

Fermiology and low energy dynamics of Fe-Pnictides

ES09

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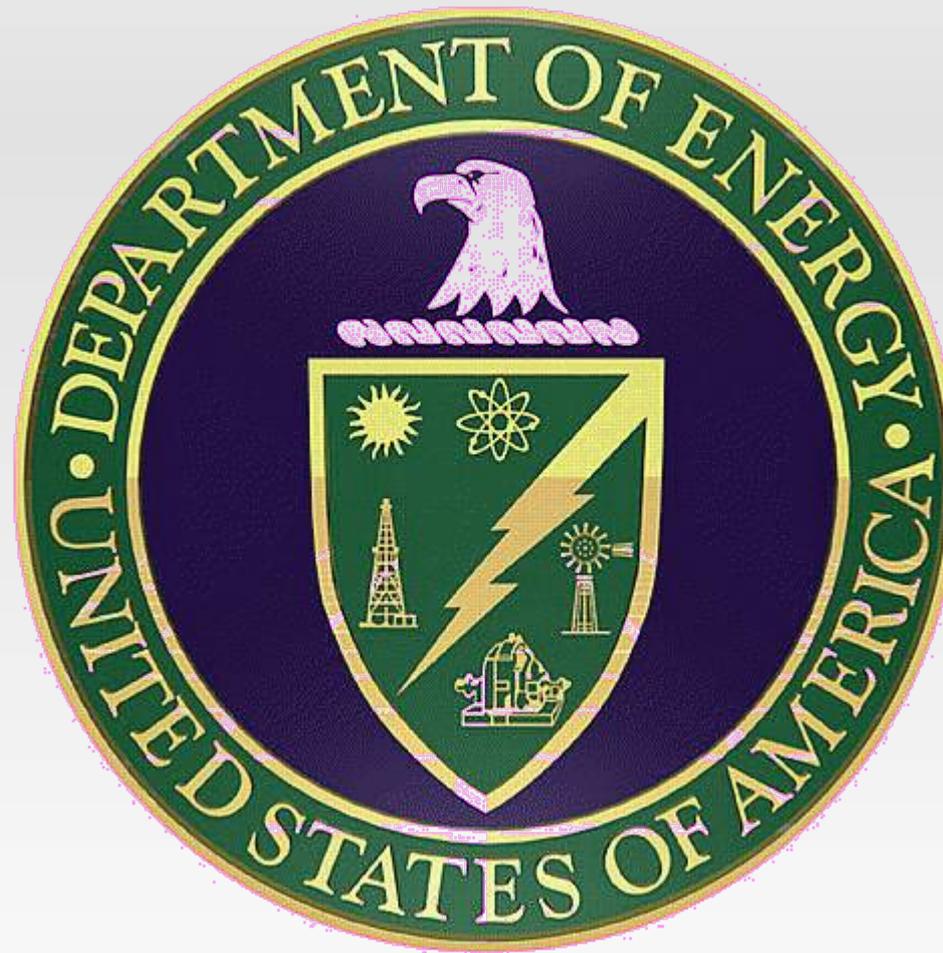
Contents: Fermiology of the pnictides

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- Part I: Summary of *some* of the experimental facts in Fe-pnictide superconductivity awaiting explanation
- Part II: Quantum oscillations and Fermiology
- Part III: Results on the AFM state
- Part IV: Results on the non-magnetic state
- Conclusions

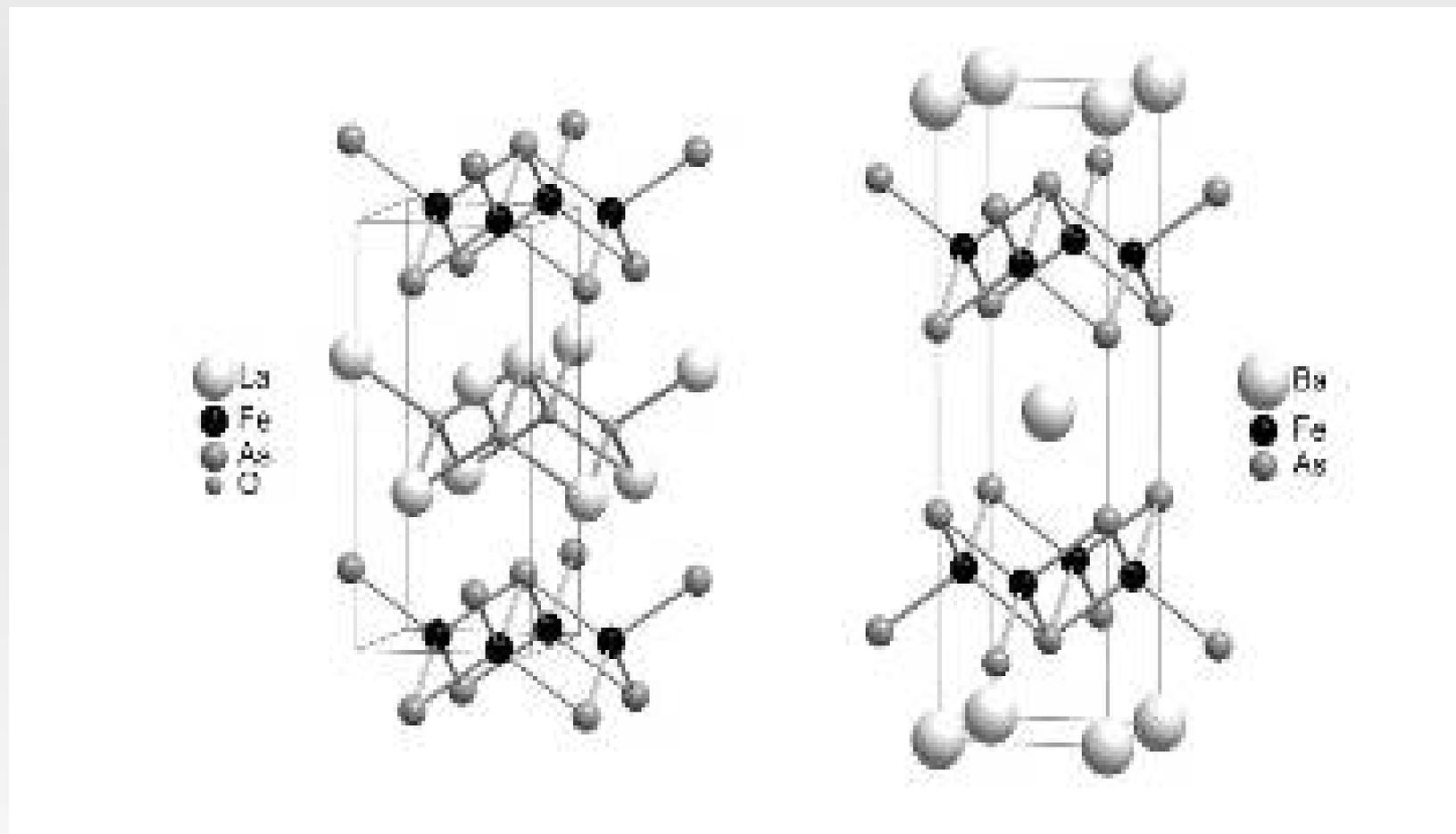
Part I: Experimental preliminaries

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The 1111s and the 122s

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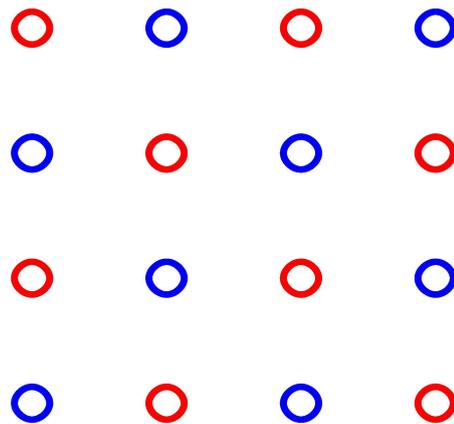
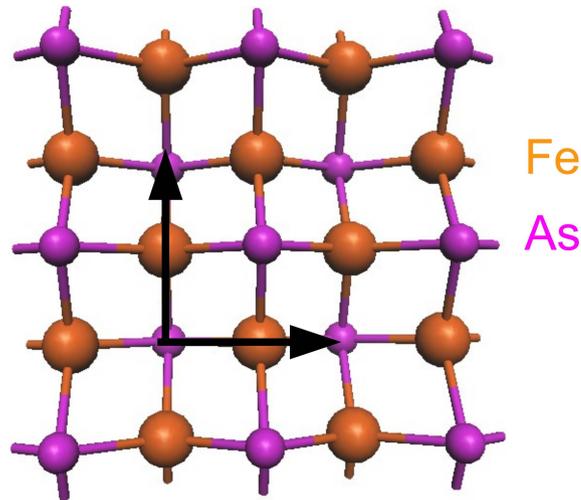


1111(As,P)

122(As,P)

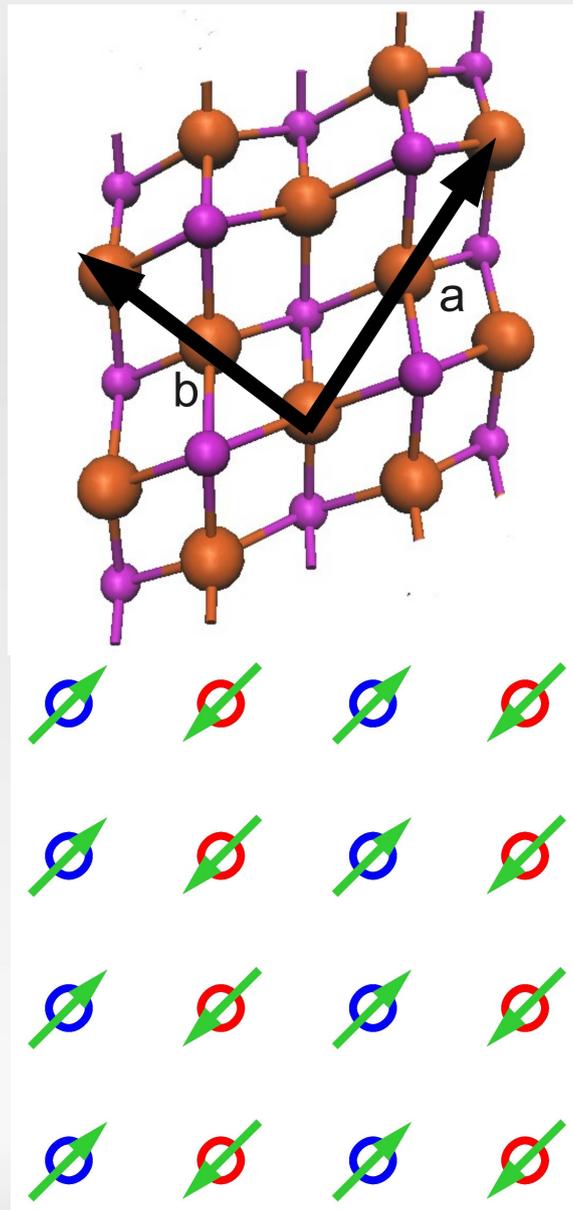
Orthorhombic and magnetic transition

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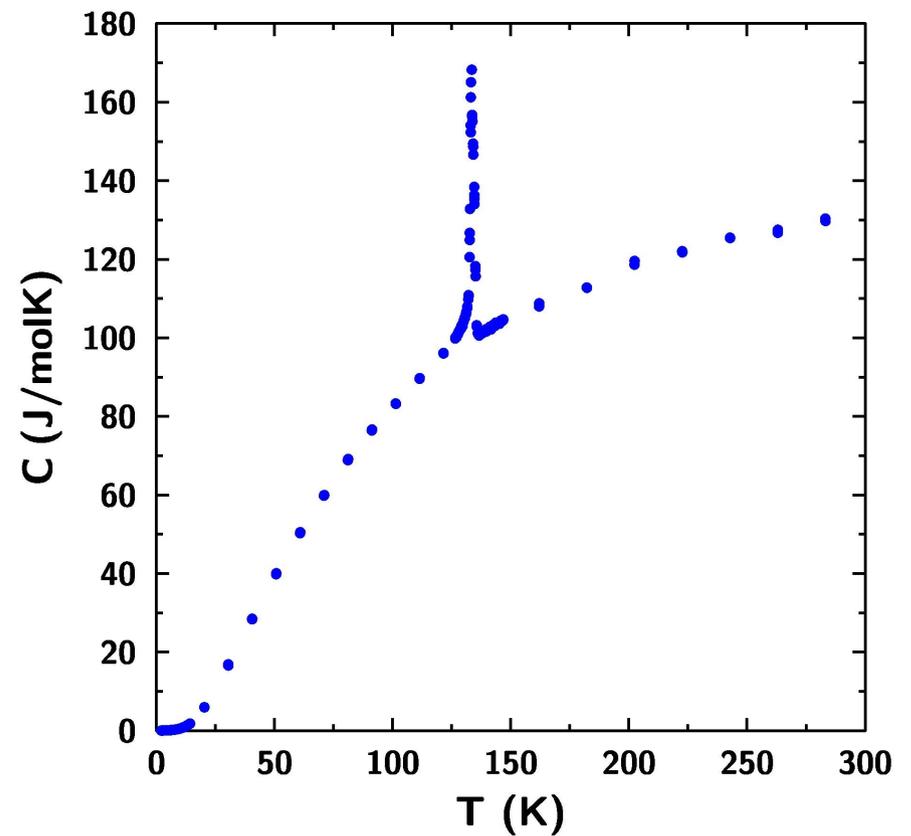
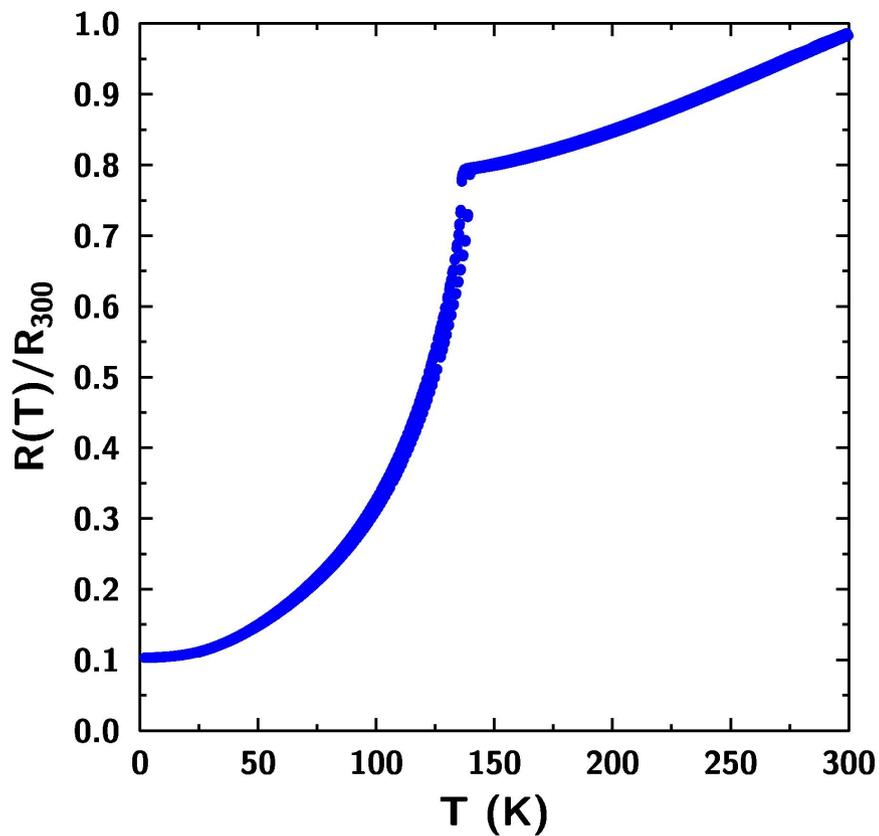
Orthorhombic and magnetic transition

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Ground state of the parent compounds

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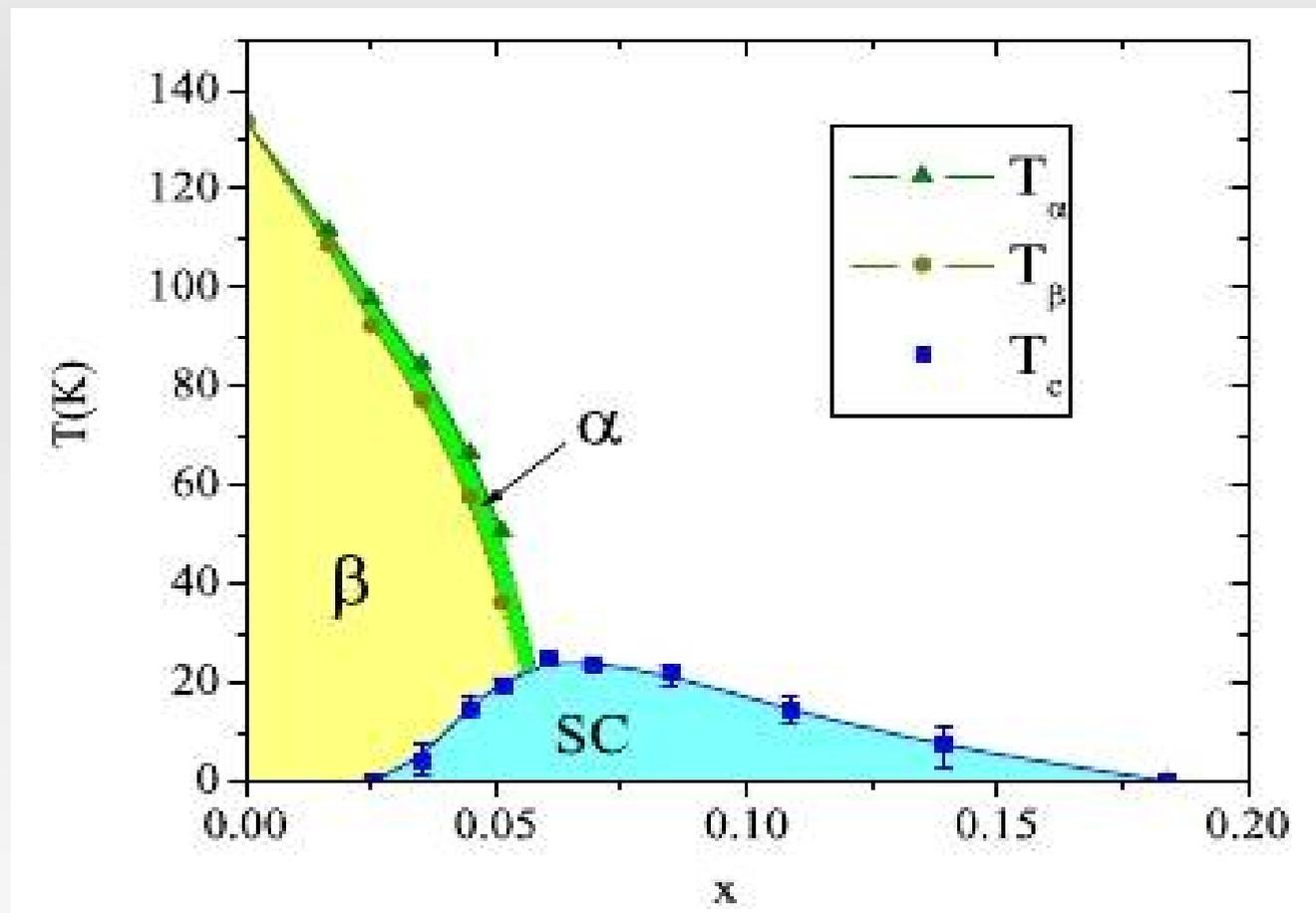
Doping in-plane

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m_e 9.1094×10^{-31} kg $m_e c^2$ 0.5110 MeV m_p 1.6726×10^{-27} kg α 1/137.036 R_∞ $10\,973\,732$ m ⁻¹ $R_\infty c$ $3.289\,842 \times 10^{15}$ Hz $R_\infty hc$ 13.6057 eV k 1.3807×10^{-23} J K ⁻¹						<input type="checkbox"/> Gases <input type="checkbox"/> Artificially Prepared		B Boron 10.811 $1s^2 2s^2 2p$ 8.2980	C Carbon 12.0107 $1s^2 2s^2 2p^2$ 11.2603	N Nitrogen 14.0067 $1s^2 2s^2 2p^3$ 14.5341	O Oxygen 15.9994 $1s^2 2s^2 2p^4$ 13.6181	F Fluorine 18.9984032 $1s^2 2s^2 2p^5$ 17.4228	I Iodine 126.90447 $[Kr] 4d^{10} 5s^2 5p^5$ 10.4513
						13 $^2P_{1/2}^o$ Al Aluminum 26.981538 $[Ne] 3s^2 3p$ 5.9858	14 3P_0 Si Silicon 28.0855 $[Ne] 3s^2 3p^2$ 8.1517	15 $^4S_{3/2}$ P Phosphorus 30.973762 $[Ne] 3s^2 3p^3$ 11.4977	16 3P_2 S Sulfur 32.065 $[Ne] 3s^2 3p^4$ 10.3600	17 $^2P_{3/2}^o$ Cl Chlorine 35.453 $[Ne] 3s^2 3p^5$ 12.9676	18 1S_0 Ar Argon 39.948 $[Ne] 3s^2 3p^6$ 15.7596		
6 VIB	7 VIIB	8 VIII			10	11 IB	12 IIB						
24 7S_3 Cr Chromium 51.9961 $[Ar] 3d^5 4s$ 6.7665	25 $^6S_{5/2}$ Mn Manganese 54.938049 $[Ar] 3d^5 4s^2$ 7.4340	26 5D_4 Fe Iron 55.845 $[Ar] 3d^6 4s^2$ 7.9024	27 $^4F_{9/2}$ Co Cobalt 58.933200 $[Ar] 3d^7 4s^2$ 7.8810	28 3F_4 Ni Nickel 58.6934 $[Ar] 3d^8 4s^2$ 7.6398	29 $^2S_{1/2}$ Cu Copper 63.546 $[Ar] 3d^{10} 4s$ 7.7264	30 1S_0 Zn Zinc 65.409 $[Ar] 3d^{10} 4s^2$ 9.3942	31 $^2P_{1/2}^o$ Ga Gallium 69.723 $[Ar] 3d^{10} 4s^2 4p$ 5.9993	32 3P_0 Ge Germanium 72.64 $[Ar] 3d^{10} 4s^2 4p^2$ 7.8994	33 $^4S_{3/2}$ As Arsenic 74.92160 $[Ar] 3d^{10} 4s^2 4p^3$ 9.7886	34 3P_2 Se Selenium 78.96 $[Ar] 3d^{10} 4s^2 4p^4$ 9.7524	35 $^2P_{3/2}^o$ Br Bromine 79.904 $[Ar] 3d^{10} 4s^2 4p^5$ 11.8138	36 1S_0 Kr Krypton 83.80 $[Ar] 3d^{10} 4s^2 4p^6$ 14.9126	
42 7S_3 Mo Molybdenum 95.94 $[Kr] 4d^5 5s$ 7.0924	43 $^6S_{5/2}$ Tc Technetium (98) $[Kr] 4d^5 5s^2$ 7.28	44 5F_4 Ru Ruthenium 101.07 $[Kr] 4d^7 5s^1$ 6.9930	45 $^4F_{9/2}$ Rh Rhodium 102.90550 $[Kr] 4d^8 5s$ 7.4589	46 1S_0 Pd Palladium 106.42 $[Kr] 4d^{10}$ 8.3369	47 $^2S_{1/2}$ Ag Silver 107.8682 $[Kr] 4d^{10} 5s$ 7.5762	48 1S_0 Cd Cadmium 112.411 $[Kr] 4d^{10} 5s^2$ 8.9938	49 $^2P_{1/2}^o$ In Indium 114.818 $[Kr] 4d^{10} 5s^2 5p$ 5.7864	50 3P_0 Sn Tin 118.710 $[Kr] 4d^{10} 5s^2 5p^2$ 7.3439	51 $^4S_{3/2}$ Sb Antimony 121.760 $[Kr] 4d^{10} 5s^2 5p^3$ 8.6084	52 3P_2 Te Tellurium 127.60 $[Kr] 4d^{10} 5s^2 5p^4$ 9.0096	53 $^2P_{3/2}^o$ I Iodine 126.90447 $[Kr] 4d^{10} 5s^2 5p^5$ 10.4513	54 1S_0 Xe Xenon 131.29 $[Kr] 4d^{10} 5s^2 5p^6$ 13.4464	
74 5D_0 W Tungsten 183.84 $[Xe] 4f^{14} 5d^4 6s^2$ 11.5483	75 $^6S_{5/2}$ Re Rhenium 186.207 $[Xe] 4f^{14} 5d^5 6s^2$ 11.6295	76 5D_4 Os Osmium 190.23 $[Xe] 4f^{14} 5d^6 6s^2$ 11.7089	77 $^4F_{9/2}$ Ir Iridium 192.217 $[Xe] 4f^{14} 5d^7 6s^2$ 11.7845	78 3D_3 Pt Platinum 195.078 $[Xe] 4f^{14} 5d^9 6s^1$ 11.8512	79 $^2S_{1/2}$ Au Gold 196.96655 $[Xe] 4f^{14} 5d^{10} 6s^1$ 11.9163	80 1S_0 Hg Mercury 200.59 $[Xe] 4f^{14} 5d^{10} 6s^2$ 11.9823	81 $^2P_{1/2}^o$ Tl Thallium 204.3833 $[Xe] 4f^{14} 5d^9 6s^2 6p$ 12.0474	82 3P_0 Pb Lead 207.2 $[Xe] 4f^{14} 5d^{10} 6s^2 6p^2$ 12.1125	83 $^4S_{3/2}$ Bi Bismuth 208.98038 $[Xe] 4f^{14} 5d^9 6s^2 6p^3$ 12.1776	84 3P_2 Po Polonium (209) $[Xe] 4f^{14} 5d^{10} 6s^2 6p^4$ 12.2427	85 $^2P_{3/2}^o$ At Astatine (210) $[Xe] 4f^{14} 5d^{10} 6s^2 6p^5$ 12.3078	86 1S_0 Rn Radon 222 $[Xe] 4f^{14} 5d^{10} 6s^2 6p^6$ 12.3729	

SDW and Superconductivity

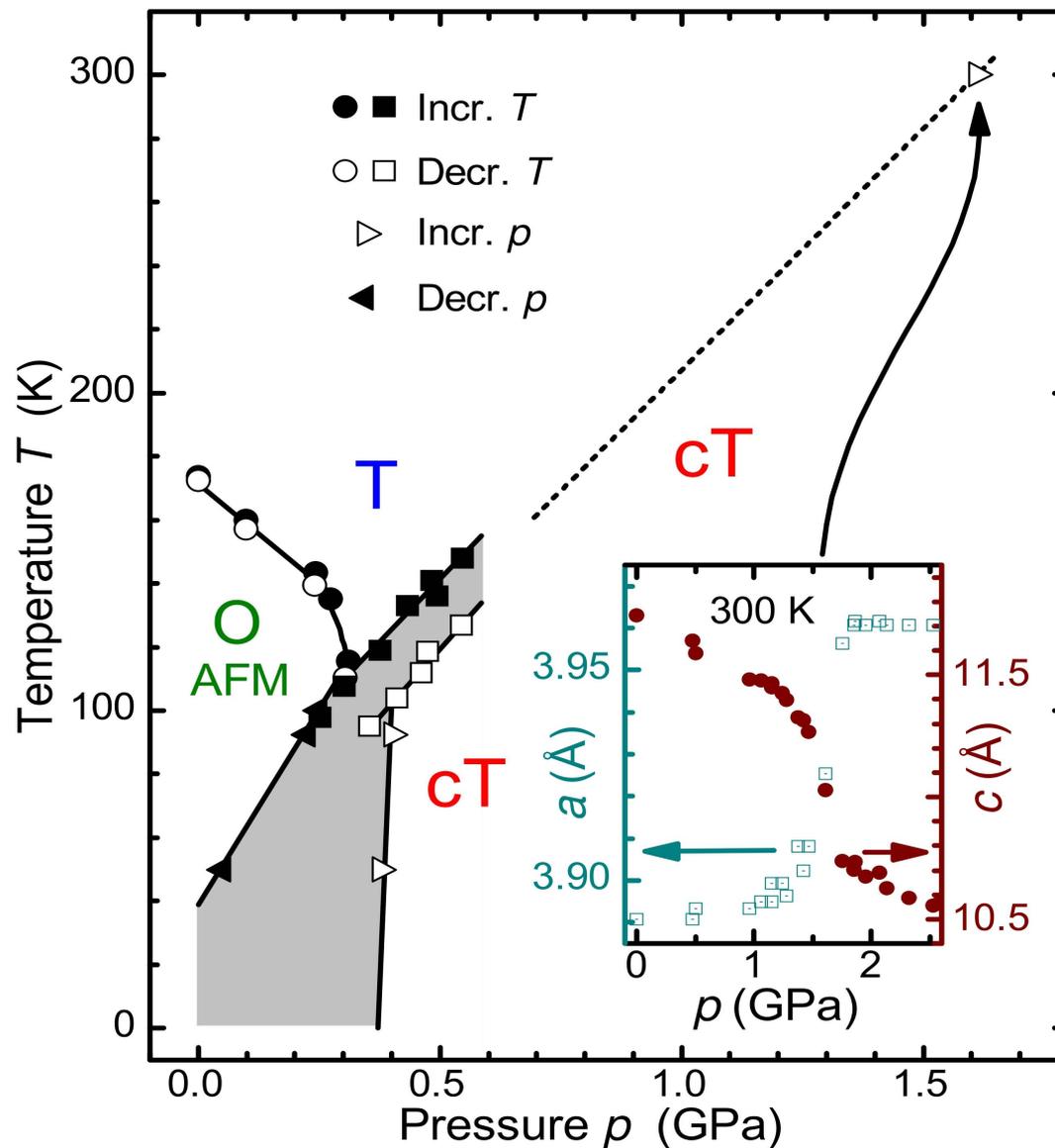
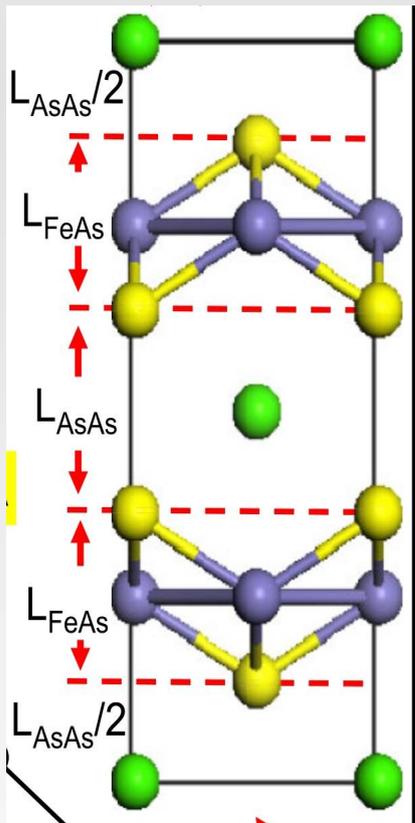
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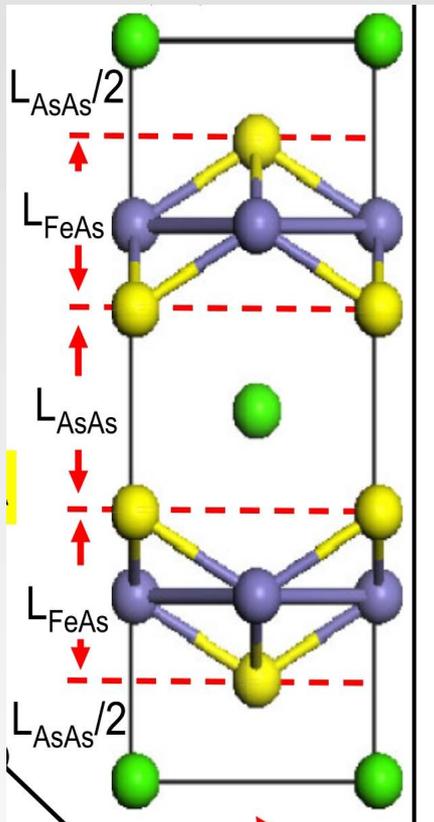
JH Chu, JG Analytis et al. PRB 2009

Ca122 – hydrostatic pressure

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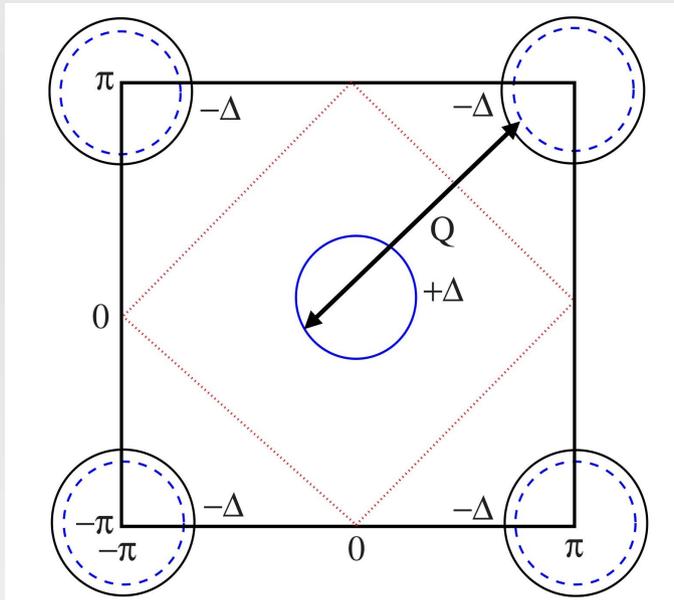
Materials



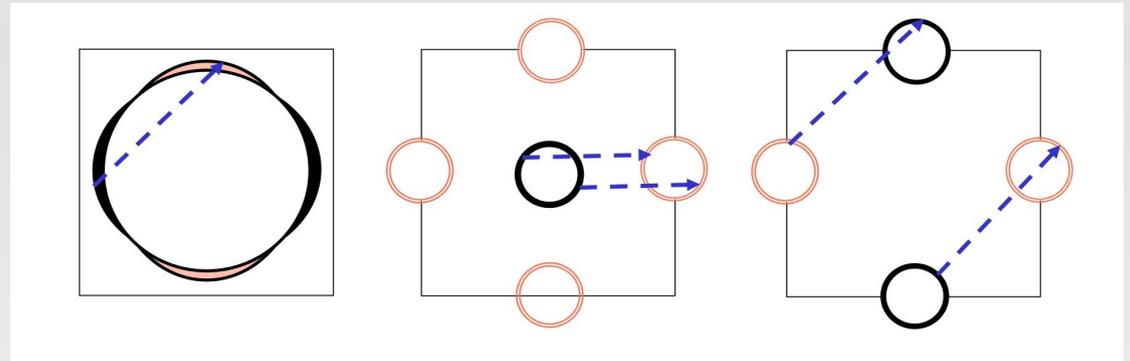
- 111s – quasi-2D, higher T_c
- 122s – more 3D, lower T_c
- Phosphides – lower T_c , non-magnetic
- Arsenides - high T_c , magnetic

- 1111s in general have higher T_c s than 122s.
- SDW is suppressed as Fe-pnictides approach optimal T_c .
- Small changes in the local structure can induce high T_c .
- Superconducting phosphides have much lower T_c than arsenides.

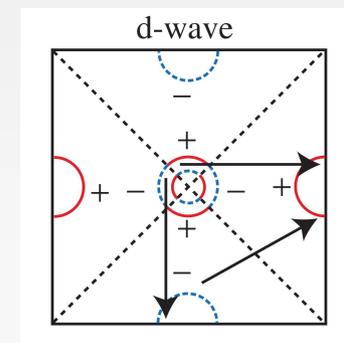
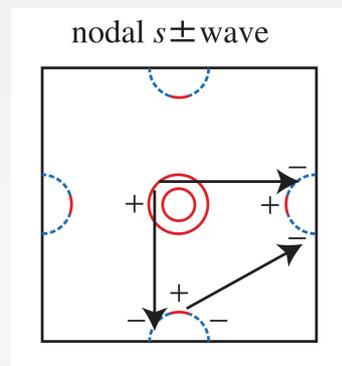
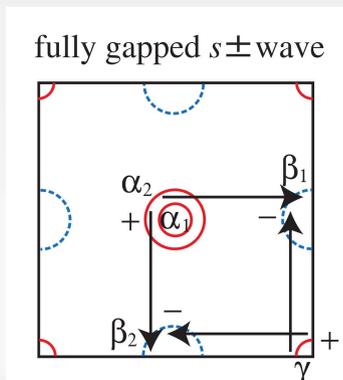
Theories for superconductivity



Chubukov 2008

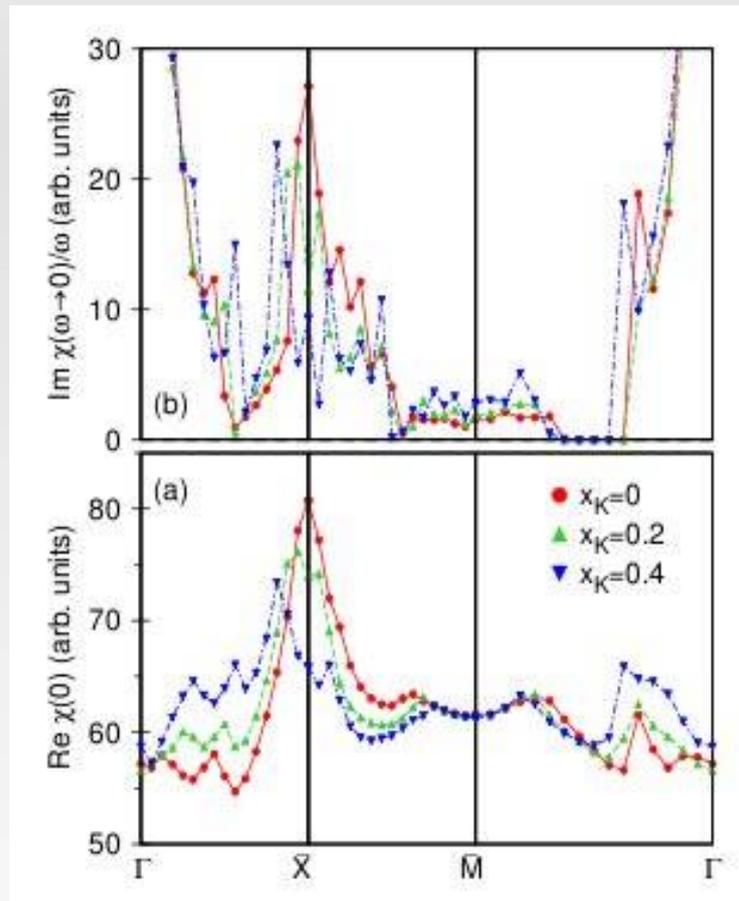


Mazin, Schmalian 2009



Kuroki, Aoki 2009

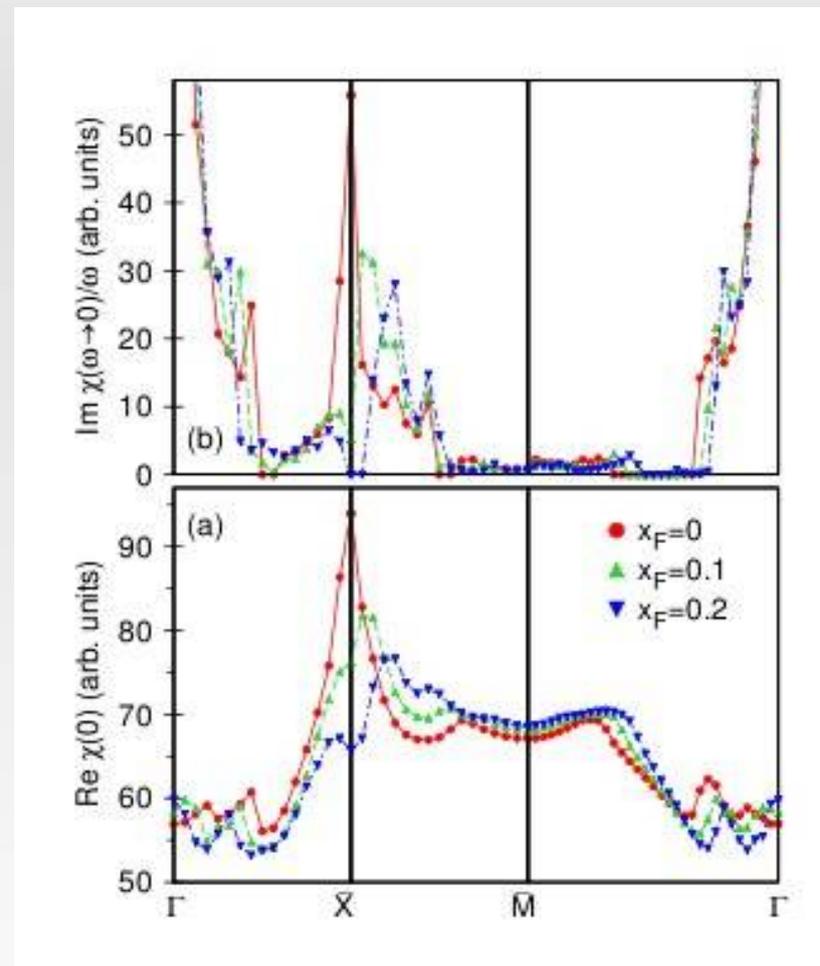
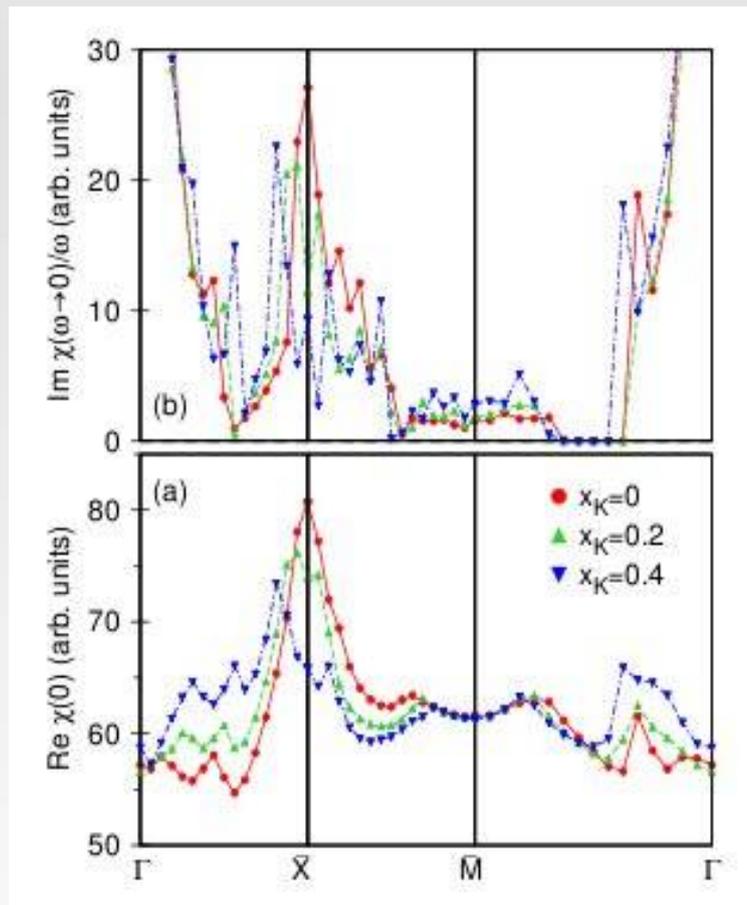
Preliminaries



Yaresko cond-mat 2008

nesting=magnetism?

Preliminaries



LaFePO?

Yaresko cond-mat 2008

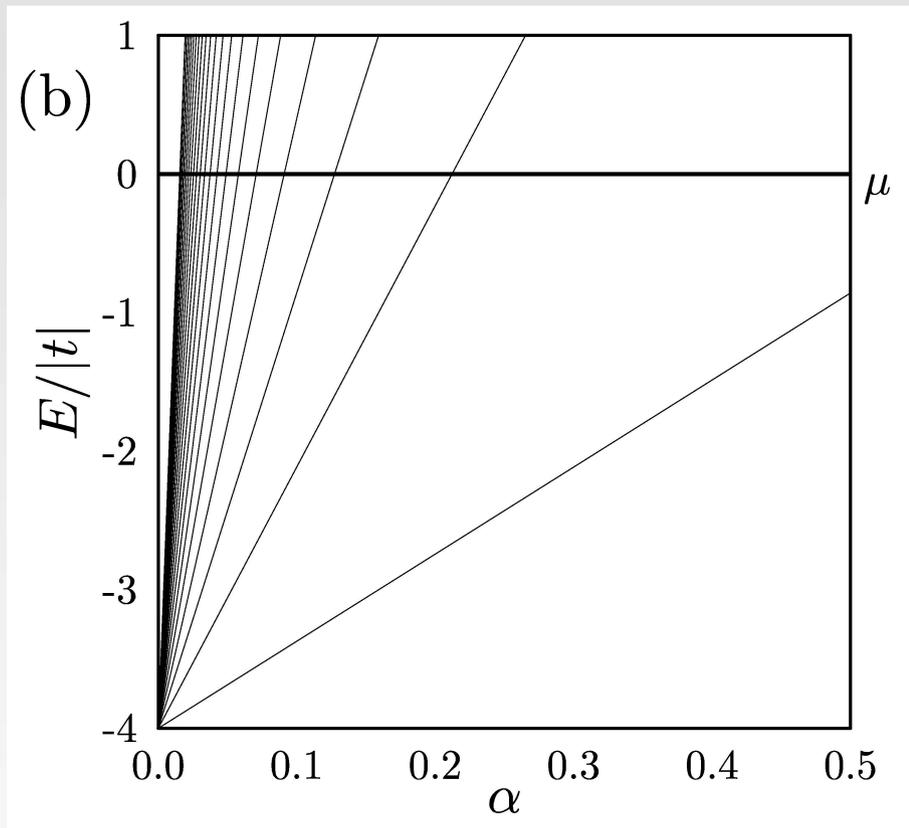
The puzzle

- What is the dimensionality of the low energy quasiparticles?
- Is the magnetism a Fermi surface nesting driven process? If not, what is the role of itineracy, if any?
- Do local lattice/magnetic interactions enhance or reduce T_c ?

Part II: Quantum Oscillations



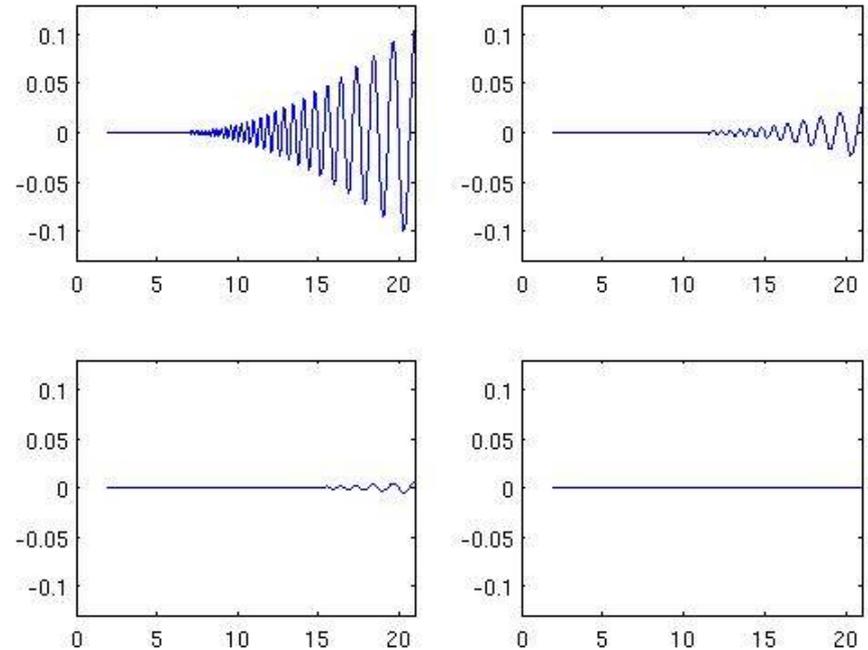
Energy quantization in field: Landau levels



- In field energy bands are quantized into Landau levels.
- As the levels sweep the Fermi energy, there are oscillations in the density of states.
- Oscillations in $1/B$
- Frequency proportional to extremal area

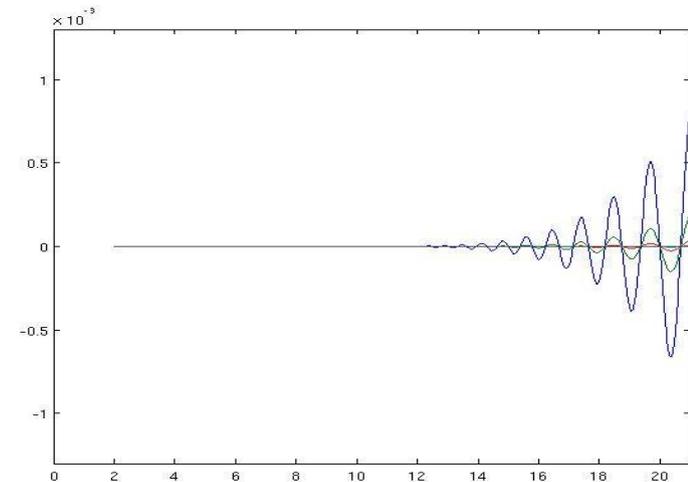
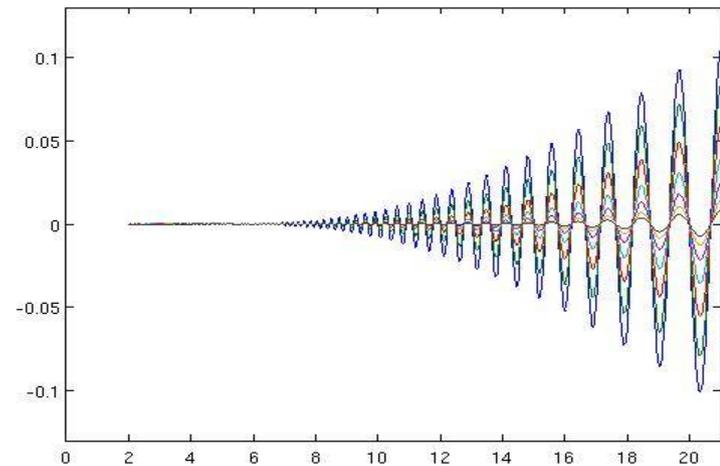
Lifschitz-Kosevich formalism

- Broadening of Landau levels due to a finite scattering time allows us to extract information about the mean-free-path.

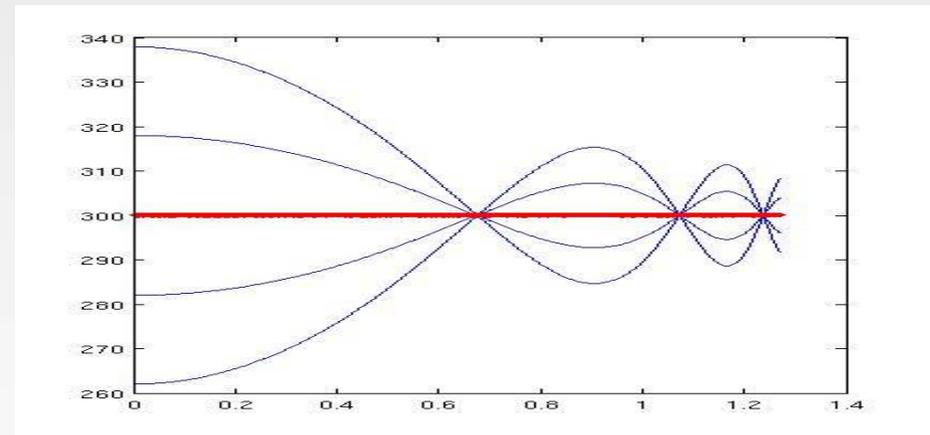
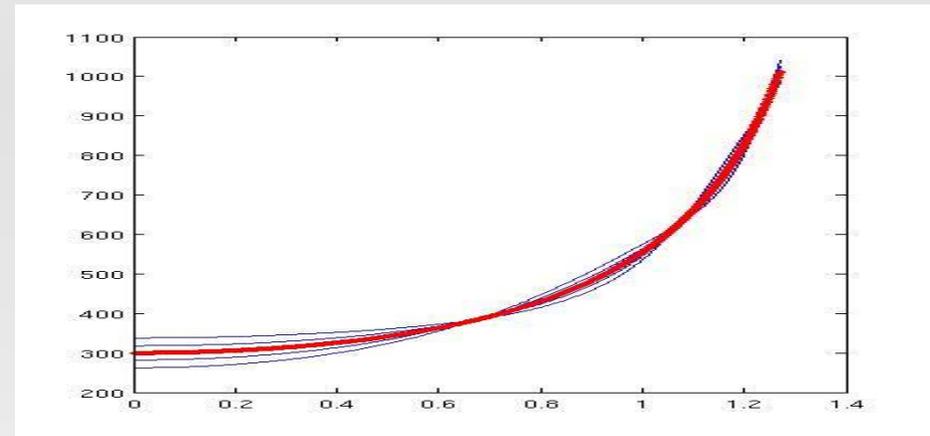
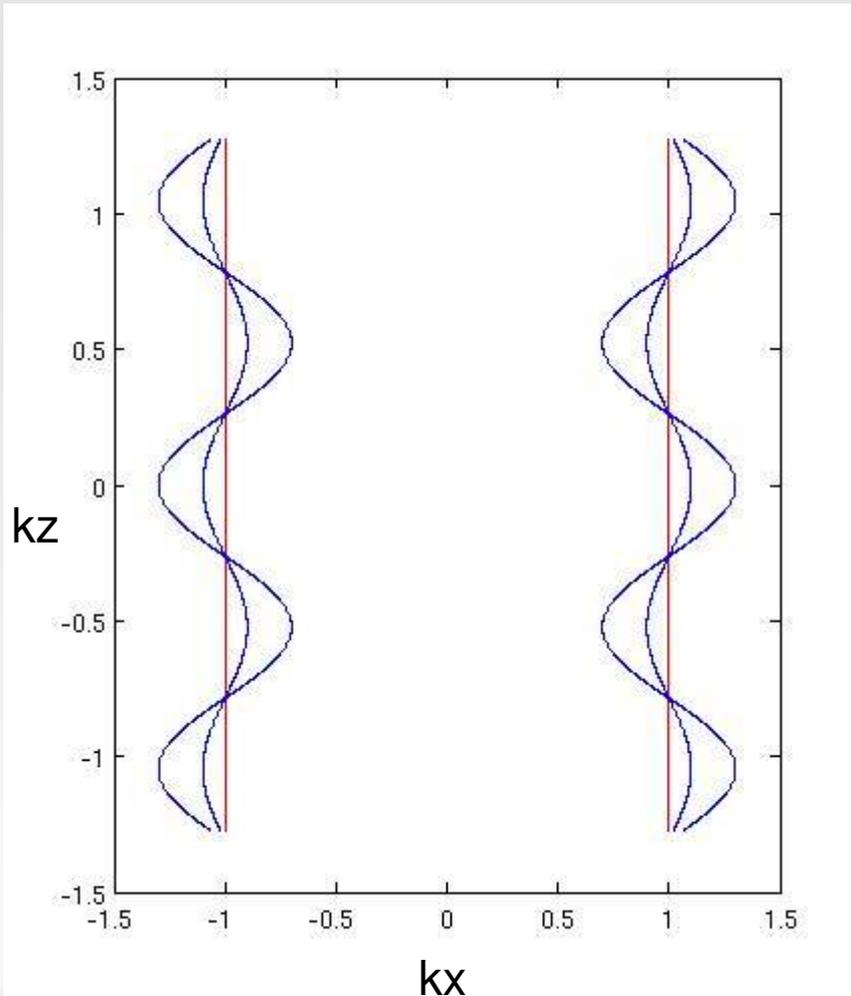


Lifschitz-Kosevich formalism

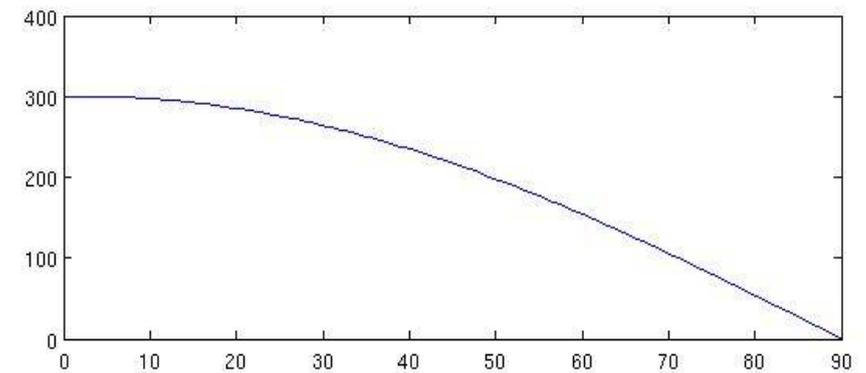
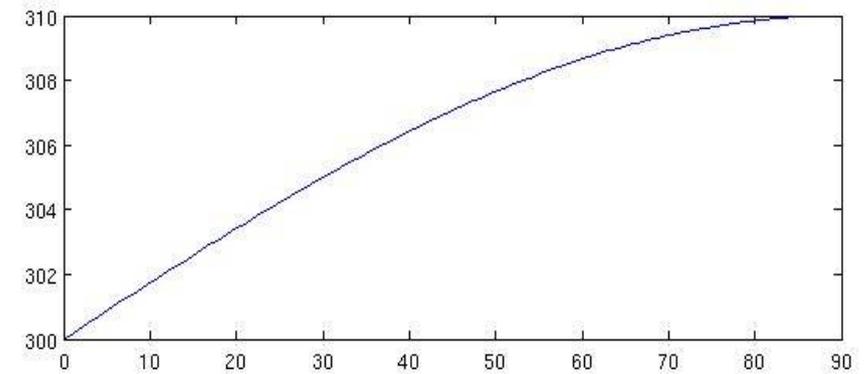
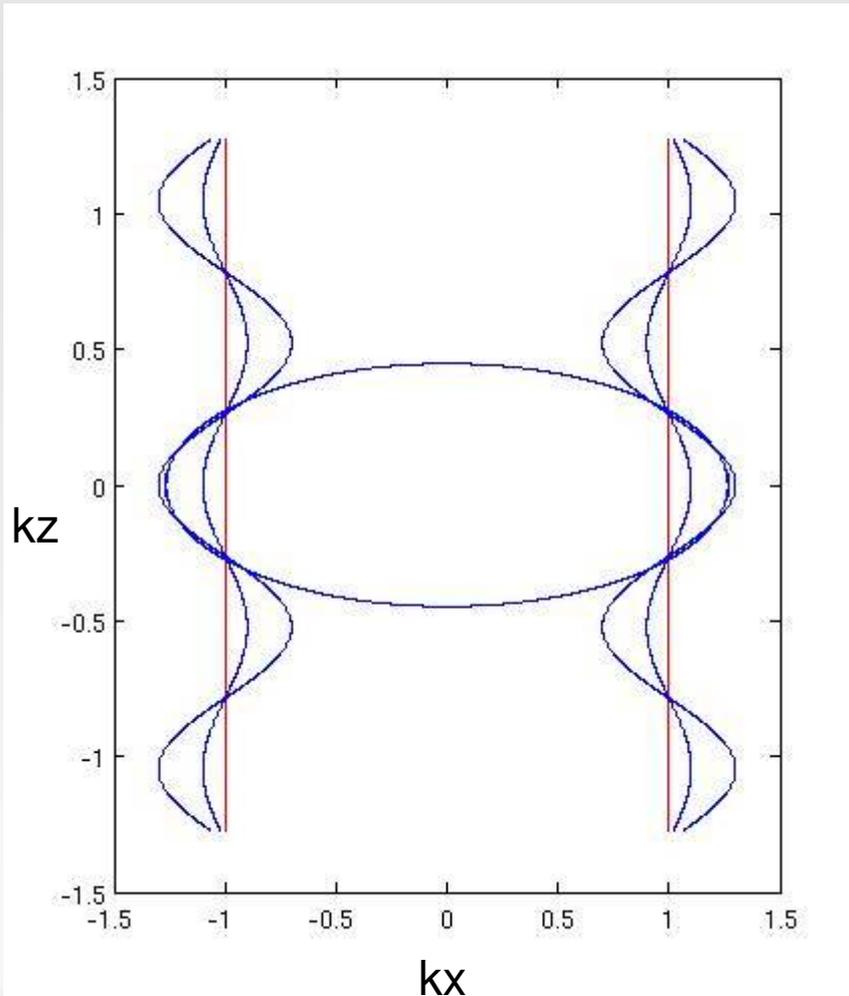
- Broadening of Landau levels due to finite temperature allows us to extract information about the effective mass m^* .



Determination of the FS topology: angle dependence



Determination of the FS topology: angle dependence

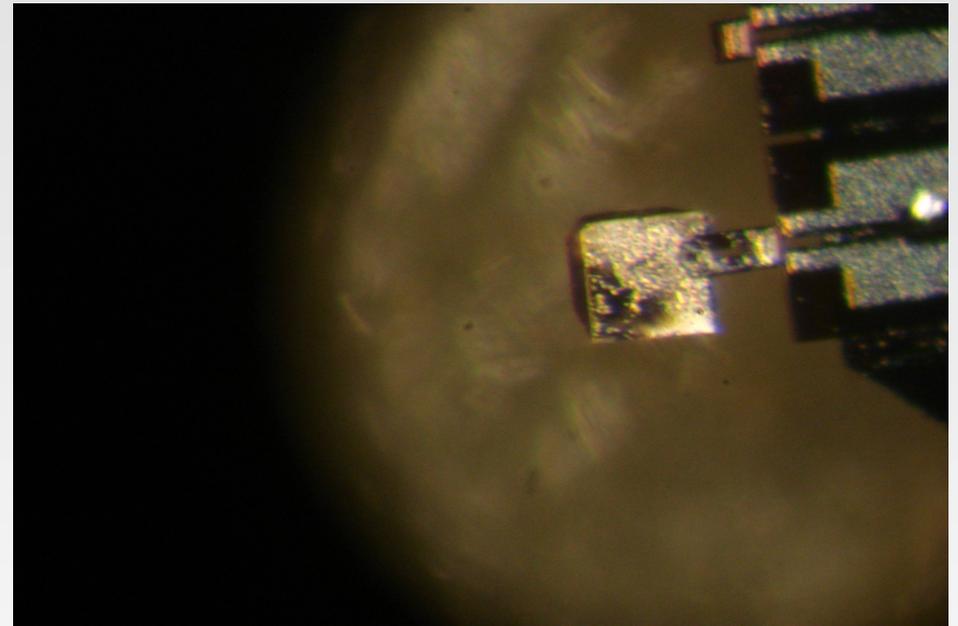


Pro's and Con's of quantum oscillations

- Very accurate determination of Fermi surface size and topology.
- Band renormalization easy to determine for each band.
- Quasiparticle lifetime easy to determine.
- Clean samples with *long* mean free paths.
- If you can't get clean samples, then you need very high field.
- Very hard to do doping studies because of both Hc_2 and disorder.
- Cannot always assign orbits

The de Haas-van Alphen effect using torque magnetometry

- Torque magnetometry
 - $\tau \propto M \times H$
- Use of piezoresistive microcantilevers
 - Balance a basic resistance bridge and measure signal on a lock-in



Use of high magnetic fields



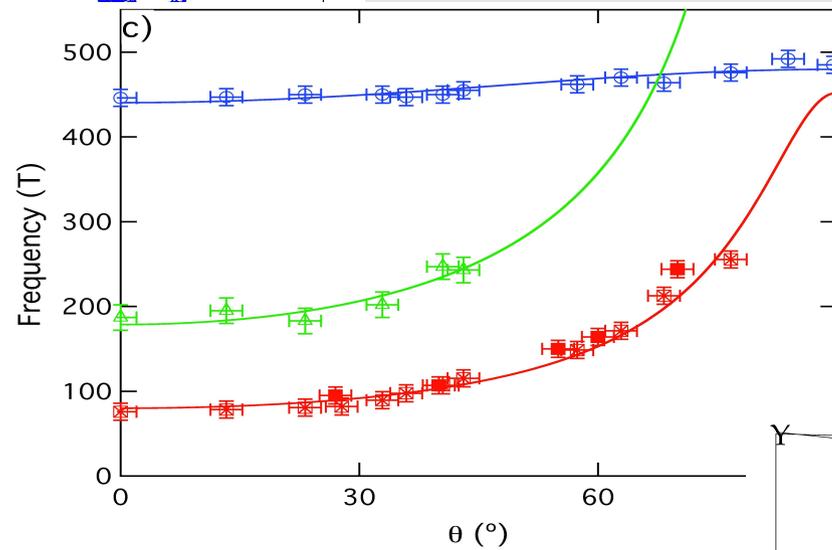
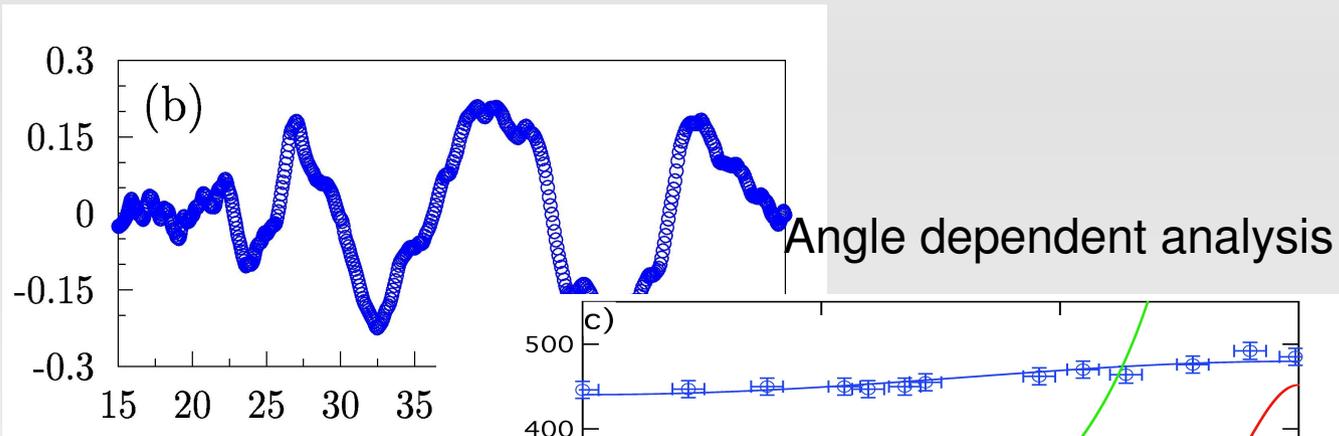
- Los Alamos national lab
 - 65 T short pulse
 - 55 T long pulse
- Nijmegen, HFML
 - 30 T DC field
- Tallahassee
 - 45 T DC field

Part III: Results on the AFM state

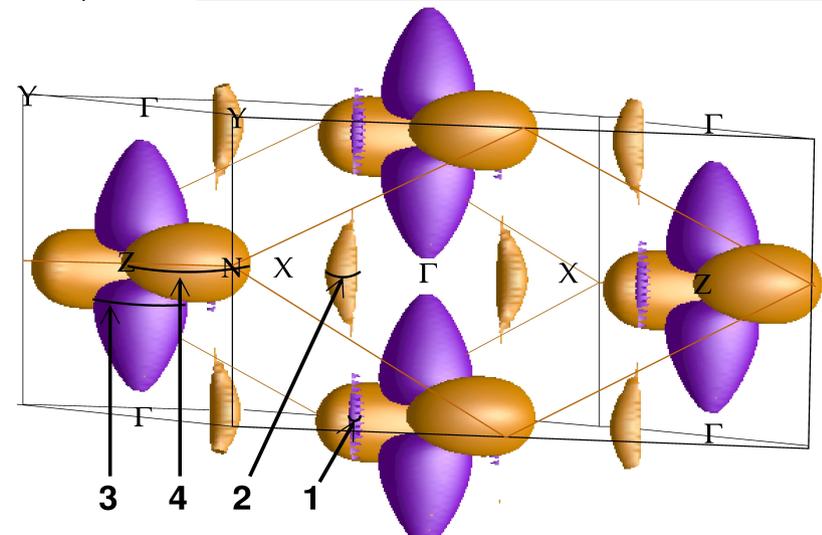


BaFe₂As₂

Background subtracted signal

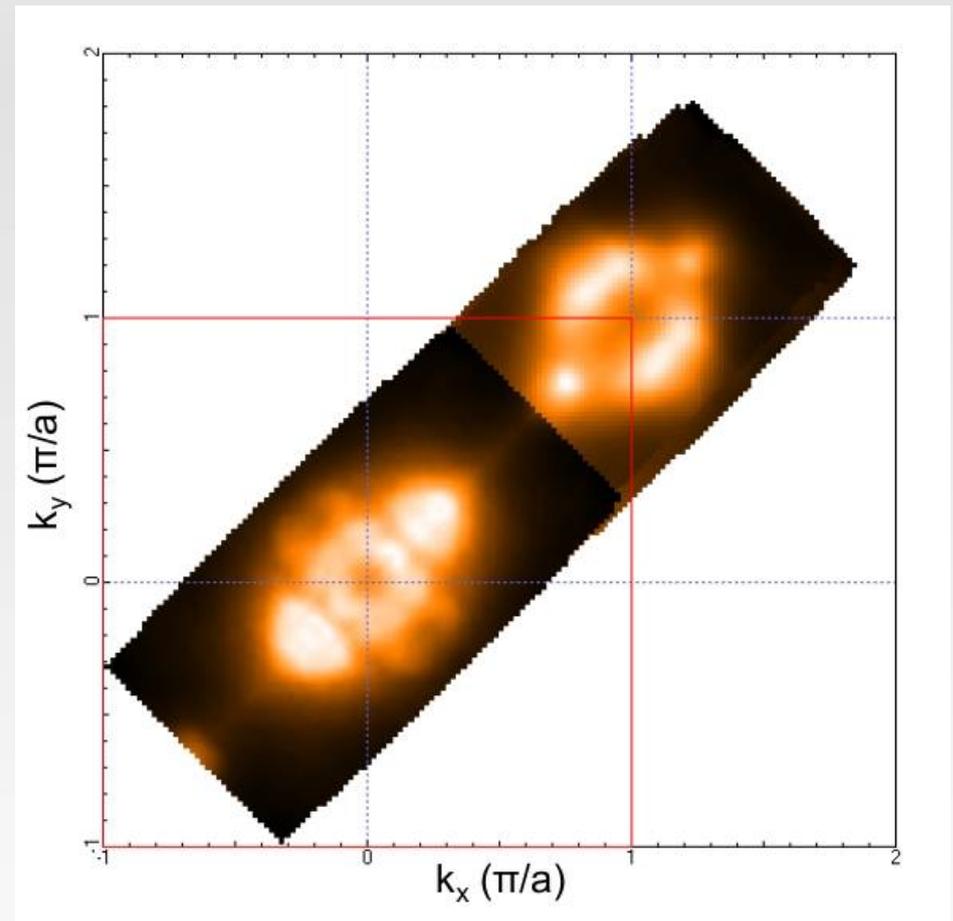


DFT calculations



Comparison to photoemission

- Comparison to recent photoemission data shows significant overlap with QO studies.
- The pockets observed place severe limits on topology and mass of any other FS sections.



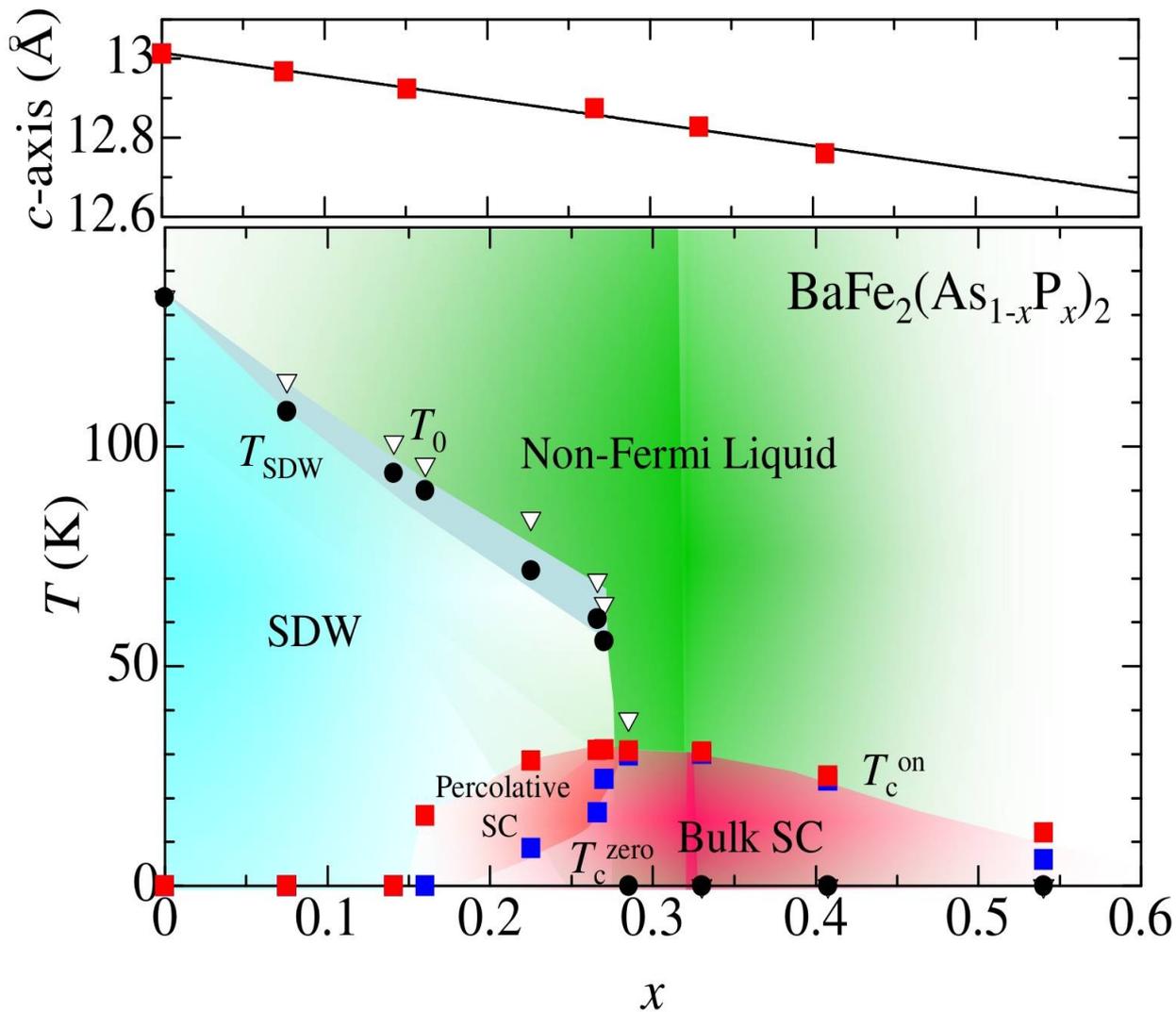
Part IV: The non-magnetic FS



How do we get to the non-magnetic state?

- For the typical mean free paths of the non-magnetic state require around 600T to complete a cyclotron orbit.
- However, by replacing As \rightarrow P, we can suppress the magnetism and increase the carrier density.
- So we can see QO in the phosphides! e.g. Sr122, Ca122, LaFePO

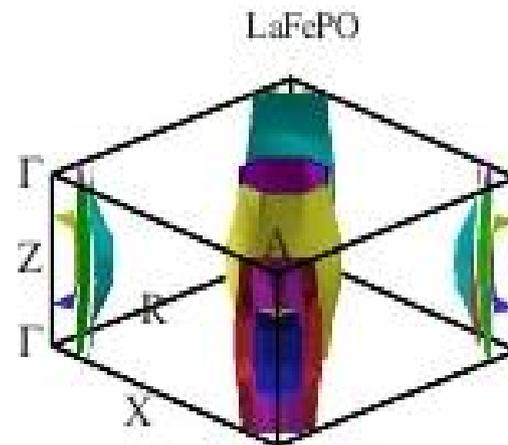
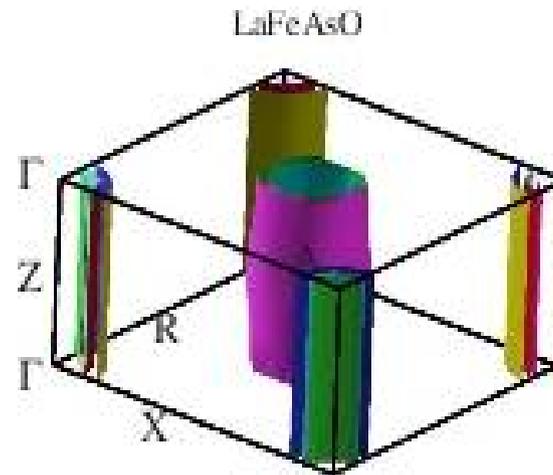
P substitution of As: phase diagram



But are they the same?

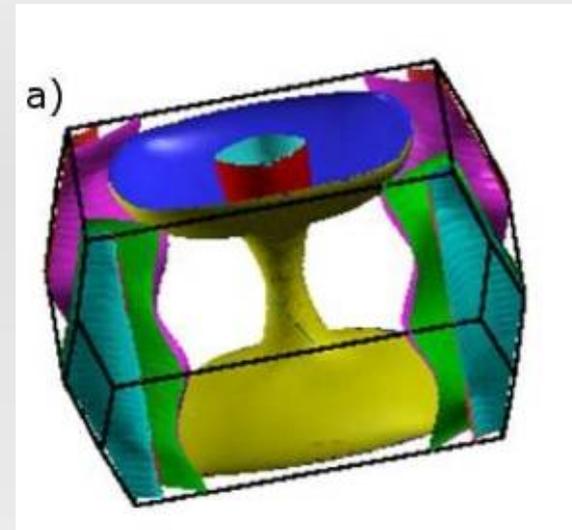
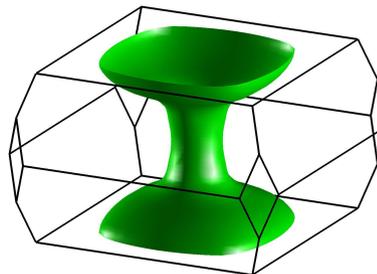
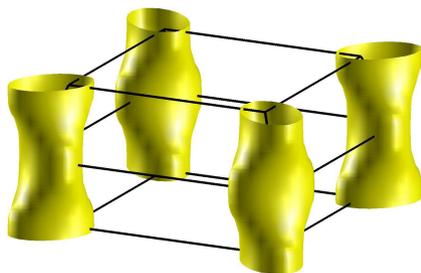
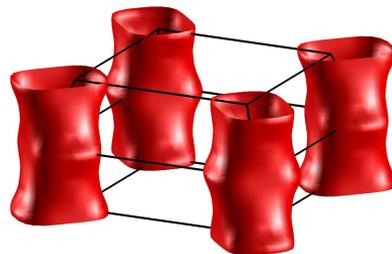
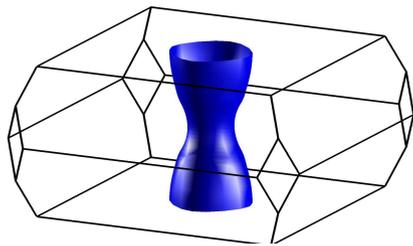
- *c*-axis smaller by 6%
- Pn-Pn distance smaller
- Polarizability smaller by 1.5
- As-Fe-As bond angle much more obtuse $\sim 109.5^\circ$ vs $\sim 116^\circ$
- *c*-axis shrinks by the same amount in arsenides
 - Ba- \rightarrow Sr- \rightarrow Ca
- Similarly the Pn-Pn distance.
- As-Fe-As bond angle seems to suppress the magnetism more than adjust the Fermiology.

But are they the same? LaFePO



Georges et al 2008

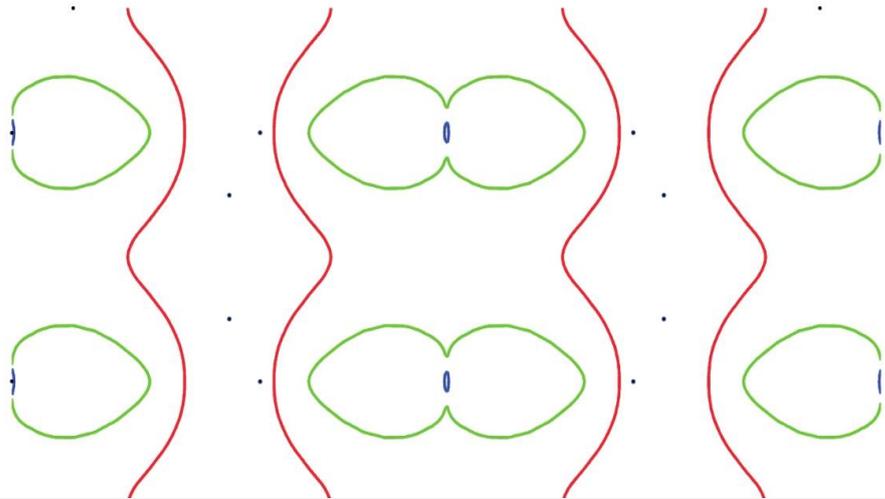
But are they the same? Sr122



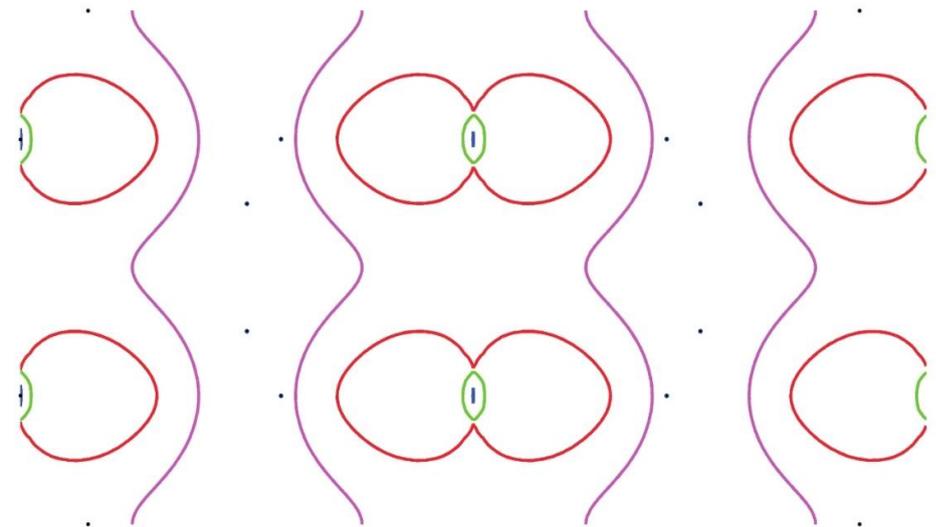
Tomsett, Lonzarich 2009

But are they the same? Ca122

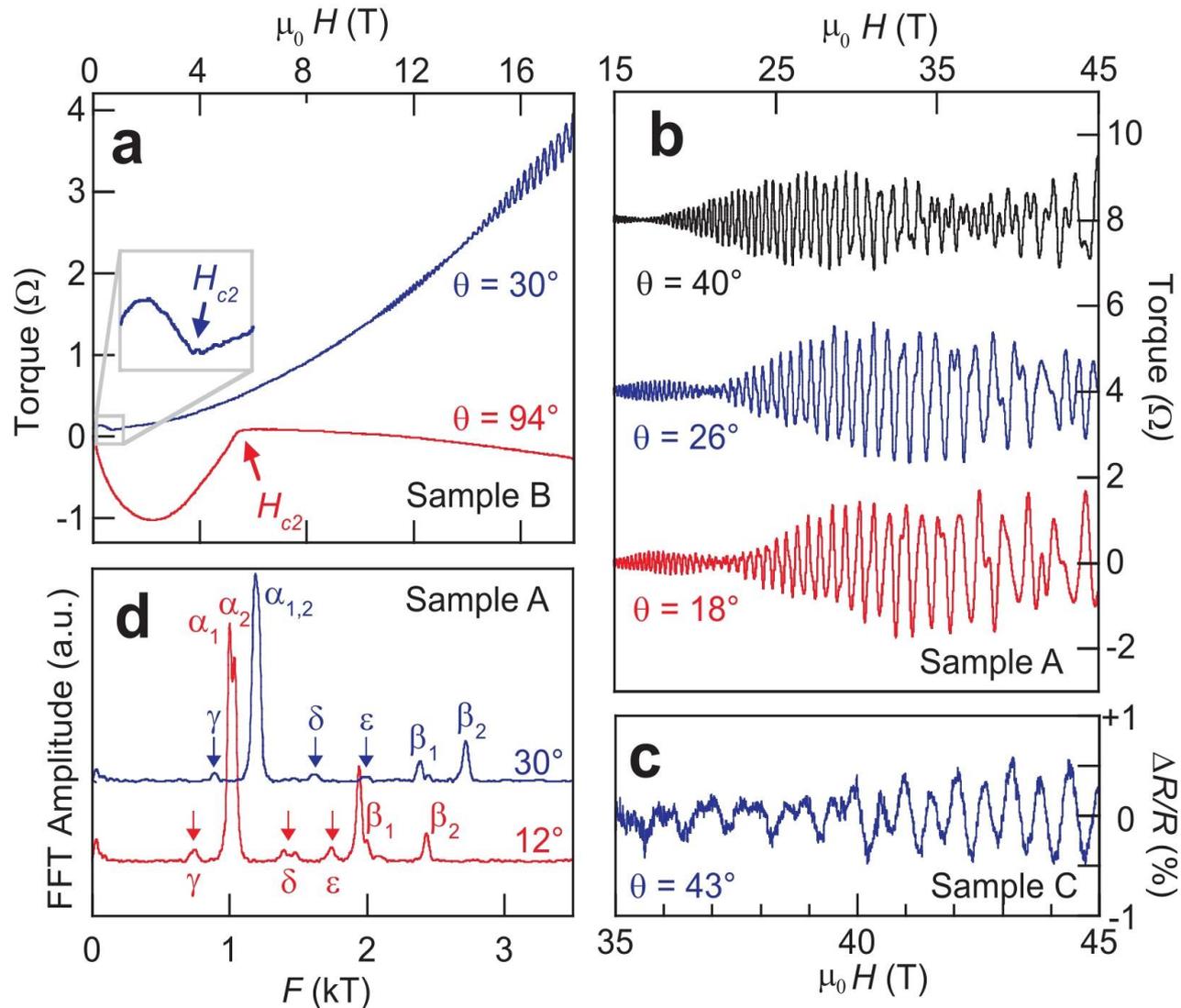
CaFe_2As_2 $P=0.63\text{GPa}$ (cT phase)



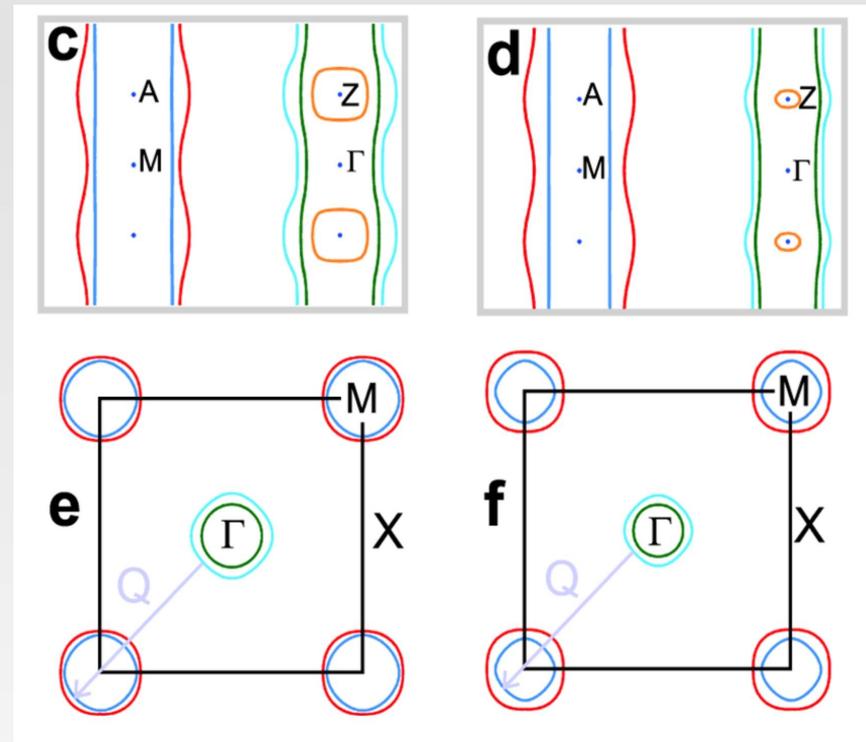
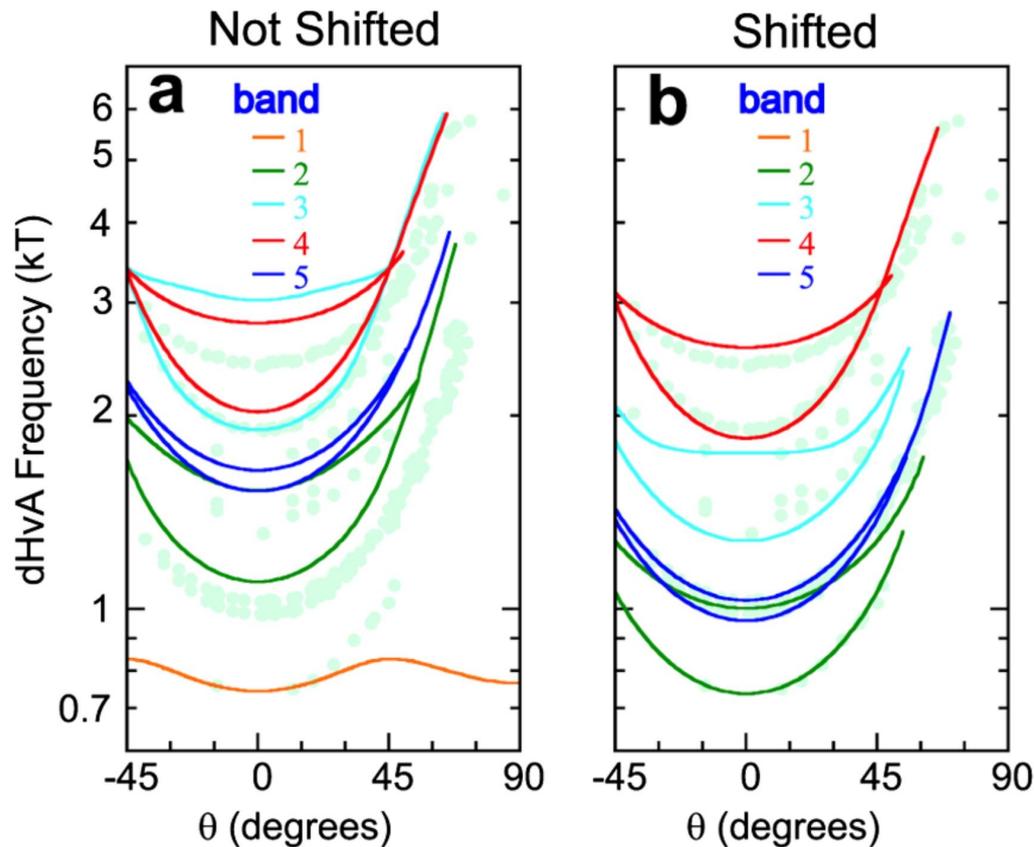
CaFe_2P_2 $P=0$



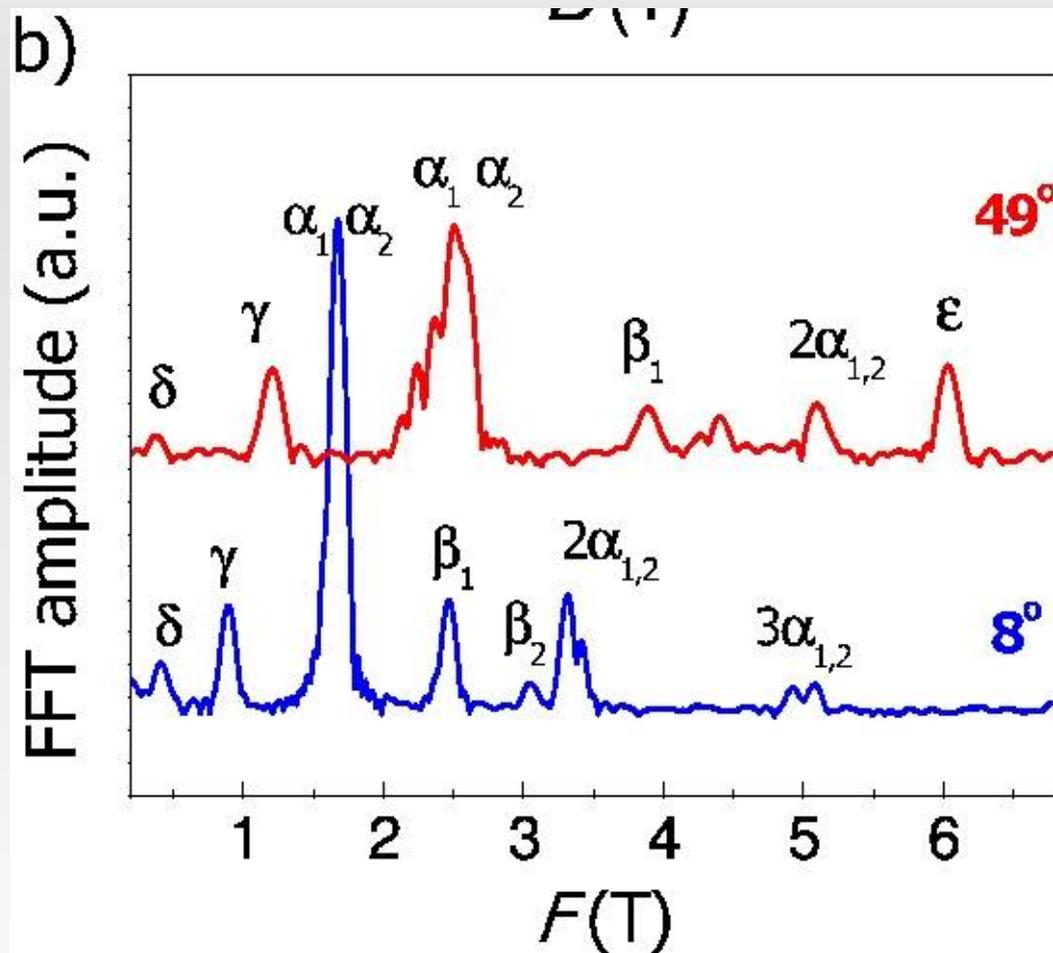
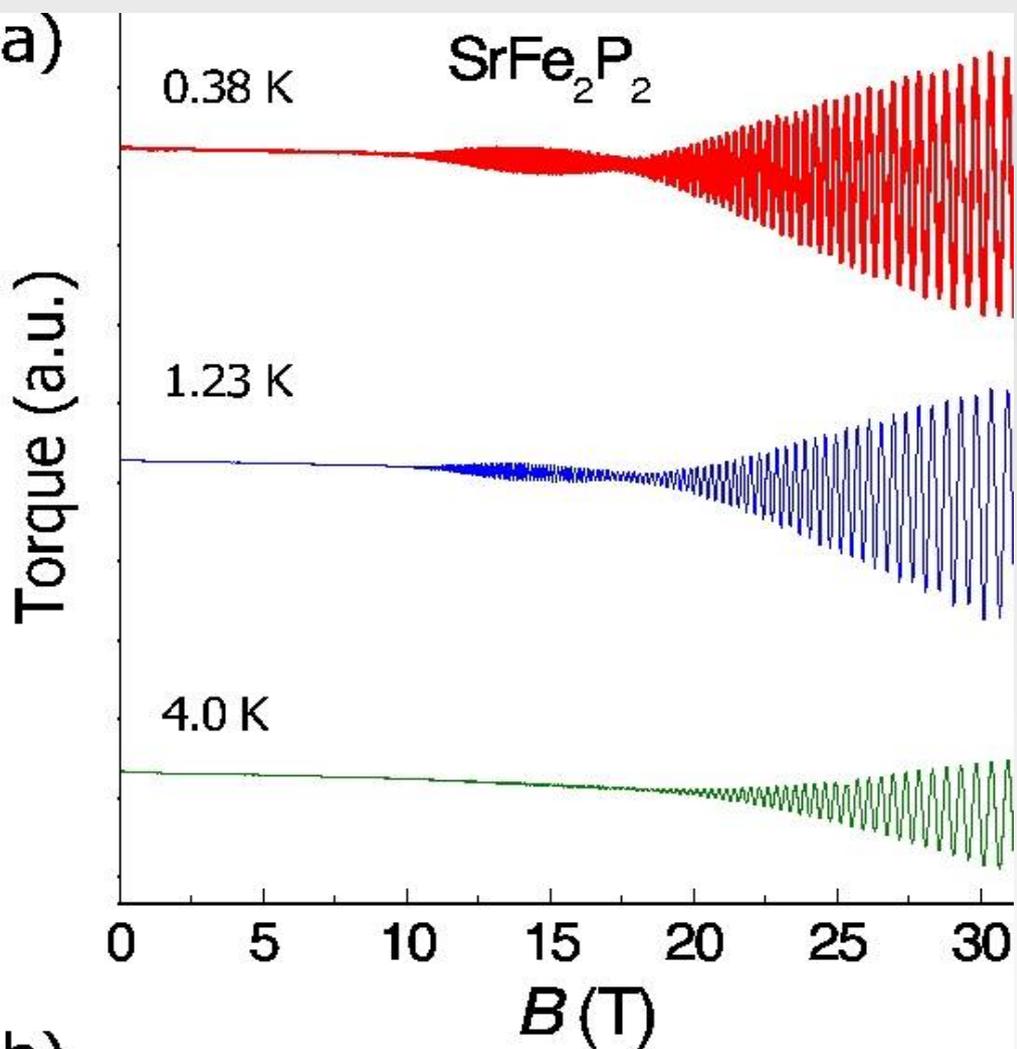
Oscillations in LaFePO



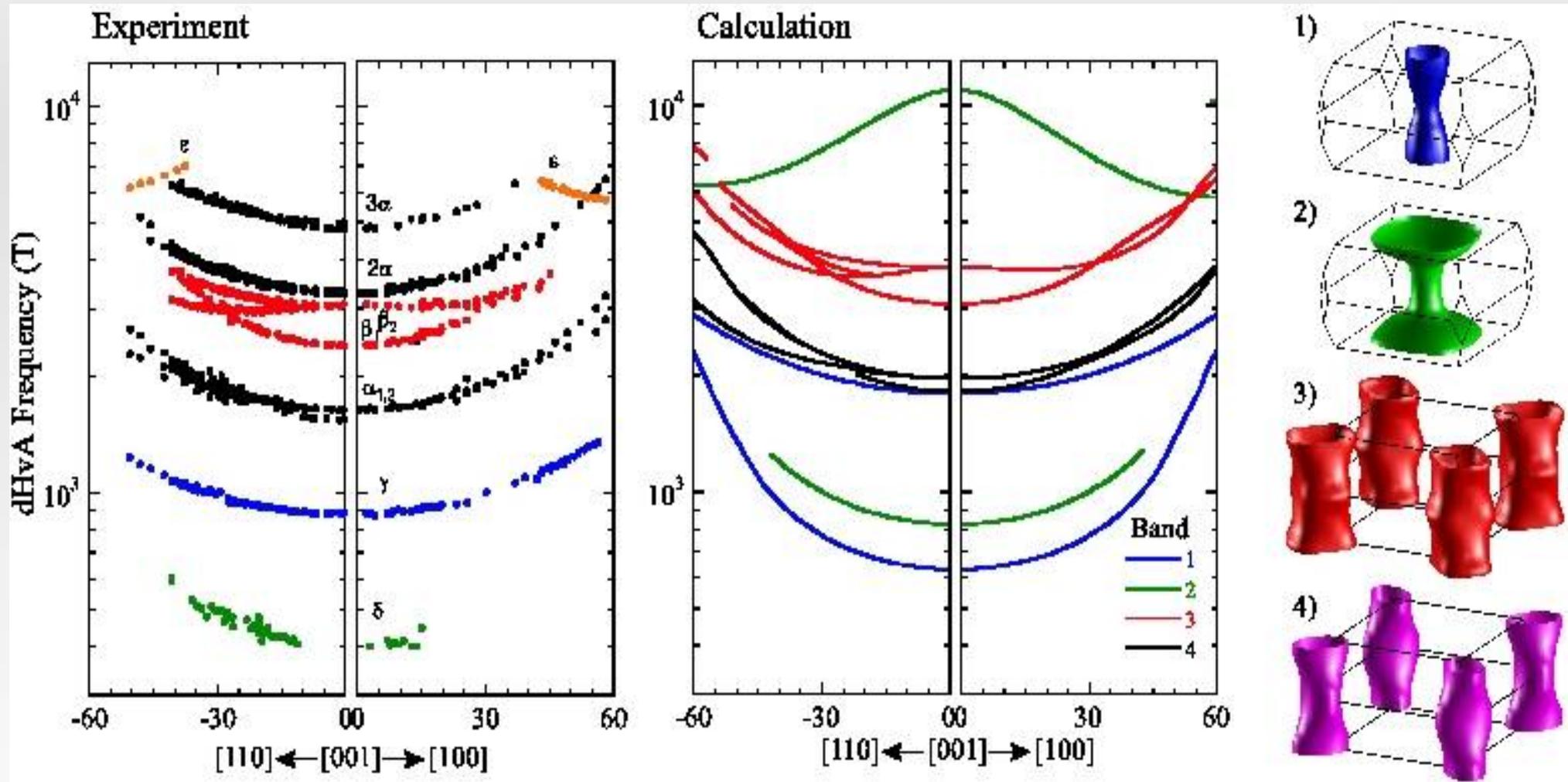
Angle dependence and bandstructure: LaFePO



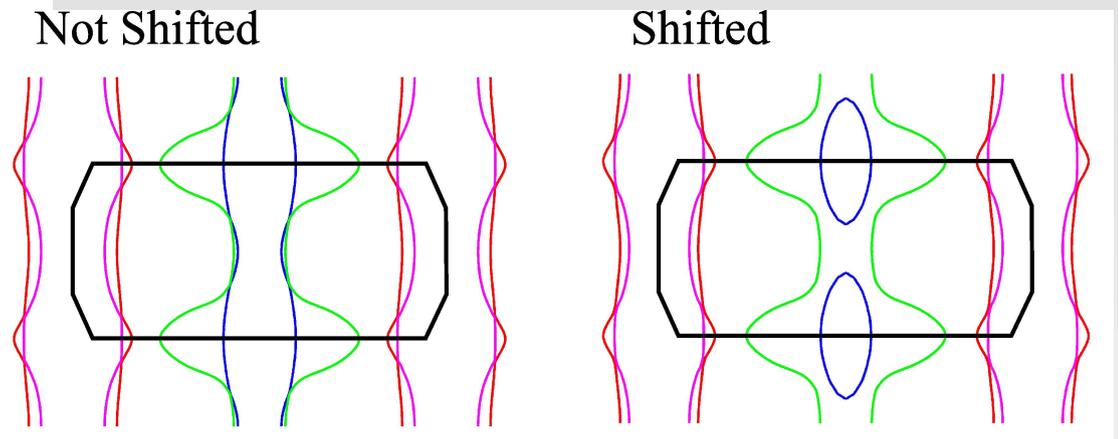
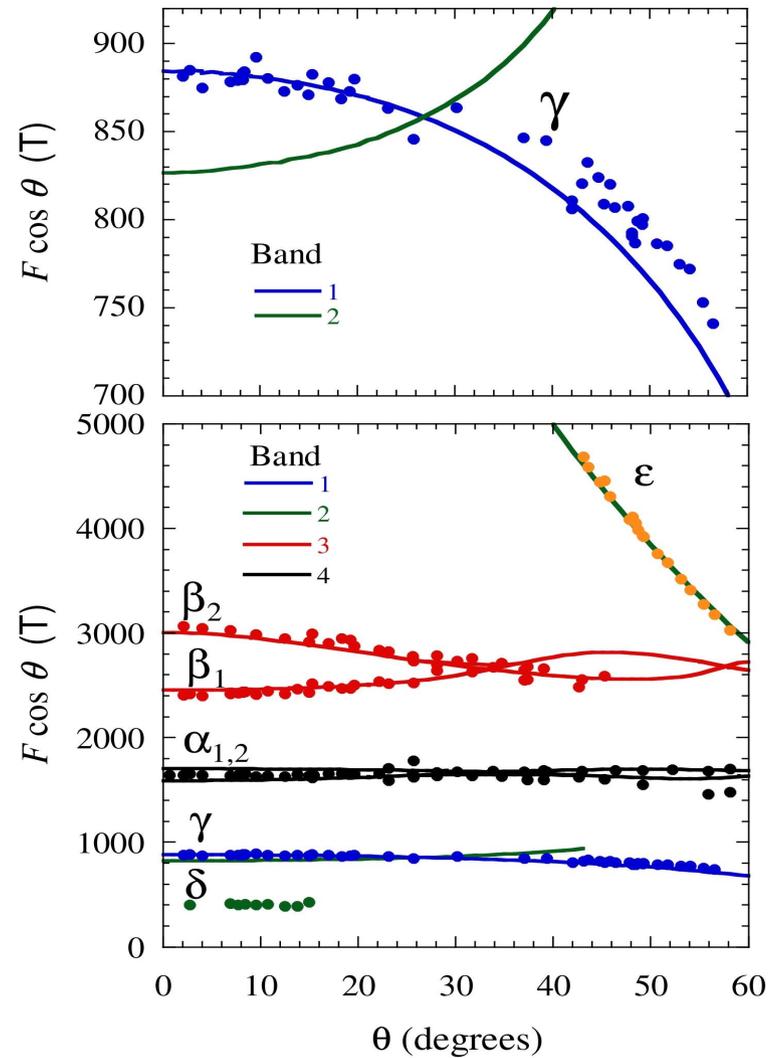
Oscillations in SrFe₂P₂



Angle dependence and bandstructure: SrFe₂P₂



Some analysis



The Fermi surface can have closed pockets!
NO (OBVIOUS) NESTING

Results summary: SrFe₂P₂/LaFePO

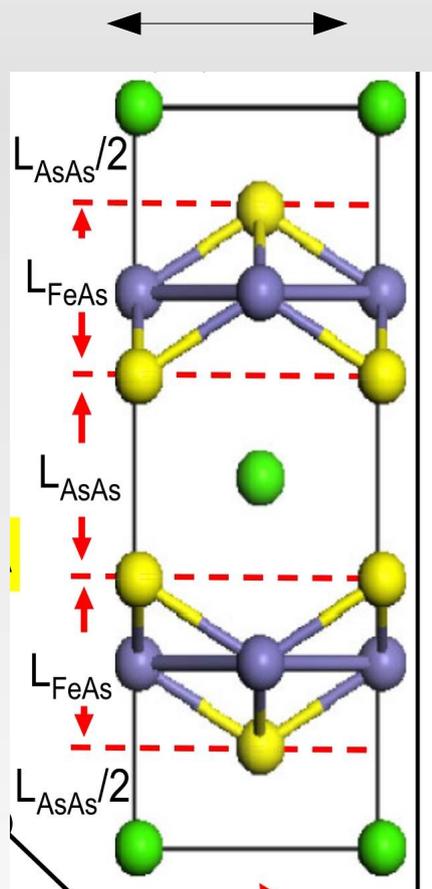
Branch	Experiment			Orbit	Calculations	
	F (kT)	m^*/m_e			Unshifted	Shifted
		A	B			
α_1	0.985(7)	1.9(2)	1.8(1)	1Z	1.0	1.9
α_2	1.025(7)	1.9(2)	1.8(1)	2 Γ	0.9	0.7
β_1	1.91(1)	1.7(2)	1.8(1)	2Z	1.2	1.1
β_2	2.41(1)	1.8(2)	1.9(1)	3 Γ	1.8	1.1

	Experiment			Orbit	Calculations		
	F (kT)	$\frac{m^*}{m_e}$	ℓ (nm)		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

2.9	2.5
0.7	0.7
0.9	0.9
0.8	0.7
0.9	0.8

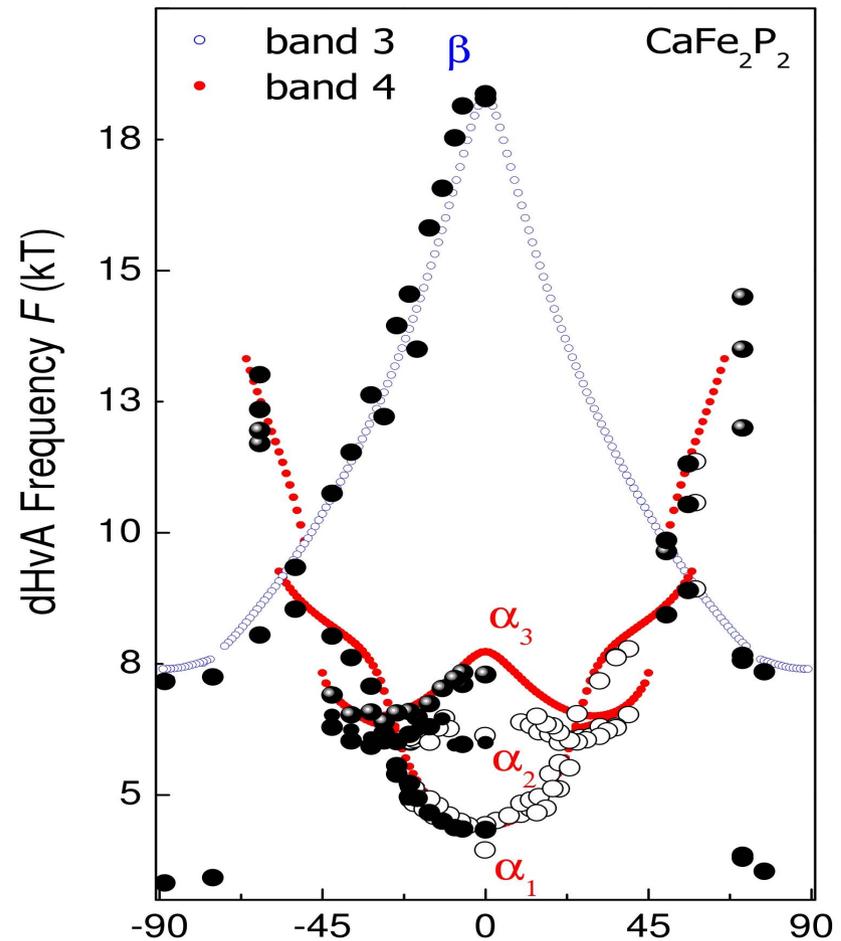
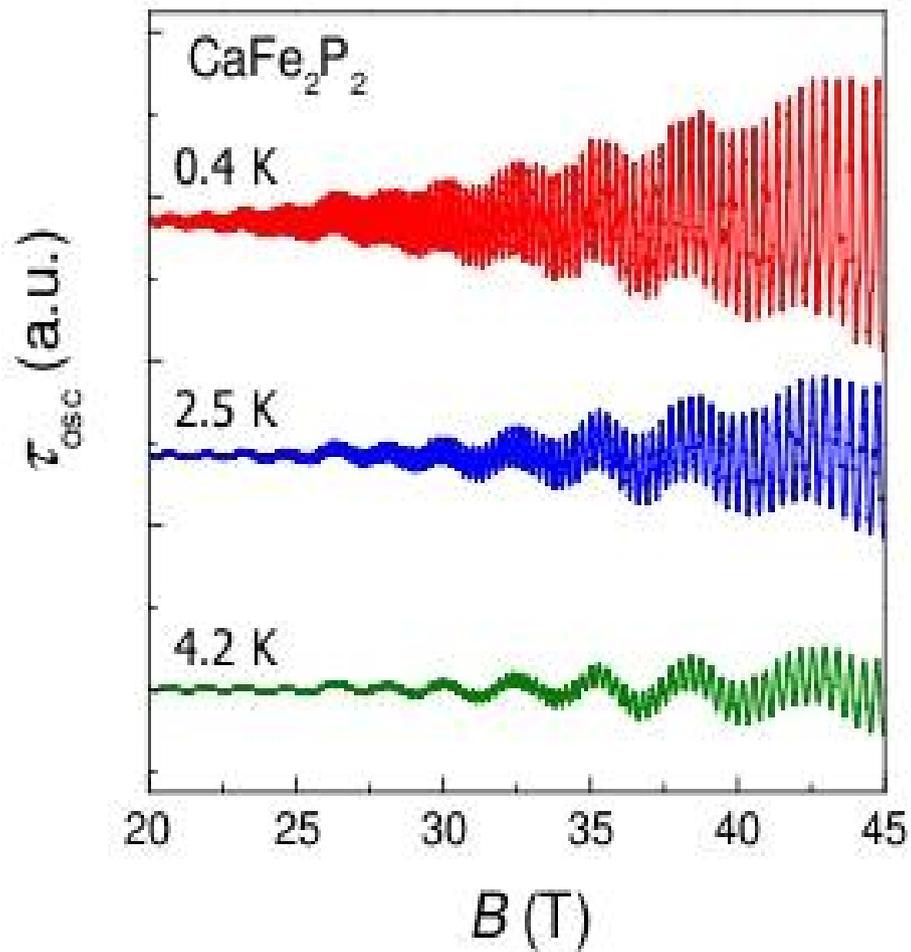
Collapsed tetragonal analogue: CaFe₂P₂

c/a
3 → 2.6



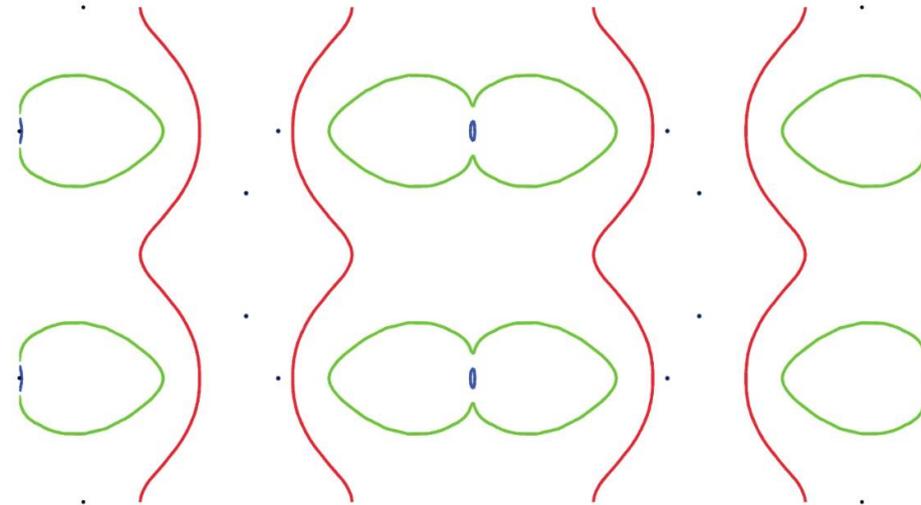
Yildirim et al 2008

Oscillations in CaFe₂P₂

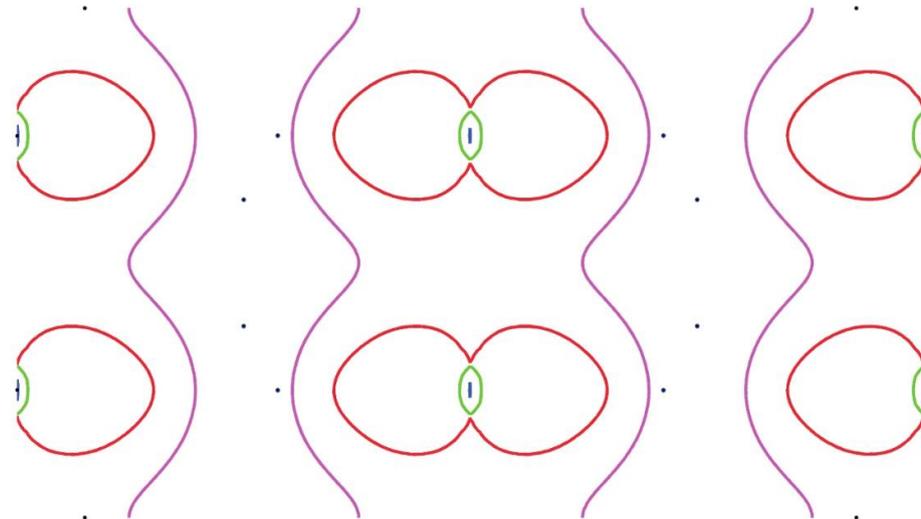


Collapsed tetragonal Fermi surface

CaFe_2As_2 $P=0.63\text{GPa}$ (cT phase)



CaFe_2P_2 $P=0$



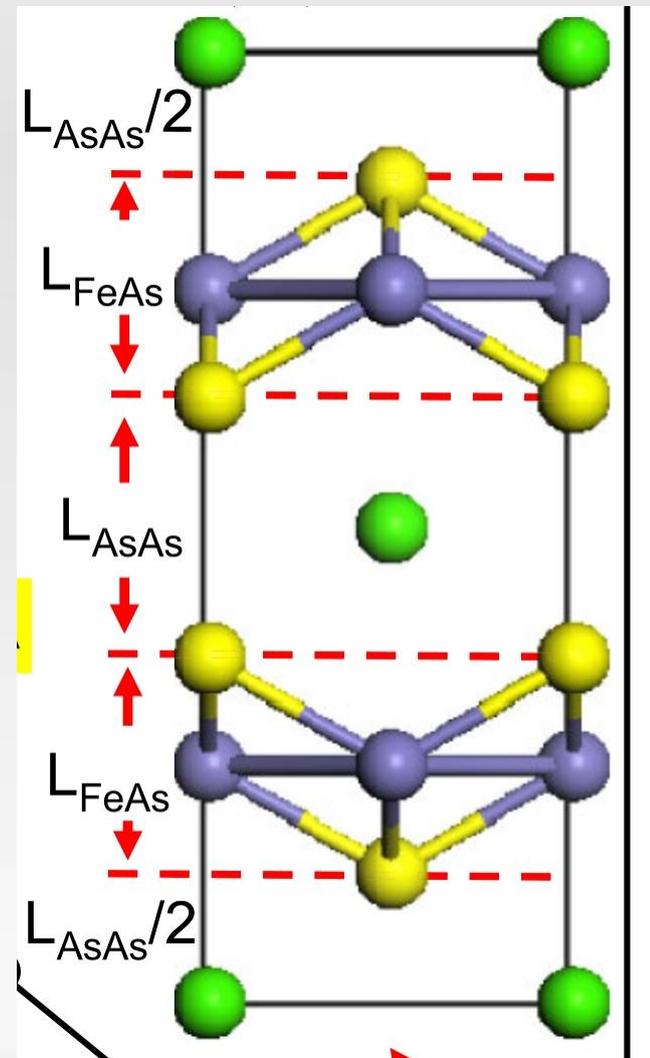
Summary of Ca122(P) data

	Experiment				Calculations		
	$F(\text{kT})$	$\frac{m^*}{m_e}$	$\ell(\text{nm})$	Orbit	$F(\text{kT})$	$\frac{m_b}{m_e}$	$\frac{m^*}{m_b}$
$\alpha_1(e)$	4.347	2.05(4)	190	4_{min}	4.439	1.38	1.49(3)
$\alpha_2(e)$	7.295	3.48(7)	71	4_{max}	7.837	2.40	1.45(3)
$\beta(h)$	18.360	4.0(2)	86	3_{min}	18.407	2.65	1.51(8)

Why are the phosphides different from the arsenides?

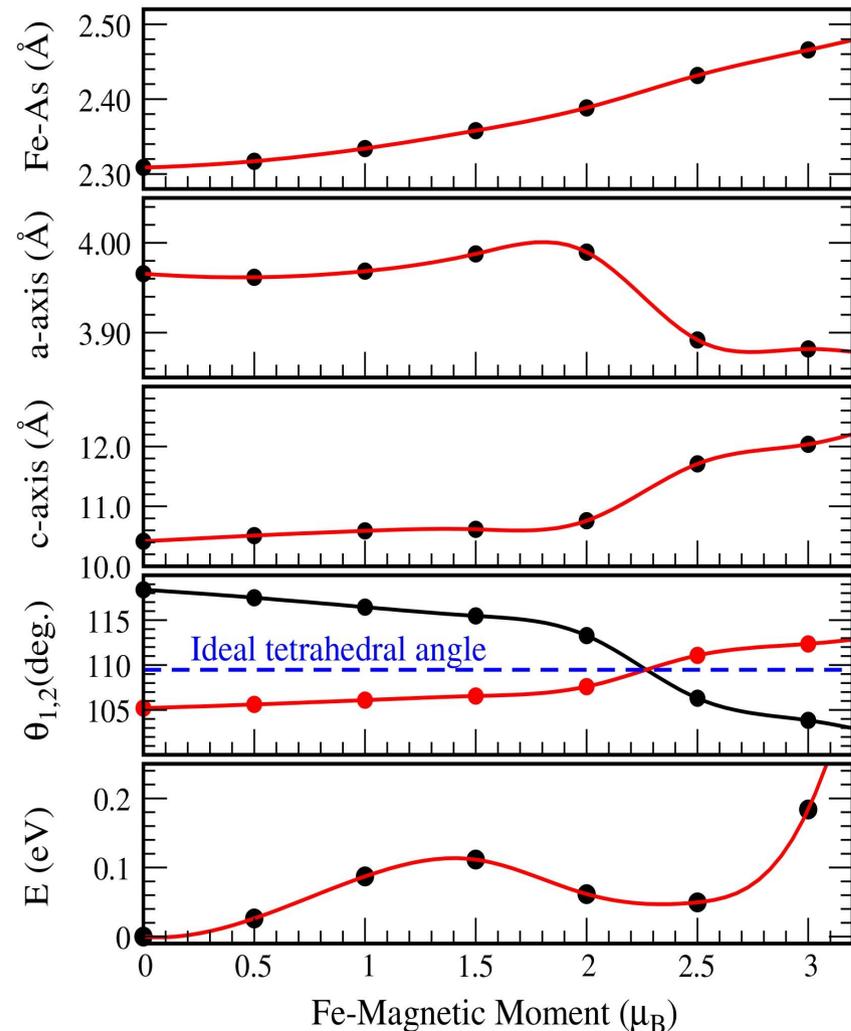
Why are the phosphides different?

- The phosphides in this talk are all Pauli paramagnets.
- The As-Fe-As bond angle is ~ 116 in the 122s and ~ 119 in the 1111s.
- In Ca122(As) this angle goes from 109.5 to 116 under pressure.

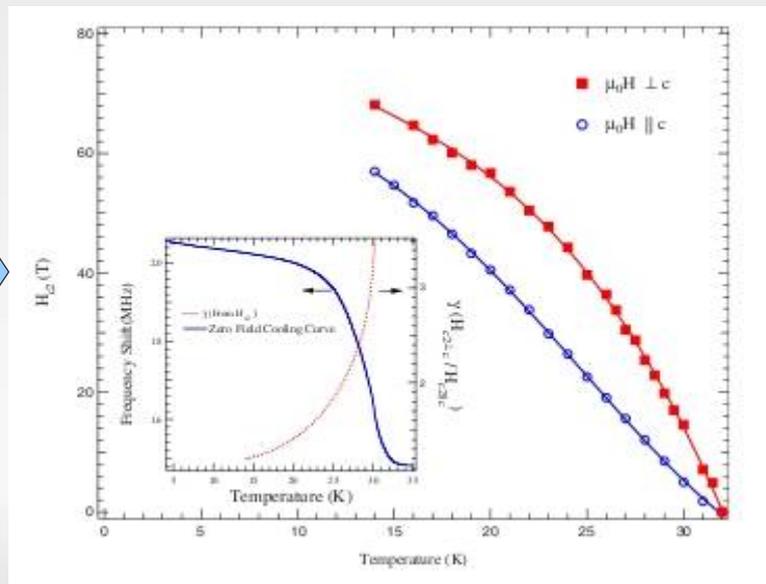
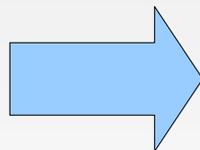
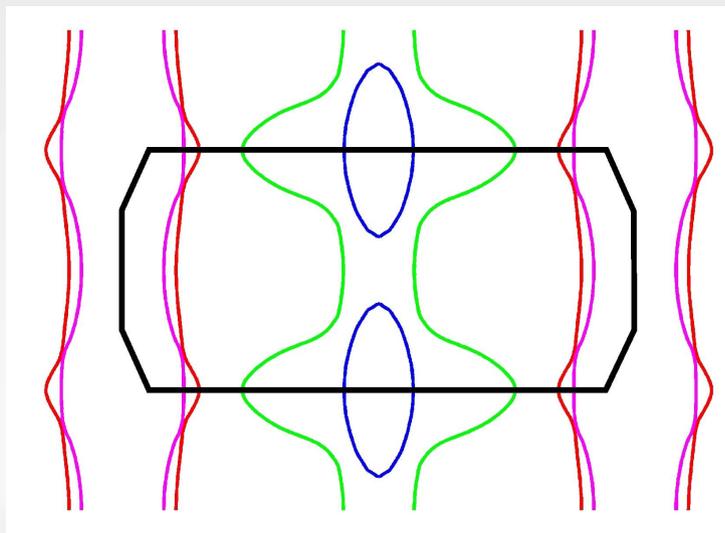
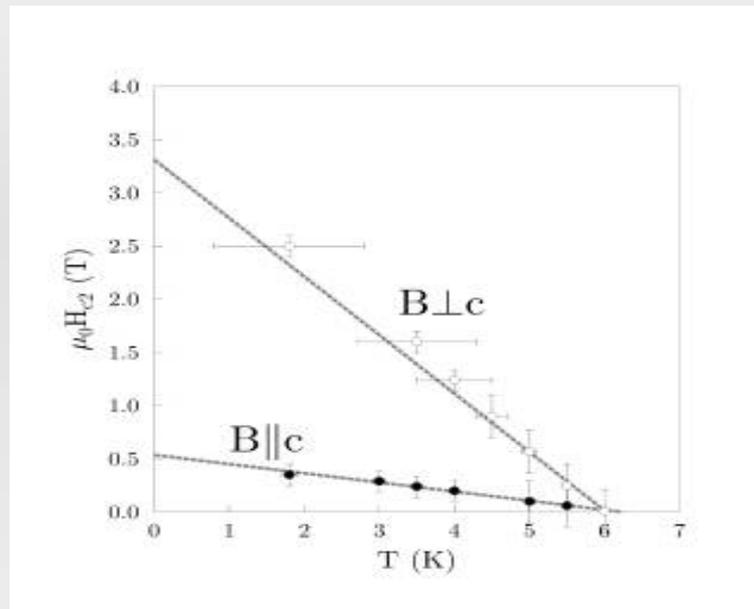
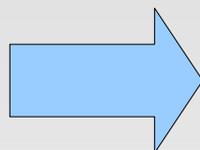
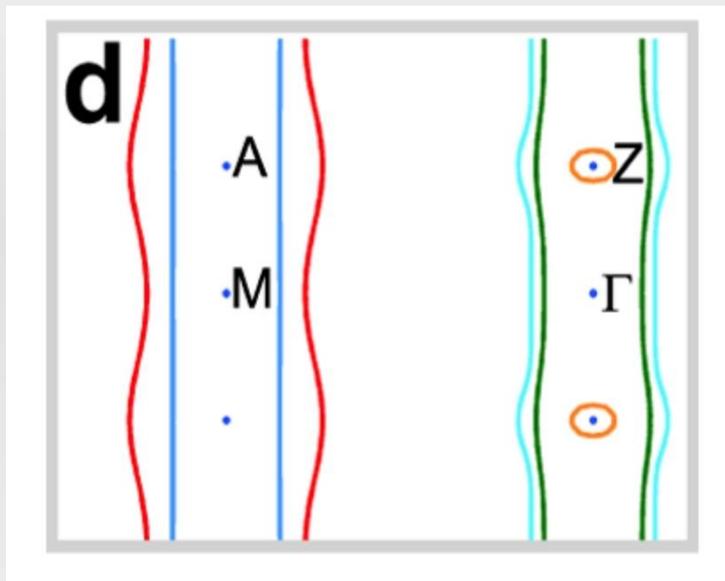


Why are the phosphides different?

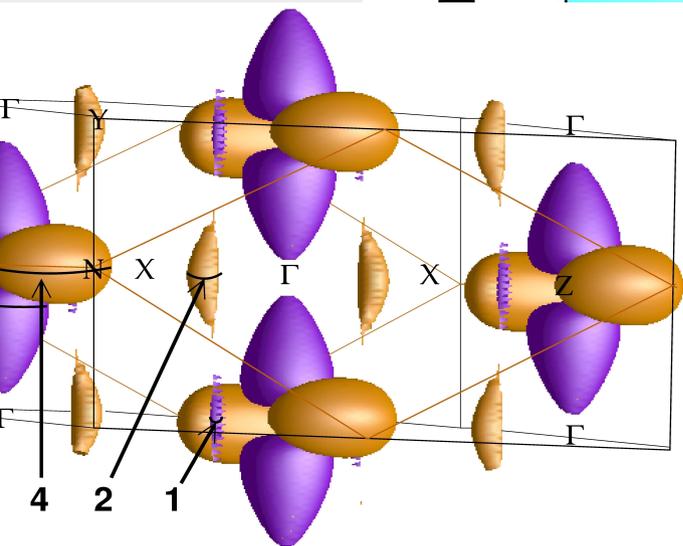
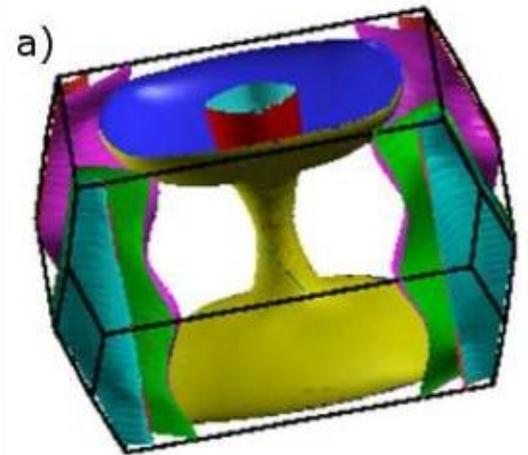
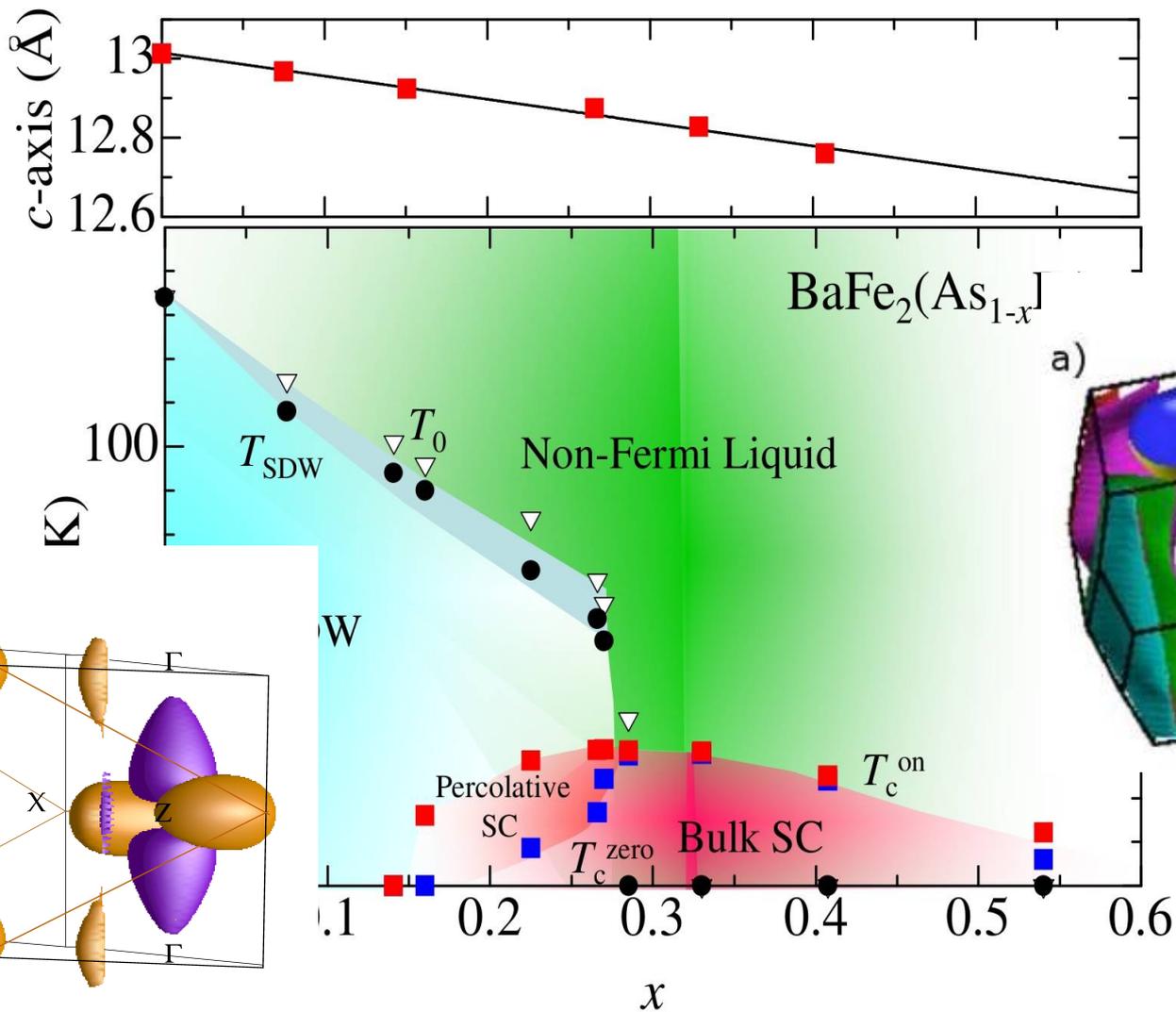
- This bond angle is likely related to the local magnetic moment. e.g. Yildirim PRL2009



Relationship to superconductivity

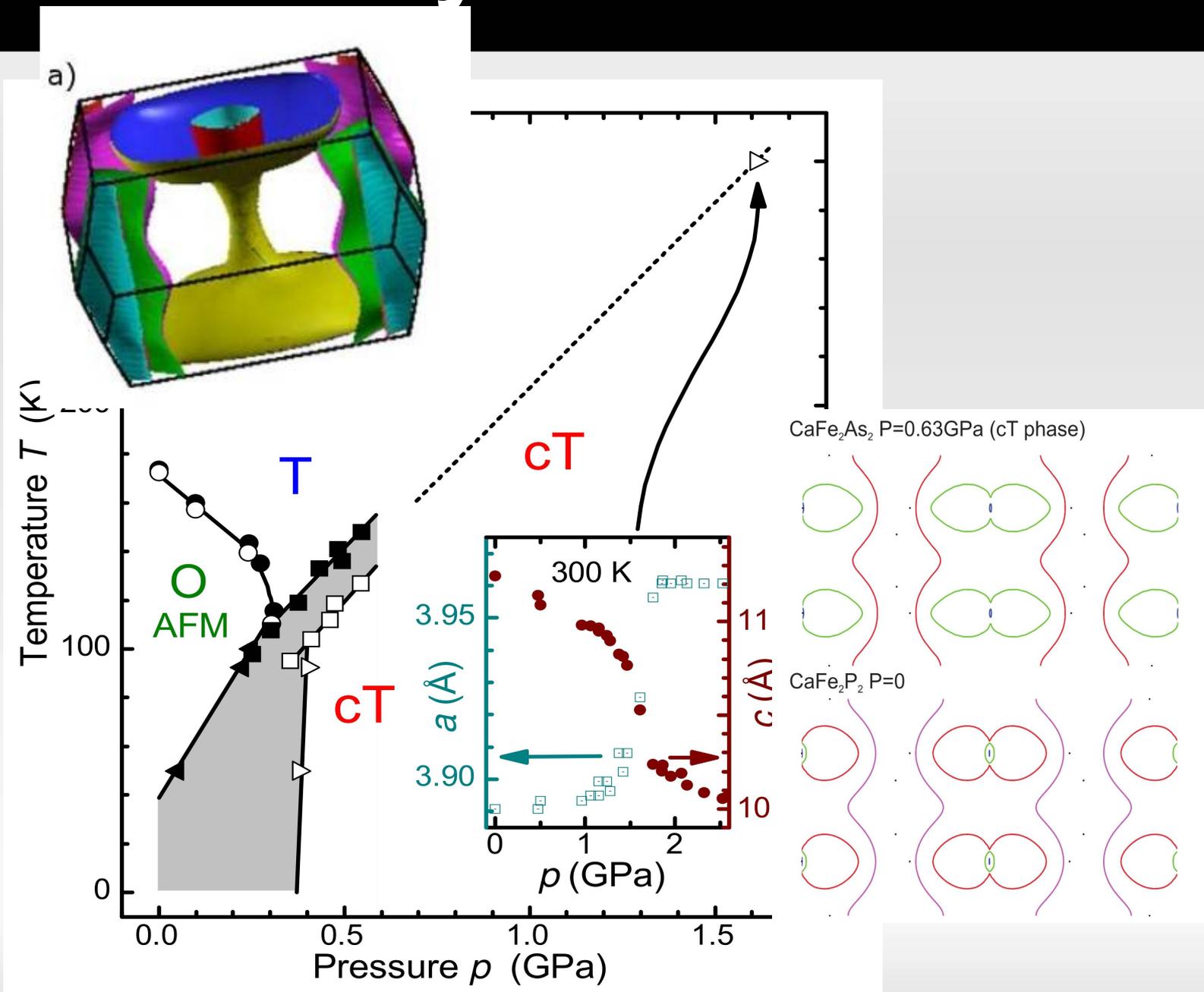


P substitution of As: phase diagram



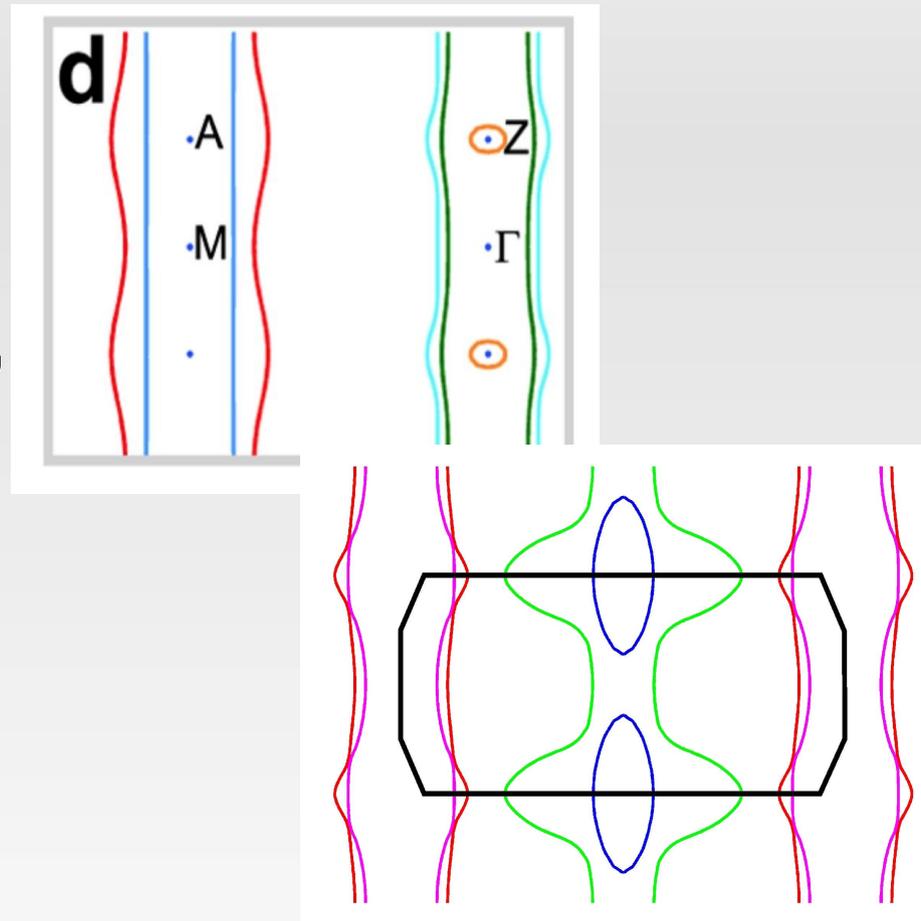
Ca122 – Summary

ES09



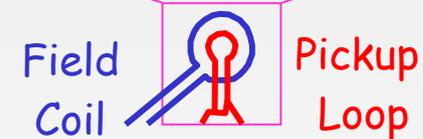
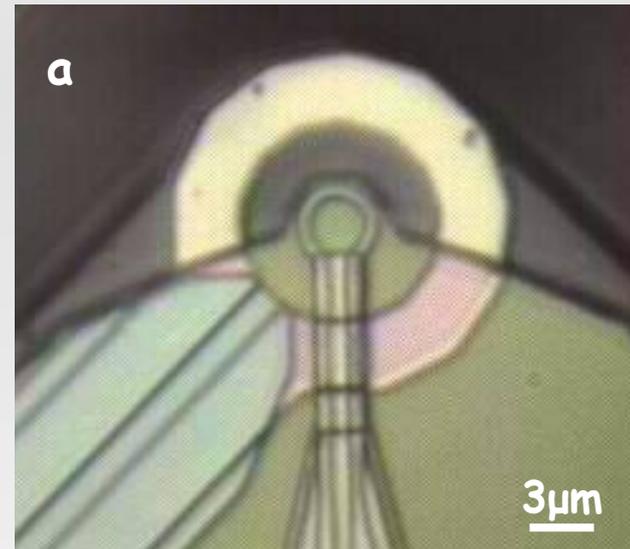
Why do the 1111 phosphides superconduct but the 122s do not?

- Note the bond angle in the 1111s is 2 degrees further than the tetrahedral angle, unlike the 122s.
- The biggest difference is nesting!
- The most 'nested' parts of the hole FS have the shortest mfp

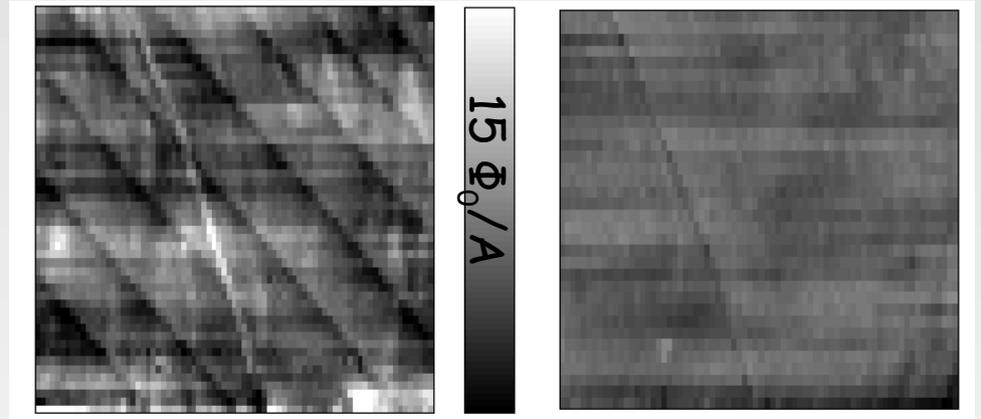
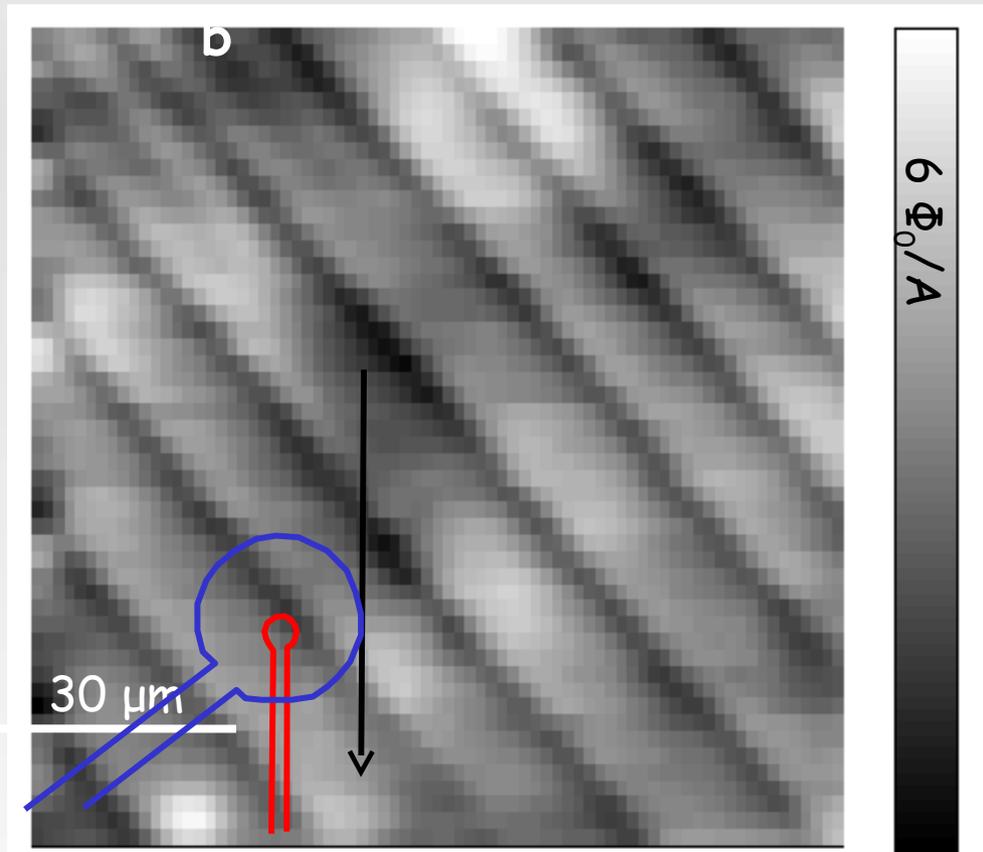


Scanning squid results

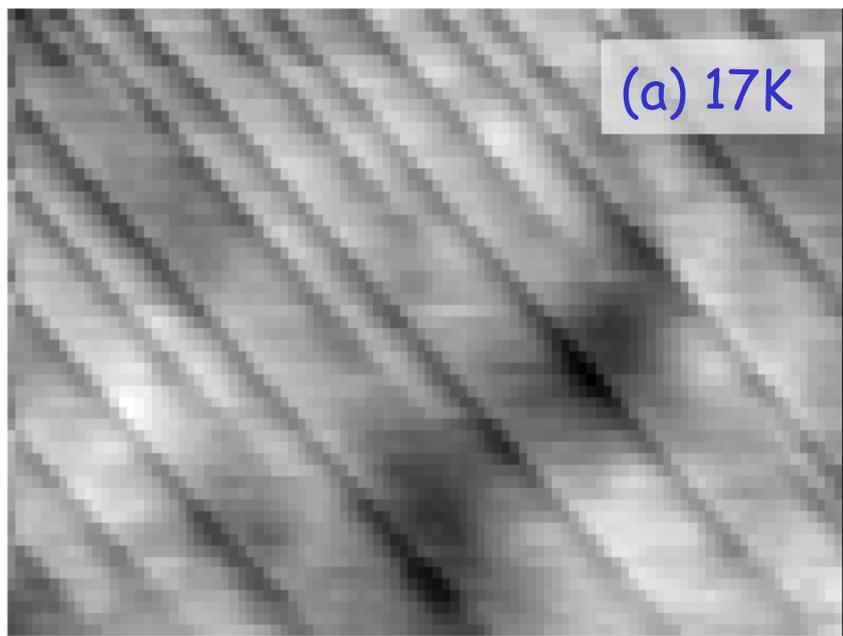
- Measuring the susceptibility as a function of position on the sample surface.



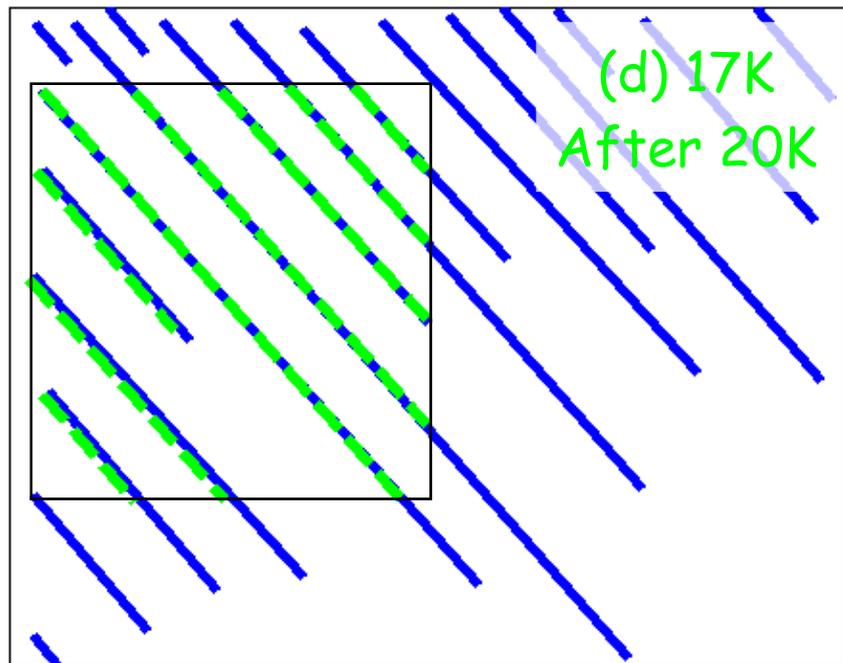
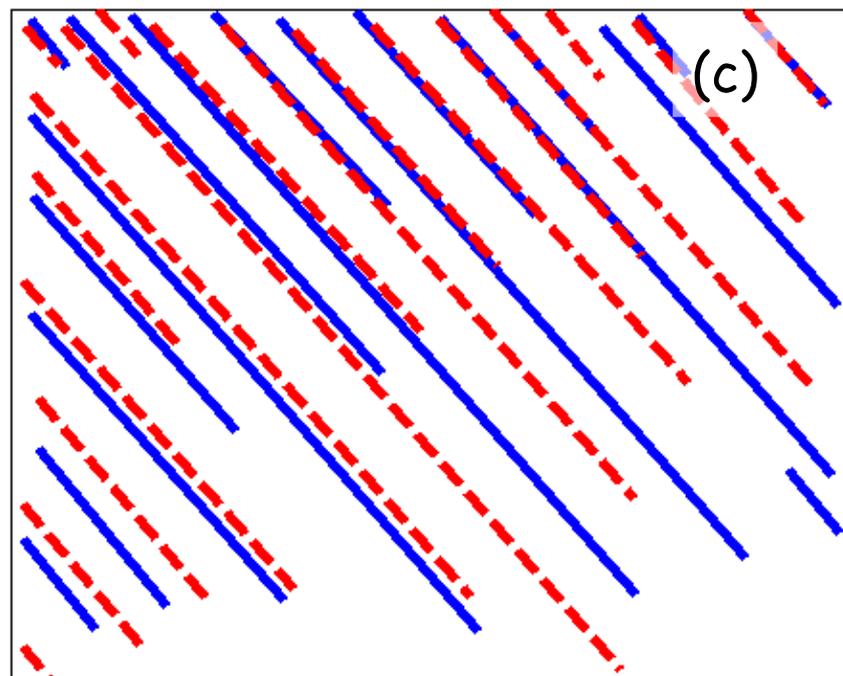
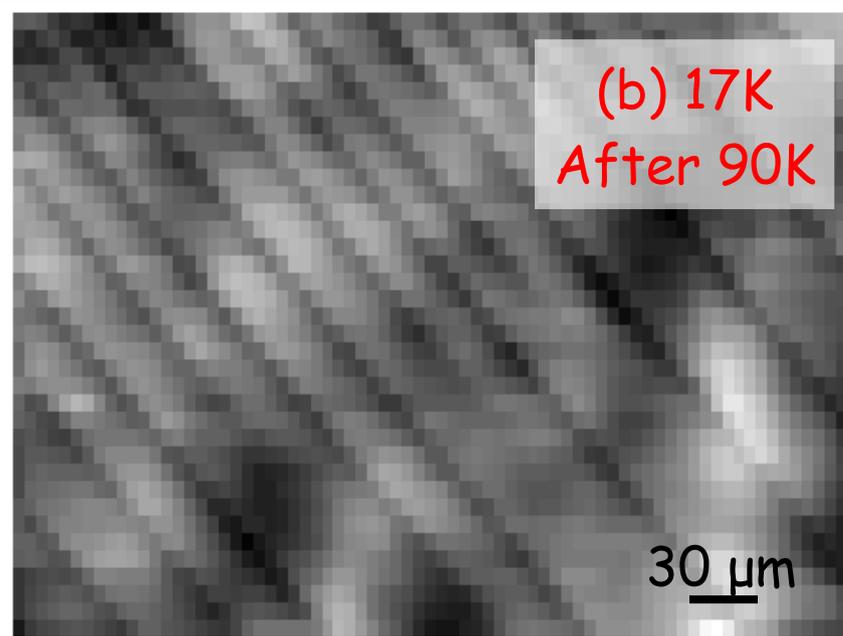
Stripes in the superfluid density!



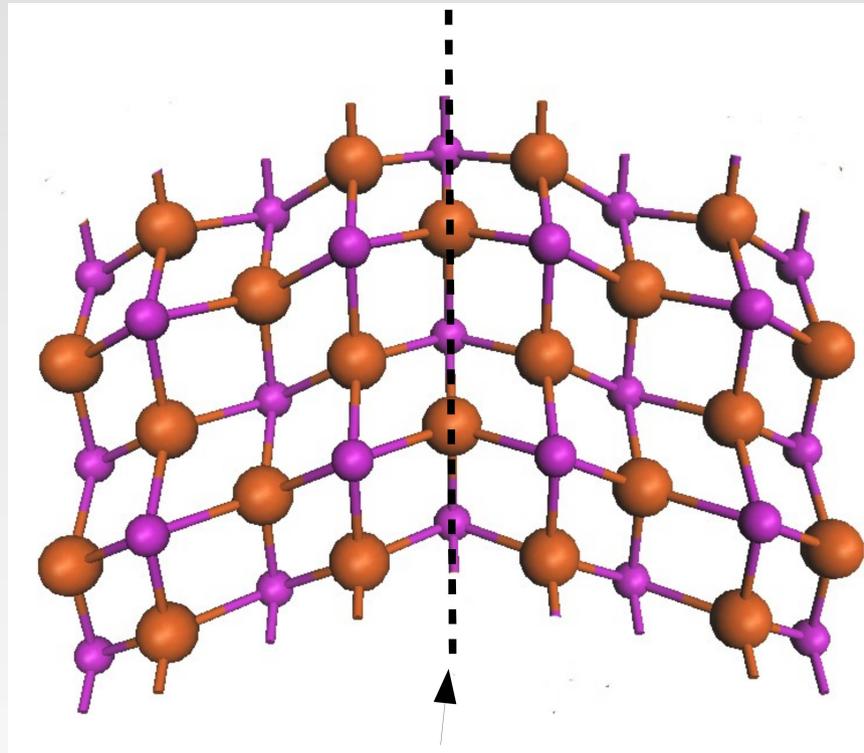
30 μm



$\downarrow 40 \Phi_0/A$
 $\uparrow 30 \Phi_0/A$



Twinning plane superconductivity?



Conclusions: non-speculative

- The Fermi surface of LaFePO is well nested, Sr122(P) is weakly nested and Ca122P is not nested at all.
- The electron pockets always tend to have the longest mean free paths and the hole pockets have the shortest.
- The effective mass renormalization seems larger for the electron pockets than for the hole pockets.
- For weak nesting electron/hole Fermi sea shrinks, but not for non-nested FS.

Conclusions: speculative

- Superconductivity emerges from quasiparticles of the tetragonal state and nesting is directly involved in the SC,
 - LaFePO is superconducting but Sr/Ca122(P) not.
 - Non-bulk SC can form at twinning boundaries
- The As-Fe-As bond angle drives the local magnetism making Sr122(As) magnetic and Sr122(P) not.
- Perhaps both local interactions and itinerant nesting drives T_c up, so that the 1111(As) have the highest T_c s of all because they have both!

Open questions

- Why is the mean free path shorter for the hole pockets than the electron pockets?
- Why is the mass renormalization greater for the electron pockets than for the holes?
- How does proximity to nesting and local interactions work together to enhance T_c ?
- What is the role of local strain fields and is the itinerant physics related?

Thanks!