Fermiology and low energy dynamics of Fe-Pnictides

ES09

Jim Analytis, Jiun-Haw Chu, Ian R. Fisher (Stanford)

Antony Carrington, Amalia Coldea , Caroline Andrew**,** Ali Bangura, N.E. Hussey (Bristol)

Ross McDonald (Los Alamos)

Ming Yi, Donghui Liu, Z. X. Shen (Stanford)

Michelle Johannes (NRL)

Beena Kalitsky, Ophir Auslander, Katherine Moler (Stanford)

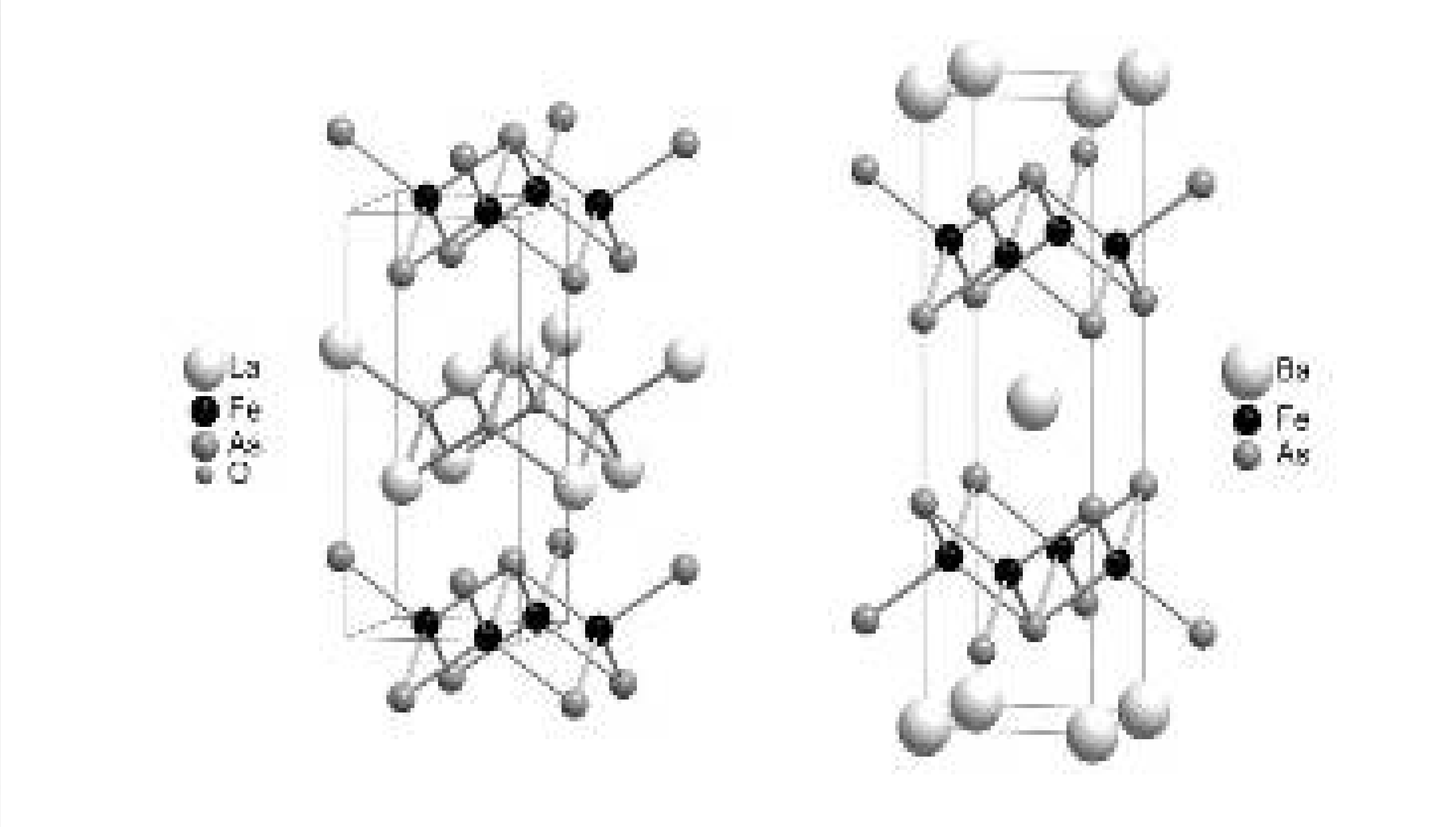
Contents: Fermiology of the pnictides

ES09

- 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

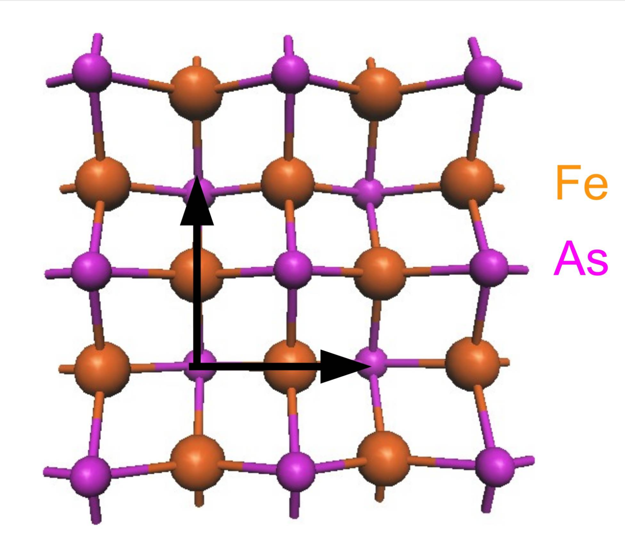
Part I: Experimental preliminaries

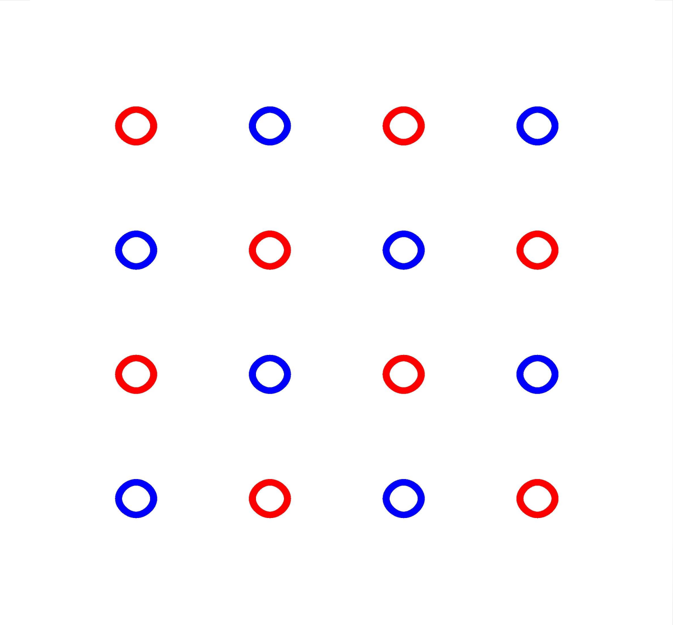
The 1111s and the 122s



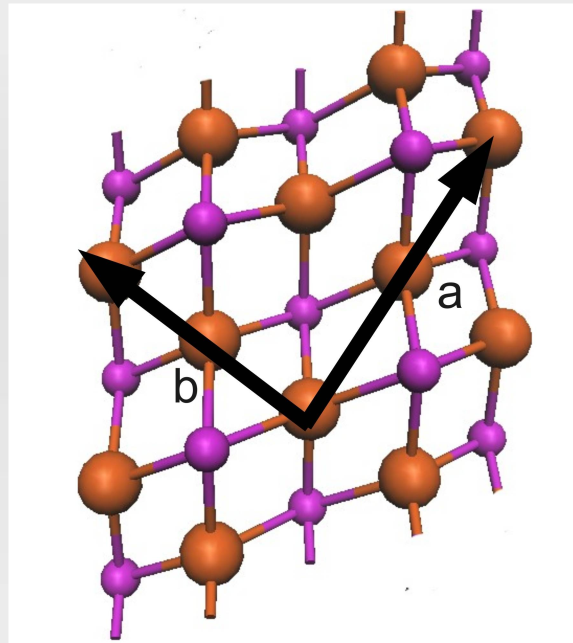
1111(As,P) 122(As,P)

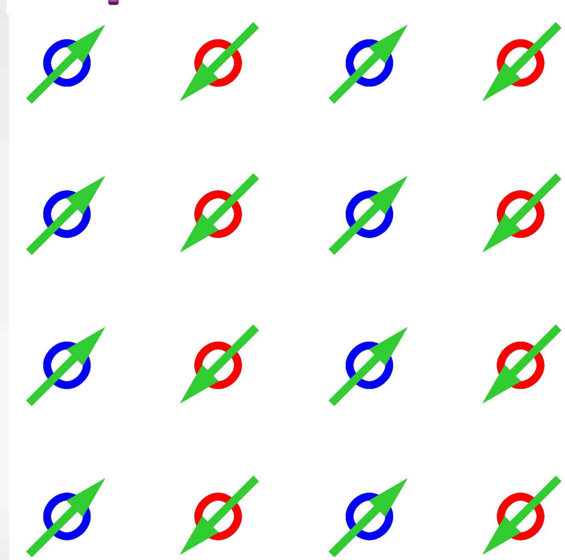
Orthorhombic and magnetic transition



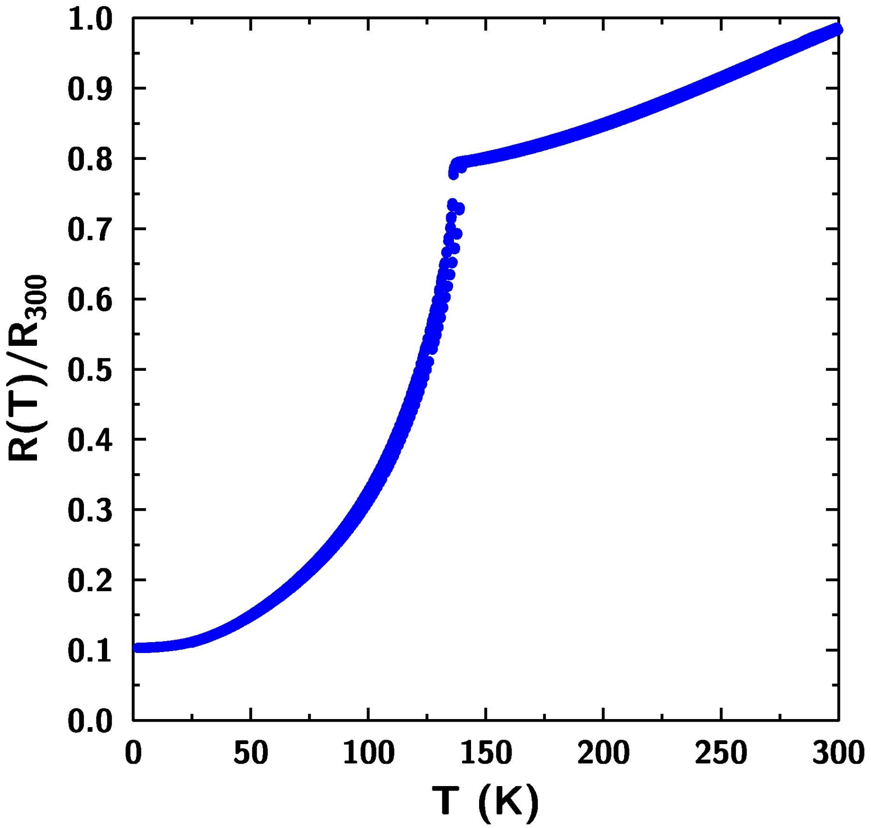


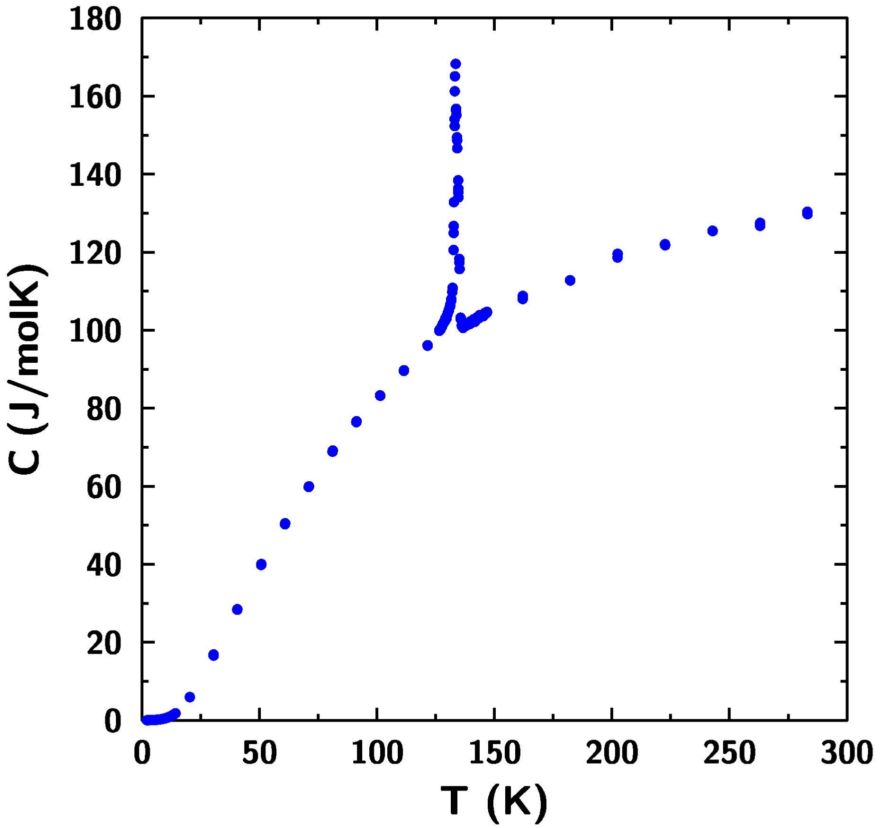
Orthorhombic and magnetic transition



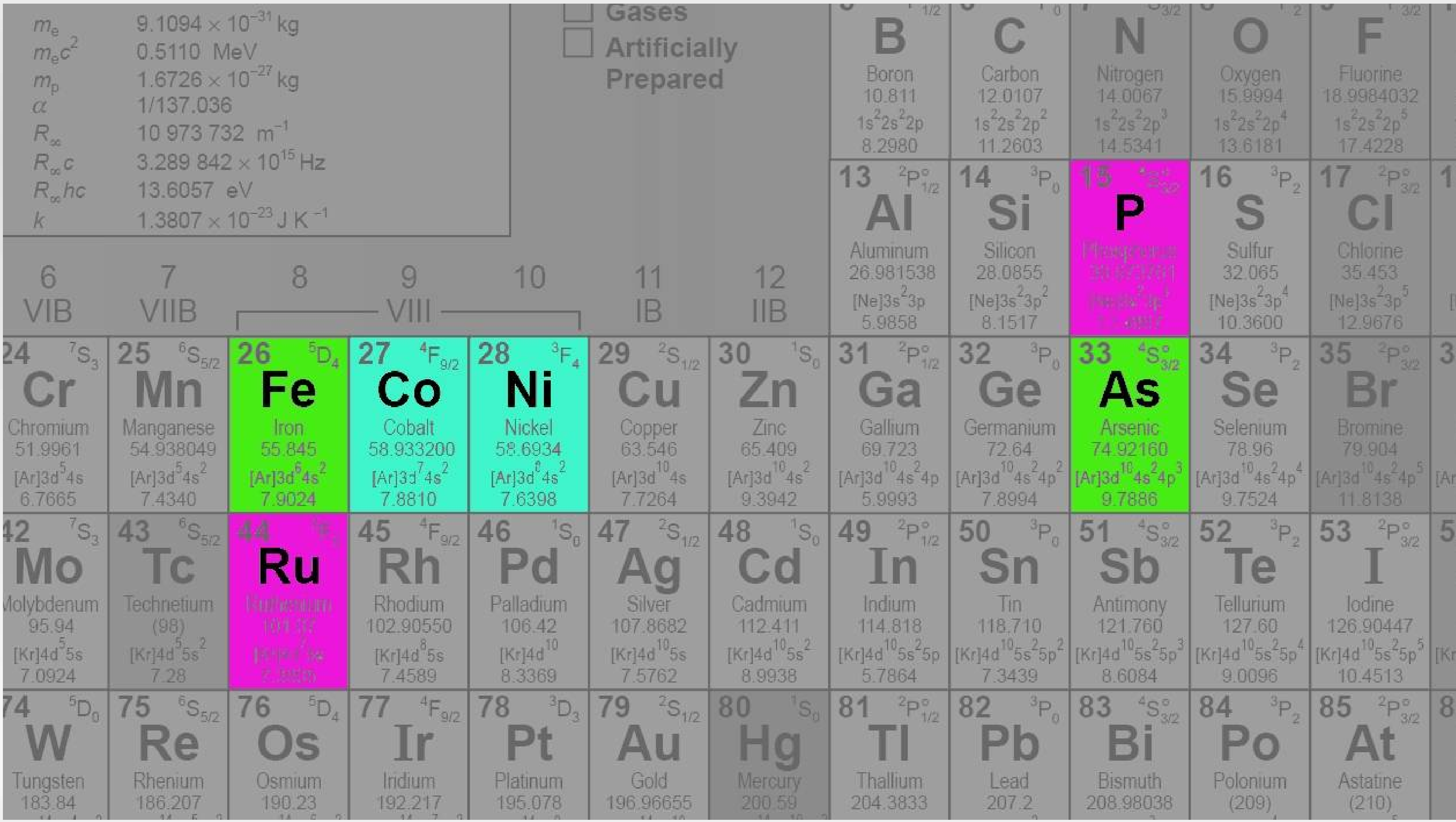


Ground state of the parent compounds

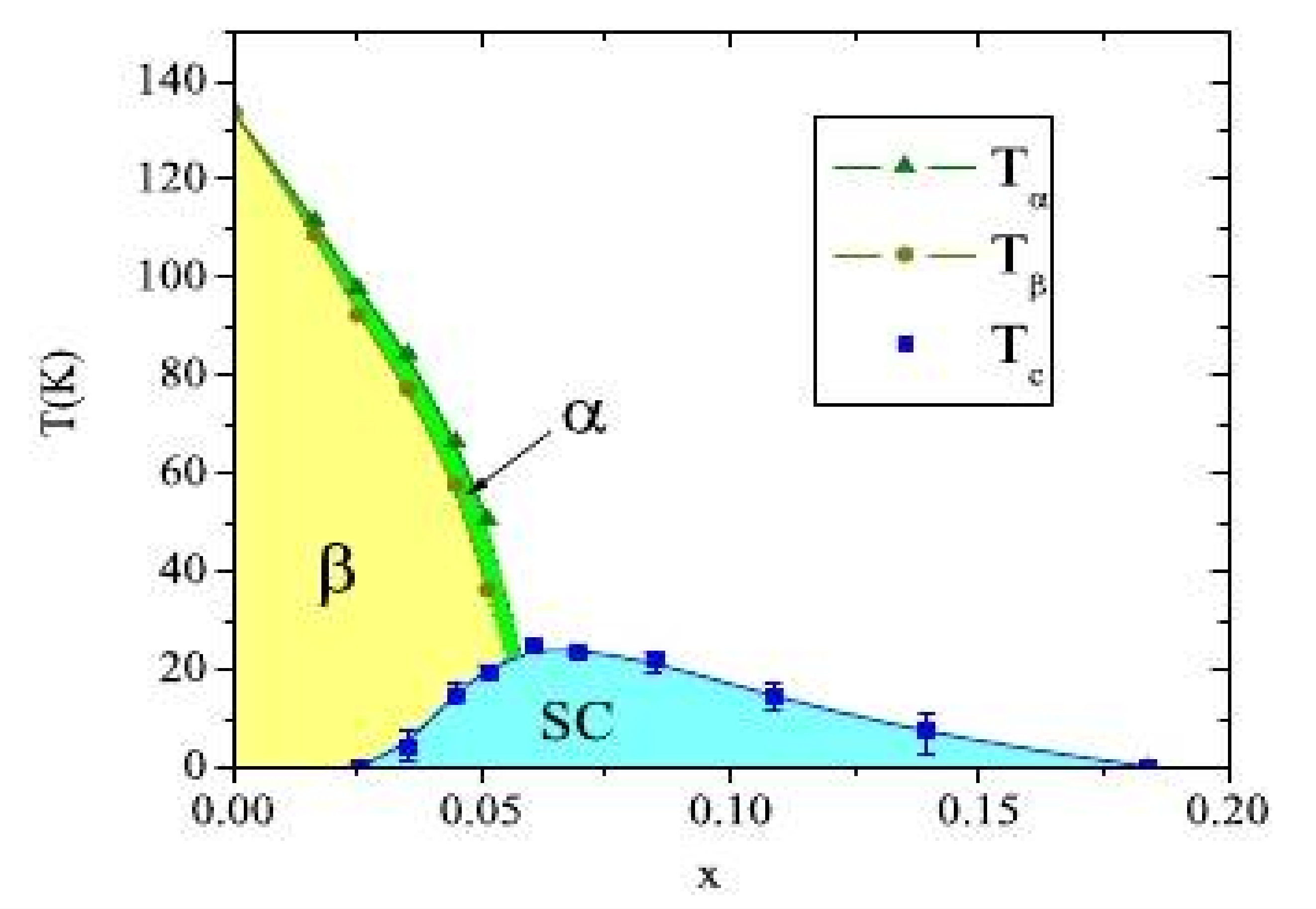




Doping in-plane

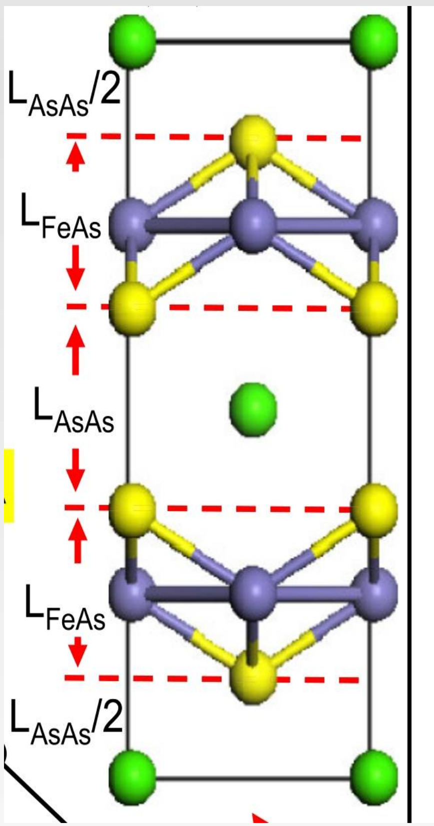


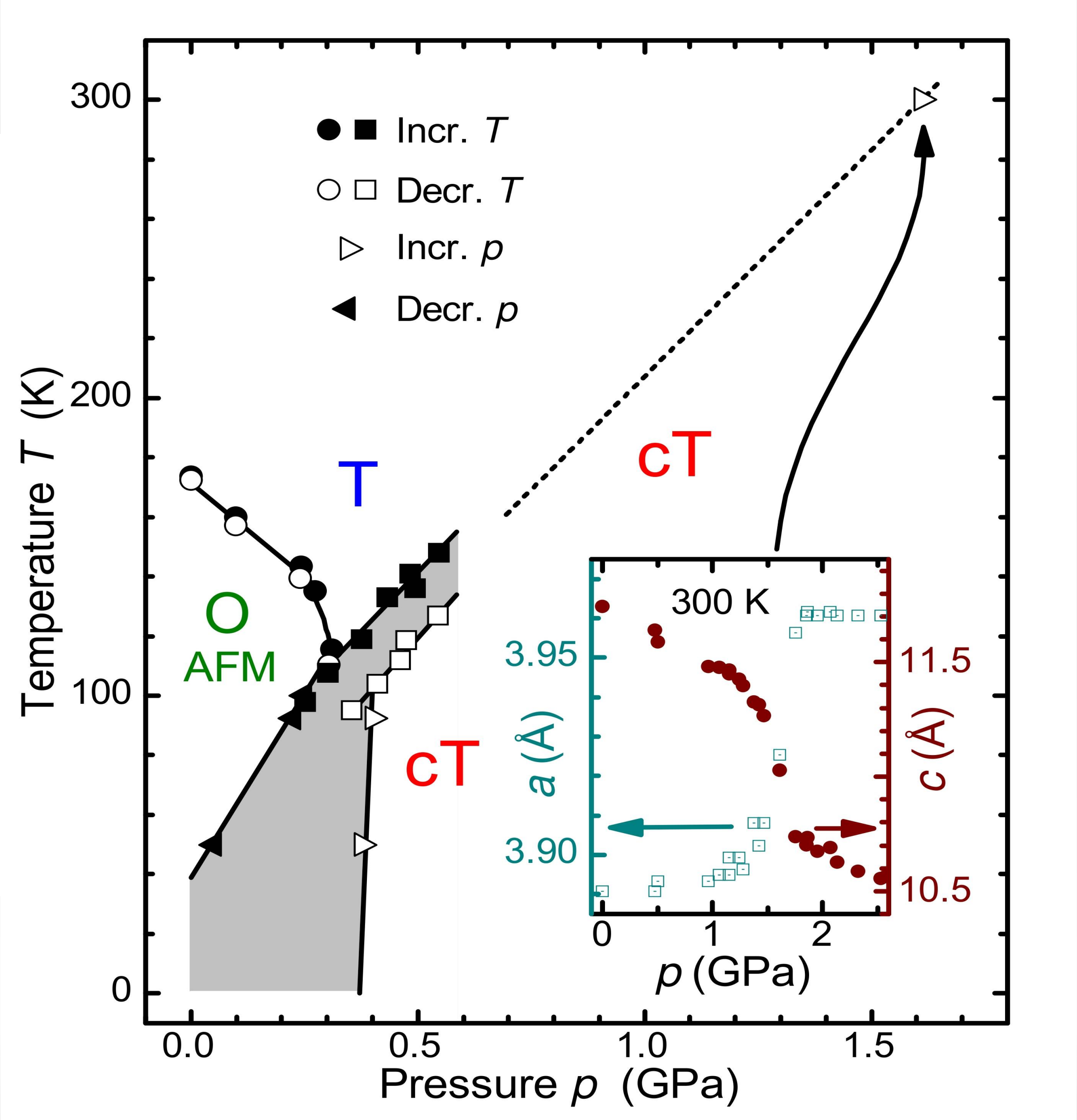
SDW and Superconductivity



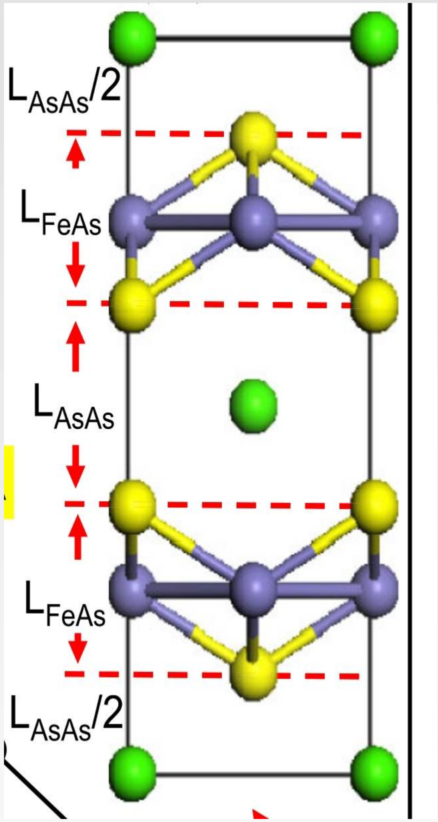
JH Chu, JG Analytis et al. PRB 2009

Ca122 – hydrostatic pressure





Materials

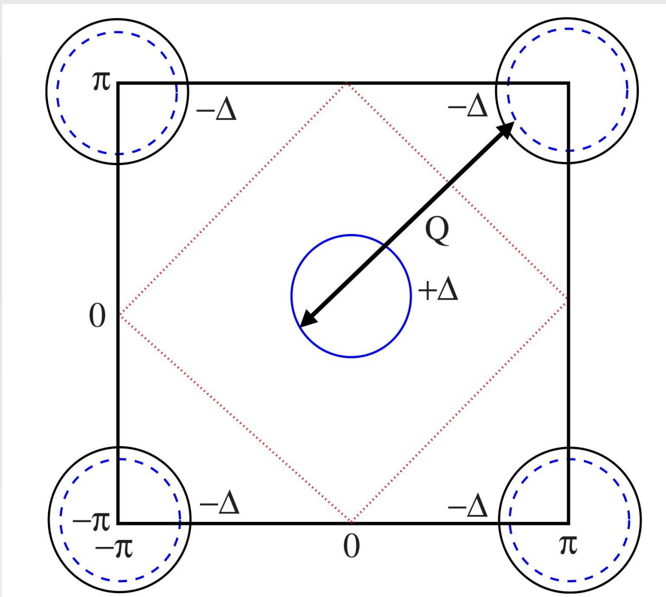


- 1111s – quasi-2D, higher Tc
- 122s – more 3D, lower Tc
- Phosphides – lower Tc, non-magnetic
- Arsenides - high Tc, magnetic

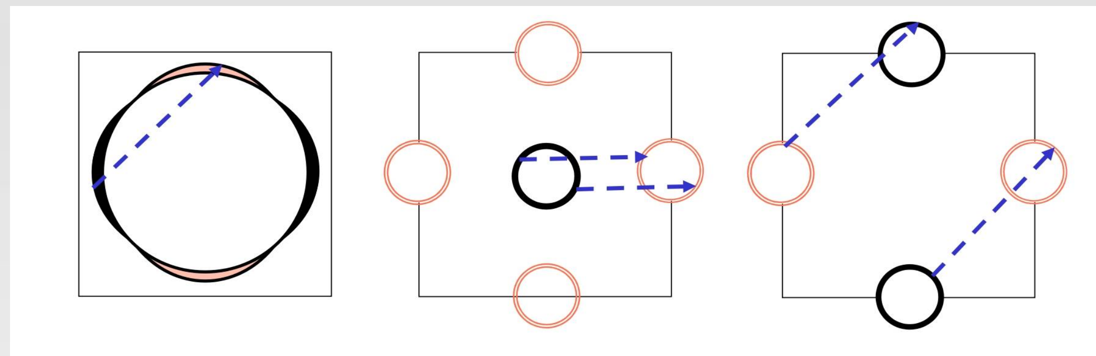
Preliminaries : Experimental

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

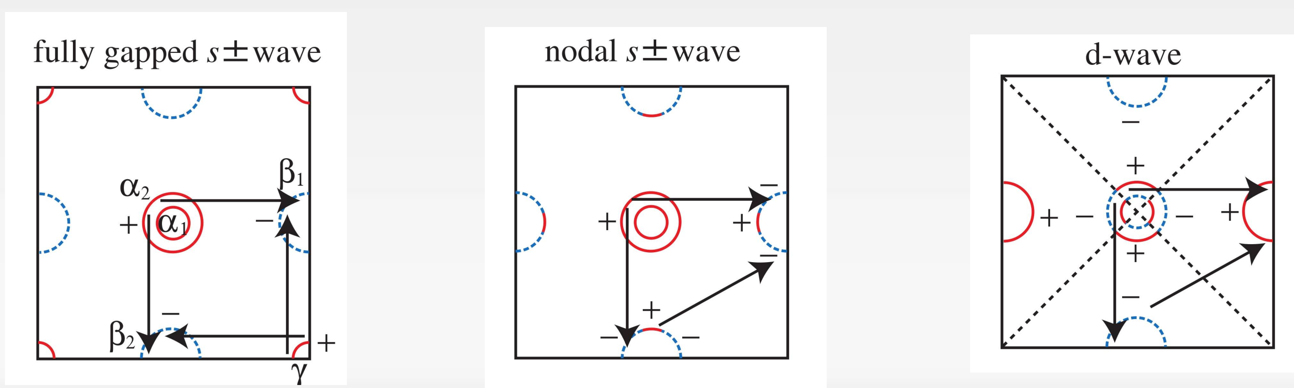
Theories for superconductivity



Chubukov 2008

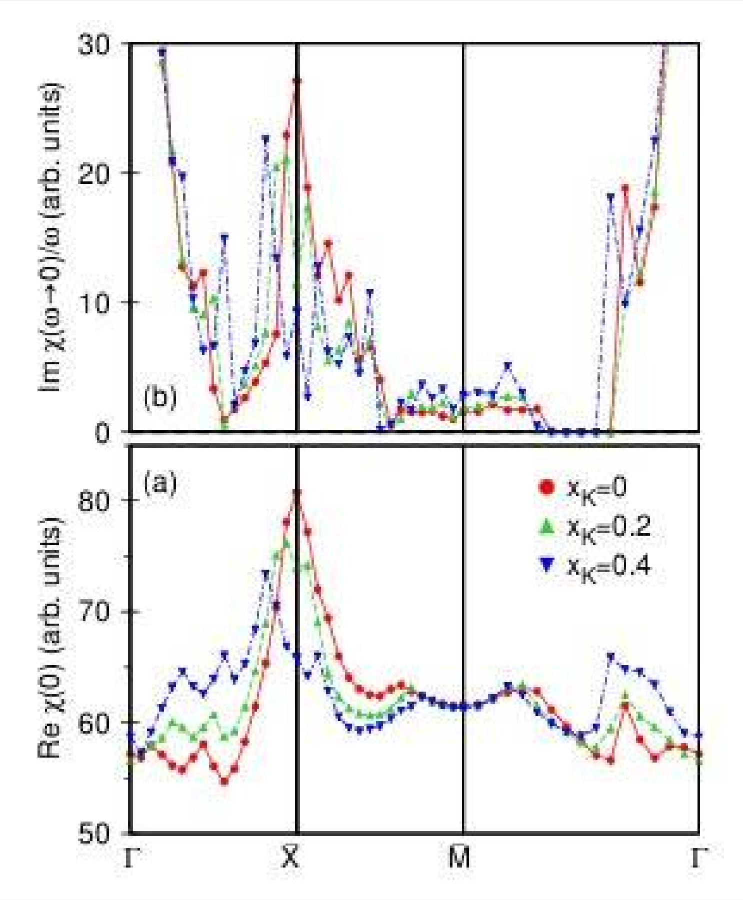


Mazin, Schmalian 2009



Kuroki, Aoki 2009

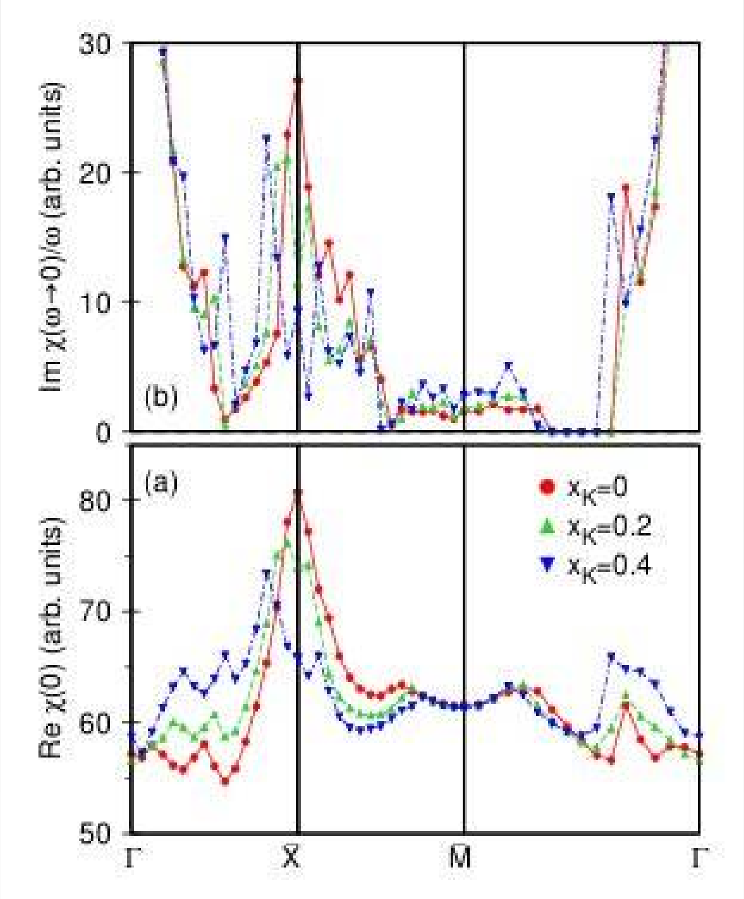
Preliminaries

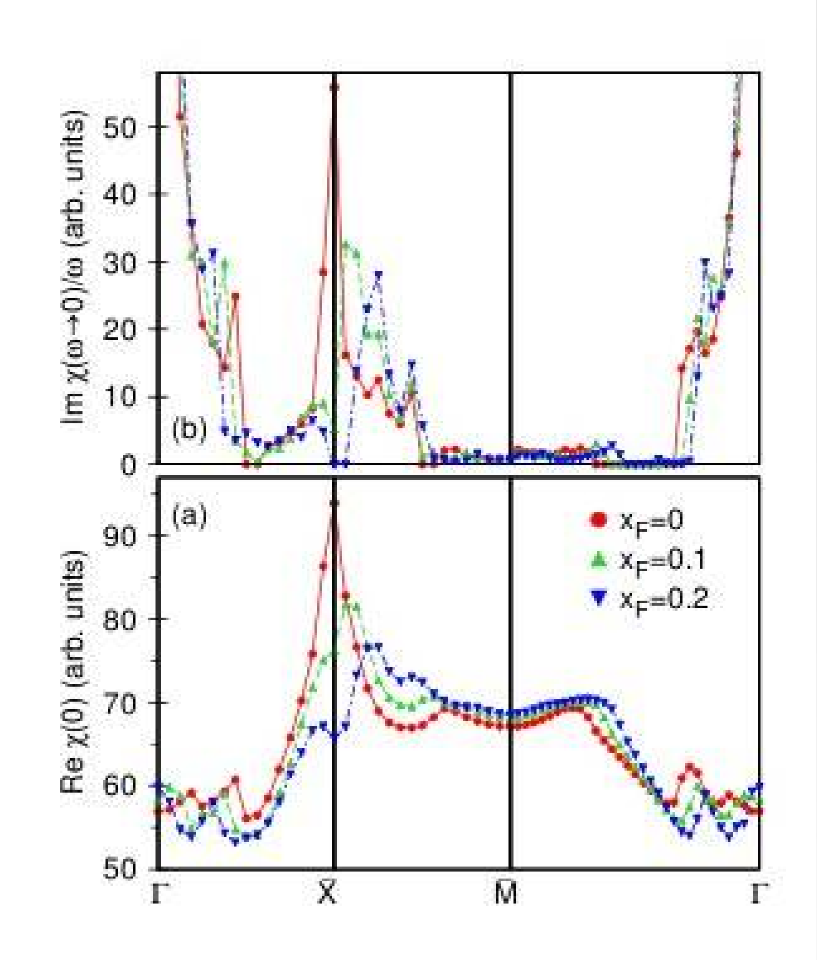


Yaresko cond-mat 2008

nesting=magnetism?

Preliminaries





LaFePO?

Yaresko cond-mat 2008

The puzzle

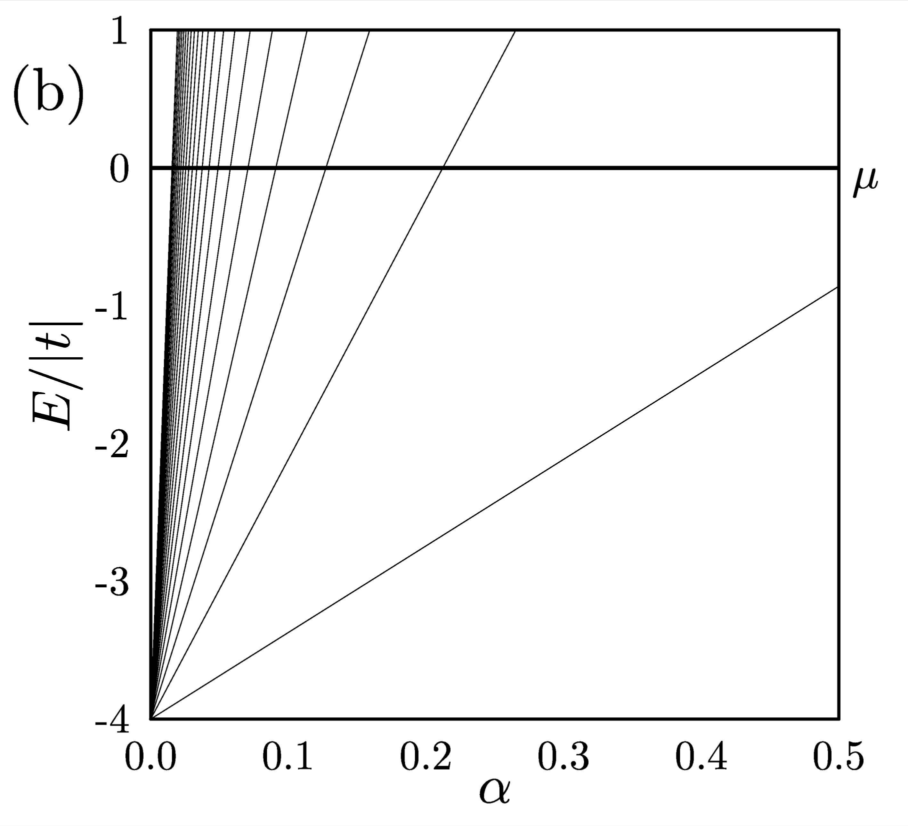
- What is the dimensionality of the low energy quasiparticles?
- Is the magnetism a Fermi surface nesting driven process? If not, what is the role of itineracy, if any?
- Do local lattice/magnetic interactions enhance or reduce Tc?

Part II: Quantum Oscillations

SLAC

NATIONAL ACCELERATOR LABORATORY

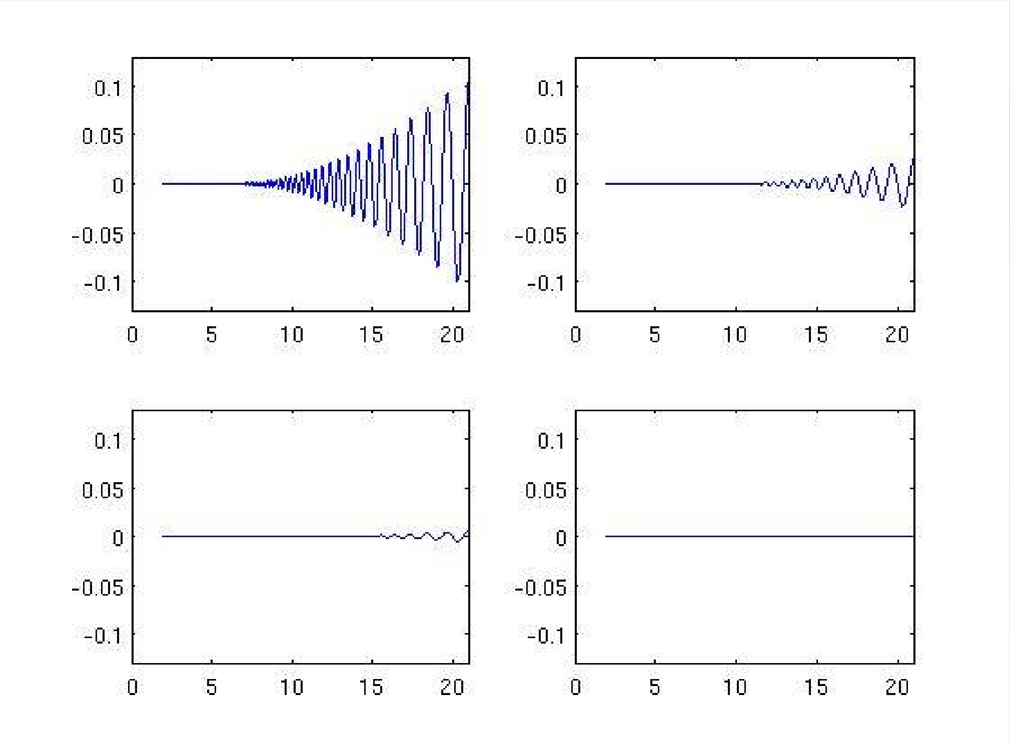
Energy quantization in field: Landau levels



- 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

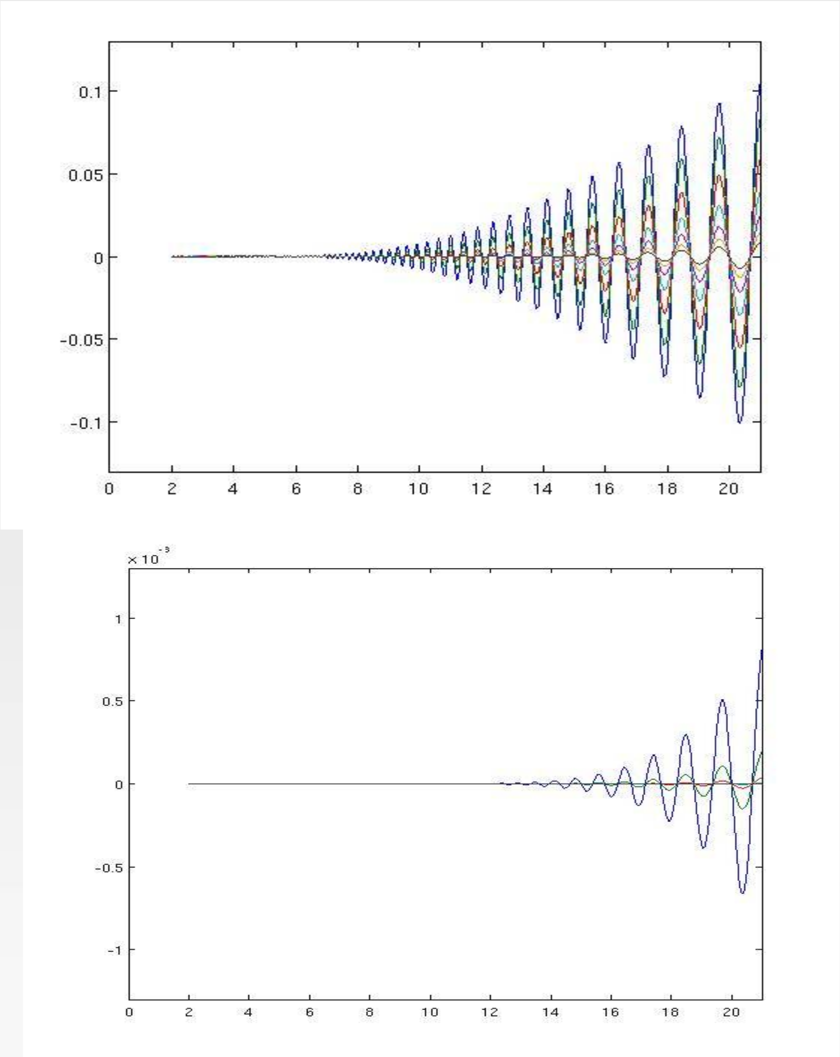
Lifschitz-Kosevich formalism

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

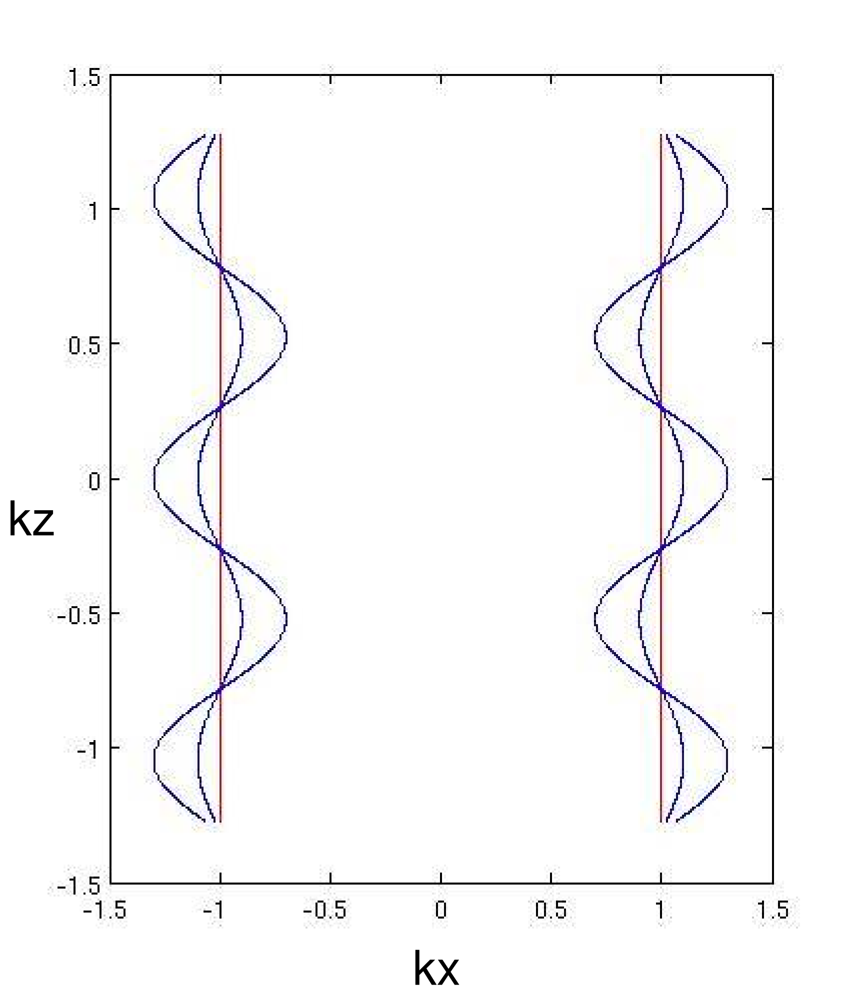


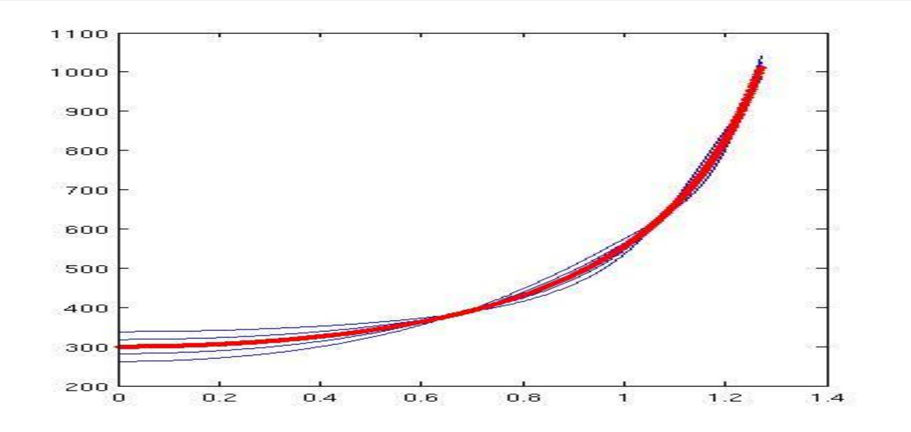
Lifschitz-Kosevich formalism

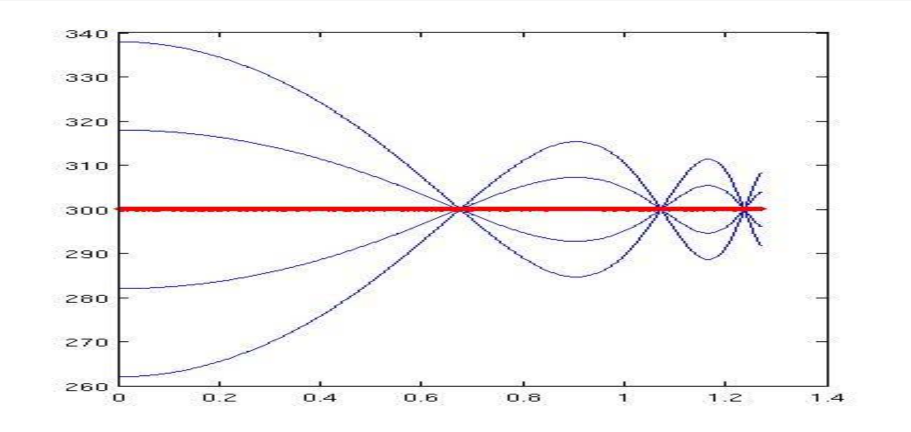
- Broadening of Landau levels due to finite temperature allows us to extract information about the effective mass m*.



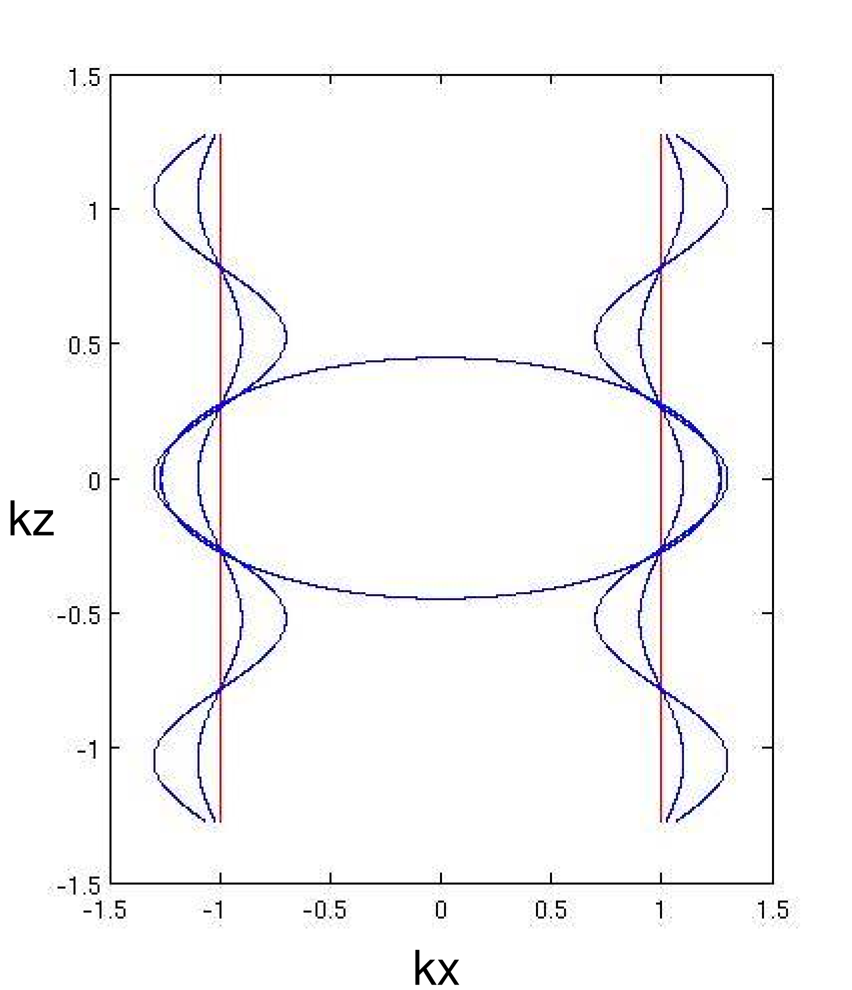
Determination of the FS topology: angle dependence

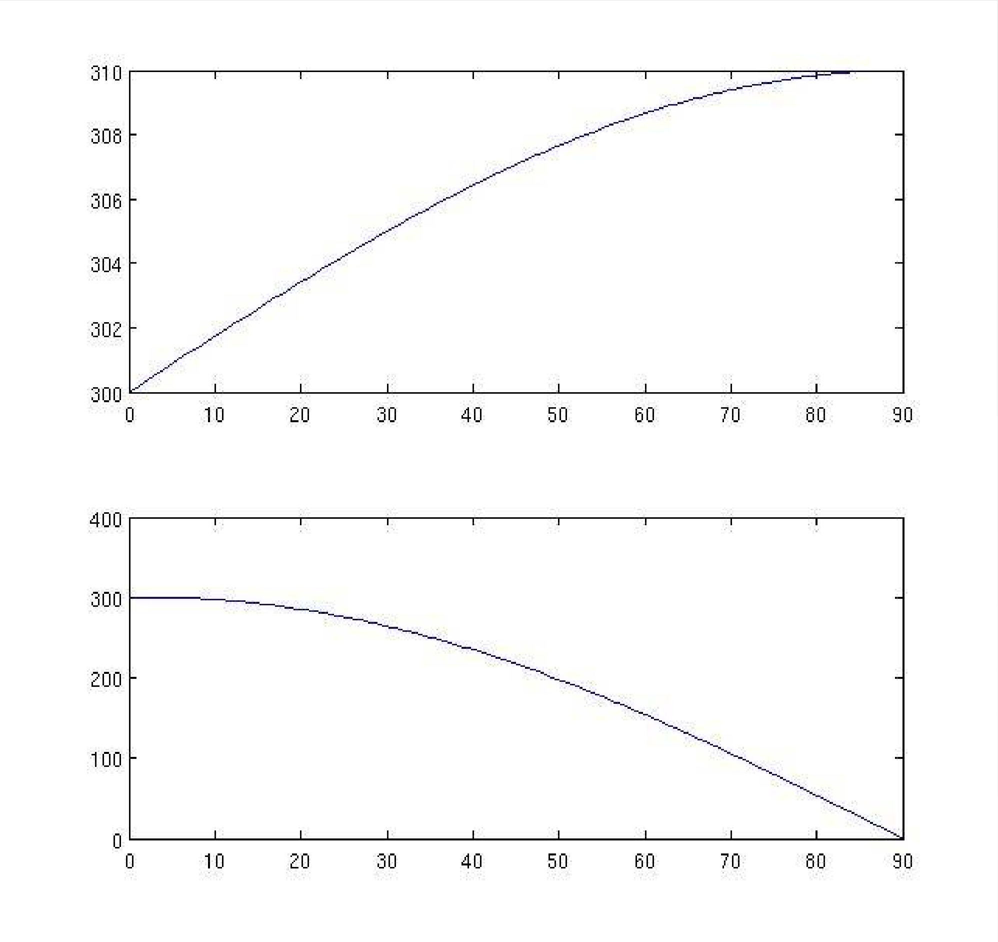






Determination of the FS topology: angle dependence





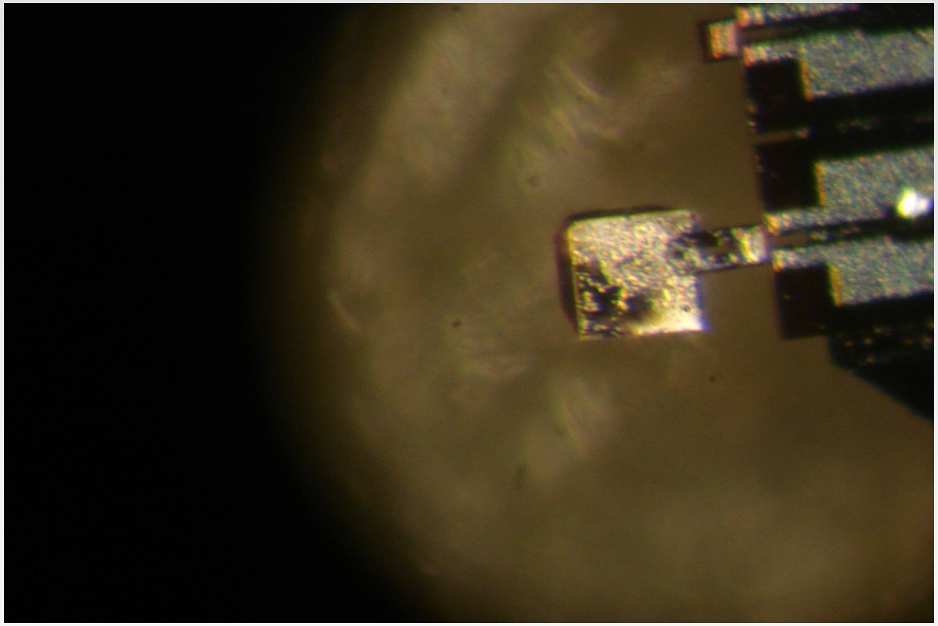
Pro's and Con's of quantum oscillations

- 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 H_{c2} 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



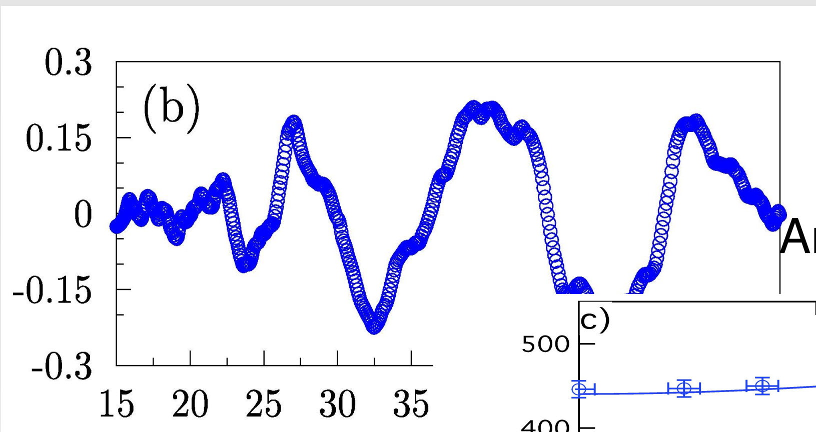
Use of high magnetic fields

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

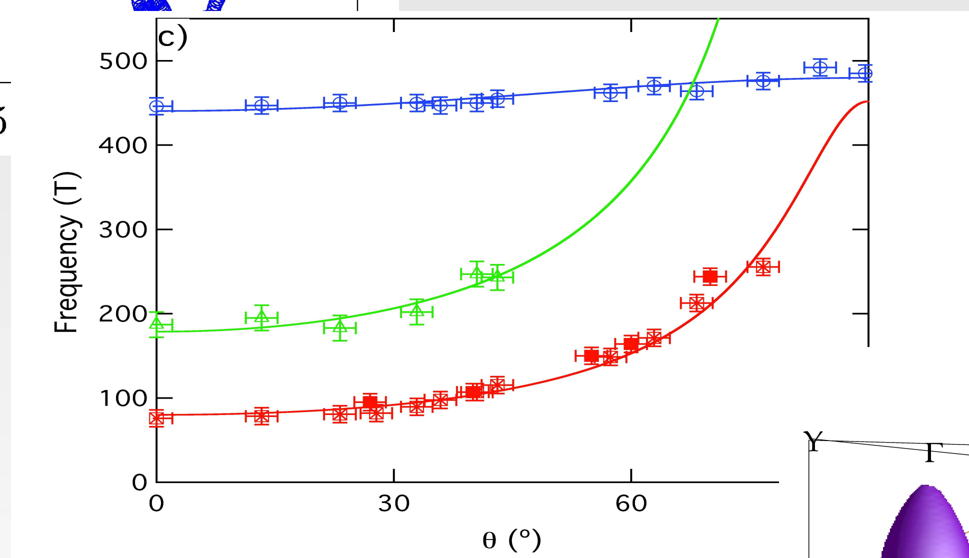
Part III: Results on the AFM state

BaFe2As2

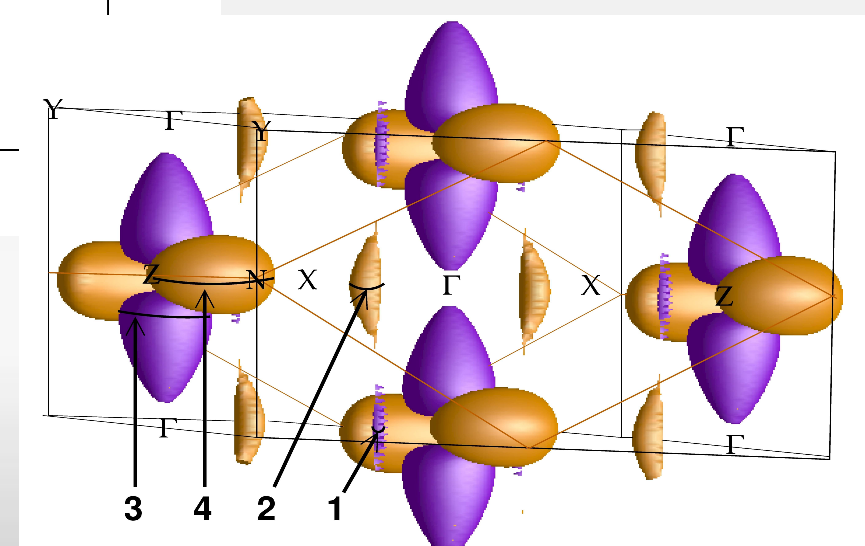
Background subtracted signal



Angle dependent analysis

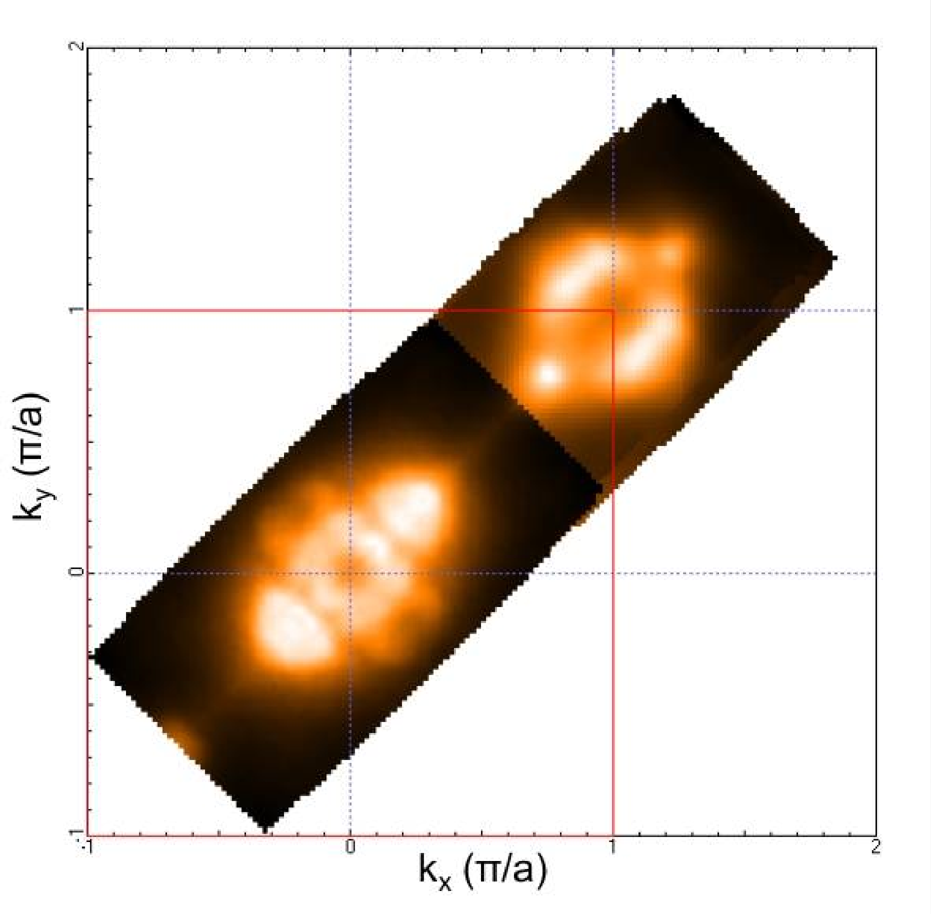


DFT calculations



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.

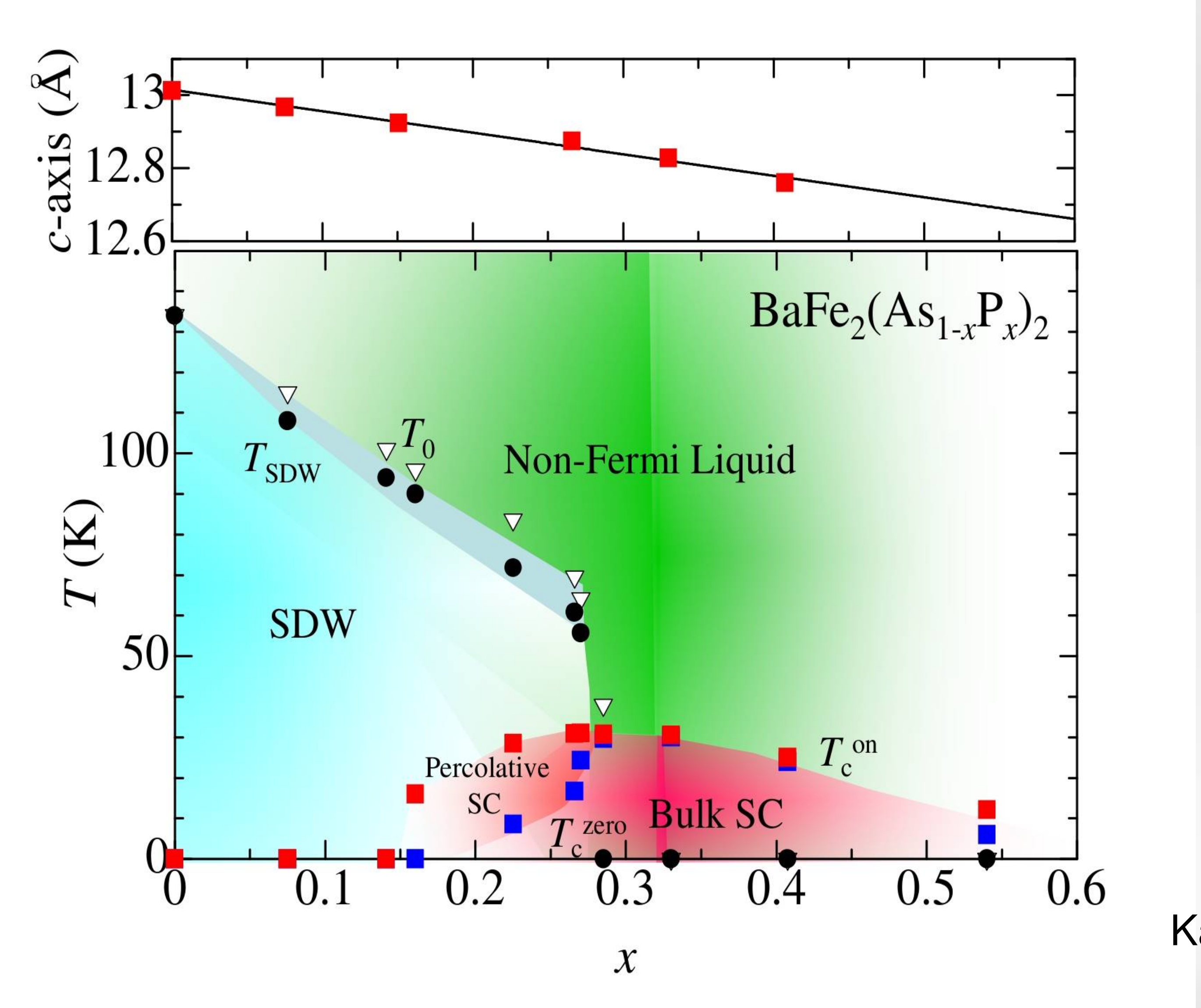


Part IV: The non-magnetic FS

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->P, we can supress 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



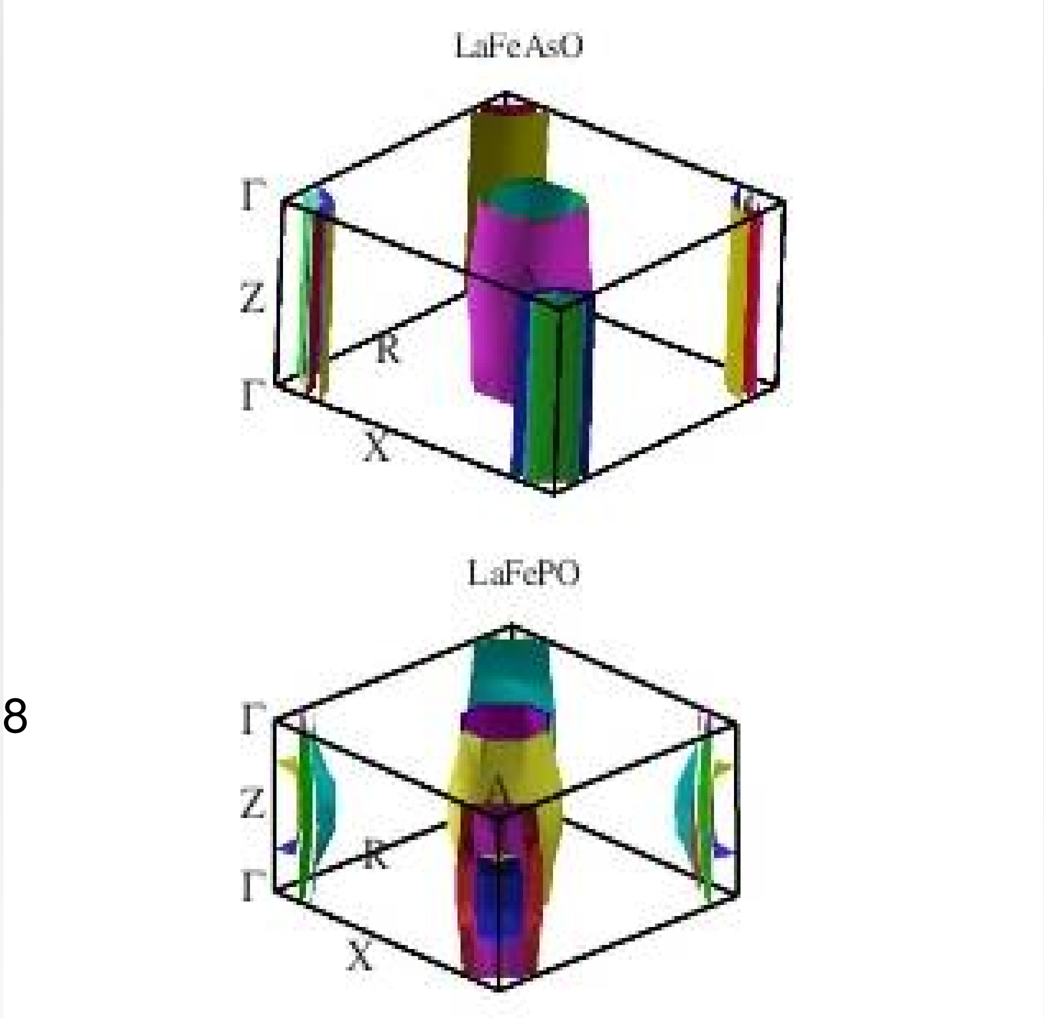
Kasahara 2009

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 ~109.5° vs ~116°

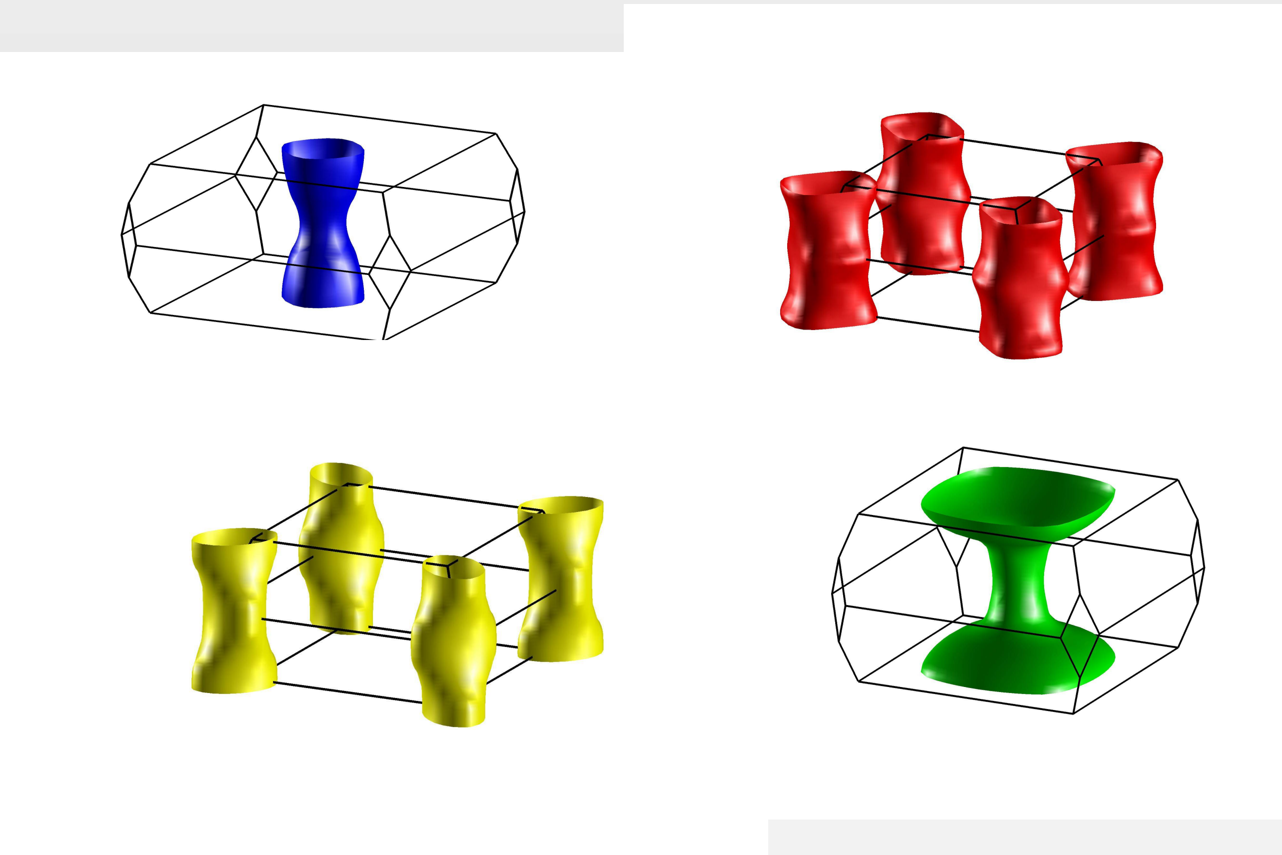
- *c*-axis shrinks by the same amount in arsenides
  - Ba->Sr->Ca
- Similarly the Pn-Pn distance.
- As-Fe-As bond angle seems to suppress the magnetism more than adjust the Fermiology.

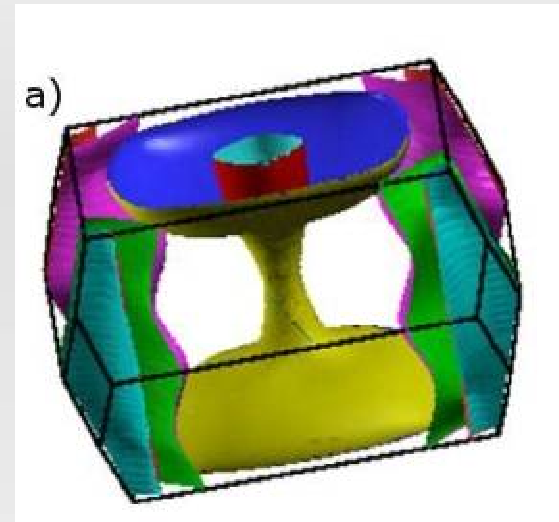
But are they the same? LaFePO



Georges et al 2008

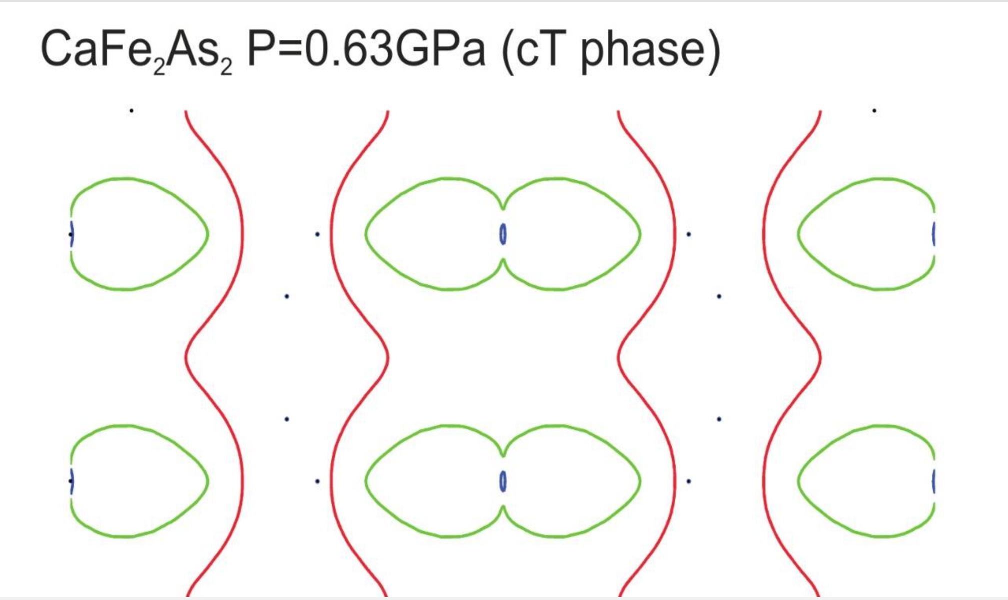
But are they the same? Sr122

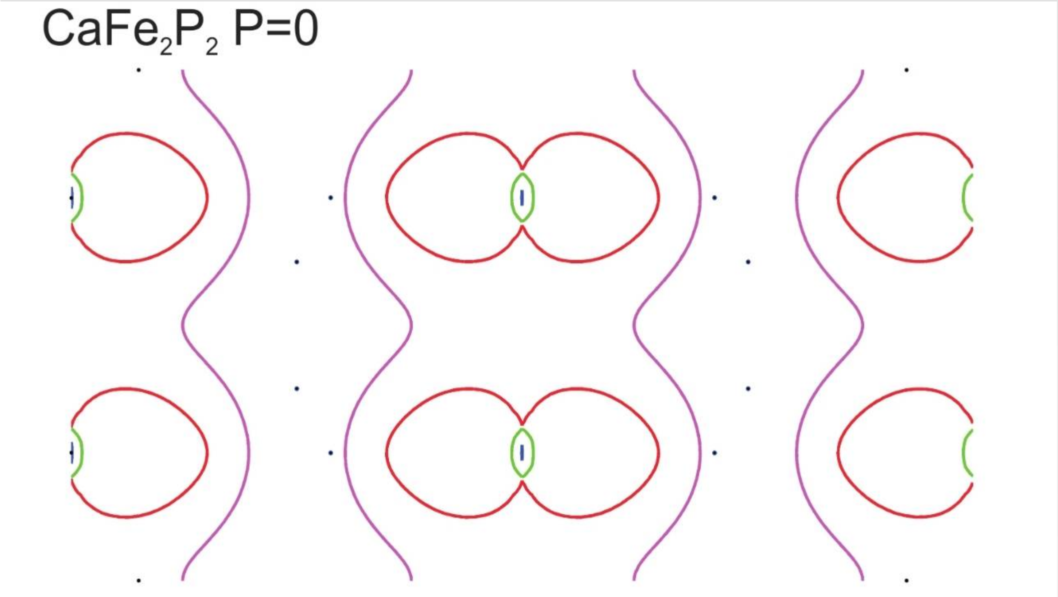




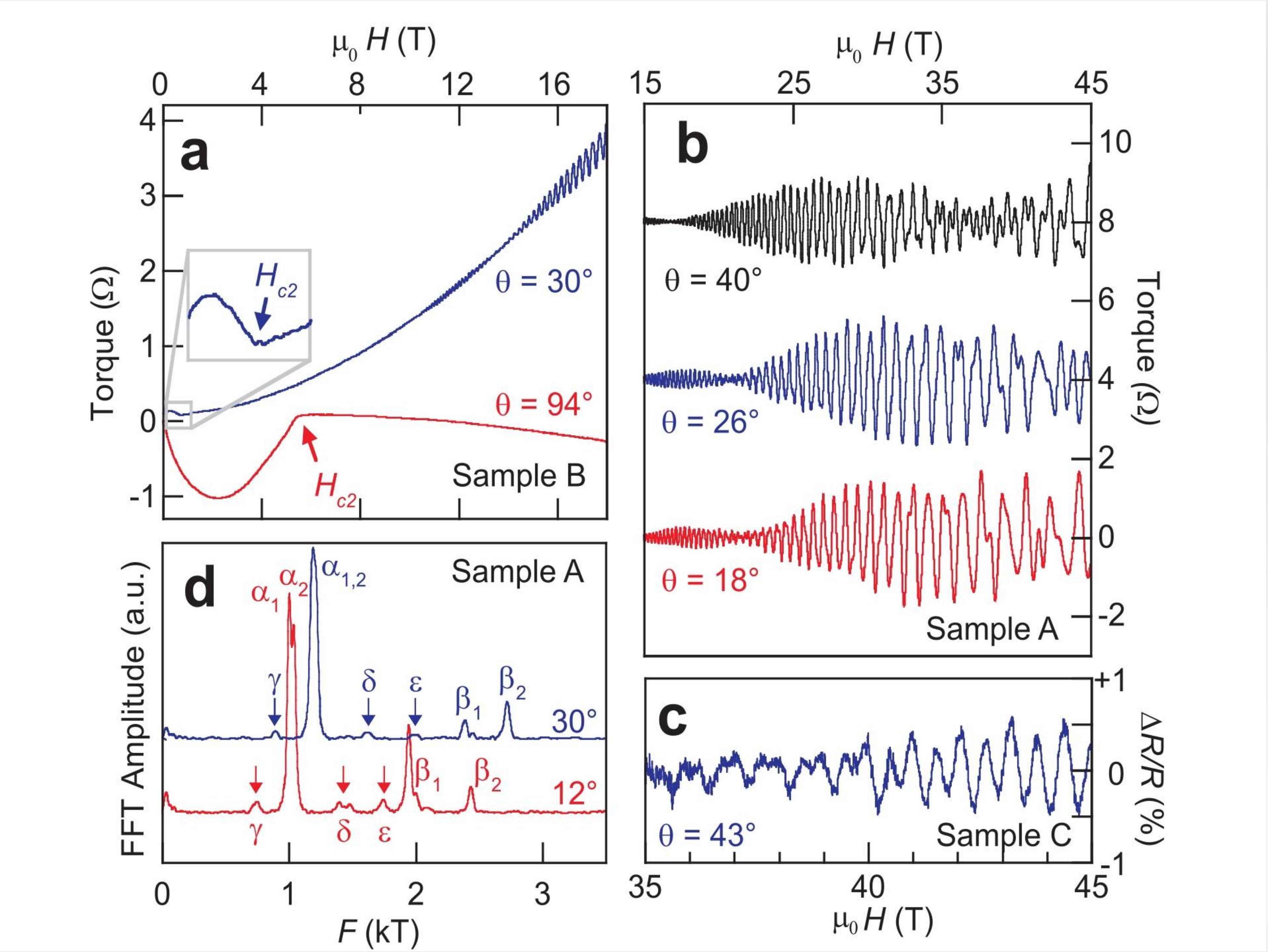
Tomsett, Lonzarich 2009

But are they the same? Ca122

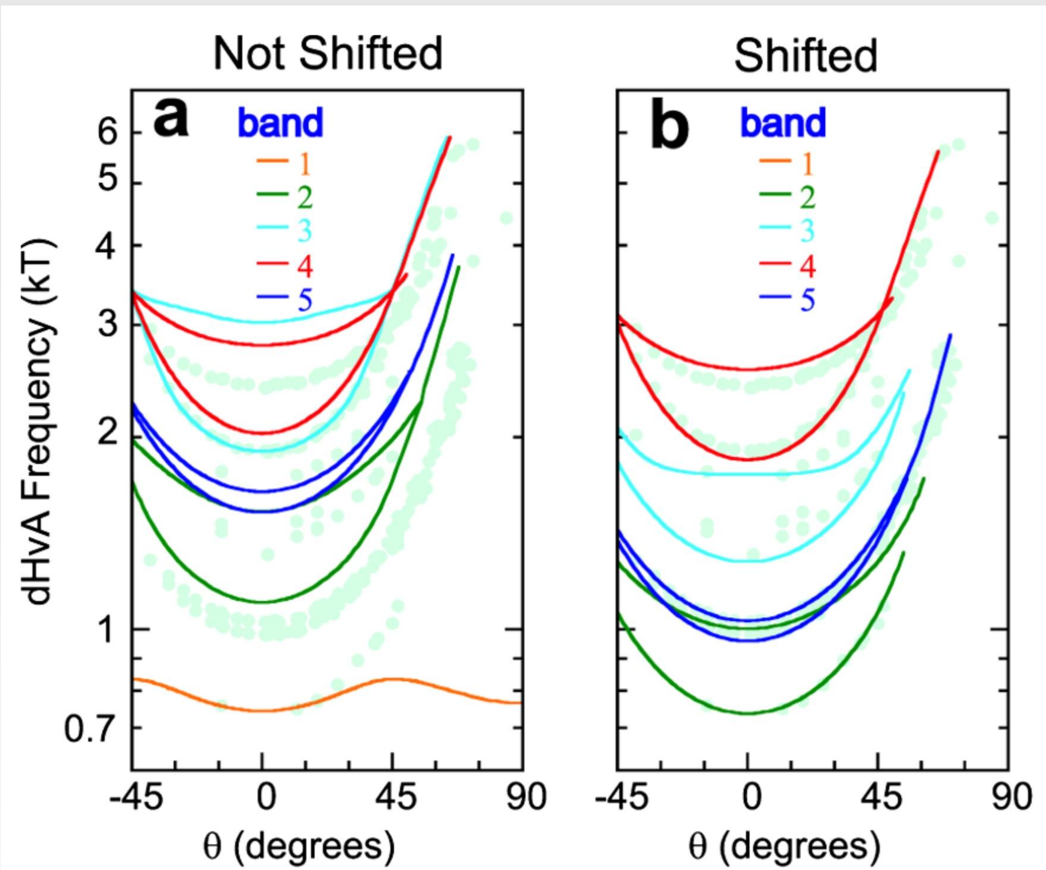


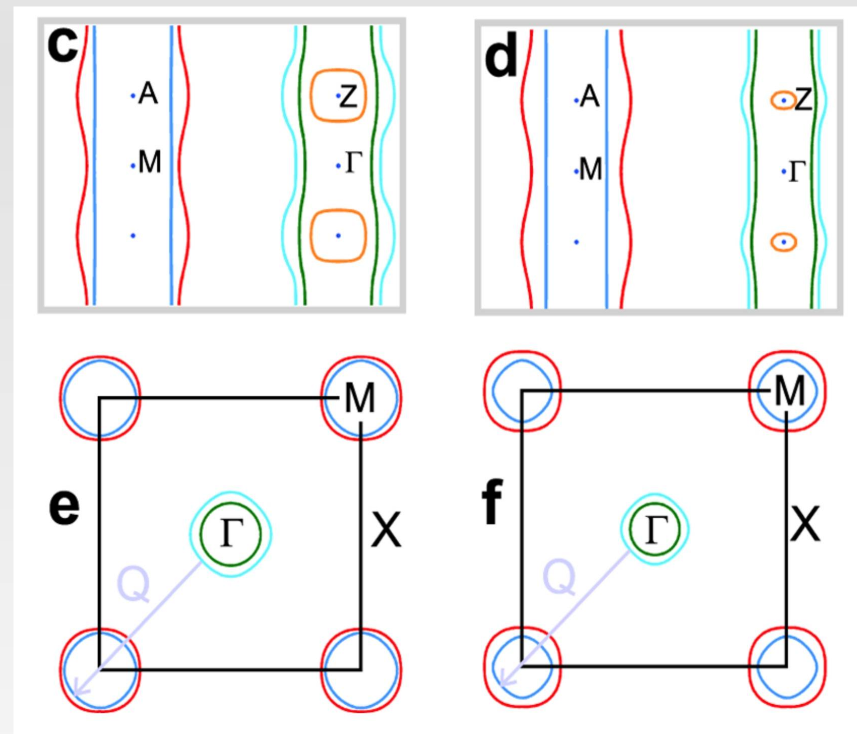


Oscillations in LaFePO

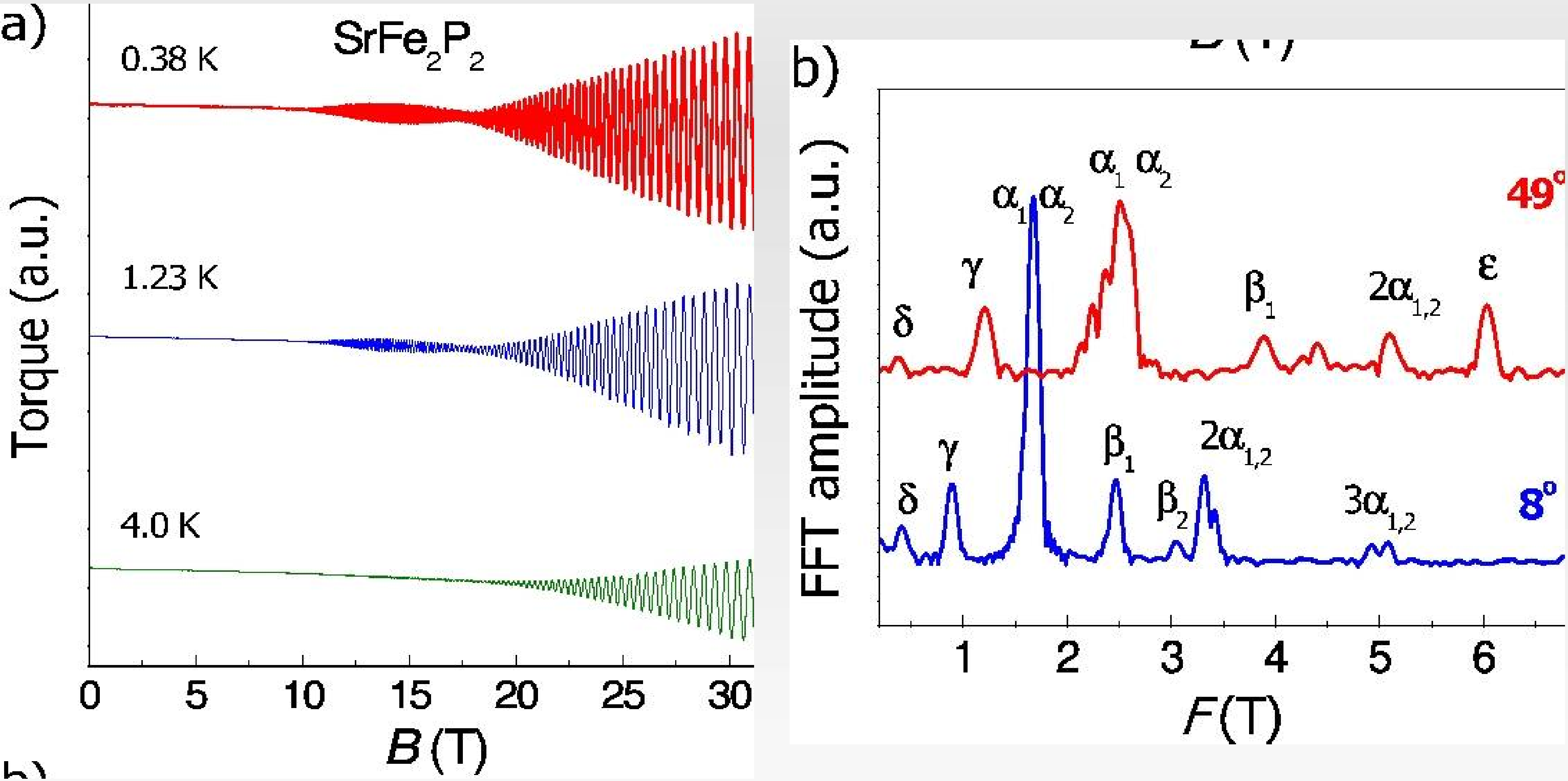


Angle dependence and bandstructure: LaFePO

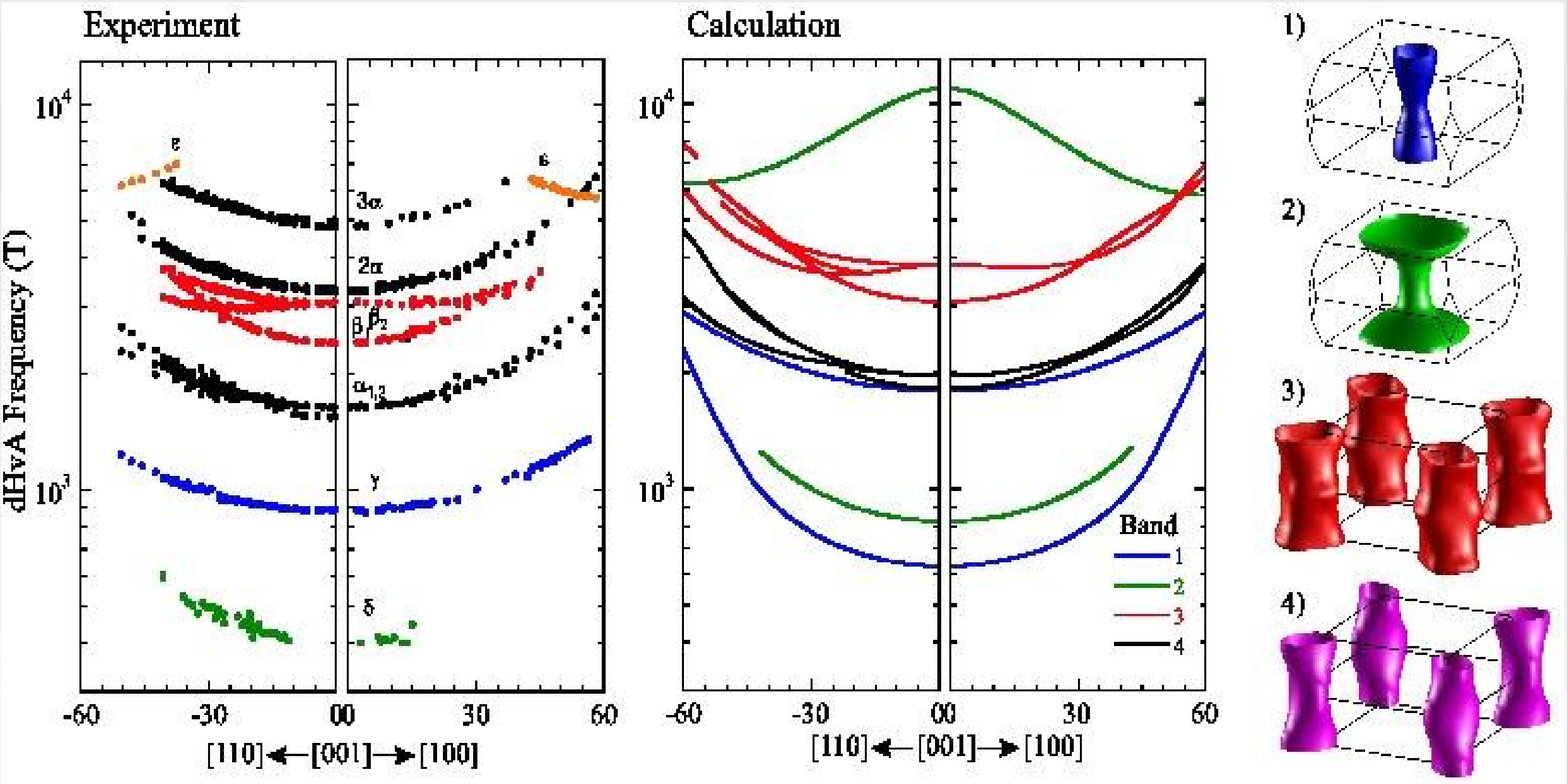




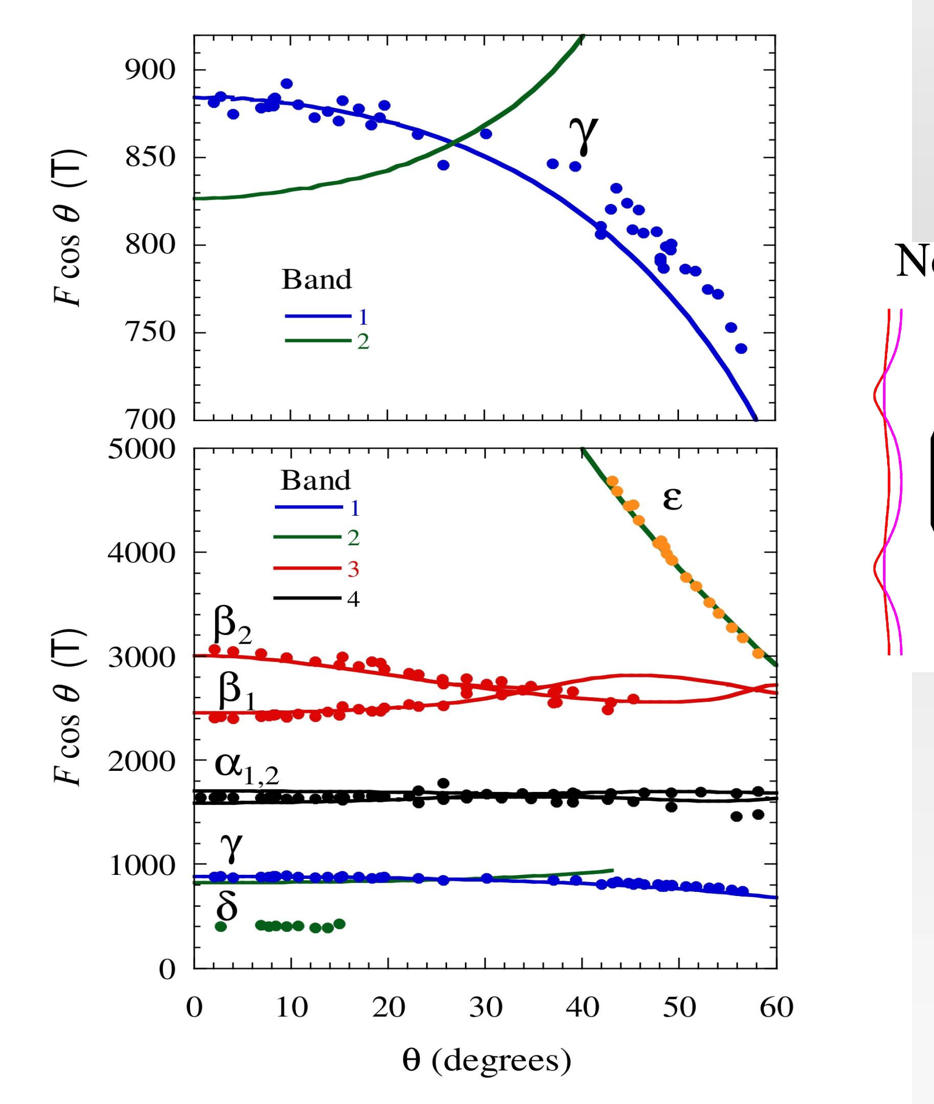
Oscillations in SrFe2P2

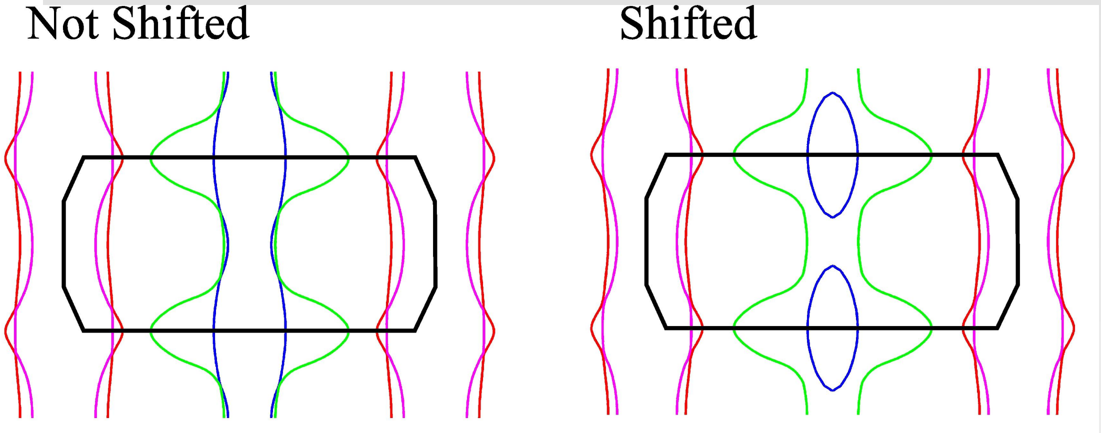


Angle dependence and bandstructure: SrFe2P2



Some analysis





The Fermi surface cas closed pockets!

NO (OBVIOUS) NESTING

Results summary: SrFe2P2/LaFePO

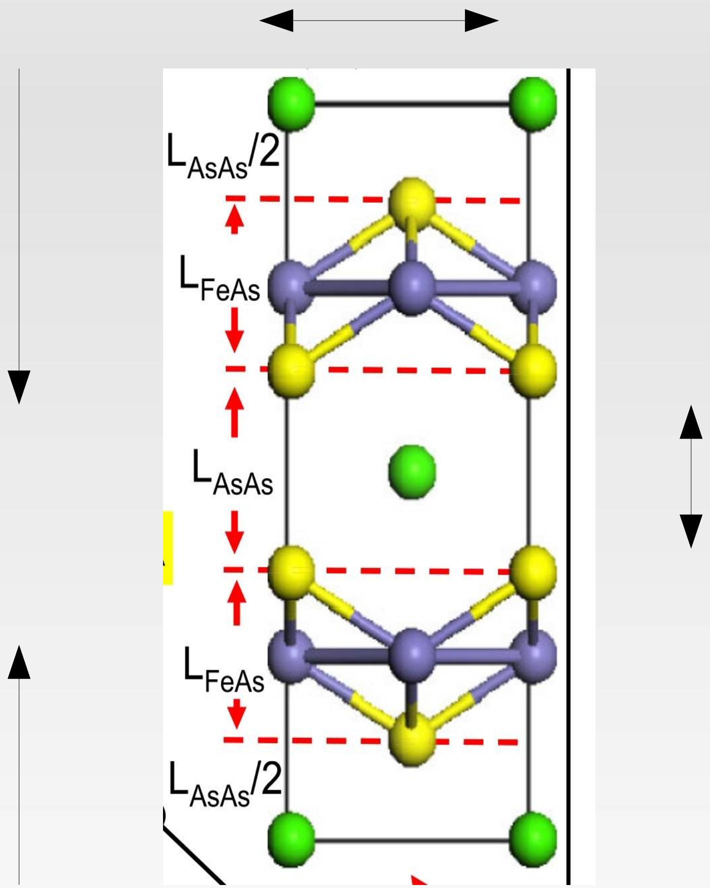
Branch	Experiment: F (kT)	Experiment: m^*/m_e A	Experiment: m^*/m_e B	Orbit	Calculations: m_b/m_e Unshifted	Calculations: m_b/m_e Shifted
α_1	0.985(7)	1.9(2)	1.8(1)	1Z	1.0	1.9
α_2	1.025(7)	1.9(2)	1.8(1)	2Γ	0.9	0.7
β_1	1.91(1)	1.7(2)	1.8(1)	2Z	1.2	1.1
β_2	2.41(1)	1.8(2)	1.9(1)	3Γ	1.8	1.1
					2.9	2.5
					0.7	0.7
					0.9	0.9
					0.8	0.7
					0.9	0.8

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

Collapsed tetragonal analogue: CaFe2P2

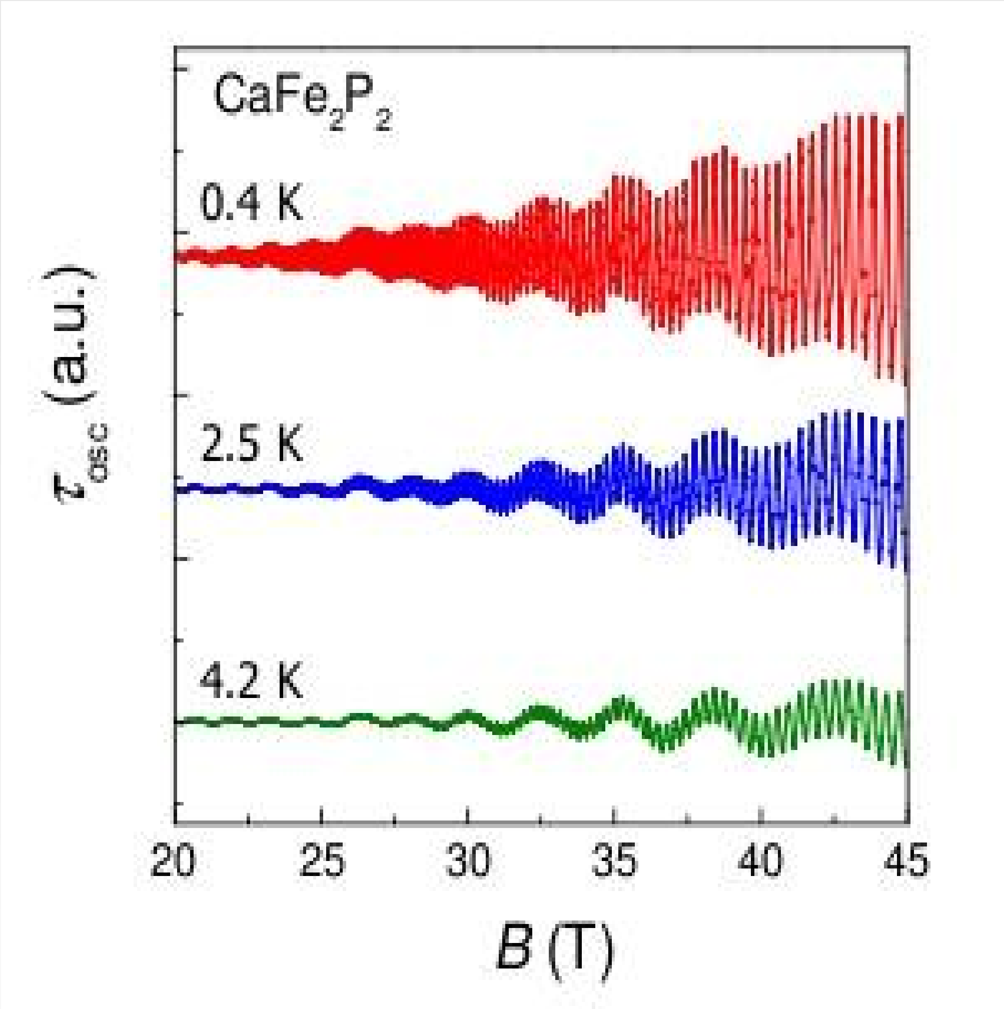
c/a

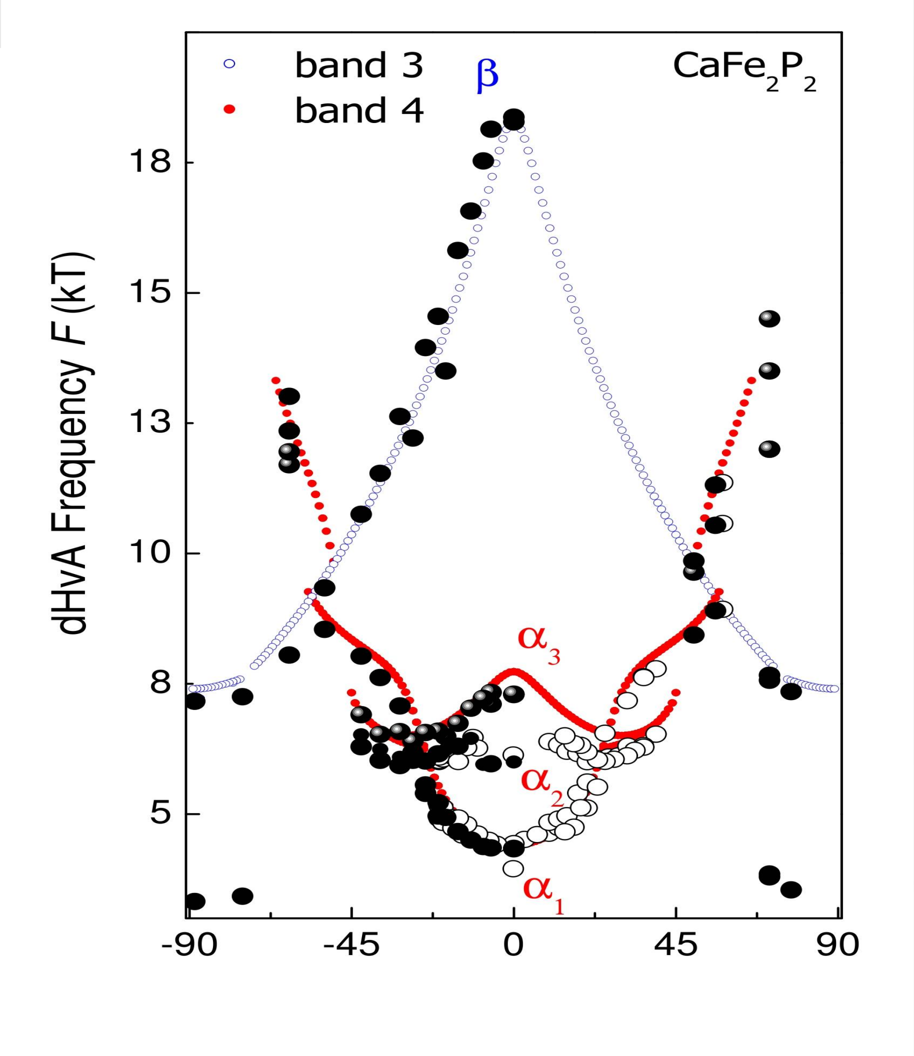
3->2.6



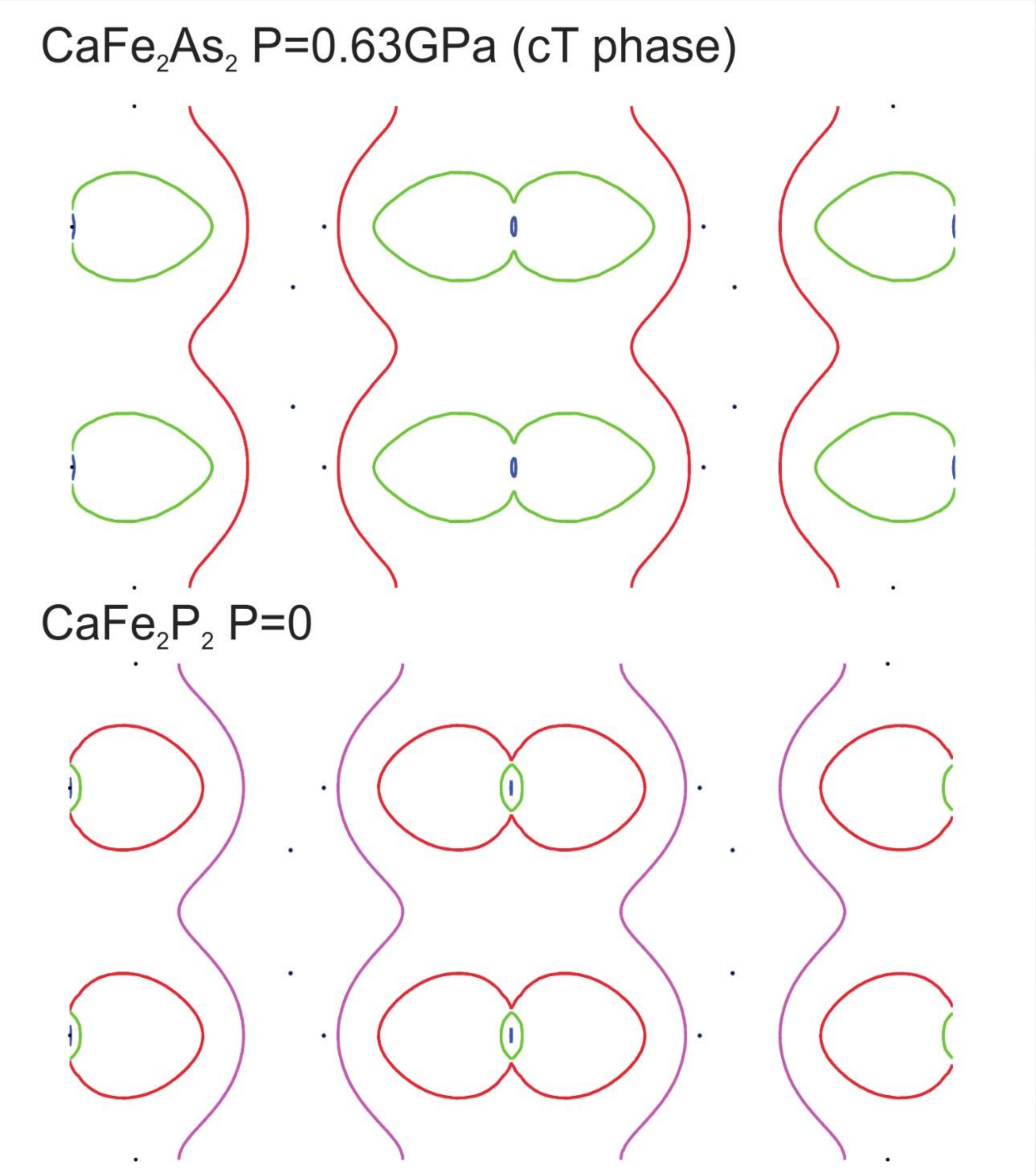
Yildirim et al 2008

Oscillations in CaFe2P2





Collapsed tetragonal Fermi surface



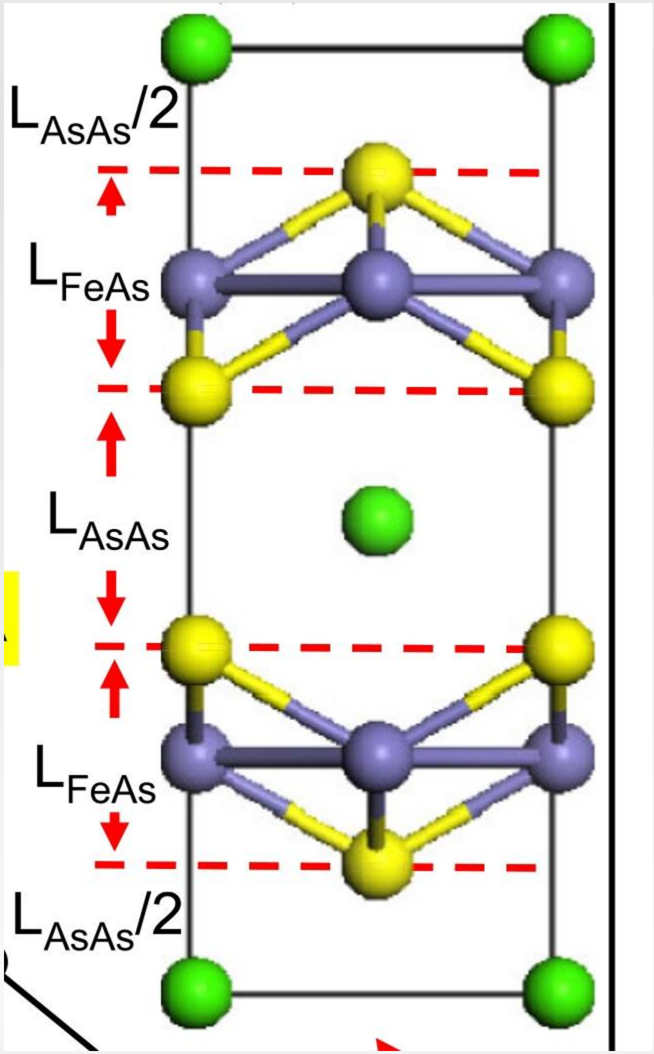
Summary of Ca122(P) data

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

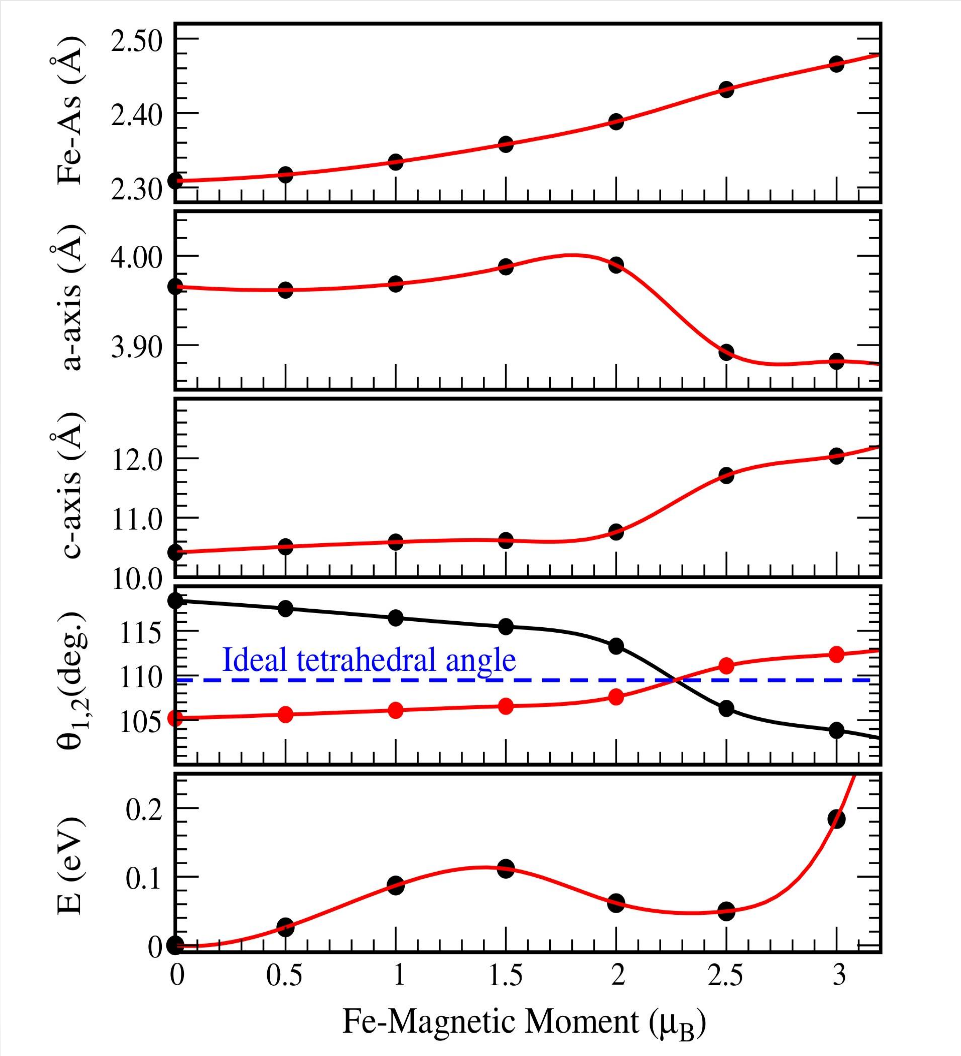
Why are the phosphides different?

- 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.

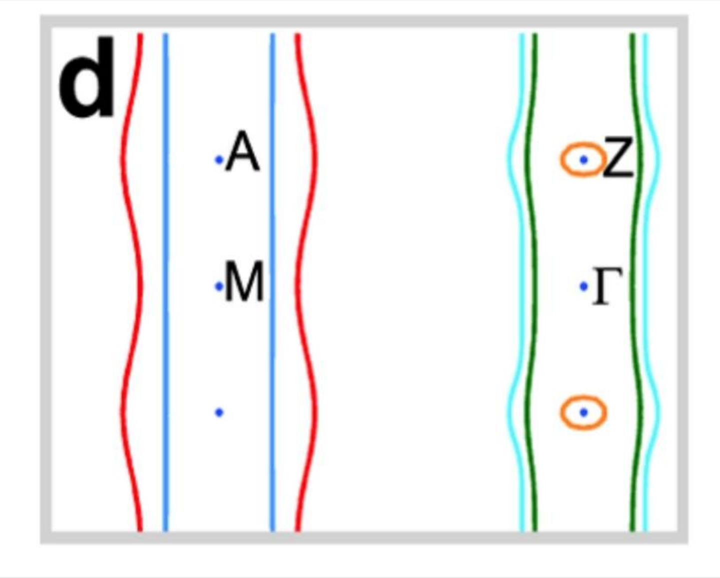


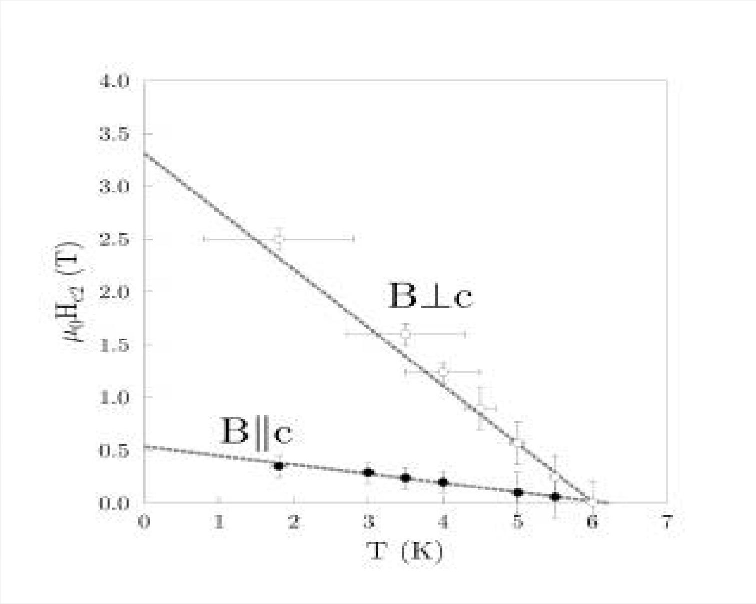
Why are the phosphides different?

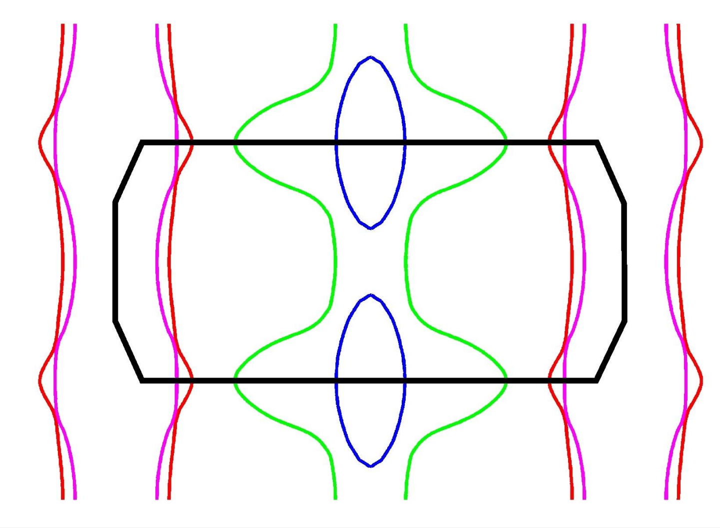
- This bond angle is likely related to the local magnetic moment. e.g. Yildirim PRL2009

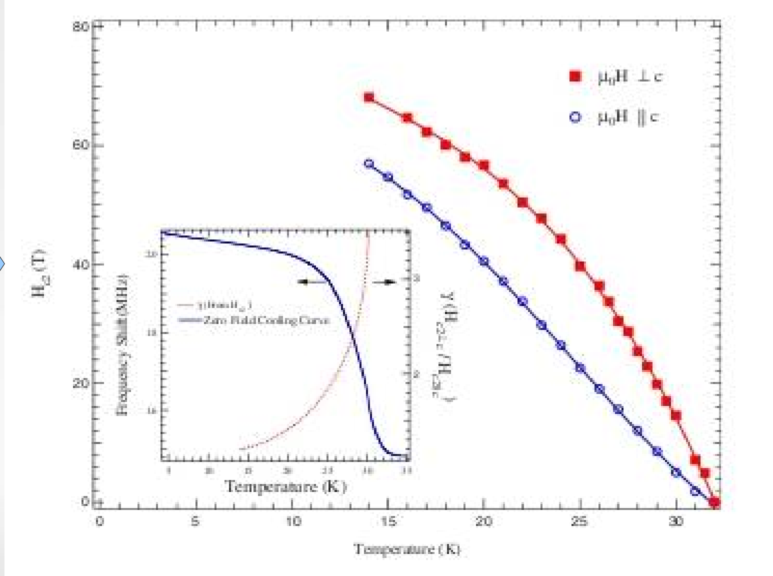


Relationship to superconductivity

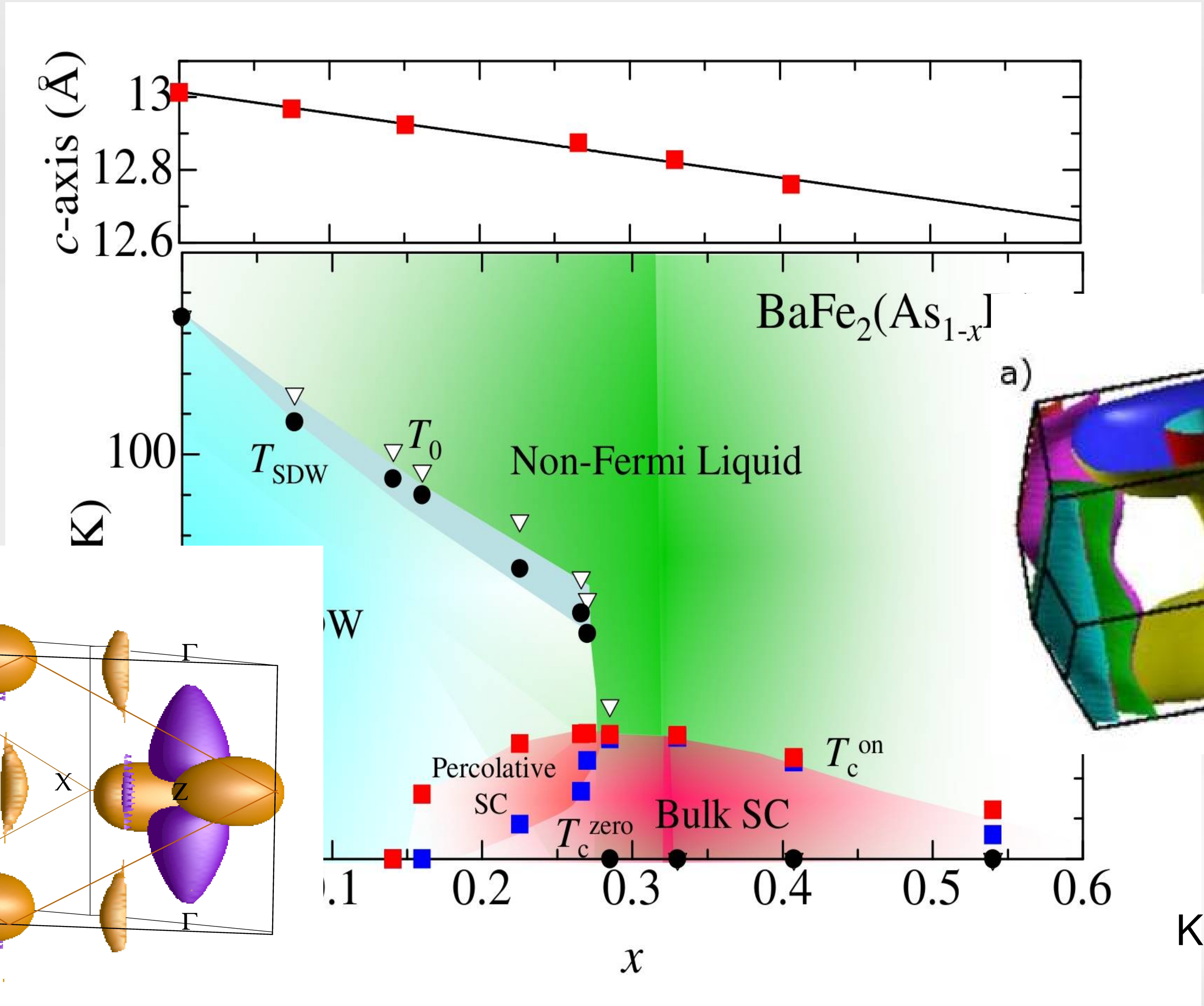


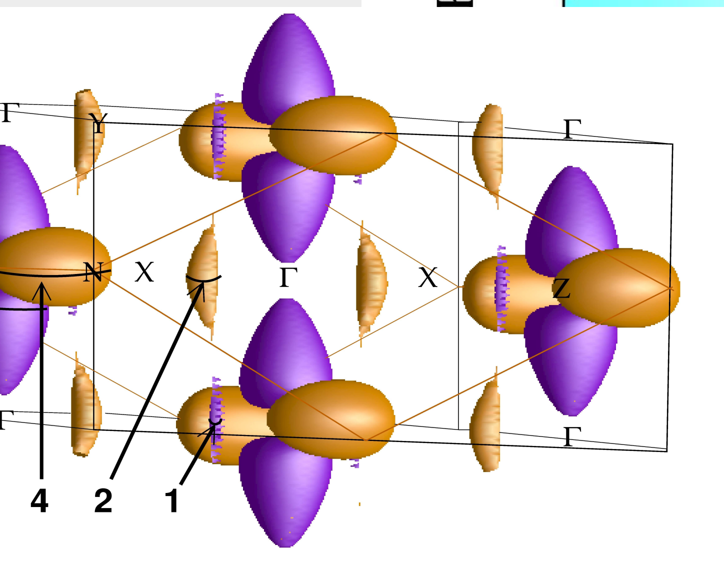


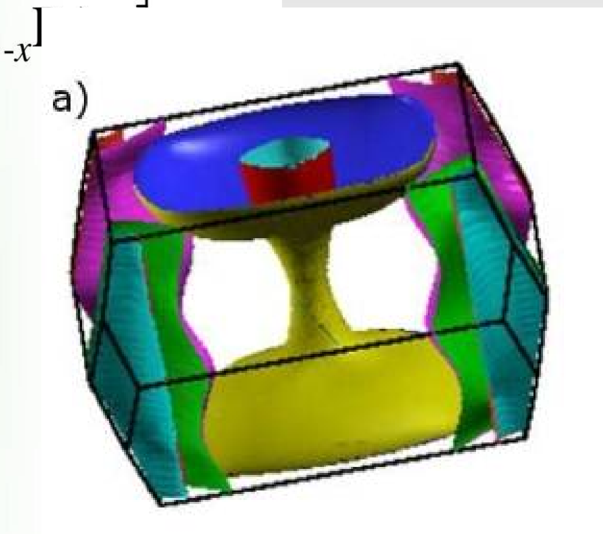




P substitution of As: phase diagram

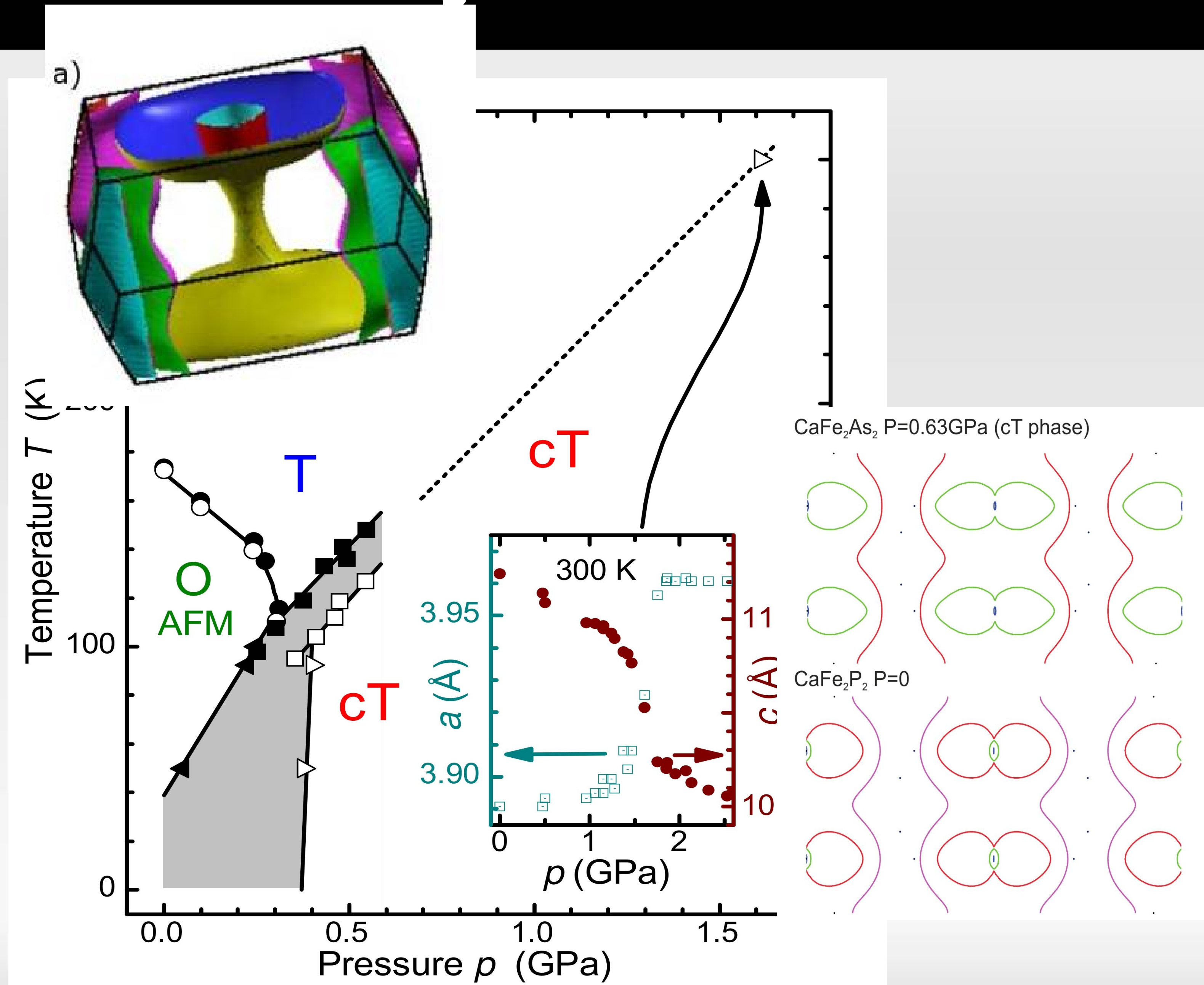






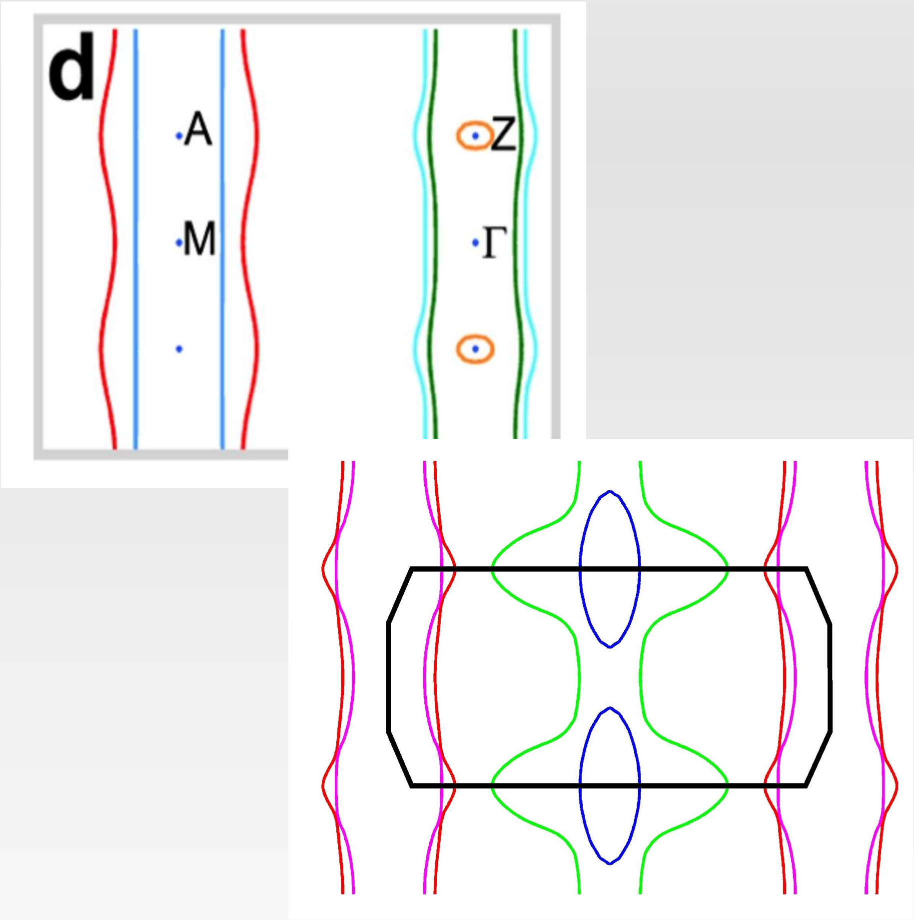
Kasahara 2009

Ca122 – Summary



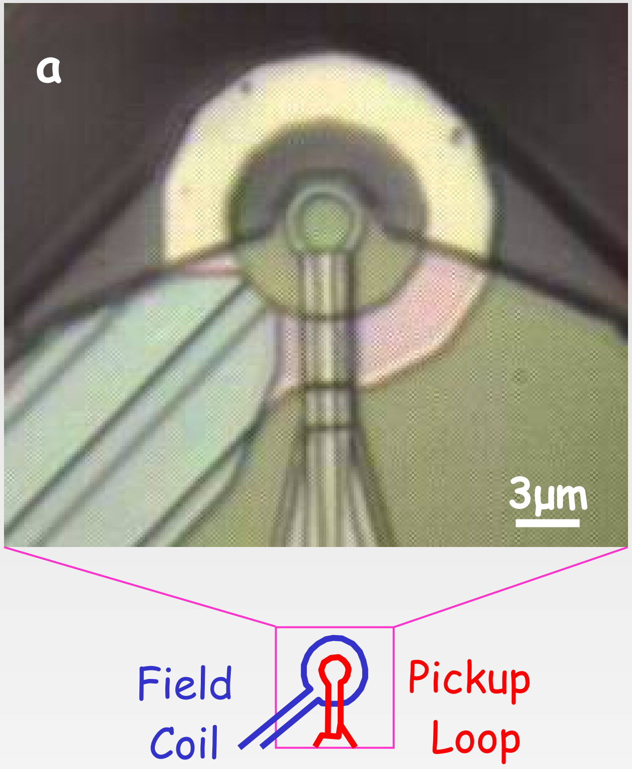
Why do the 1111 phosphides superconduct but the 122s do not?

- 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

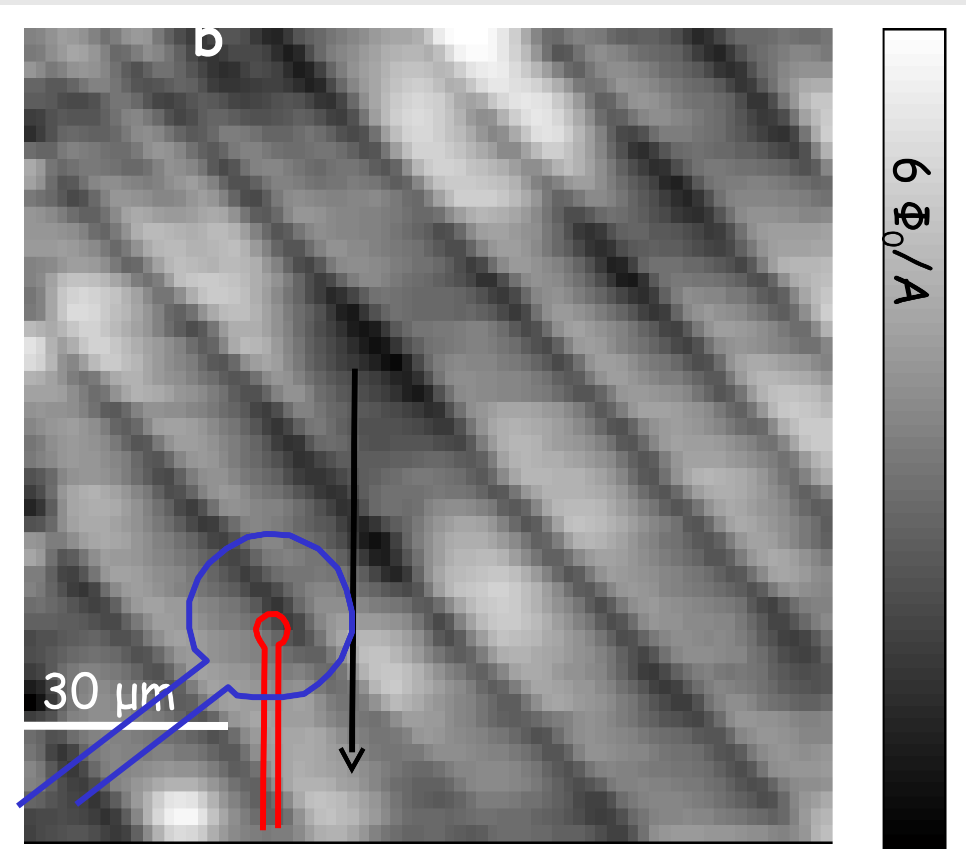


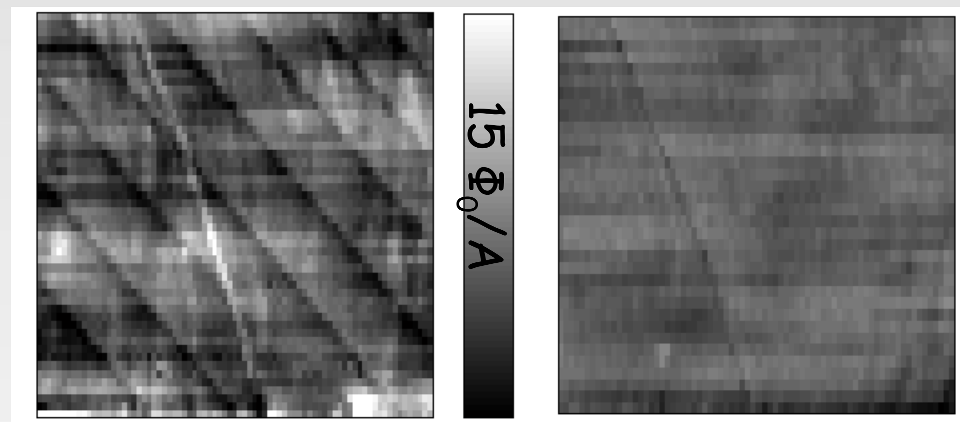
Scanning squid results

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

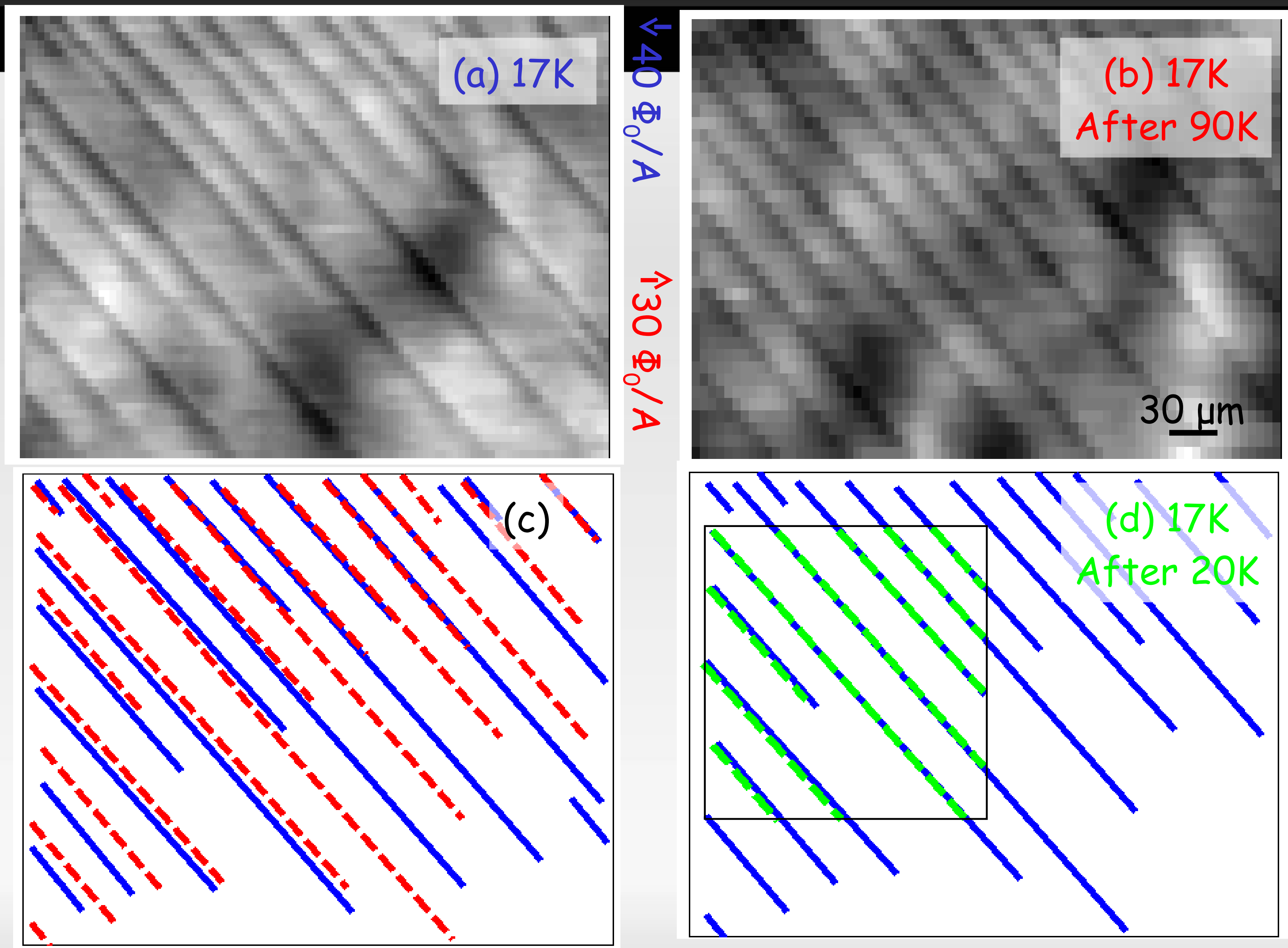


Stripes in the superfluid density!

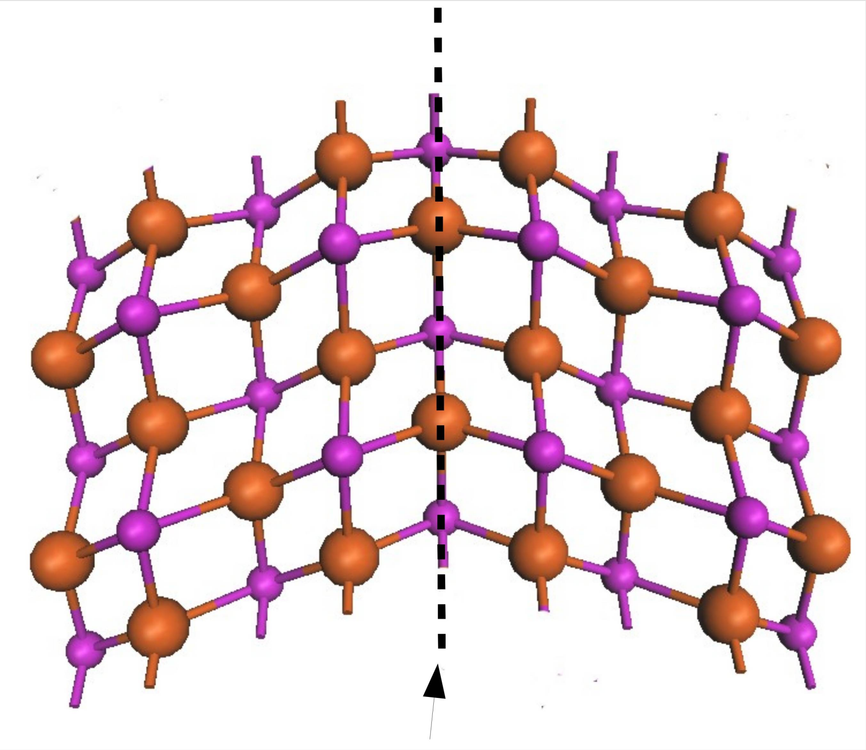




30 µm


(a) 17K
40 Φ0/A
30 Φ0/A
(b) 17K
After 90K
30 µm
(c)
(d) 17K
After 20K

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 quasipaticles 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 Tc up, so that the 1111(As) have the highest Tcs 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 Tc?
- What is the role of local strain fields and is the itinerant physics related?

Thanks!