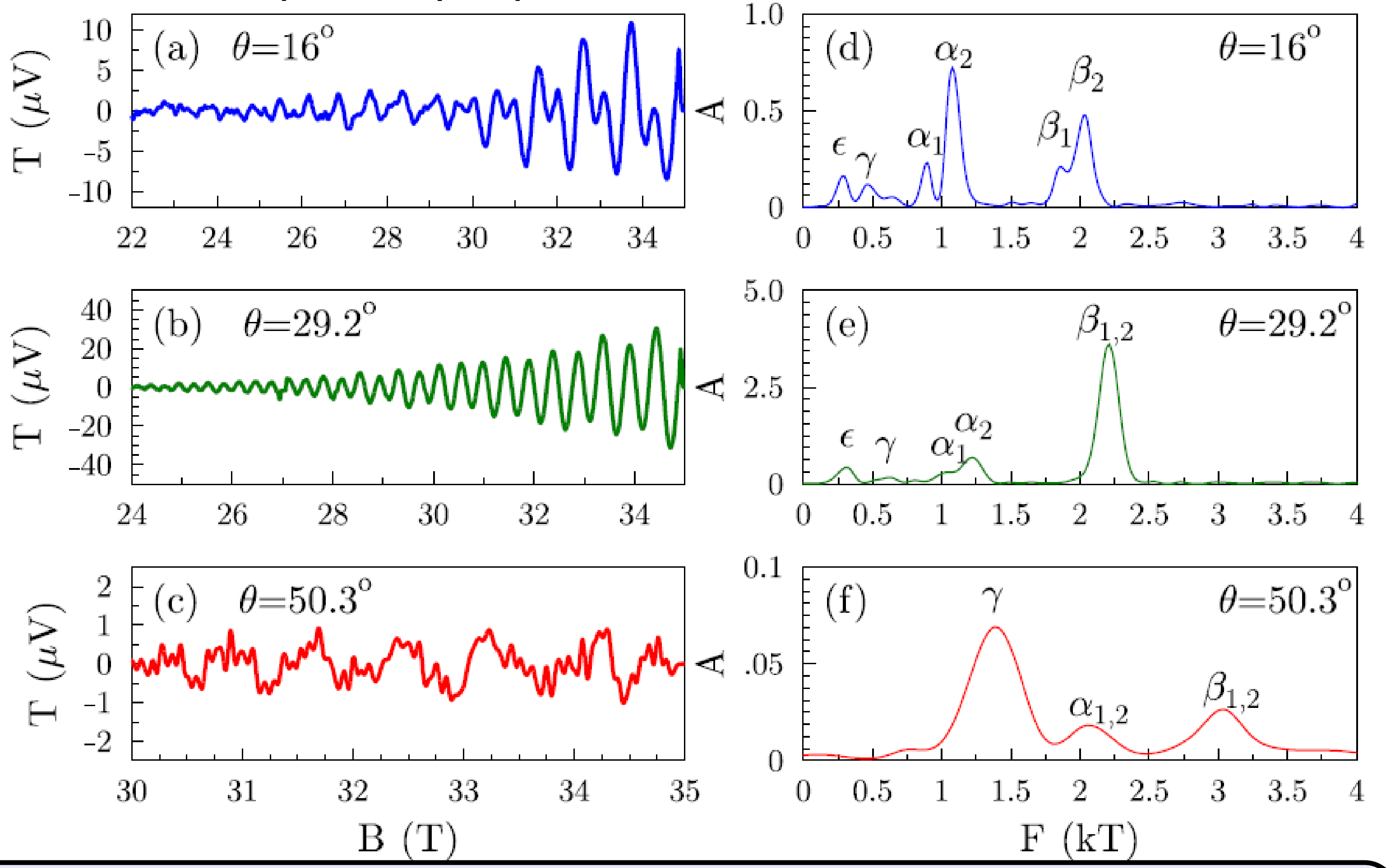
Question:
How does this change with As doping?

Matsuda et al, arXiv 0907.4399



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

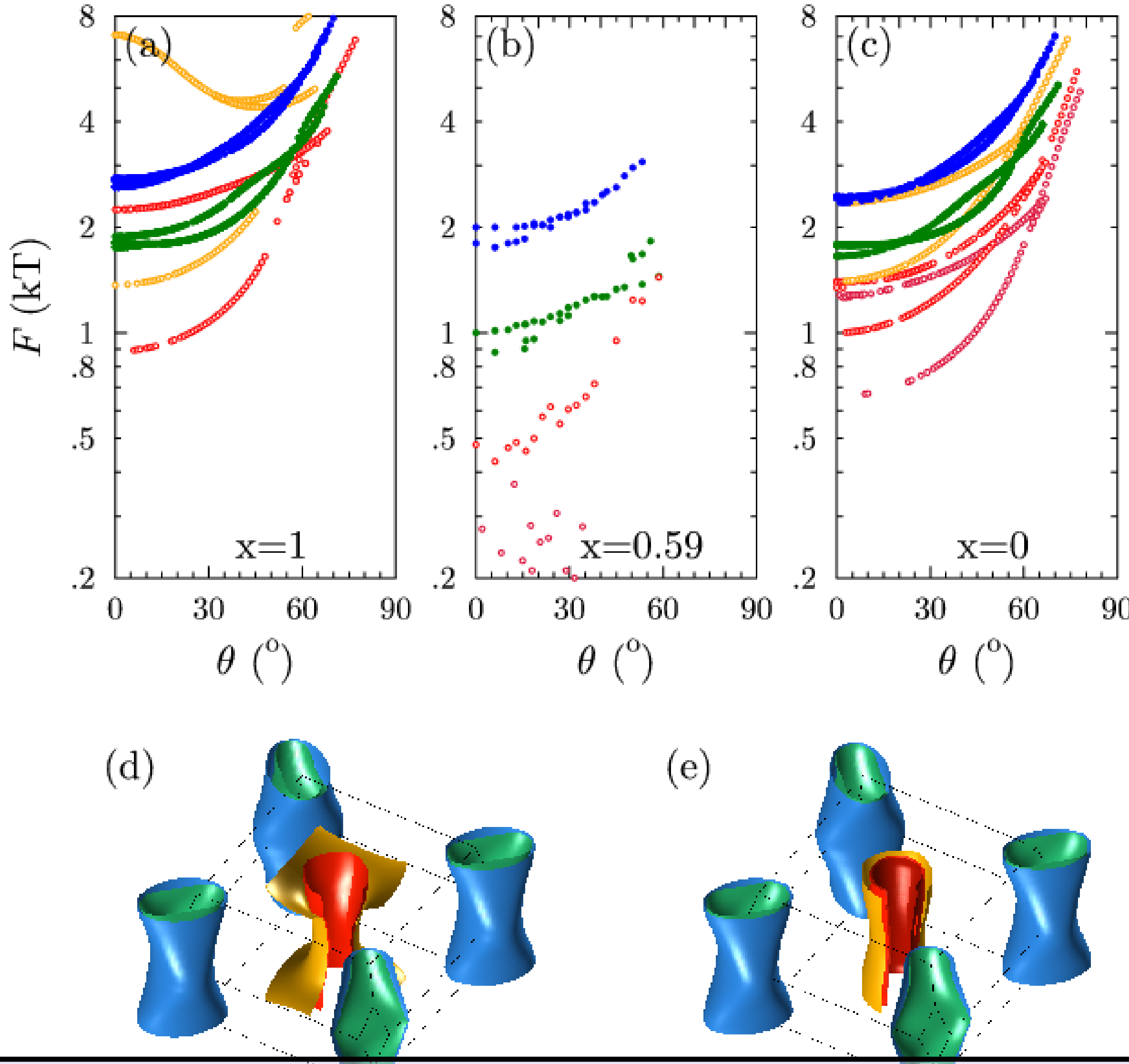
x=0.63, Tc = 9 K (overdoped):-



Analytis et al, ArXiv 1002.1304

- Beautiful wiggles! (In an alloy!)
- Assign α and β orbits as electron pockets (larger mean free path)
- Additional frequency – hole pocket

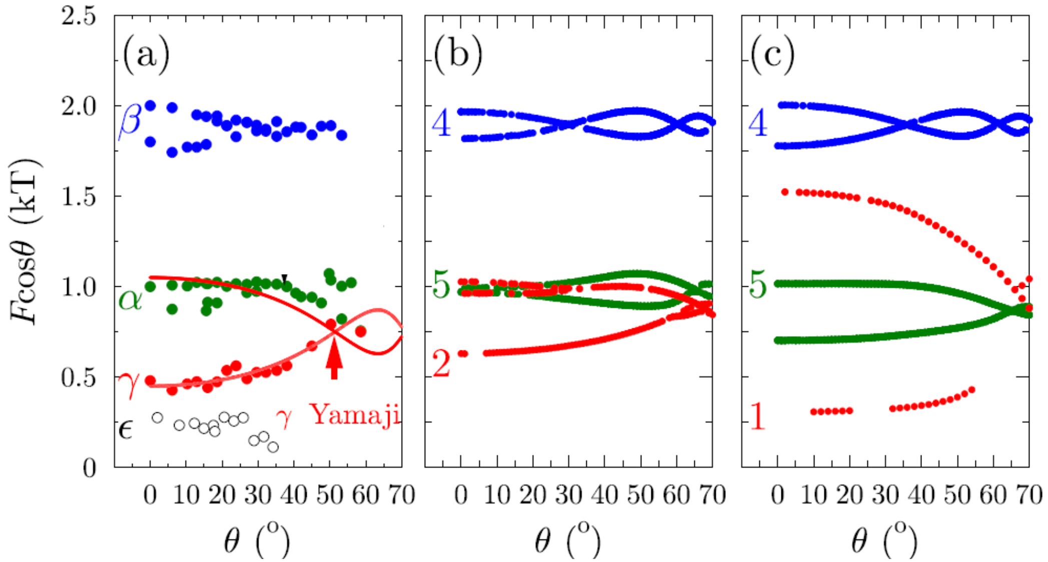
(c) $BaFe_2(As_{1-x}P_x)_2$

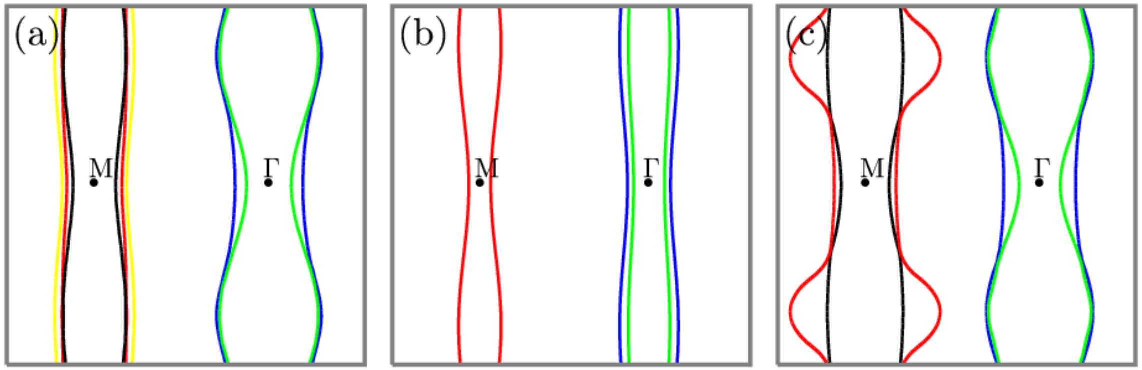


Analytis et al, ArXiv 1002.1304

- Observed frequencies cannot be fit by LDA bands for either end member

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

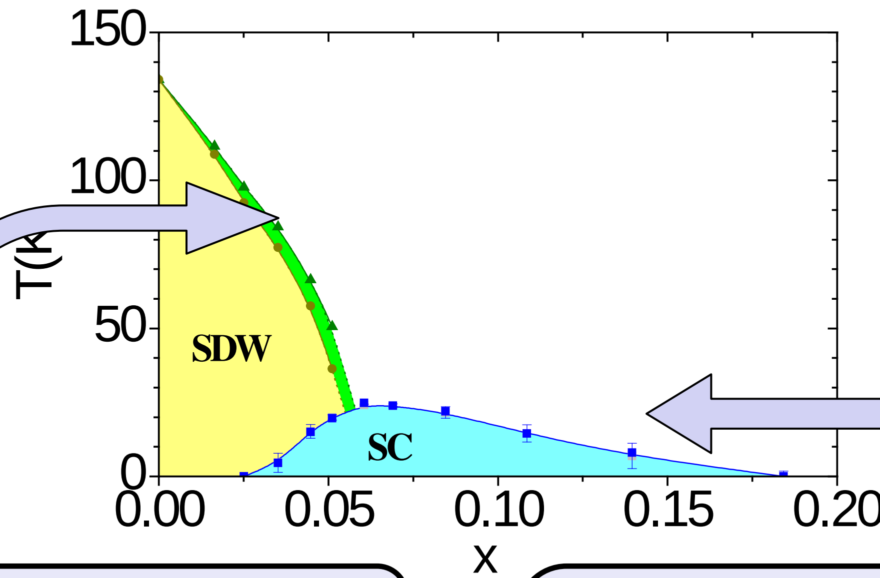




Analytis et al, ArXiv 1002.1304

- FS has smaller volume & much less c-axis dispersion than LDA predicts
- Significantly improved nesting between inner hole and electron pockets
- **Main point:** FS morphology significantly changes on doping As in to $BaFe_2P_2$ – substantially increased potential for nesting

Summary



- Dramatic electronic anisotropy
- Origin and effect on FS unknown

- Correlation between FS nesting and superconductivity
- Key feature of spin-fluctuation pairing

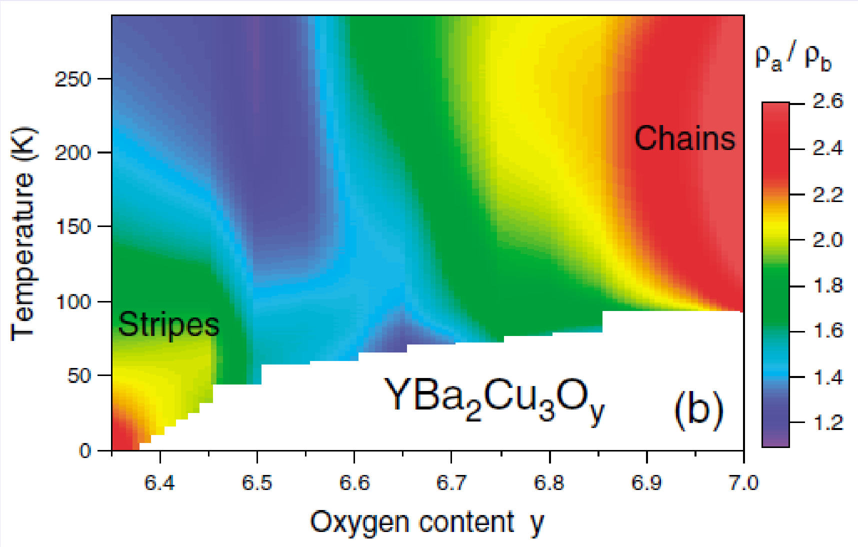
Phase diagram
Chu et al, PRB **79**, 014506 (2009).
Hayden et al, PRB **79**, 144523 (2009).

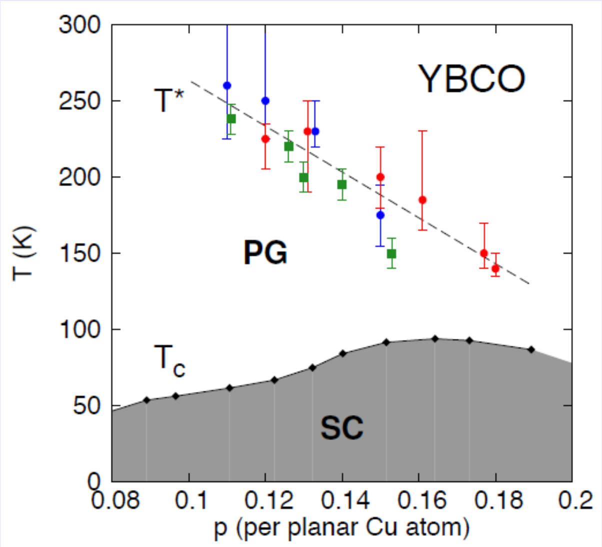
Quantum oscillations
Coldea et al, PRL **101**, 216402 (2008).
Carrington et al, Physica C **469**, 459 (2009).
Analytis et al, PRB **80**, 064507 (2009).
Coldea et al, PRL **103**, 026404 (2009).
Analytis et al, PRL **103**, 076401 (2009).
Analytis et al, ArXiv 1002.1304

In-plane anisotropy
Chu *et al*, arXiv 0911.3878
Chu *et al*, arXiv:1002.3364

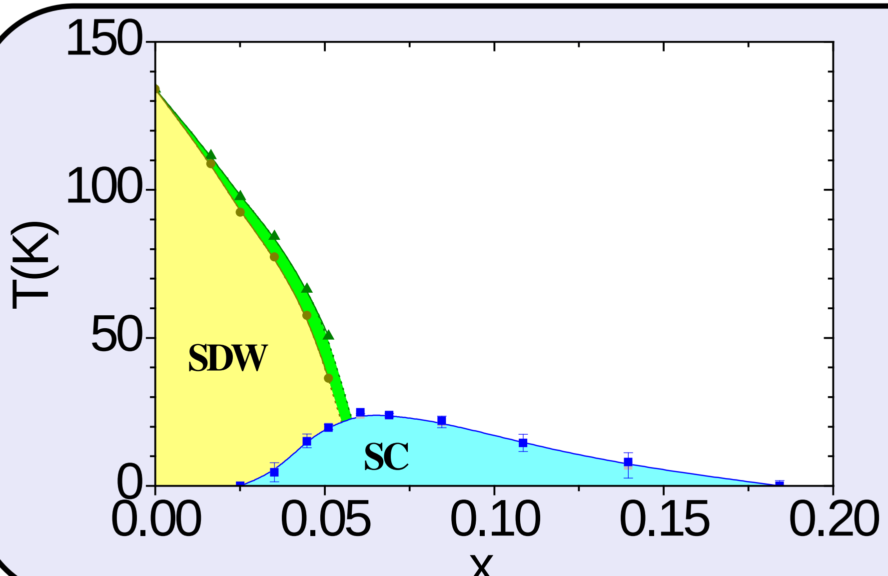
Aside: correspondence to underdoped cuprates?

Y. Ando *et al*, PRL **88**, 137005 (2002).





L . Taillefer *et al*, arXiv 0909.4430



- Succession of nematic order followed by broken translational symmetry in *both* systems

- Cuprates: ill-defined cross-over
- Fe arsenides: with well-defined phase transitions