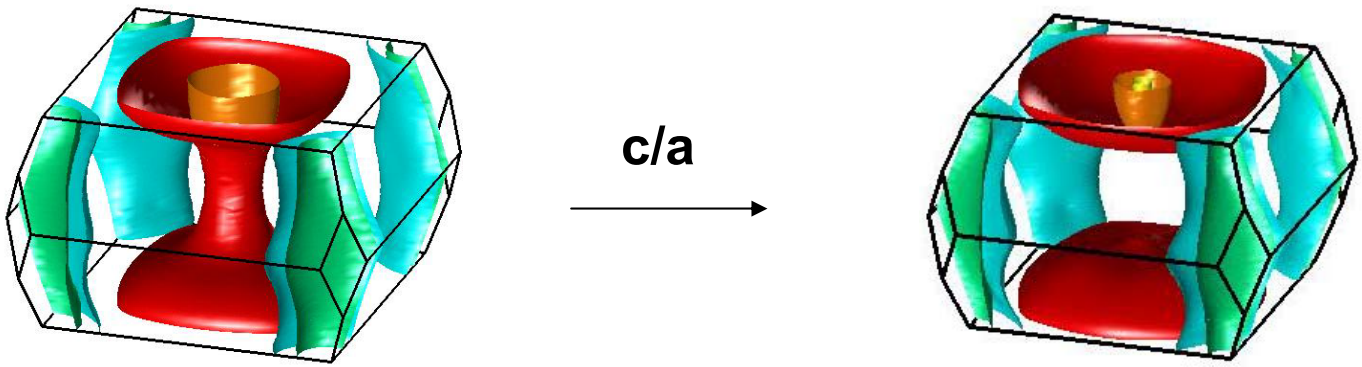
Topological changes of the Fermi surface and the effect of electronic correlations in iron pnictides

Amalia Coldea

Oxford University



http://www.physics.ox.ac.uk/users/coldeaa

KITP, Santa Barbara, Jan 2011

Collaborators

Antony Carrington, Caroline Andrew, Jon Fletcher, A. Bangura
H. H. Wills Physics Laboratory, University of Bristol, **UK**

Ian Fisher, James Analytis, Jiun-Haw Chu, Hsueh-Hui Kuo
Geballe Laboratory for Advanced Materials, Stanford University, **USA**

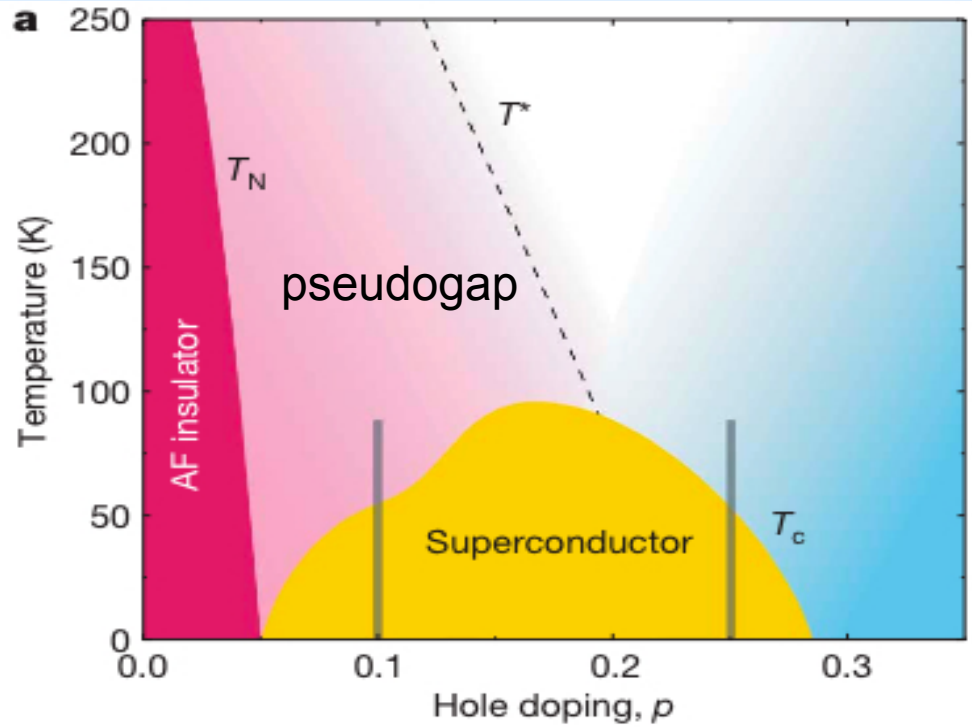
S. Kasahara, H. Shishido, K. Hashimoto, T. Shibauchi, Y. Matsuda
Department of Physics, Kyoto University, **Japan**

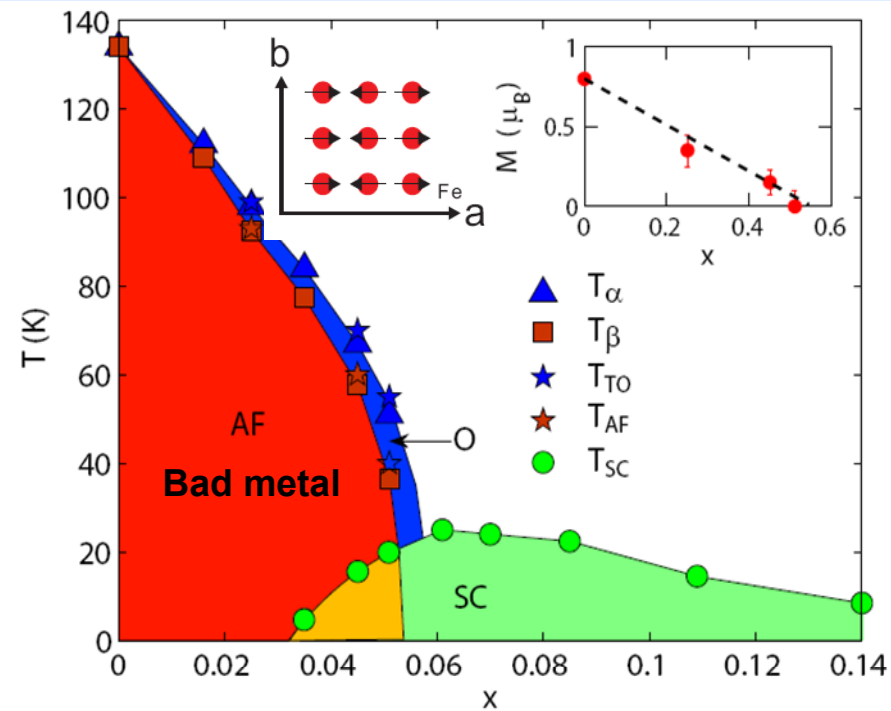
Ross McDonald
National High Magnetic Field Laboratory,
Los Alamos National Laboratory, **USA**

Alix McCollam
High Magnetic Field Laboratory,
Nijmegen, **The Netherlands**

D. Vignolles, C. Proust, B. Vignolle
Laboratoire National des Champs Magnetiques Intenses, Toulouse,
France

Phase diagrams: cuprates vs pnictides





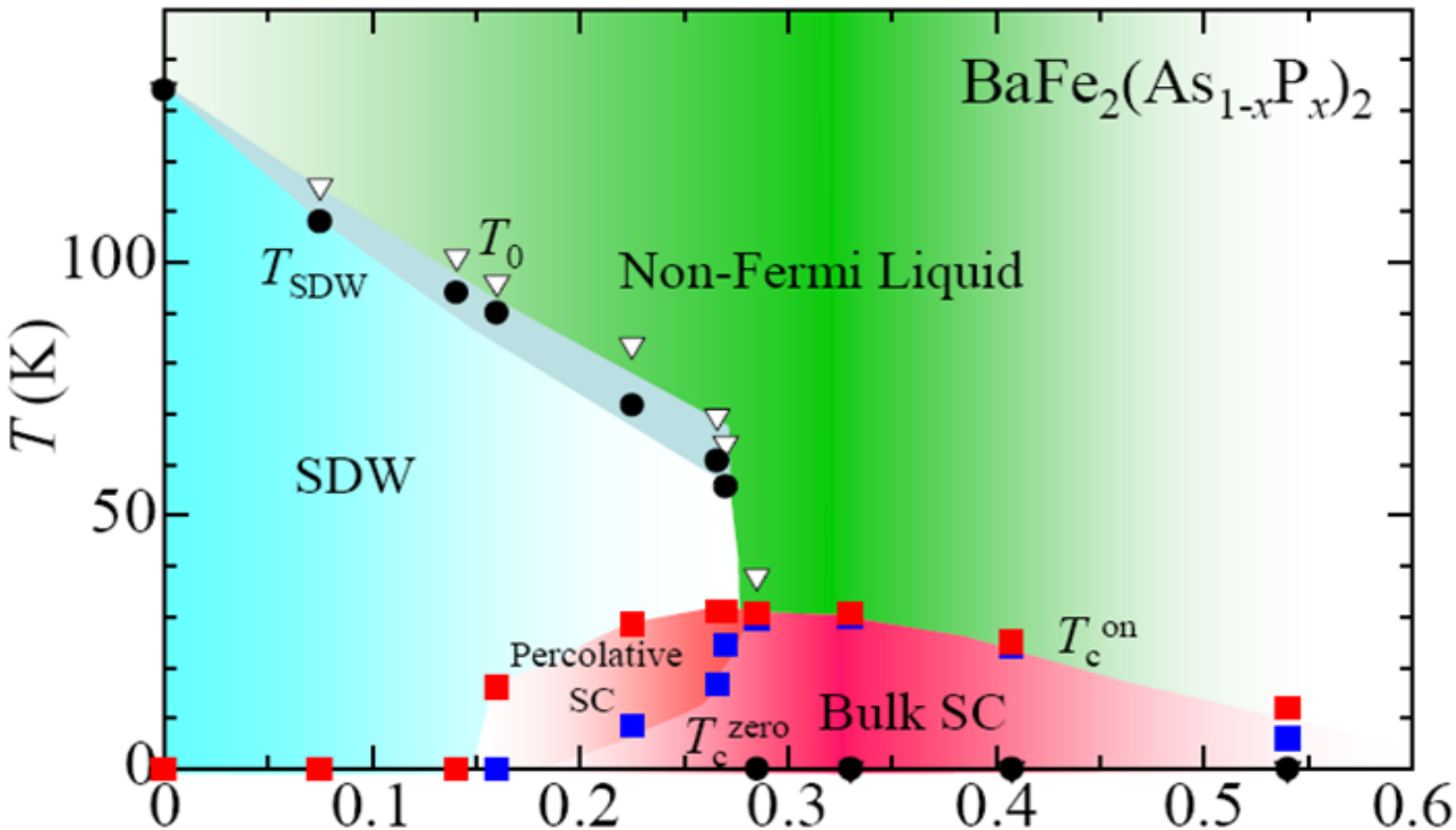
- AFM ordering - Mott-insulator;
- Strong electronic correlations;
- pseudogap;
- Cu^{2+} -O_{2p} $3d_{x2-y2}$ single band;

- AFM ordering– Bad metals;
- small carrier density ;
- Fe^{2+} - As^{3-} (d^6); all five d orbitals important;
- high density of states N(EF), prone to magnetic instabilities;

Doiron-Leyraud et al, Nature, **447** 565 (2007)

C. Lester et al, Phys. Rev. B 79, 144523 (2009)

Effect of chemical pressure: P substitution

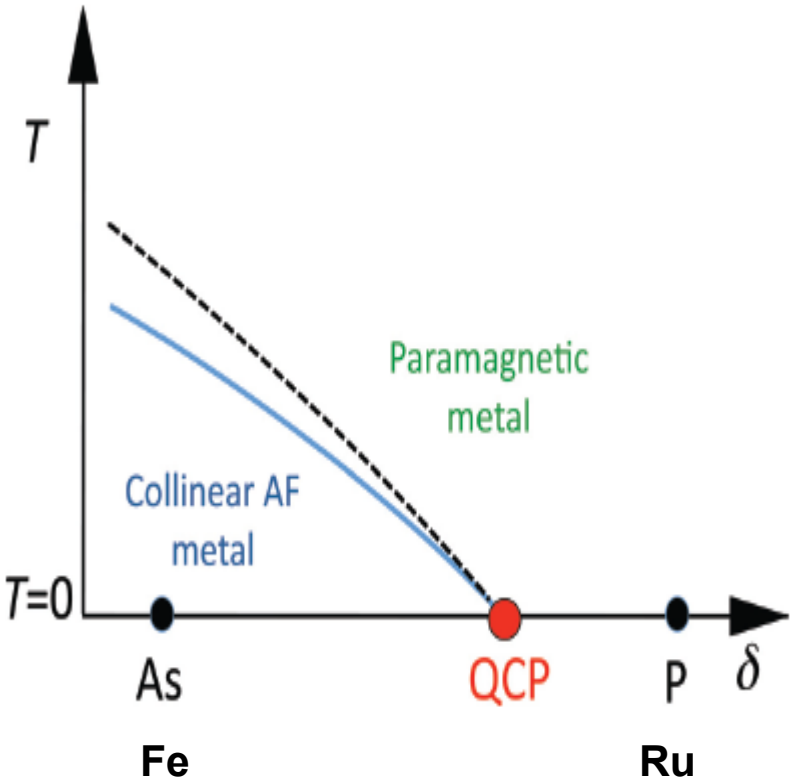


• suppression of magnetism and the presence of superconductivity through chemical substitutions: As replaced by P, or Fe replaced by 4*d* and 5*d* elements: Rh, Ir and Pd; other examples $SrFe_{1-x}Ru_xAs_2$, $LaFeAs_{1-x}P_xO$ and $EuFe_2As_{2-x}P_x$.

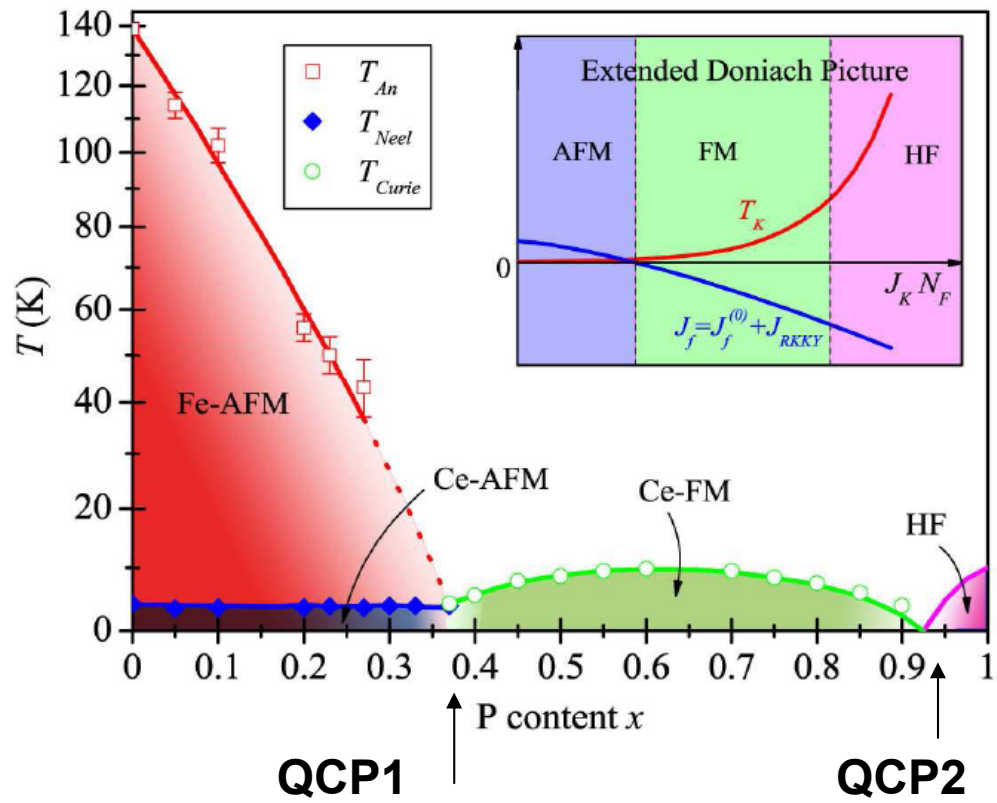
S. Jiang, *et al*., arXiv:0901.3227 (2009)

S. Kasahara *et al*. , PRB **81**, 134422 2010

Criticality determined by As/P substitution



$CeFeAs_{1-x}P_xO$:



• suppression of magnetism by chemical substitution As/P, unique role of P-doping in suppressing the *d*-electron correlations.

J. Dai *et al.* , PNAS, 106, 4118 (2009)

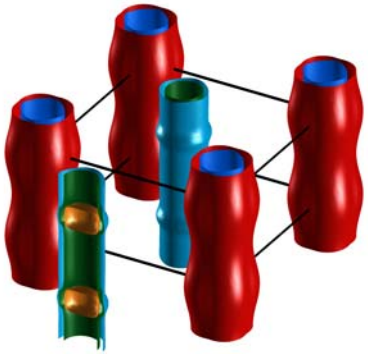
Y. Luo, *et al.*, arXiv:0907.2961 (2009)

Plan of my talk

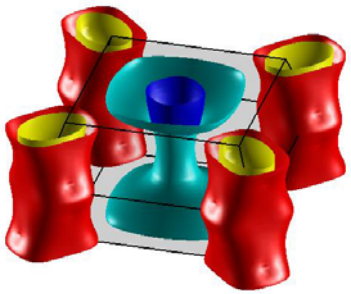
- Quantum oscillations to determine the Fermi surface and comparison with band structure calculations.
- the superconducting **LaFePO**; role of nesting ;

- Role of dimensionality on the Fermi surface: the case of **$SrFe_2P_2$**;
- Fermi surface shrinking and enhanced correlations in **$BaFe_2(As_{1-x}P_x)_2$**

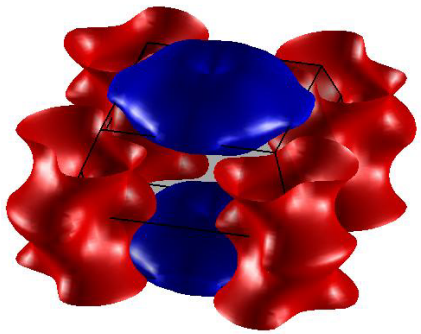
- Topological change of the Fermi surface with c/a ratio: the case of **$CaFe_2P_2$.**
- Conclusions



1111
LaFePO
T_c~ 6K



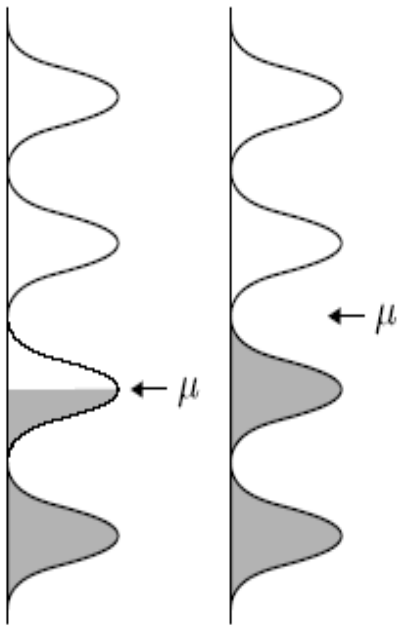
122
$SrFe_2P_2$
***c/a*=3.04**

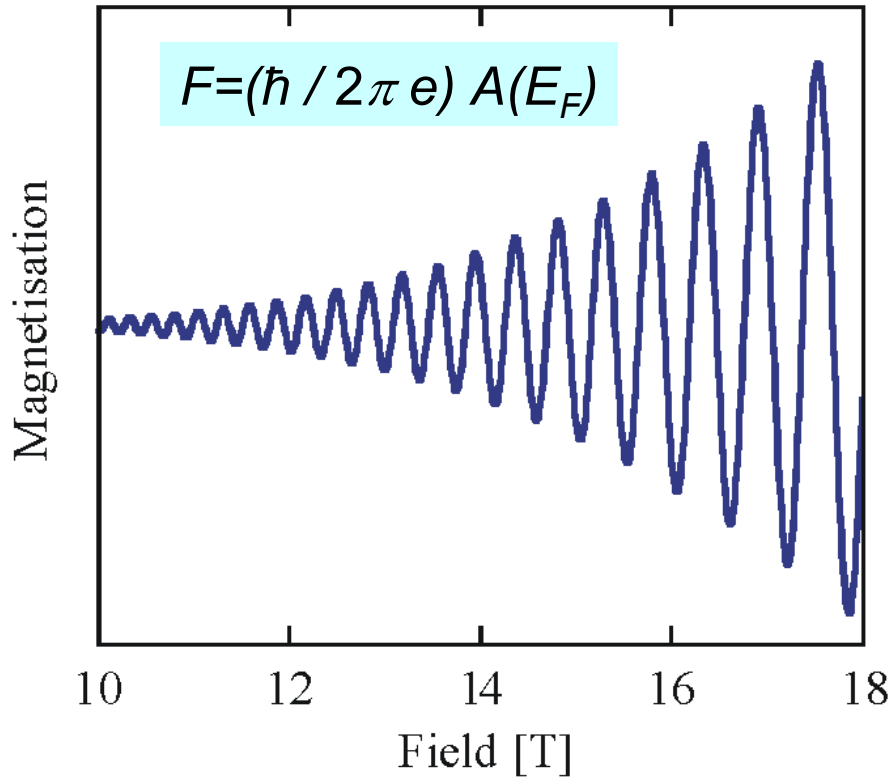


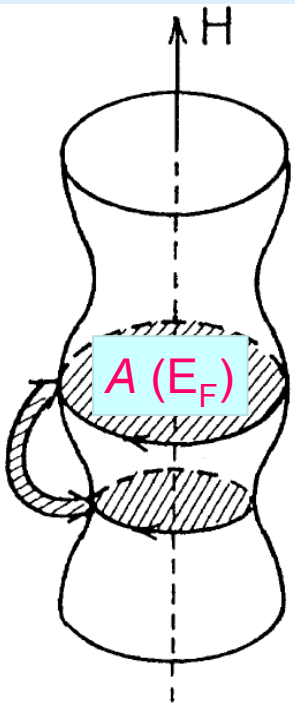
122
$CaFe_2P_2$
***c/a*=2.65**

Quantum oscillations map out the Fermi surface

- oscillations of the density of states in magnetic field;



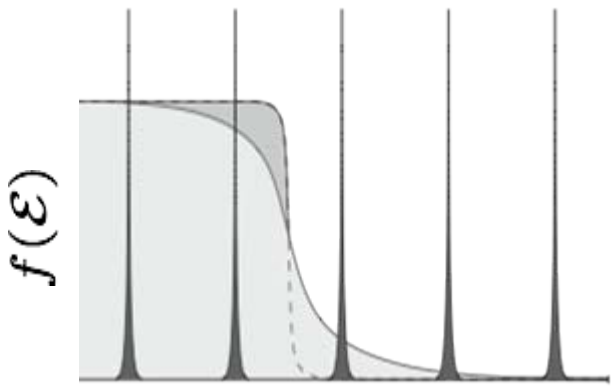




- **'k-space microscopy': 0.1% IBZ; 3D map of the Fermi surface;**
- **bulk probe; no sensitive to surface effects like ARPES;**

Shoenberg, *Magnetic oscillations in metals*, (1984)

Lifshitz-Kosevich formalism



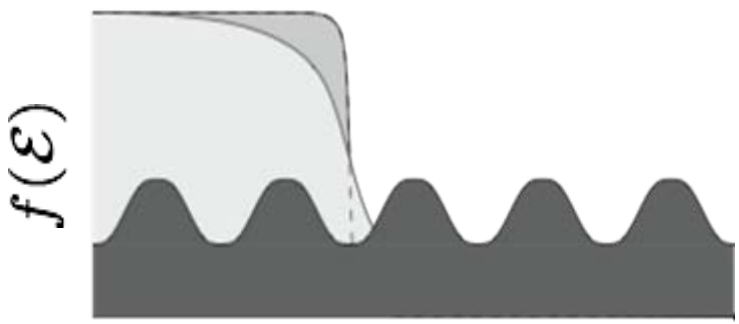
$$M_{\rm osc} \propto R_T\, R_D\, R_s\, R_{sc} \sin\left(\frac{2\pi F}{B} + \gamma\right)$$

Temperature - low temperatures

$$R_T = \frac{2\pi^2 p k_B T m^* / e\hbar B}{\sinh\left(2\pi^2 p k_B T m^* / e\hbar B\right)}$$

Finite scattering time – clean samples

$$R_D = e^{-2\pi^2 p k_B T_D m^* / e\hbar B}$$



Superconducting state –random vortex lattice

$$R_{SC} = \exp\left[-\pi^{\frac{3}{2}} \left(\frac{\Delta_E(B)}{\hbar\omega_c}\right)^2 \left(\frac{B}{F}\right)^{\frac{1}{2}}\right]$$

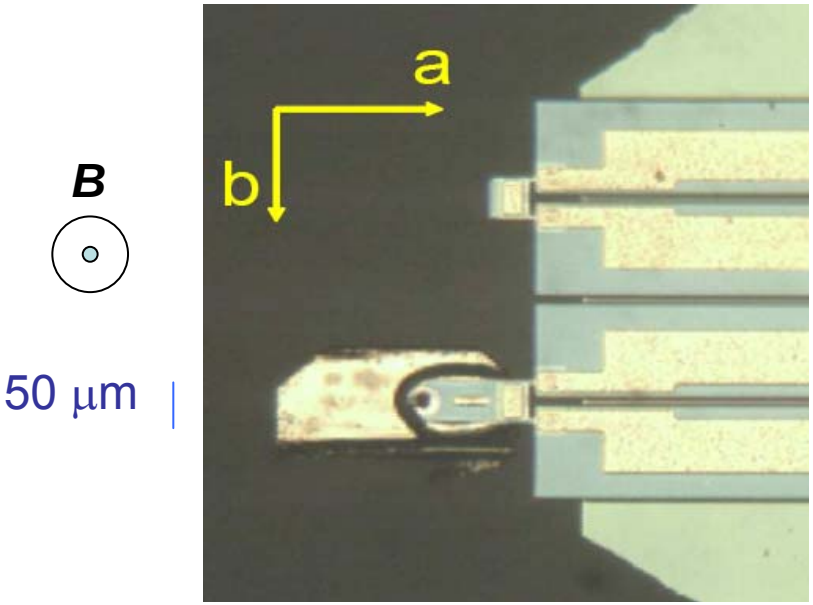
• extracted parameters: quasiparticle effective mass ***m**** **(band renormalization near the Fermi energy),** scattering rates ~ $T_D = \hbar / (2pk_B t)$, spin-splitting factor g^*

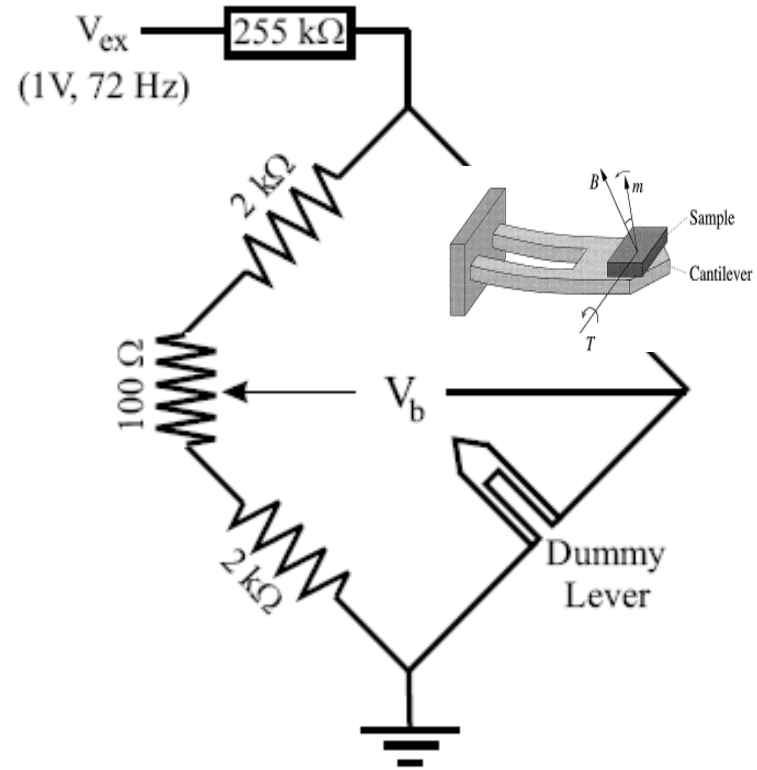
$$m^*/m_b = (1+\lambda_{\text{el-ph}})(1+\lambda_{\text{el-el}}) \sim 1+\lambda_{\text{el-ph}} + \lambda_{\text{el-el}}$$

$$\frac{\Gamma m_b}{m_b} = \frac{1 + F_1^s/3}{1 + F_0^a}$$

Shoenberg, *Magnetic oscillations in metals*, (1984)

Torque measurements with AFM cantilevers

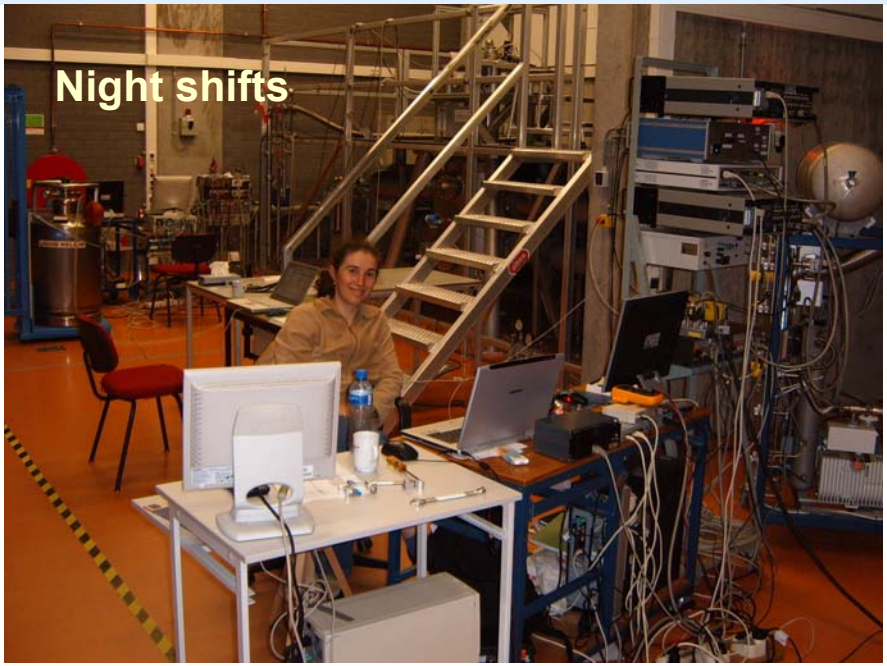




$$\tau = \mathbf{m} \times \mathbf{B}, \quad \tau = mB\sin(\theta)$$

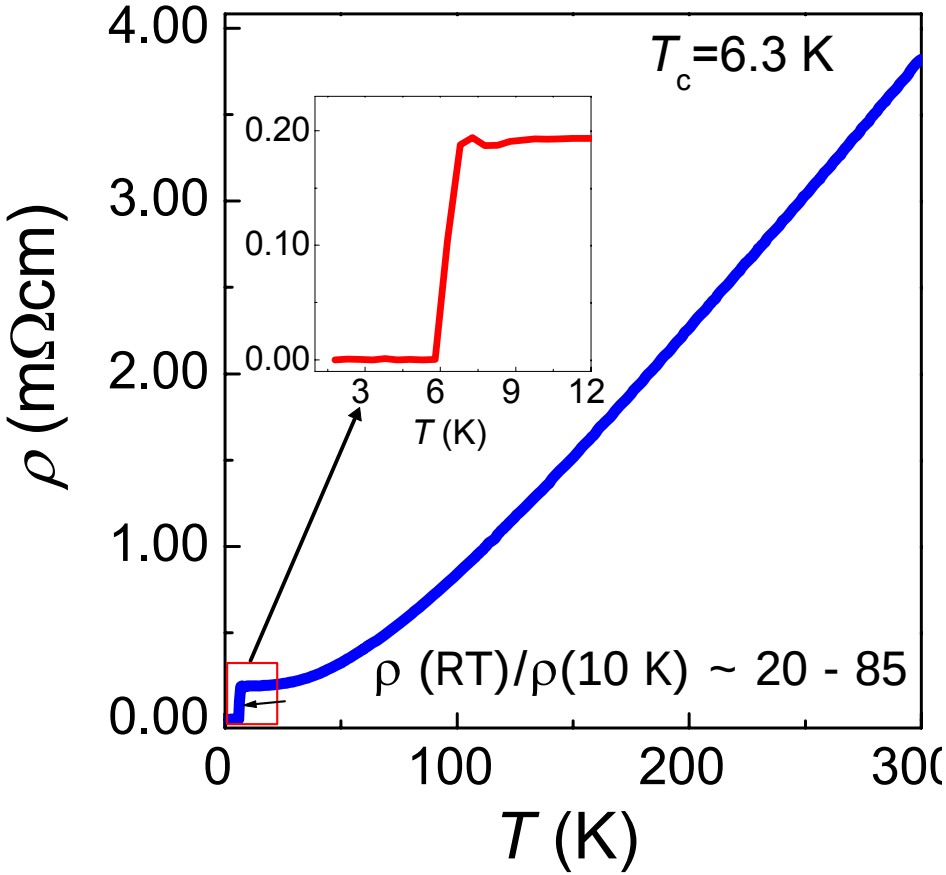
The resistance of the active piezocantilevers (SEIKO) is measured with respect to that of the dummy using a conventional *ac* Wheatstone bridge circuit.

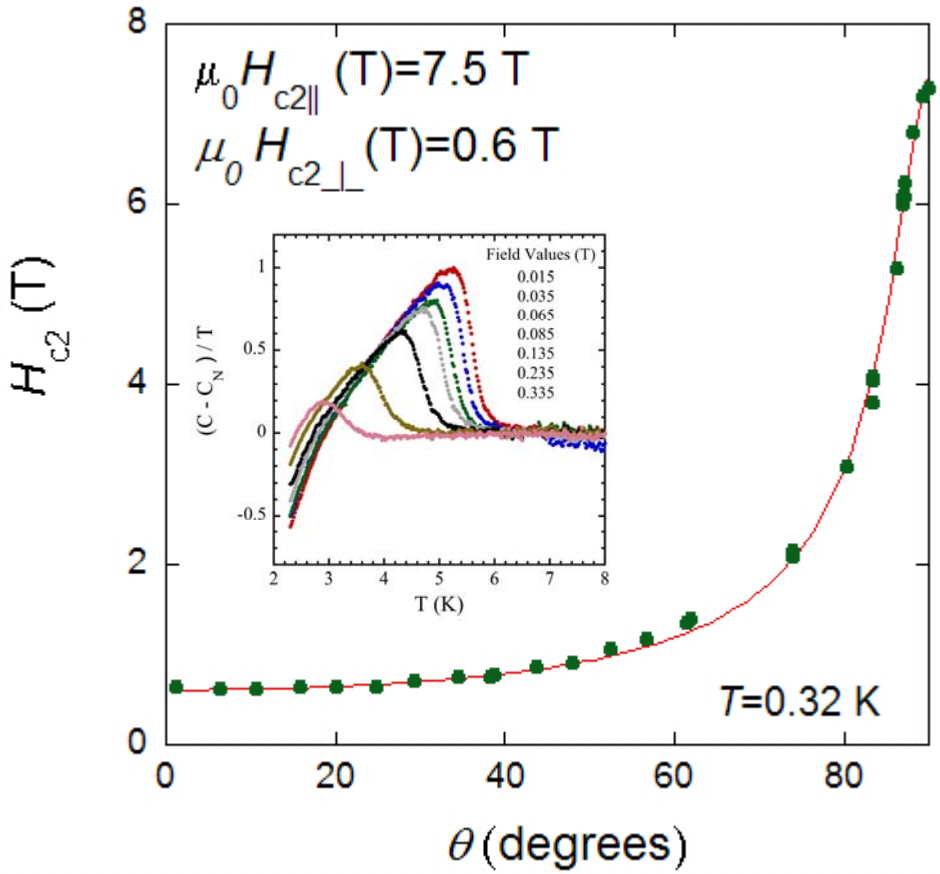
High magnetic field and low temperatures



Low temperatures (0.3 K < T < 4 K), **high magnetic fields** (0 < B < 55 T) at NHMFL, Tallahassee, USA, Nijmegen, The Netherlands and Toulouse, France; **rotation in field** ($-90^0 < \theta < 90^0$);

Bulk superconductivity in LaFePO



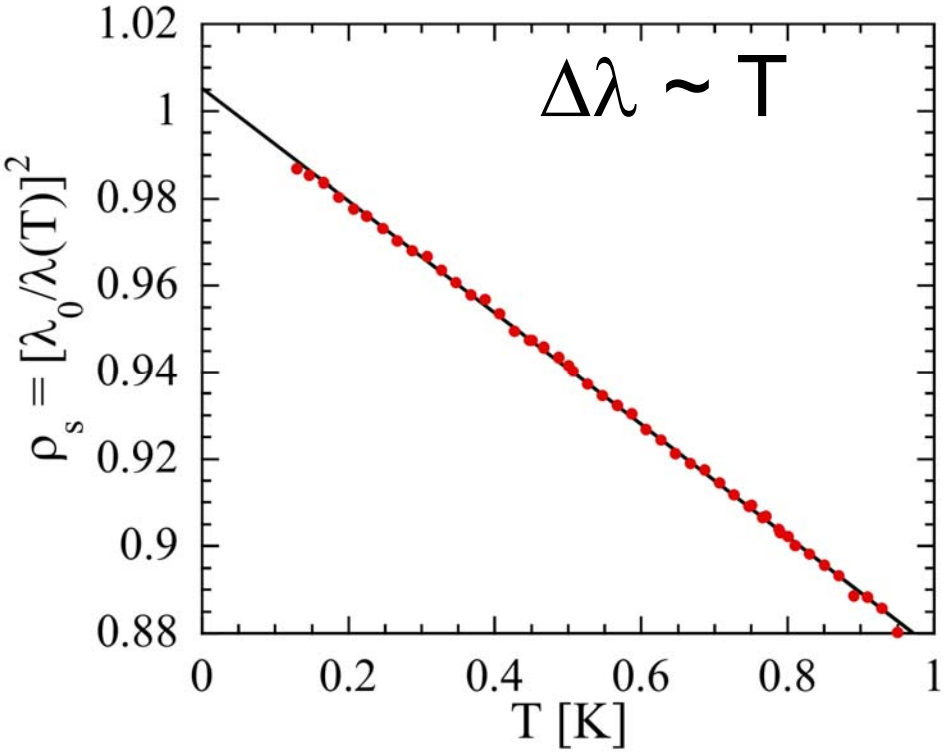


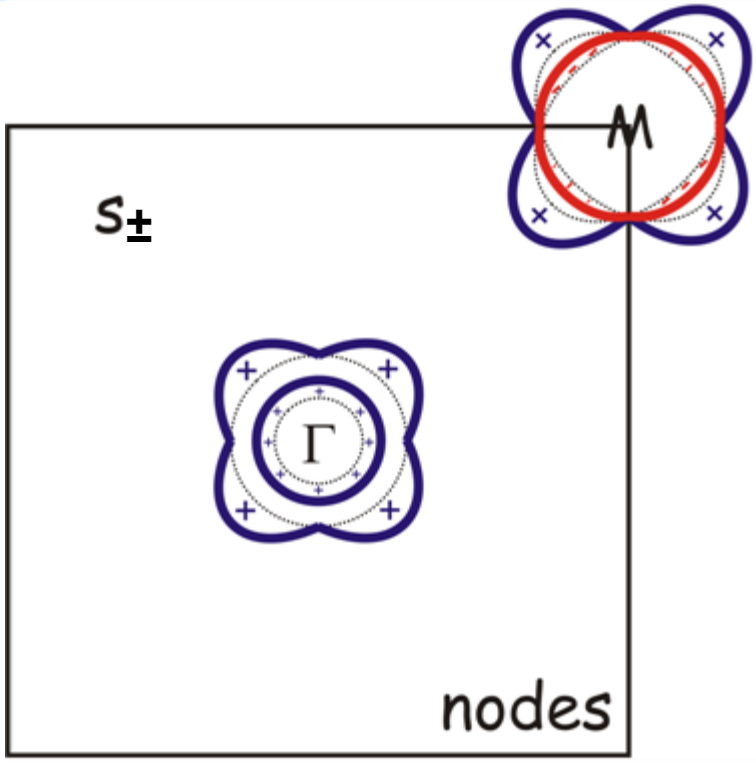
- High residual resistivity ratio: ~ 85; low H_{c2};
- Anomaly in specific heat: bulk superconductor; non-magnetic; 0.07 μ_B/Fe;
- reversible signal - weak pinning; **anisotropy ~10 ;**

J. Analytis, *et. al.,* arXiv:0810.5368 (2008)

C. Andrew, PhD Thesis (2010)

Superconducting order parameter with line nodes in LaFePO



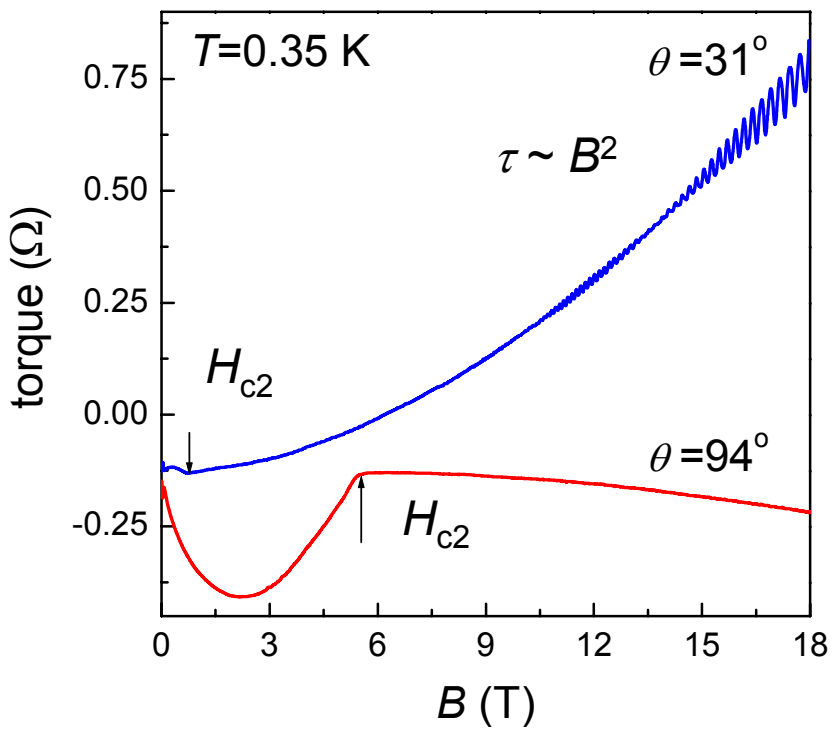


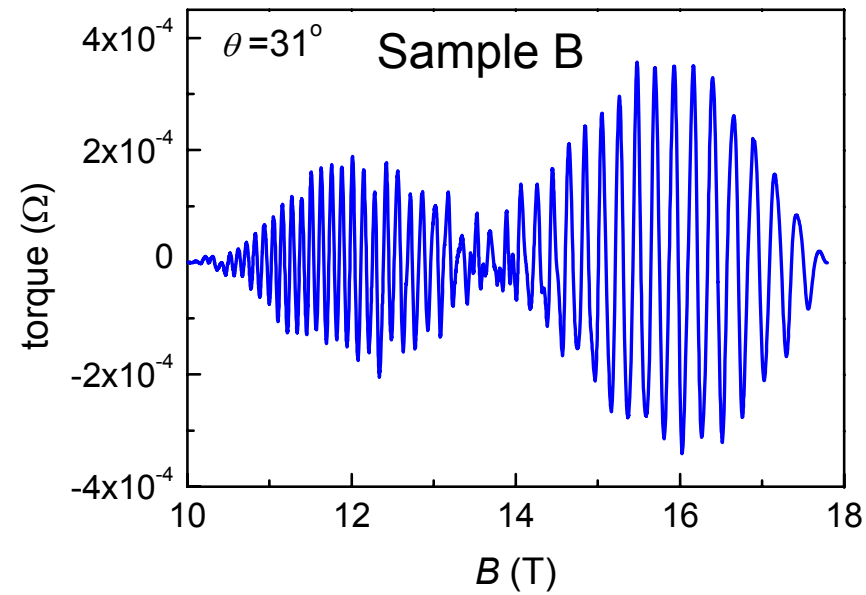
- Clean superconductor: Superfluid density show linear dependence down to 100 mK suggesting the presence of **nodes** in the symmetry of the superconducting gap;

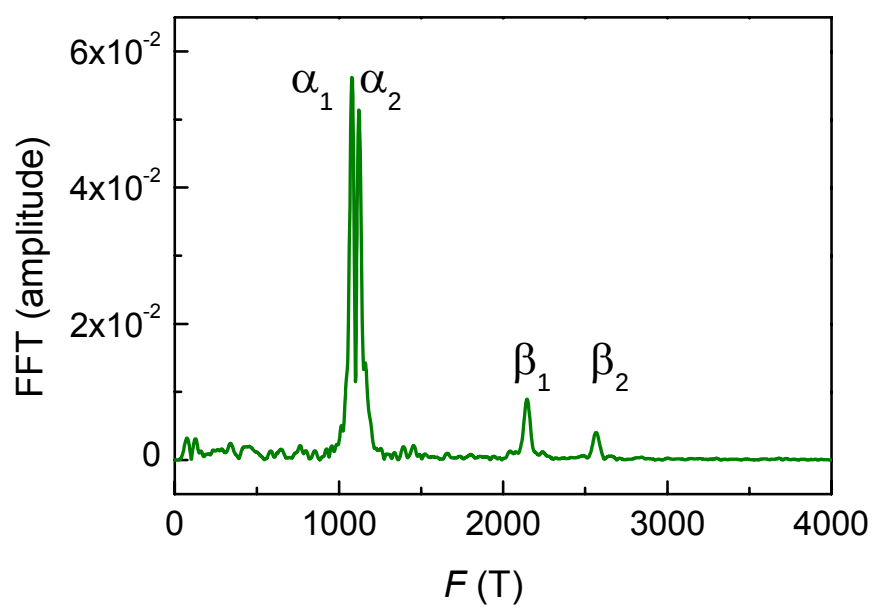
J. Fletcher, *et. al.,* PRL **102**, 147001 (2009)

New J. Phys. 11, 025016 (2009)

de Haas-van Alphen effect in LaFePO



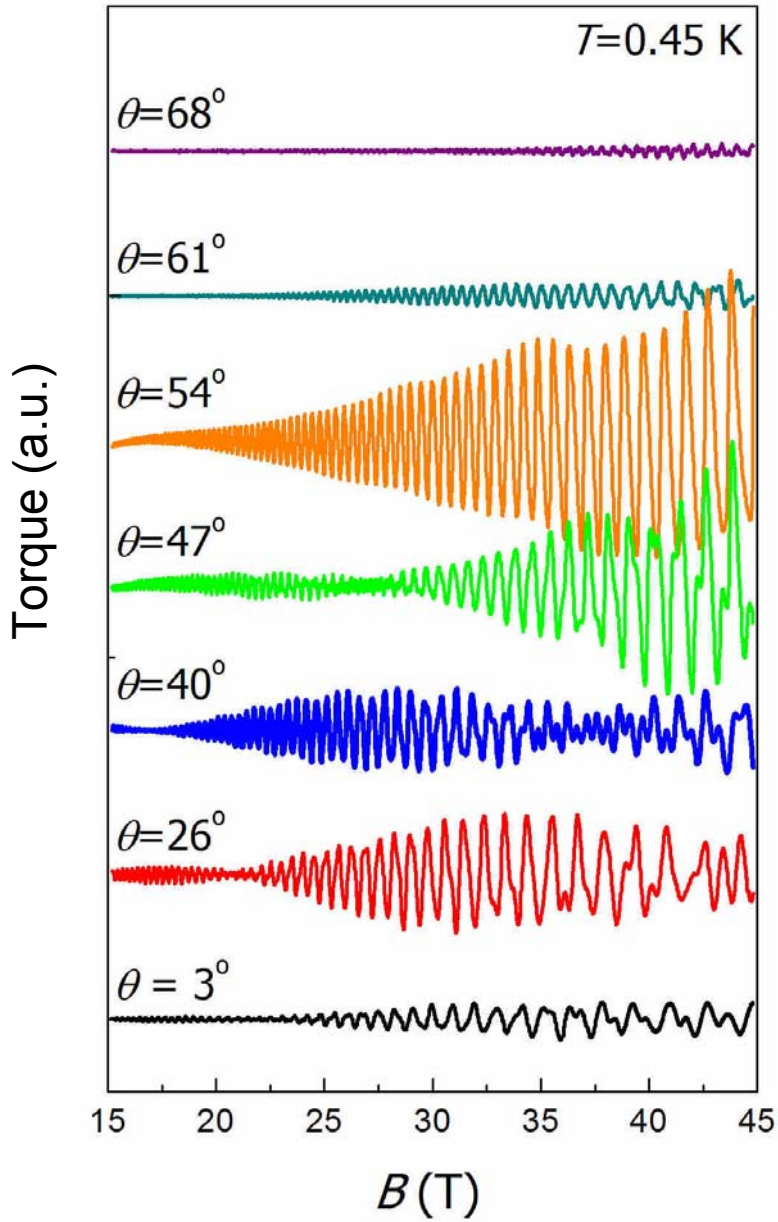


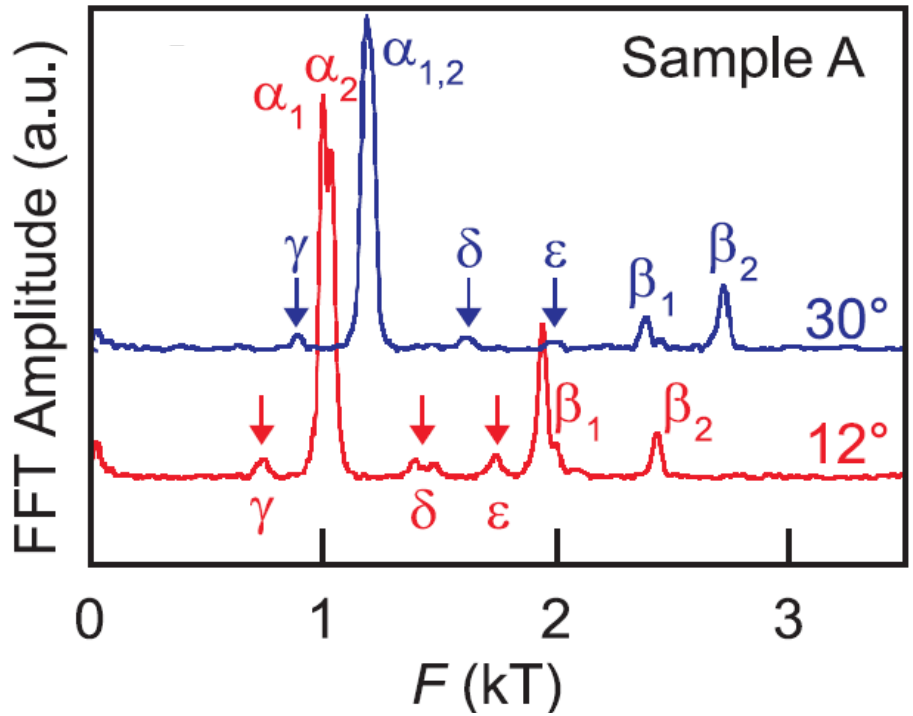


- **high *B***: normal state; oscillations periodic in inverse field, de Haas-van Alphen effect.
- $\tau \sim B^2$ –characteristic to a paramagnet;
- a simple corrugation of the Fermi cylinder leads to a **beat pattern** in the magnetization.

A.I. Coldea *et al.*, PRL, 101,216402 (2008)

de Haas-van Alphen effect in LaFePO



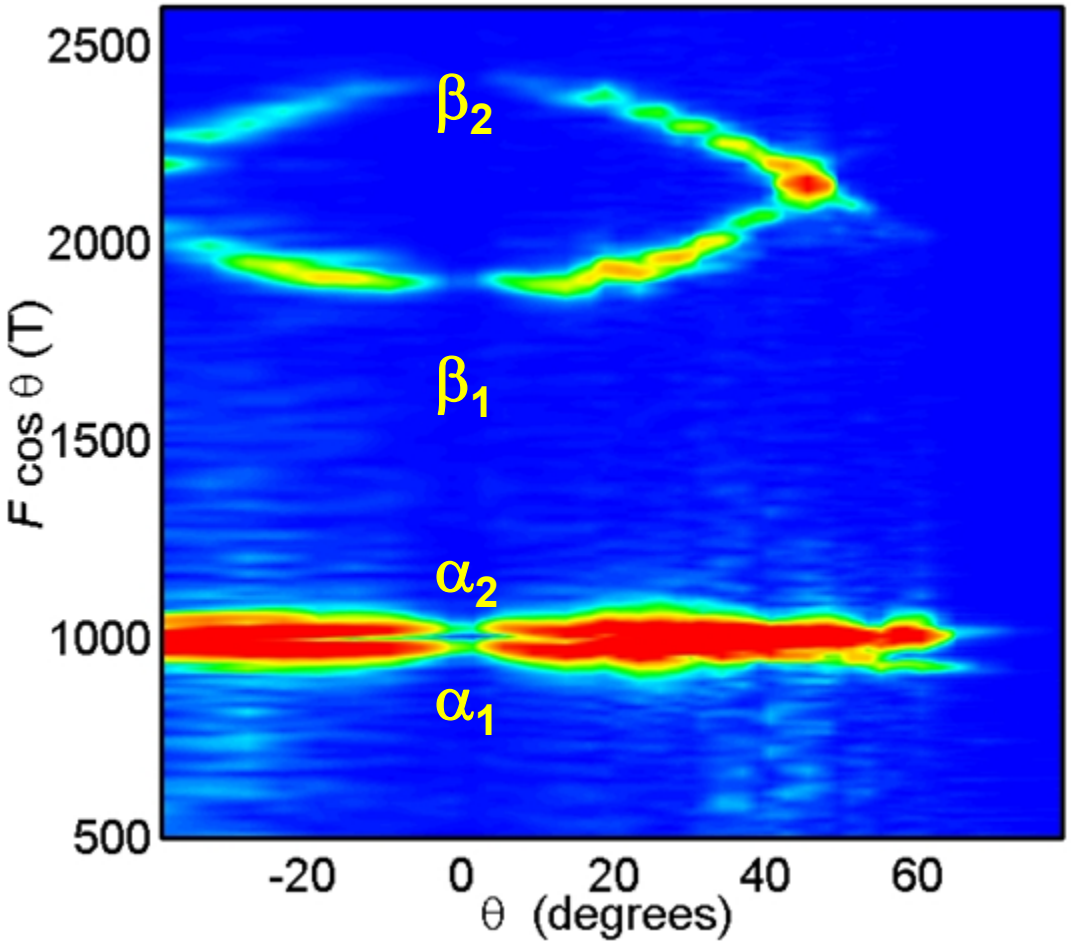


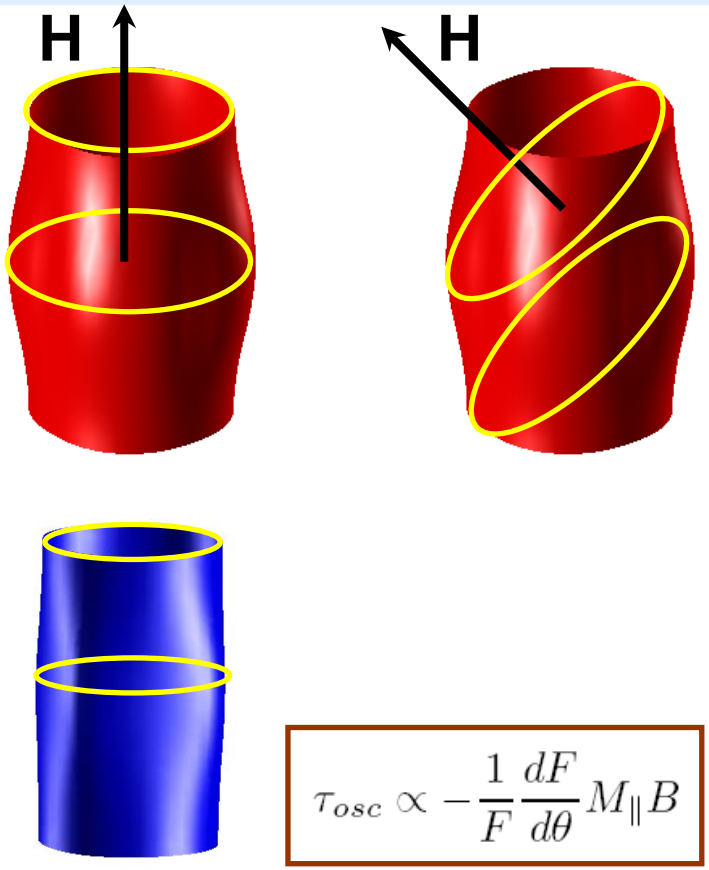
$F=(\hbar / 2\pi e)\, A(E_F)$

Different frequencies correspond to extremal areas of the Fermi surface perpendicular to the applied magnetic field for a particular orientation;

A.I. Coldea *et al.*, PRL, 101,216402 (2008)

Fermi surface warping and Yamaji angle





$$\tau_{osc} \propto -\frac{1}{F}\frac{dF}{d\theta} M_{\parallel} B$$

$F(\theta)=F(0)/\cos\theta$
Quasi-two dimensional cylinder;

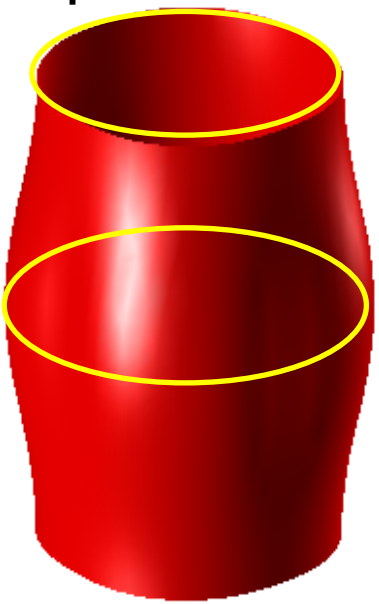
$\Delta F_{\alpha}/F_{\alpha} \sim 4\%$;
$\Delta F_{\beta}/F_{\beta} \sim 23\ \%$;

At Yamaji angles all Fermi surface cross sections have equal areas; their magnetization contributions interfere constructively=peak effect.

K. Yamaji, J. Phys. Soc. Jpn. **58**, 1520 (1989)

Significant c-axis warping: of the Fermi surface
3D Fermi surfaces in 1111 compounds

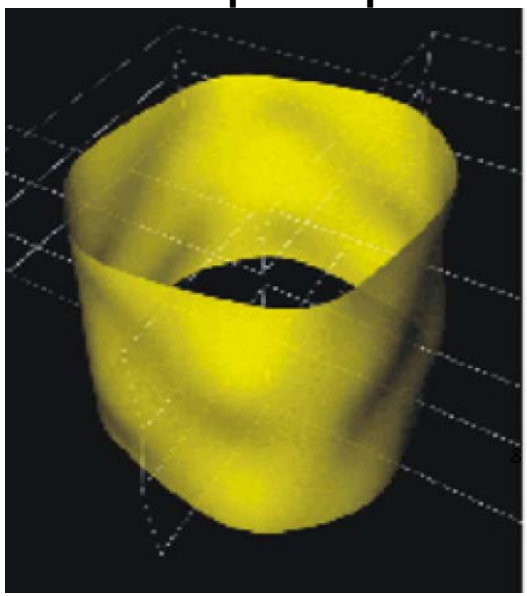
pnictides



LaFePO

$\Delta F_\alpha/F_\alpha \sim 4\%$;
$\Delta F_\beta/F_\beta \sim 23\ \%$;
$\rho_c/\rho_{ab} \sim 10$

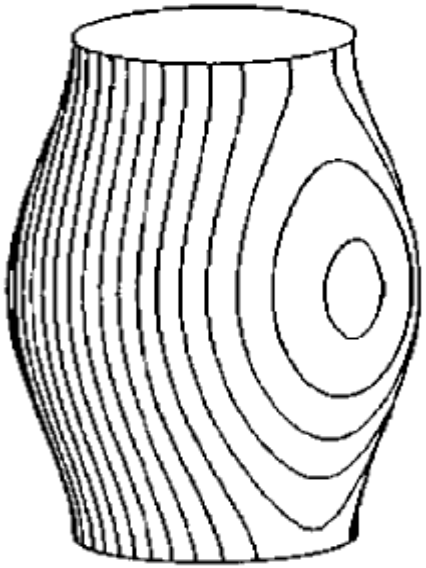
overdoped cuprates



$Tl_2Ba_2CuO_{6+\delta}$

$\Delta F/F < 1\%$;
$\rho_c/\rho_{ab} \sim 10^3$

organics



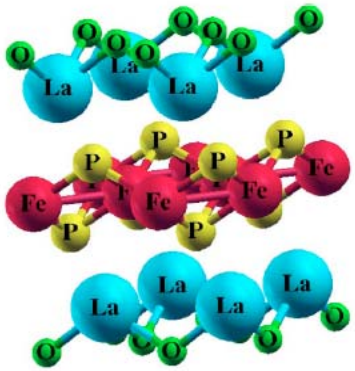
β-(BEDT-TTF)$_2$IBr$_2$

$\Delta F/F < 1.3\%$;
$\rho_c/\rho_{ab} \sim 10^4$

$$\frac{2t_\perp}{\epsilon_F} = \frac{\Delta F}{2F}$$

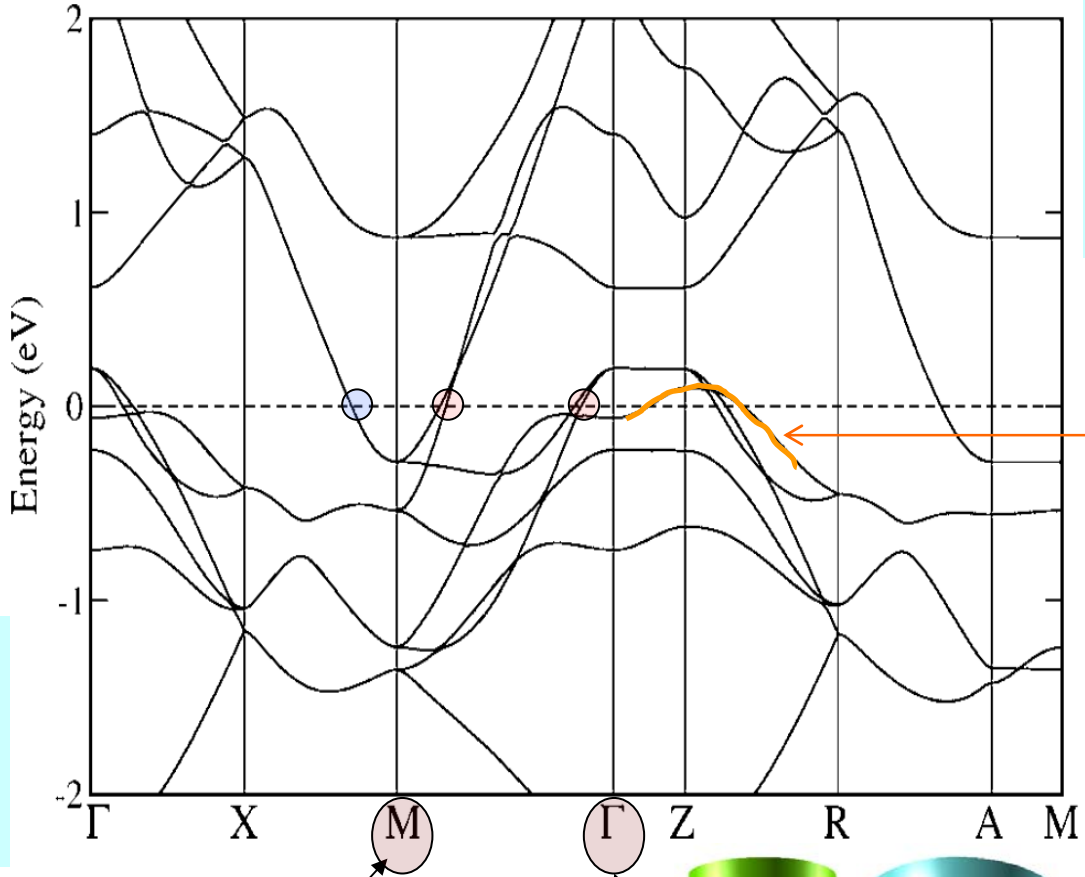
N. Hussey *et al., Nature* **425,** 814 (2003); M. Kartsovnik et al., Chem. Rev., **104**, 5737 (2004)

Band structure of LaFePO: spaghetti



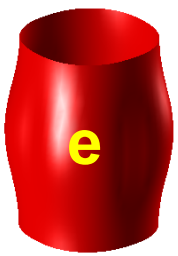
Conduction FeP layer

Electron pockets centred at **M** point: *d*xz, *d*yz



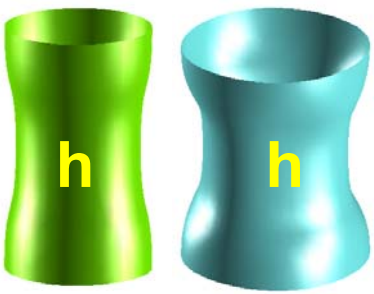
3D d_{z^2} hole pocket at Z most susceptible to P position and doping;

band 1



band 4

band 5

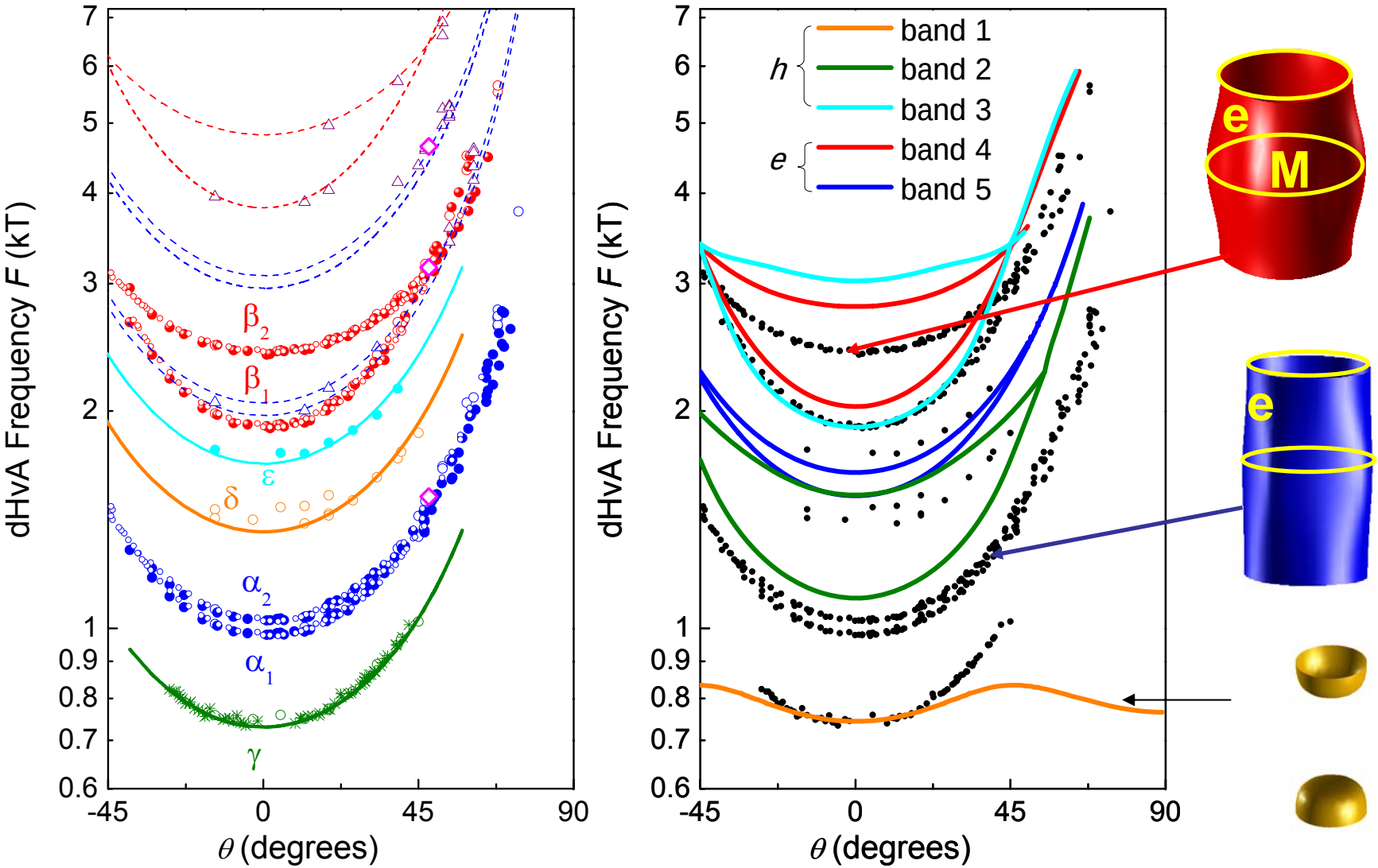


Hole pockets centred at Γ point:dxz,dyz

bands 2 and 3

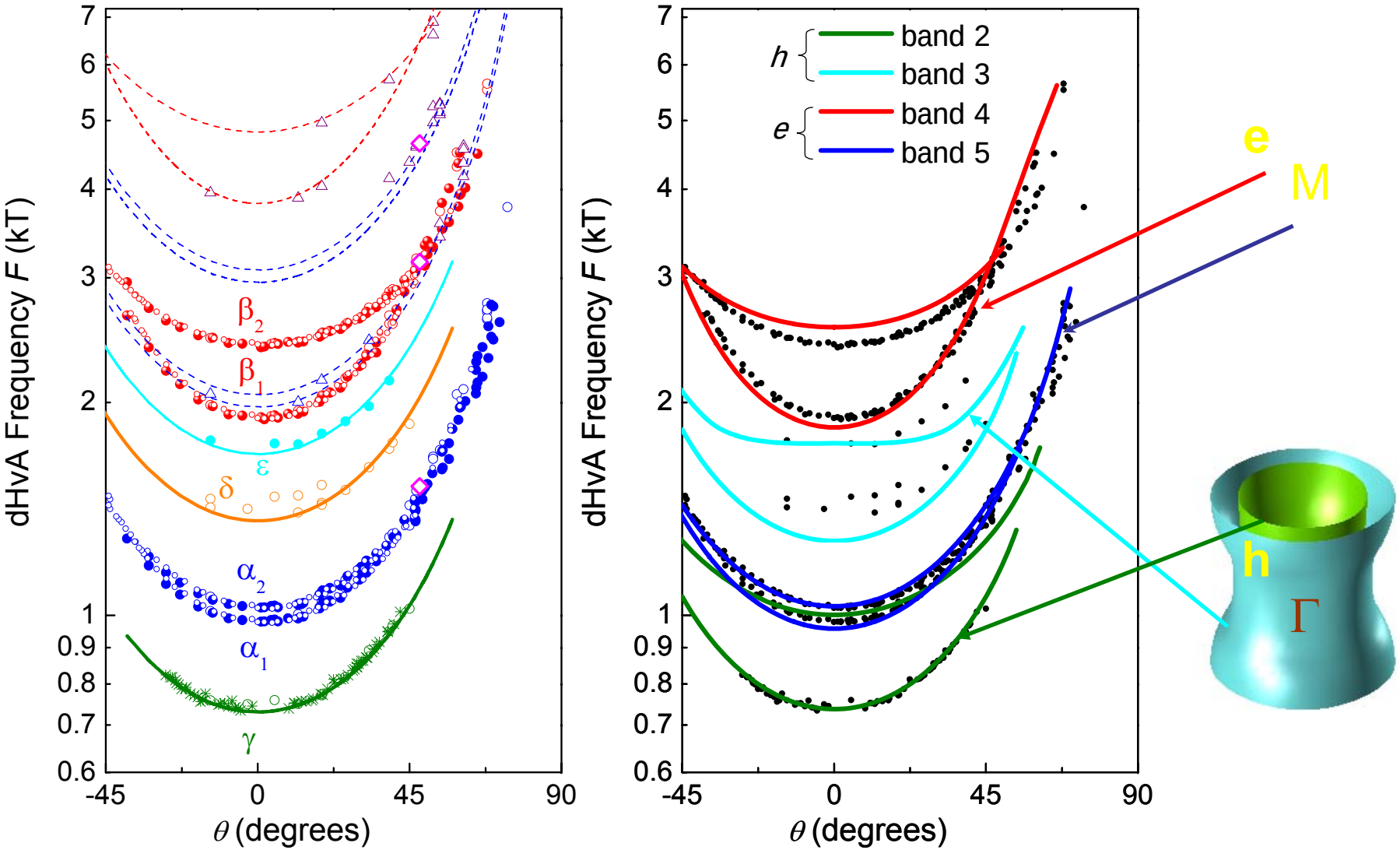
S. Lebègue, Phys. Rev. B 75, 035110 (2007)

dHvA data versus band structure calculations



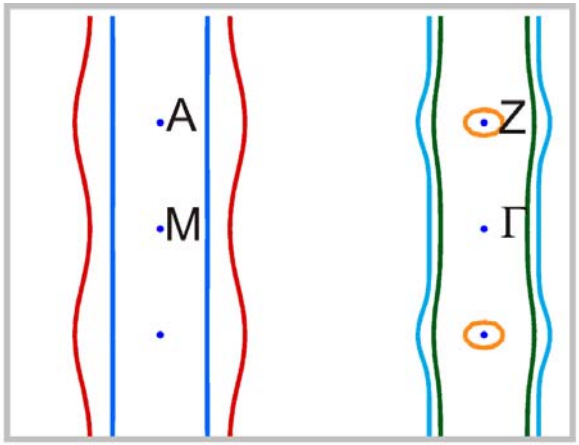
- electronic branches show similar dispersion to the experimental α and β pockets;
- no experimental branch matches the weak dispersion due to the 3D hole pocket;

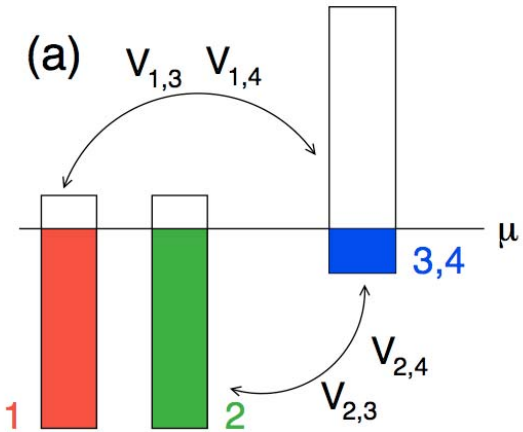
Band shifting and charge balance

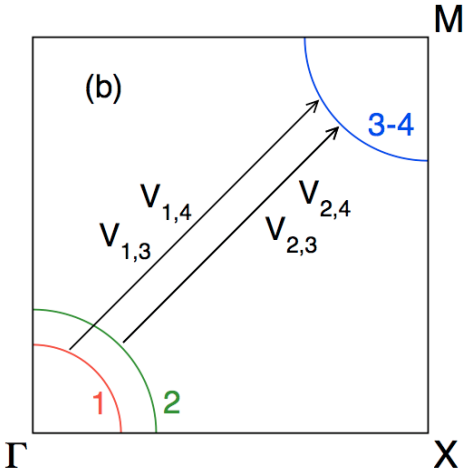


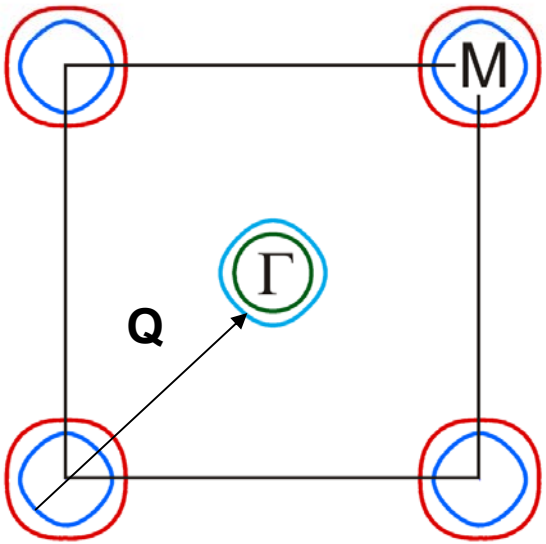
Electron bands shifted by ΔE=+85 meV (band 5), +30 meV (band 4); hole bands all shifted by ΔE=-53 meV; Charge imbalance ~0.034 el/fu; ~1.7% oxygen deficiency in LaFePO.

Shrinking of the Fermi surface in LaFePO





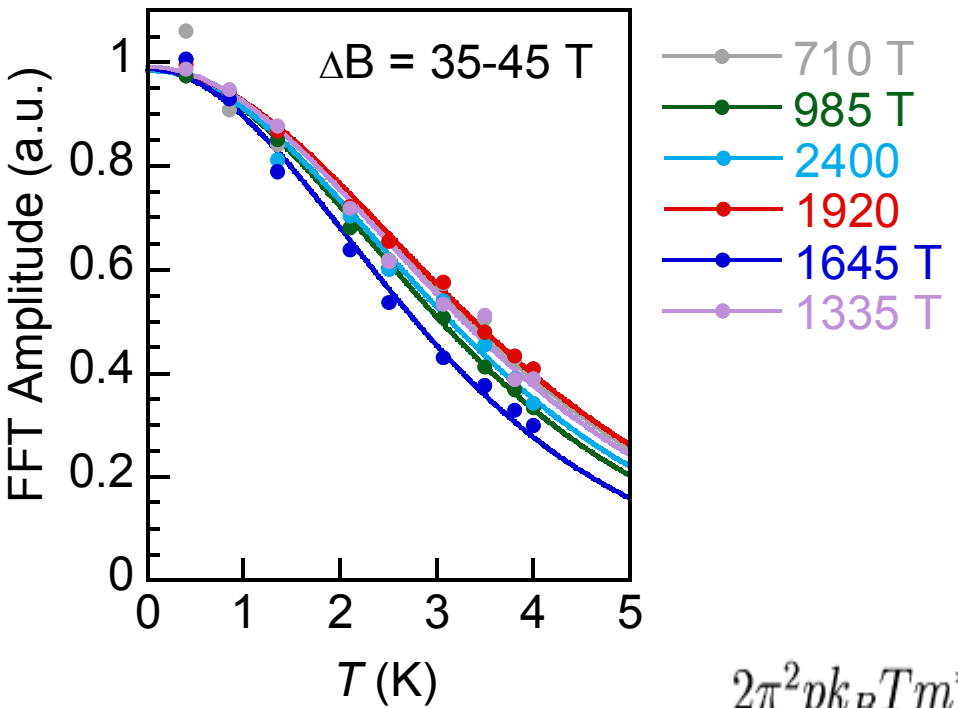


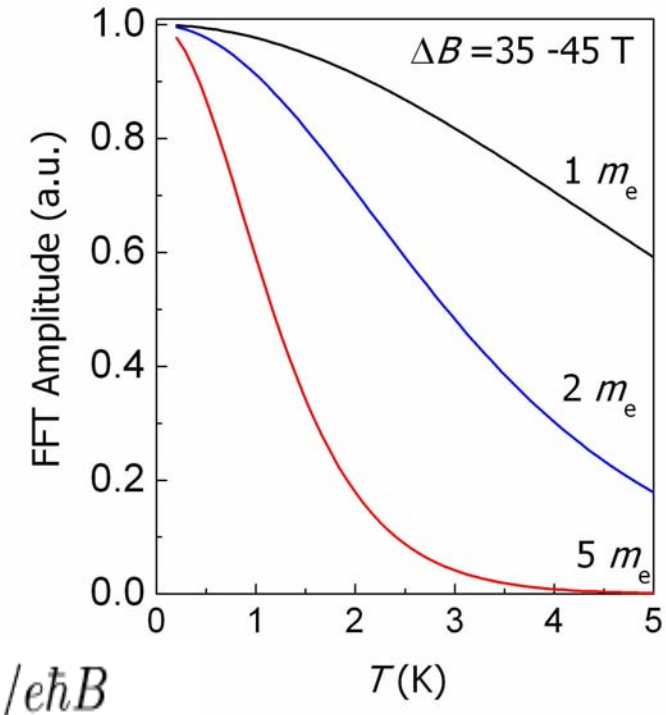


experimental observation of upward shift of the electron bands and of a downward shift of the hole band may be evidence of dominance of interband scattering (nesting);

L. Ortenzi *et al.*, PRL 103, 046404 (2009).

Moderate mass enhancement in LaFePO





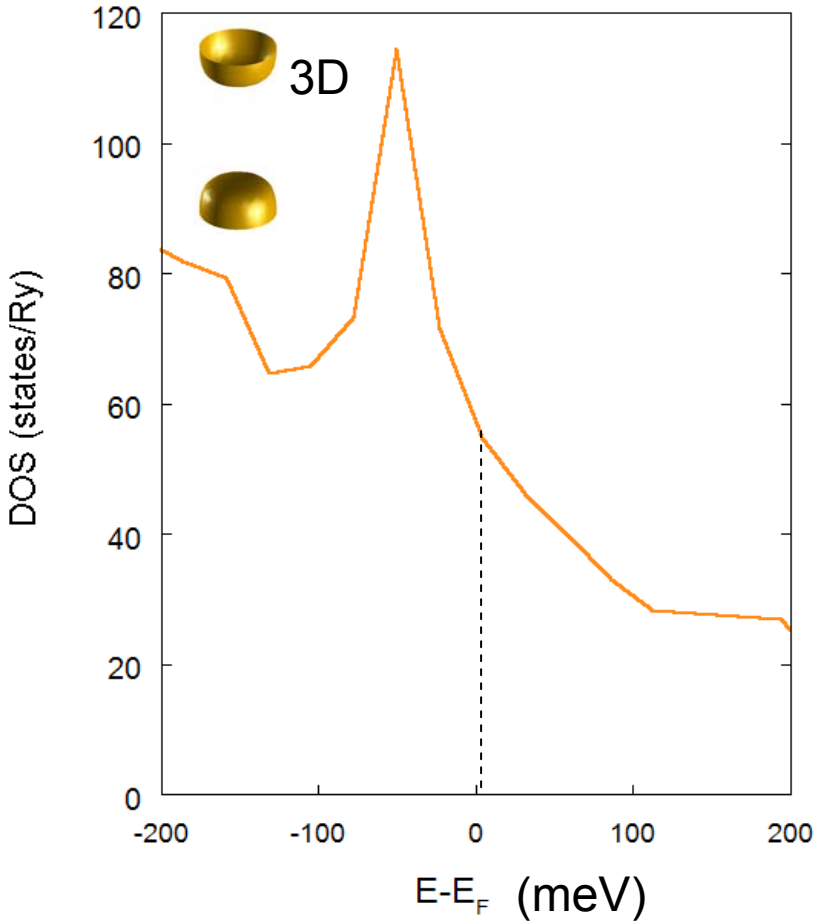
$$R_T = \frac{2\pi^2 p k_B T m^* / e\hbar B}{\sinh\left(2\pi^2 p k_B T m^* / e\hbar B\right)}$$

$$m^*/m_b = (1 + \lambda) \approx 2.$$

(el-el + el-ph)

- the effective masses between 1.7-2.1 m_e for both electrons and holes;
- moderate mass enhancement for the electronic bands;

Electronic contribution to the specific heat



E_F lies just above a peak in the DOS, which leads to a rapidly decreasing DOS with energy.

$$\frac{C}{T} = \frac{\pi k_B^2 N_A a^2}{3\hbar^2} \times \sum m_i^*$$

γ_{exp_powder} ~7 -12 mJ/mol K^2;

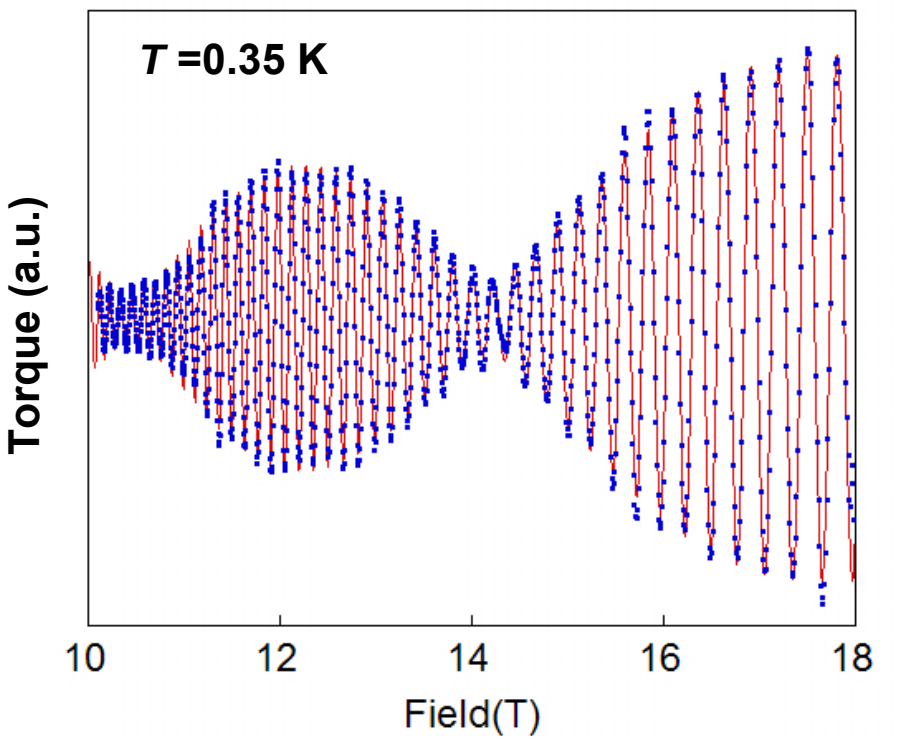
γ_{dHvA} = 6 mJ/mol K^2 ;

Assuming 4 quasi-two dimensional cylinders with m^*~2 m_e;

3D pocket absent?

Advances in Physics, 2003, Vol. 52, No. 7, 639–725

Quasiparticle scattering rates in LaFePO



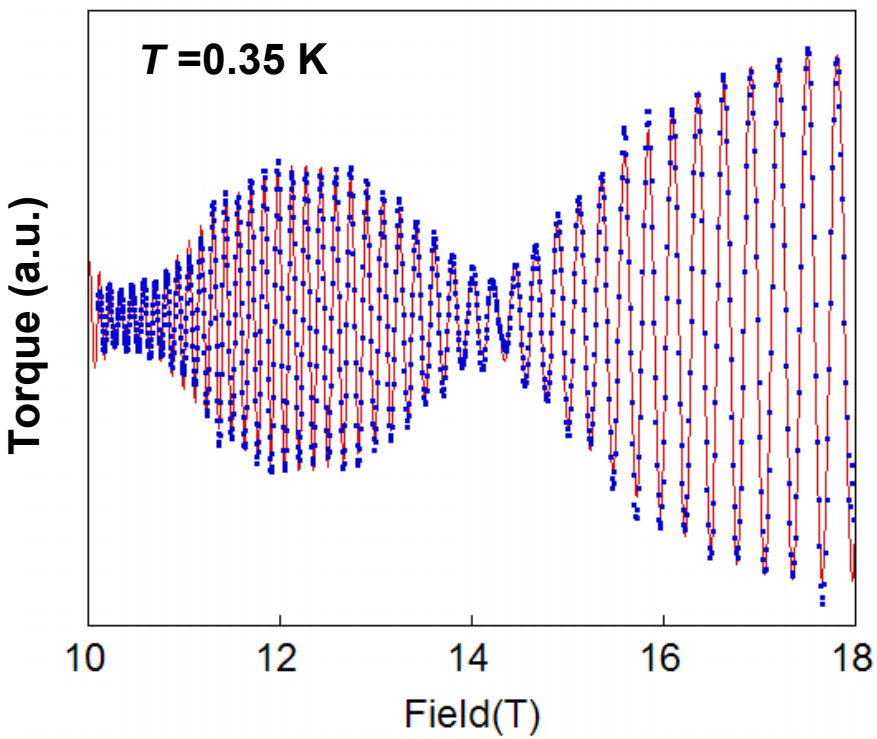
$$R_D = \exp(-\pi k_F / eB\ell)$$

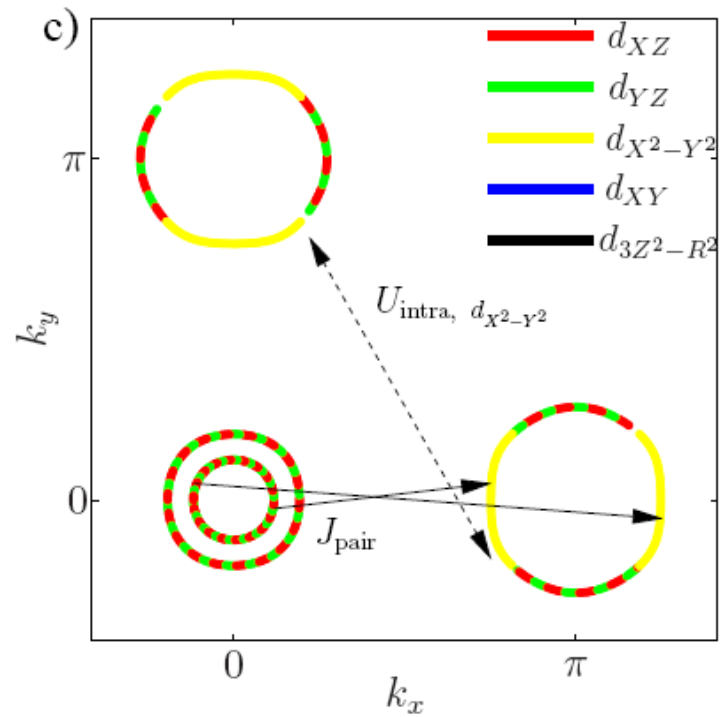
k_F is the orbitally averaged Fermi wavevector for the particular Fermi surface orbit;

l_α ~1300 Å
inelastic quasiparticle mean free-path (small and large angle scattering from impurities)

- mean free path: electrons l_α ~1300 Å and l_β~ 800 Å; scattering for **hole ~ factor 2 larger**;

Relevance of the orbital character of bands





$$R_D = \exp(-\pi k_F / eB\ell)$$

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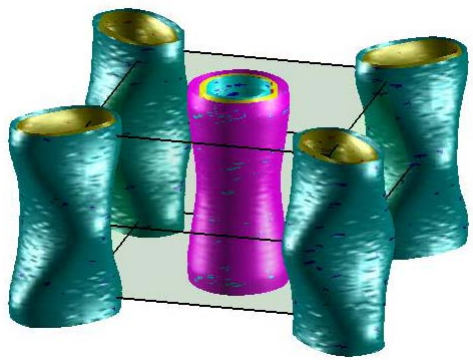
(small and large angle scattering from impurities)

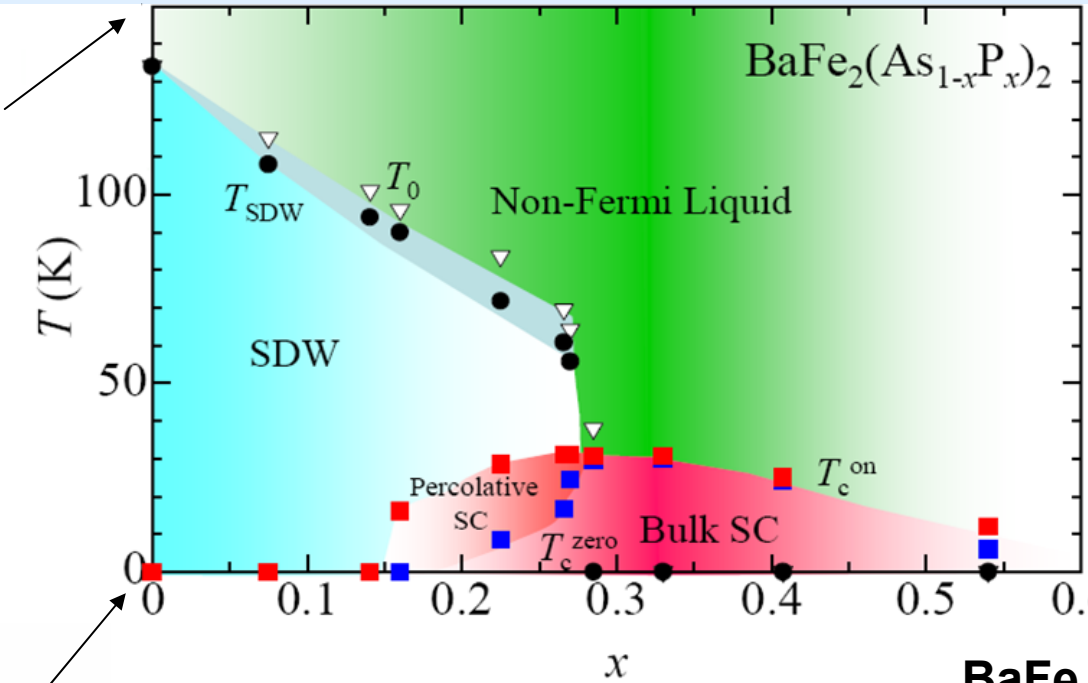
- mean free path: electrons l_α ~1300 Å and l_β~ 800 Å; scattering for **hole ~ factor 2 larger**;

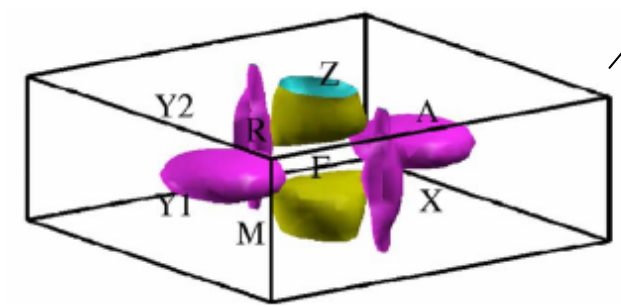
K. Kuroki *et al*. Phys. Rev. B 79, 224511 (2009)
S. Gaser et al., arxiv.1003.0133 (2010)

Effect of chemical pressure: P substitution



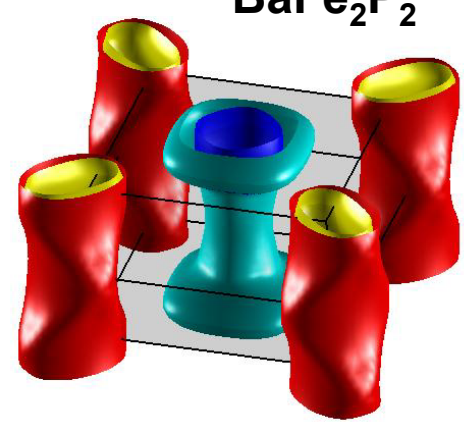
$BaFe_2As_2$





Low temperature Fermi surface of $BaFe_2As_2$

$BaFe_2P_2$

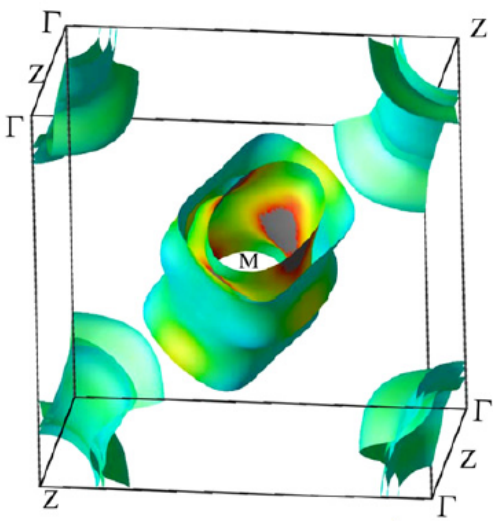


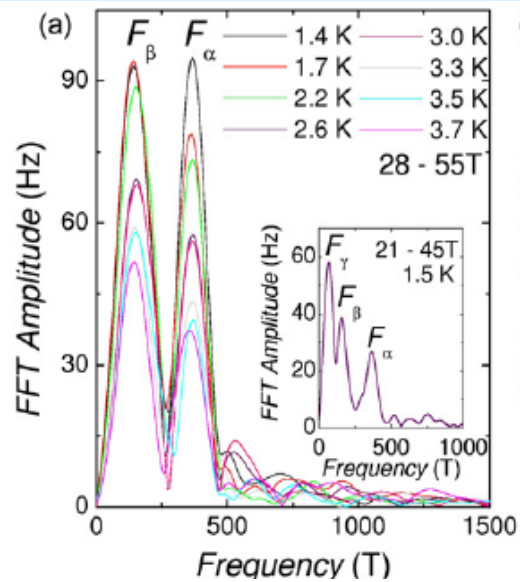
W. Xie, PRB **79**, 115128 (2009)

S. Kasahara et al. , PRB **81**, 134422 2010

Reconstructed Fermi surface in the AFM phase

PM

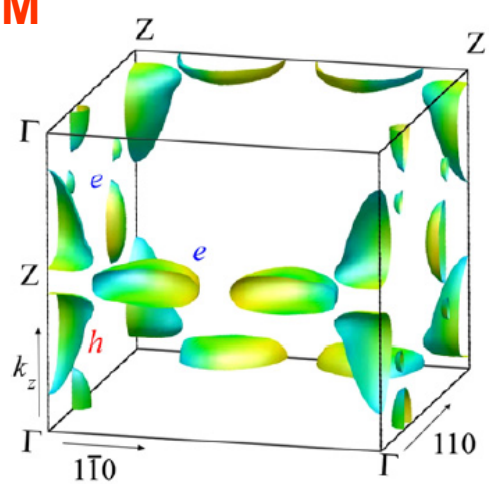


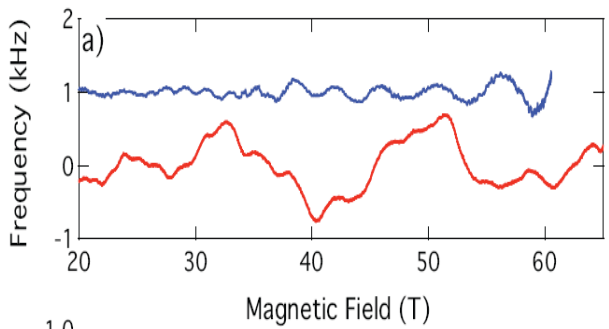


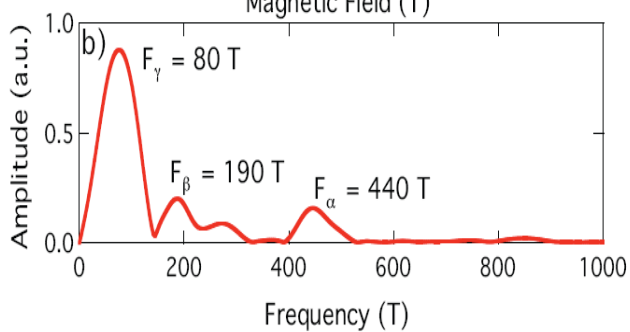
$SrFe_2As_2$

S. Sebastian *et al.*,
J. Phys.: Cond. Mat. 20 (2008) 422203

AFM



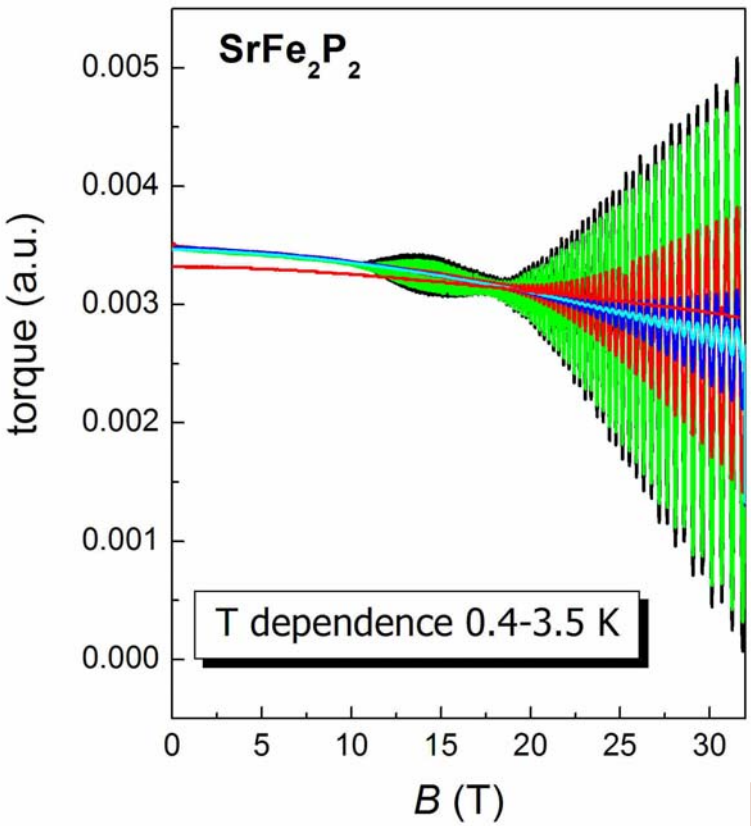


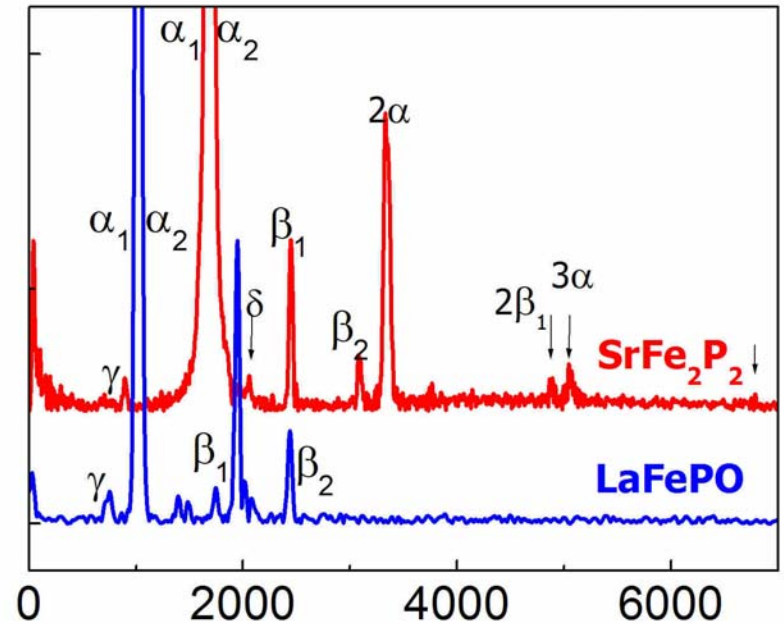


$BaFe_2As_2$

J. Analytis *et al.*,
arXiv: 0902.1172 (2009)

Quantum oscillations in $SrFe_2P_2$



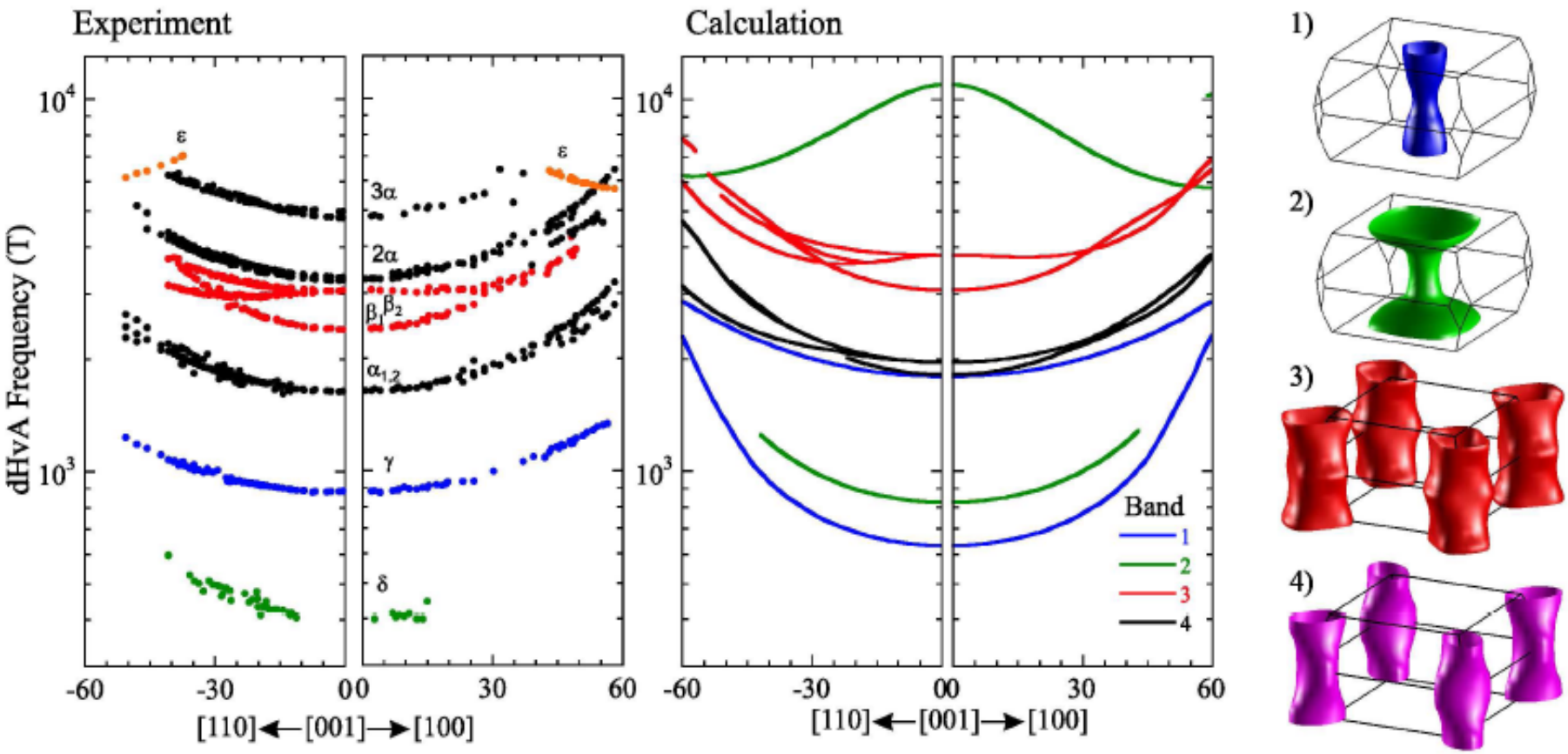


$SrFe_2P_2$ is non-magnetic and non-superconducting with bond angle **116.34°** (away from a perfect tetrahedron with **109.47**)

Electronic bands α and β shows the largest amplitude; the least affected by scattering (if masses the same);

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

Fermi surface of $SrFe_2P_2$

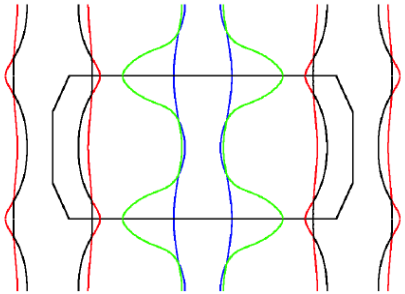


Electronic bands in very good agreement with band structure calculations; band shifts still needed. Nesting?

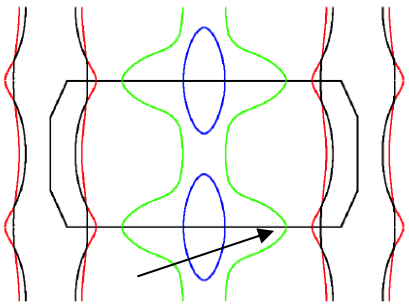
J.G. Analytis *et al.*, PRL **103**, 076401 (2009)

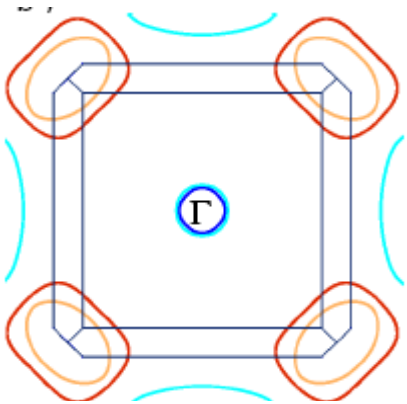
Fermi surface of $SrFe_2P_2$

Not Shifted



Shifted



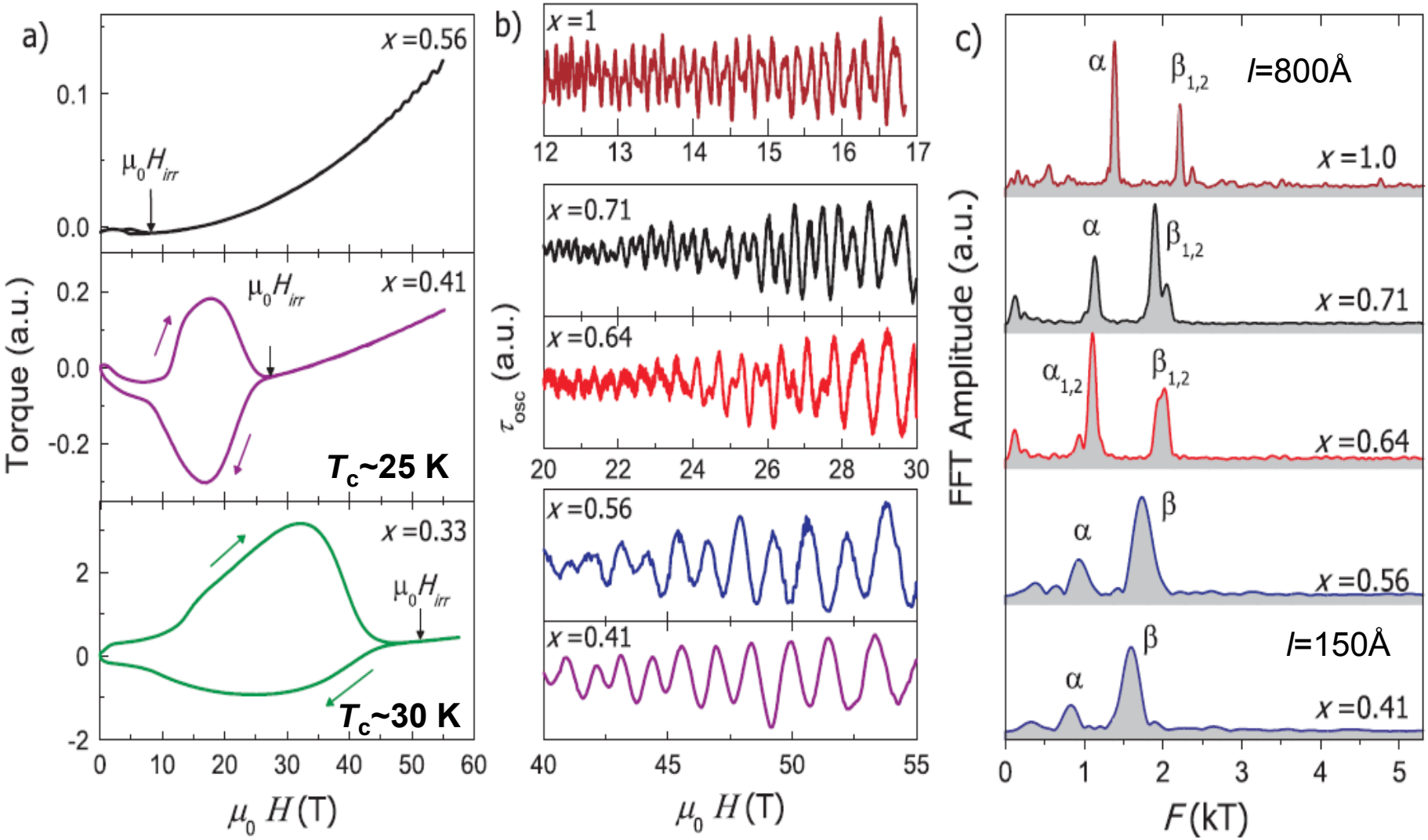


		Experiment			Calculations			
		F(kT)	$\frac{m^*}{m_e}$	ℓ(nm)	Orbit	F(kT)	$\frac{m_b}{m_e}$	$\frac{m^*}{m_b}$
					$1_{\min}$	0.632	0.97	
holes	γ	0.89	1.49(2)	58	$1_{\max}$	1.804	1.07	1.4
holes	δ	0.41	1.6(1)	21	$2_{\min}$	0.828	1.24	1.3
holes	ϵ	6.02^*	$3.41(5)^*$	90	$2_{\max}$	10.95	2.30	1.7
electrons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

- Moderate mass enhancement sheet dependent and anisotropy in scattering;
- Nesting strongly diminished-strongly warped cylinders and a three-dimensional hole pocket; some nesting may be possible along k_z;

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

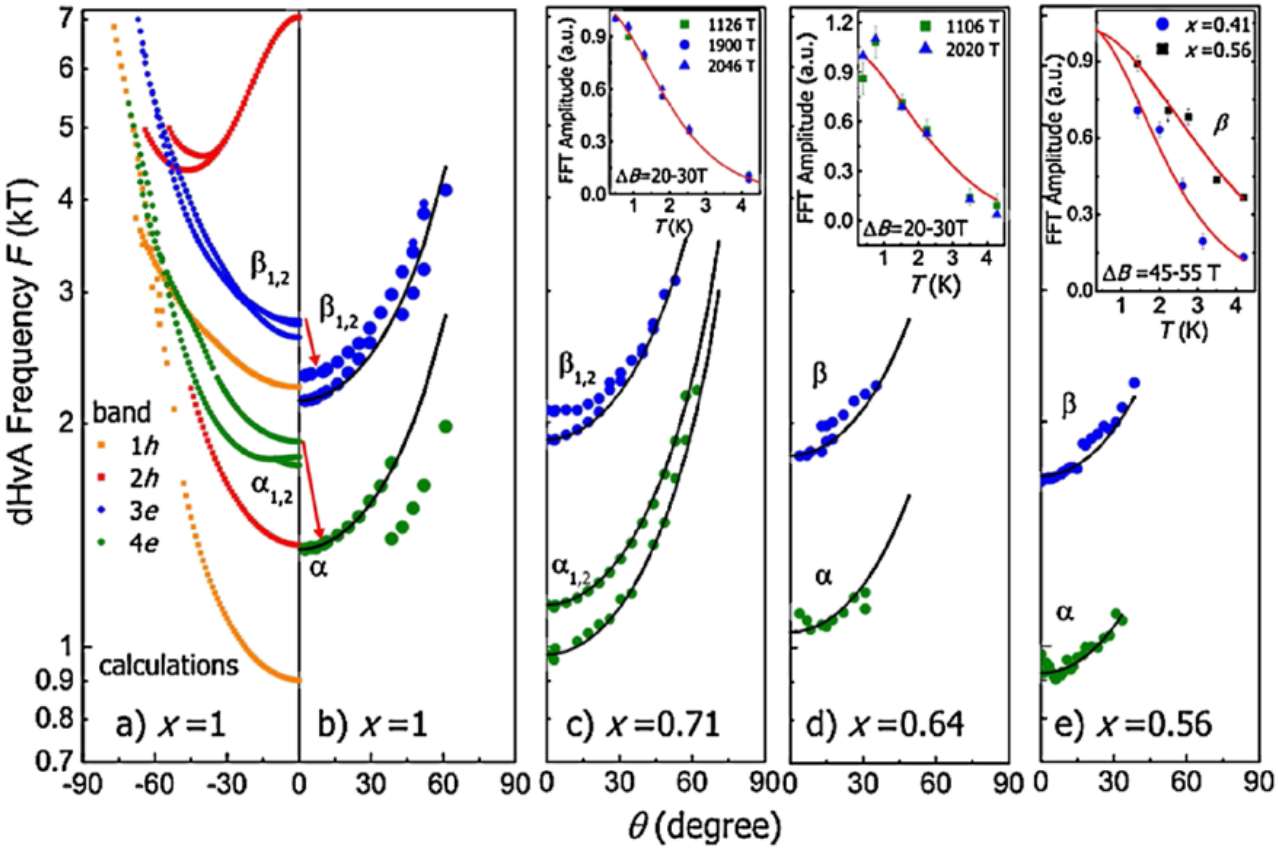
Evolution of Fermi surface in $BaFe_2(As_{1-x}P_x)_2$

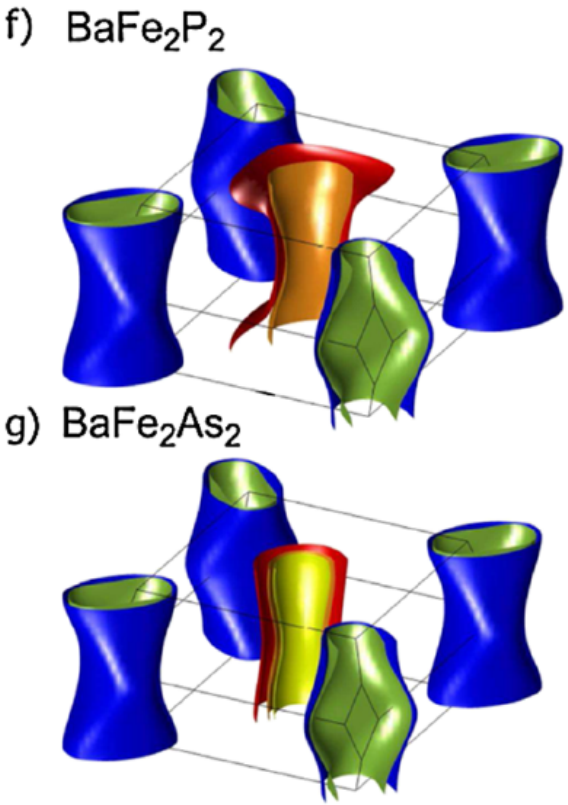


oscillations observed for materials with *Tc* = 0 – 25 K; T_{max}=30 K for *x* = 0.33;

H. Shishido *et al.*, PRL 104, 057008 (2010)

Evolution of electronic pockets in $BaFe_2(As_{1-x}P_x)_2$

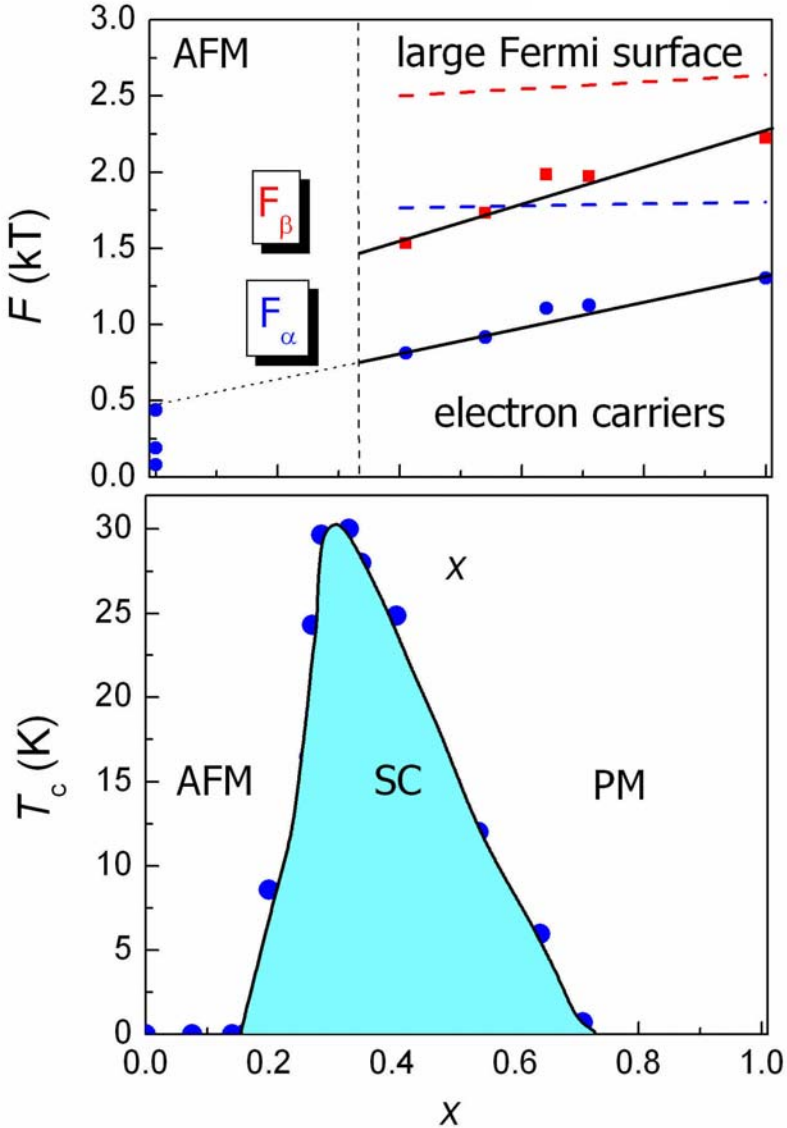


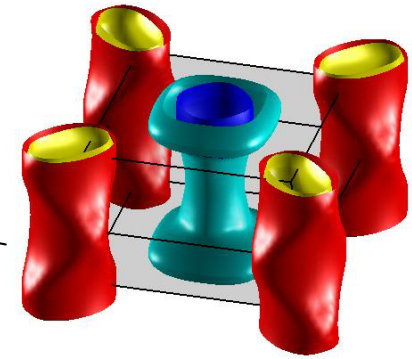


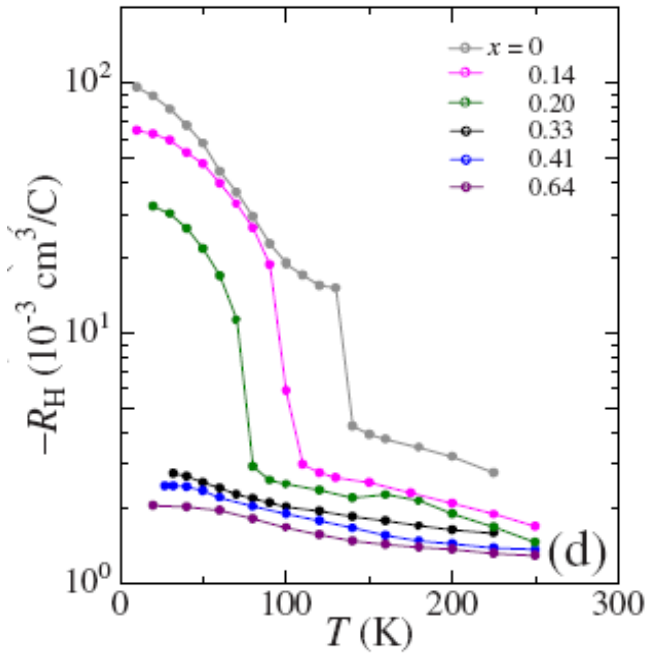
- **Two electron cylindrical Fermi surfaces;**
- **Volume: Decrease with decreasing *x* (no doping);**

H. Shishido *et al.*, PRL 104, 057008 (2010)

Fermi surface shrinking in $BaFe_2(As_{1-x}P_x)_2$

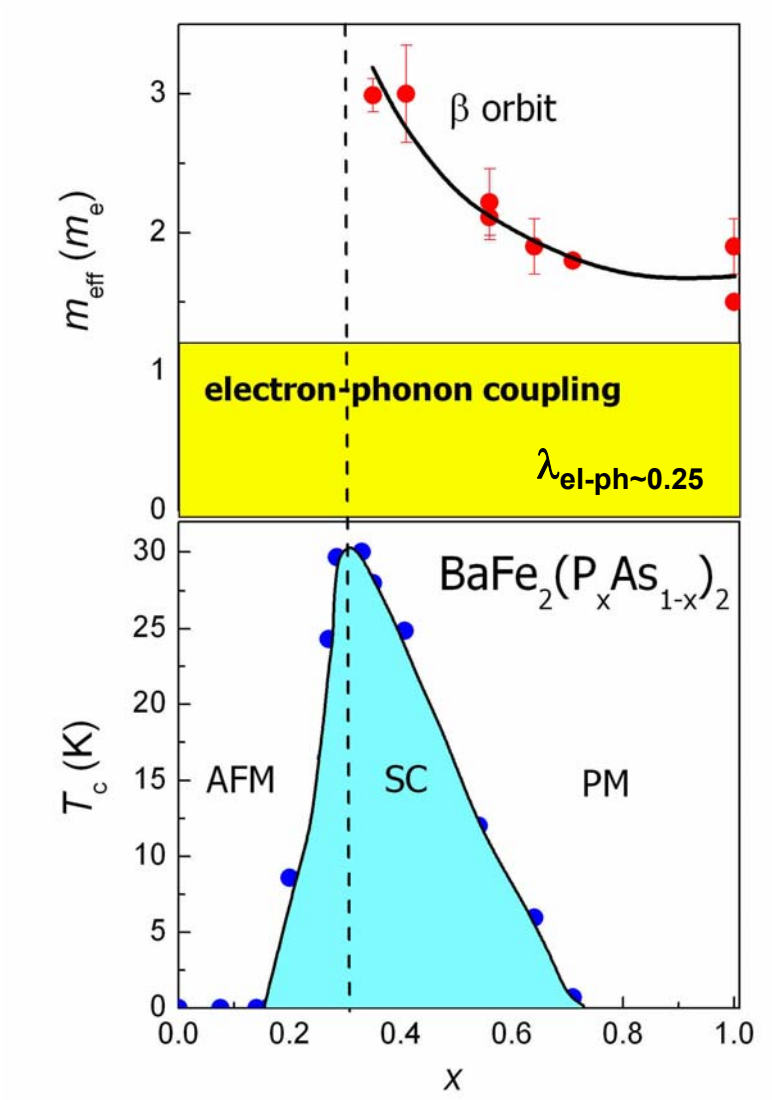






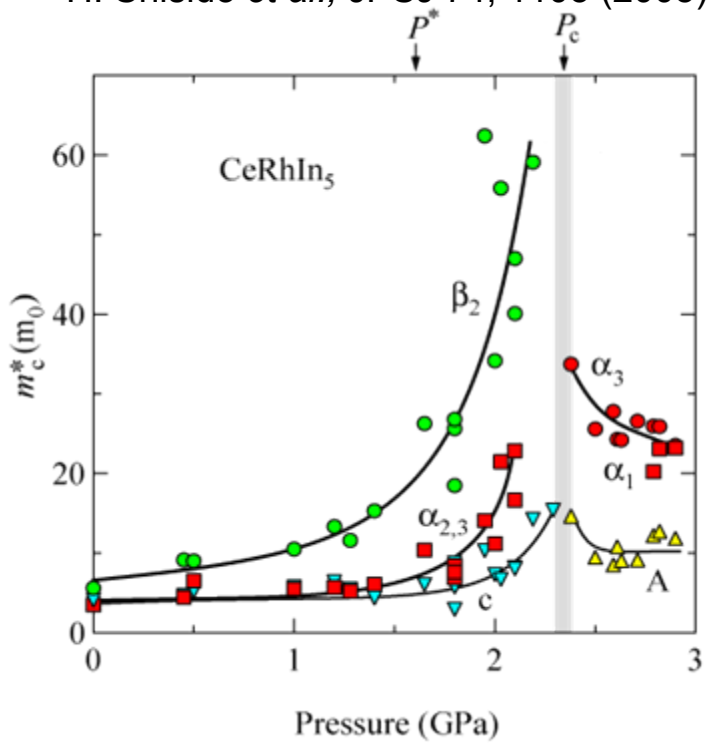
S. Kasahara *et al.*, *PR*B 81, 184519 (2010)

Enhancement of the effective mass in $BaFe_2(As_{1-x}P_x)_2$



Outer electron cylinder

H. Shisido *et al.*, JPSJ 74, 1103 (2005)



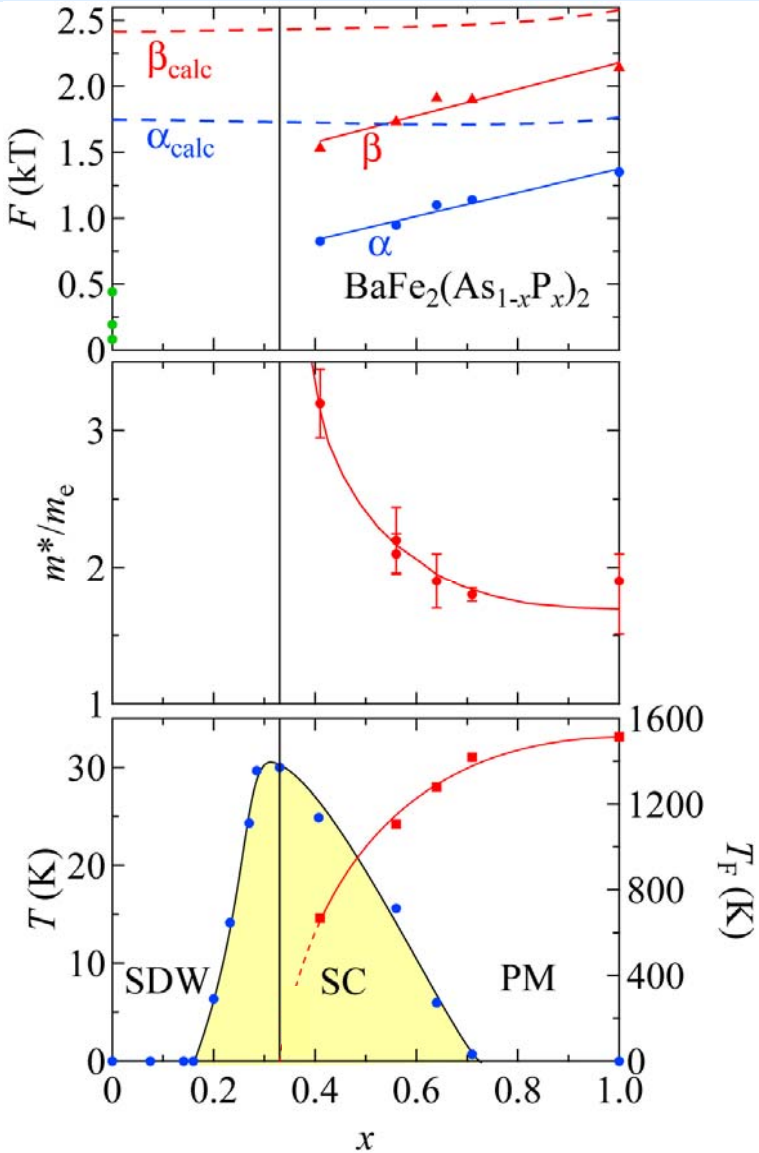
Increase of effective mass due to many-body interactions; Decrease of T_F

$$T_F = \frac{\hbar e F}{m^* k_B}$$

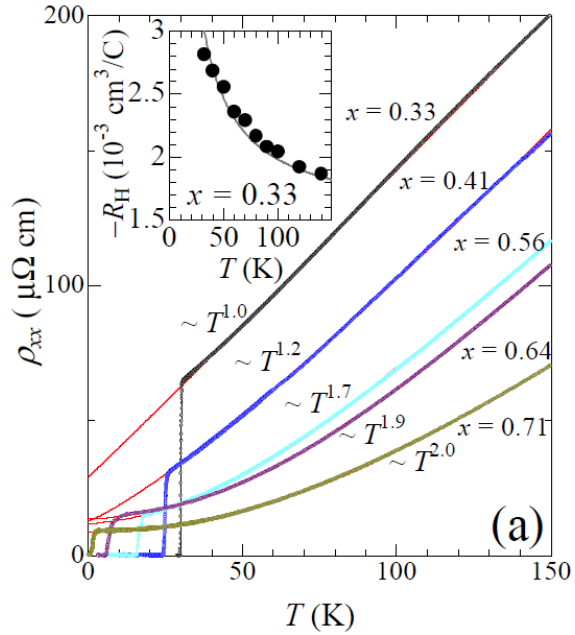
Quantum critical behavior ?

γ_{expr} **~18 mJ/mol K²** (x=0.38); (arXiv:1002.3355)

Spin fluctuations in $BaFe_2(As_{1-x}P_x)_2$

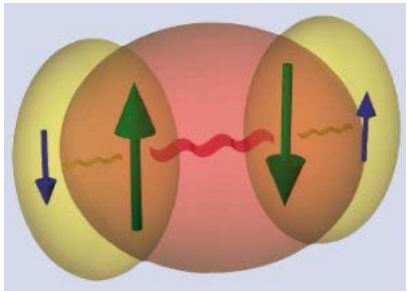


H. Shishido *et al.*, PRL 104, 057008 (2010)

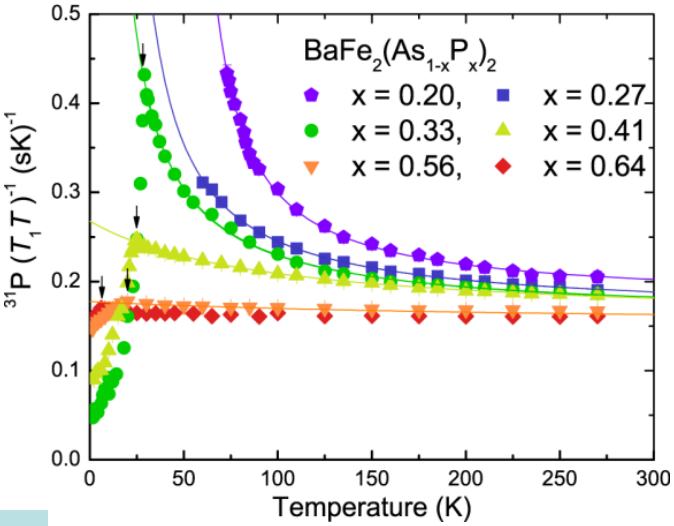


$\rho = \rho_0 + AT^{\alpha}$

S. Kasahara *et al.*, *PR*B 81, 184519 (2010)



Antiferromagnetic spin fluctuations close to QCP

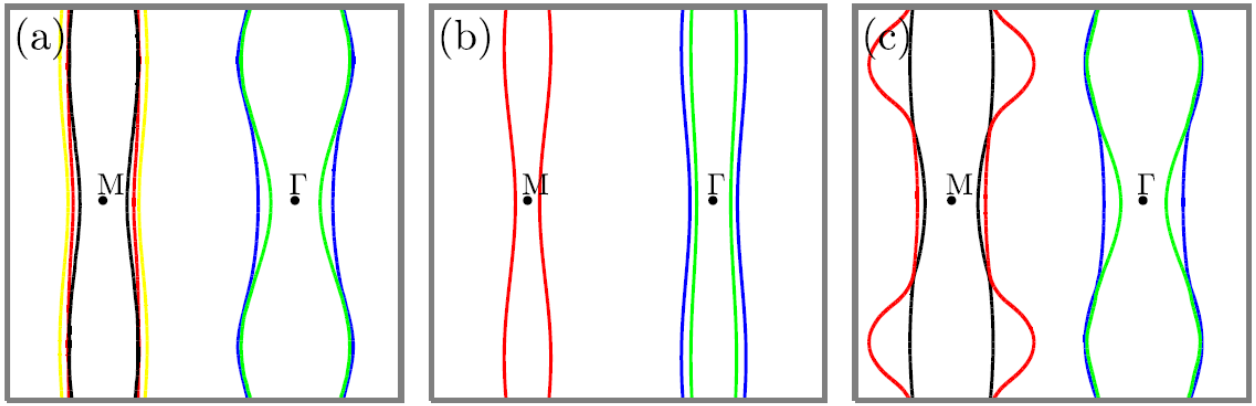


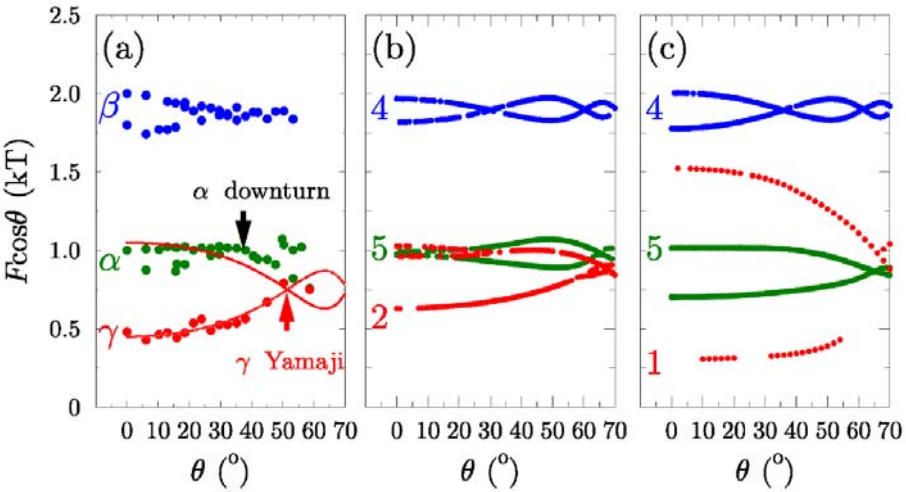
$1/T_1T \sim 1/(T+\theta)$

Y. Nakai, *et al.* arXiv:1005.2853 (2010)

Enhanced nesting towards maximum Tc ?

$BaFe_2As_2$ **x~0.63 (T_c~ 9 K)** **$BaFe_2P_2$**



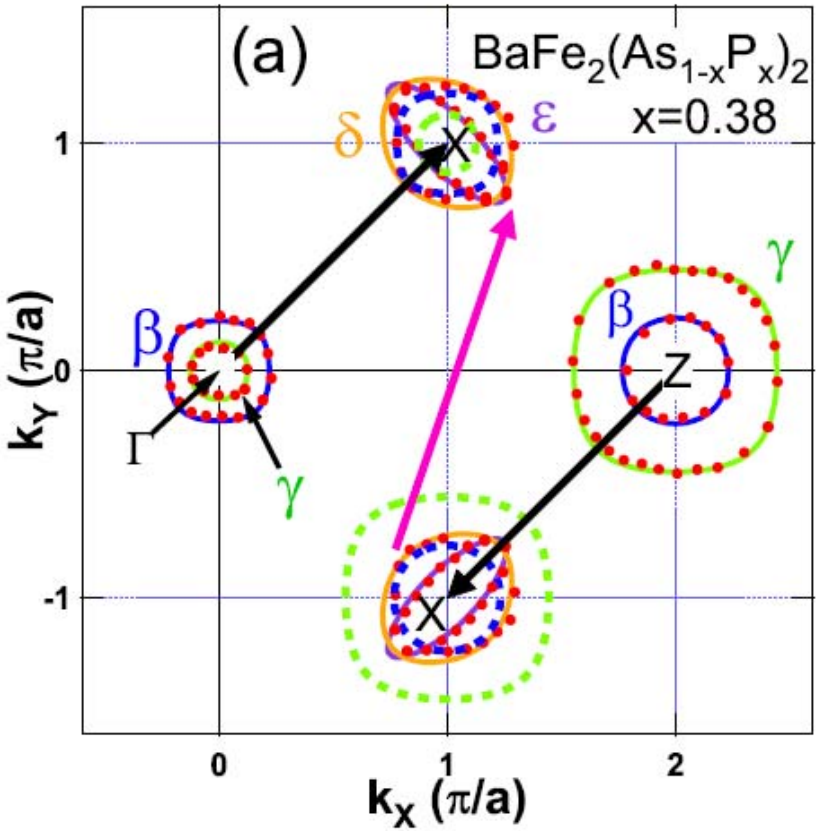


	Experiment			Calculations			
	F(kT)	$\frac{m^*}{m_e}$	ℓ(nm)	Orbit	F(kT)	$\frac{m_b}{m_e}$	$\frac{m^*}{m_b}$
γ	0.45	4.5(5)	12	2_{min}	.53	1.24	3.6
				2_{max}	0.86	1.72	
α_1	.89	2.3(1)	-	5_{min}	1.02	1.25	1.8
α_2	1.10	2.10(5)	48	5_{max}	1.04	1.31	1.6
β_1	1.80	2.1(1)	-	4_{min}	1.81	1.17	1.8
β_2	2.01	2.0(5)	57	4_{max}	1.95	1.30	1.5

- **One further HEAVY hole pocket observed; inner electron pocket and inner hole pocket have similar sizes ; shrinking of the electronic bands;**

J.G. Analytis *et al.*, PRL **105**, 207004 (2010)

ARPES studies in $BaFe_2(As_{1-x}P_x)_2$ (x=0.38)



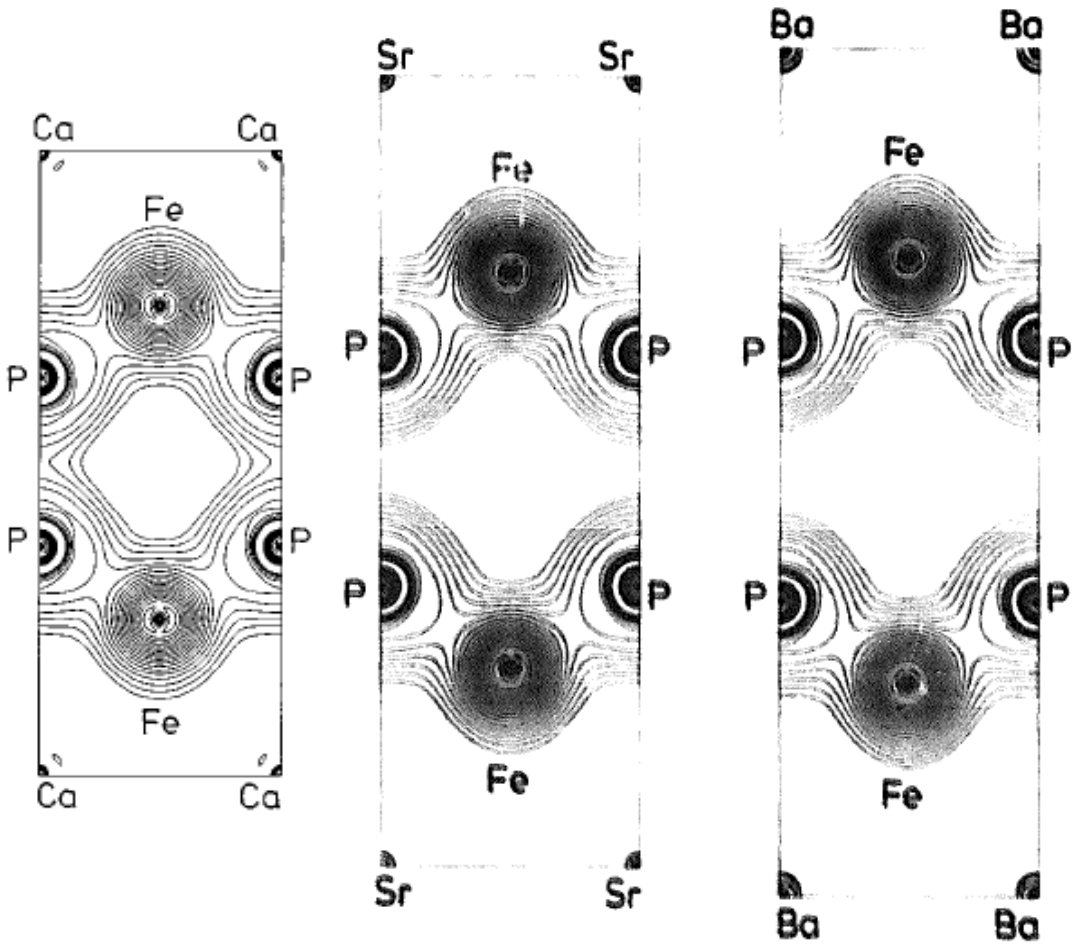
FS		3D volume	k_z	2D area	m^*/m_e	m_b/m_e	m^*/m_b
β	h	3.9	Γ	3.9	3.8	1.3	2.9
			Z	3.8	2.5	1.2	2.1
γ	h	6.0	Γ	1.0	2.6	0.9	2.9
			Z	16.3	3.9	2.3	1.7
δ	e	5.3	X	5.3	2.8	0.71	3.9
ϵ	e	3.4	X	3.0	2.0	0.93	2.1

Mass enhancement for all orbits varies between 2 - 3.9

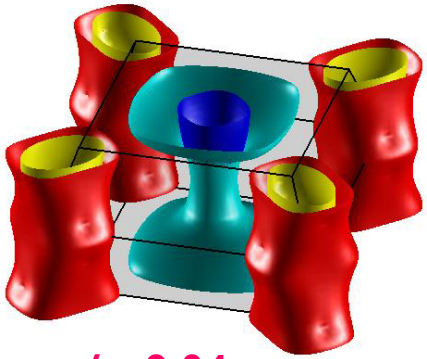
• one quasi-two dimensional electron and hole pockets have similar size and shape inplying good nesting but they have different orbital character ($d_{xz/yz}$ for hole and d_{xy} for the electron sheet) so weak contribution to the spin susceptibility;

T. Yoshida *et al.*, arXiv:1008.2080 (2010)

Significant pnictogen bonding affects FS

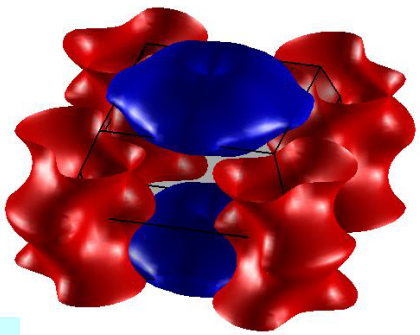


SrFe2P2



c/a=3.04

CaFe2P2

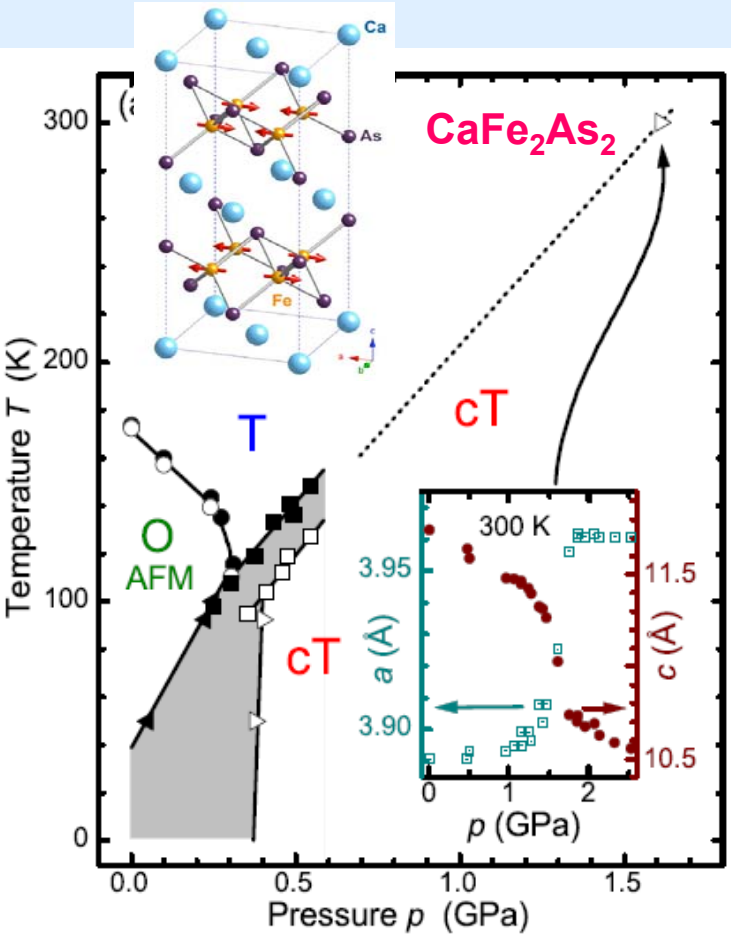


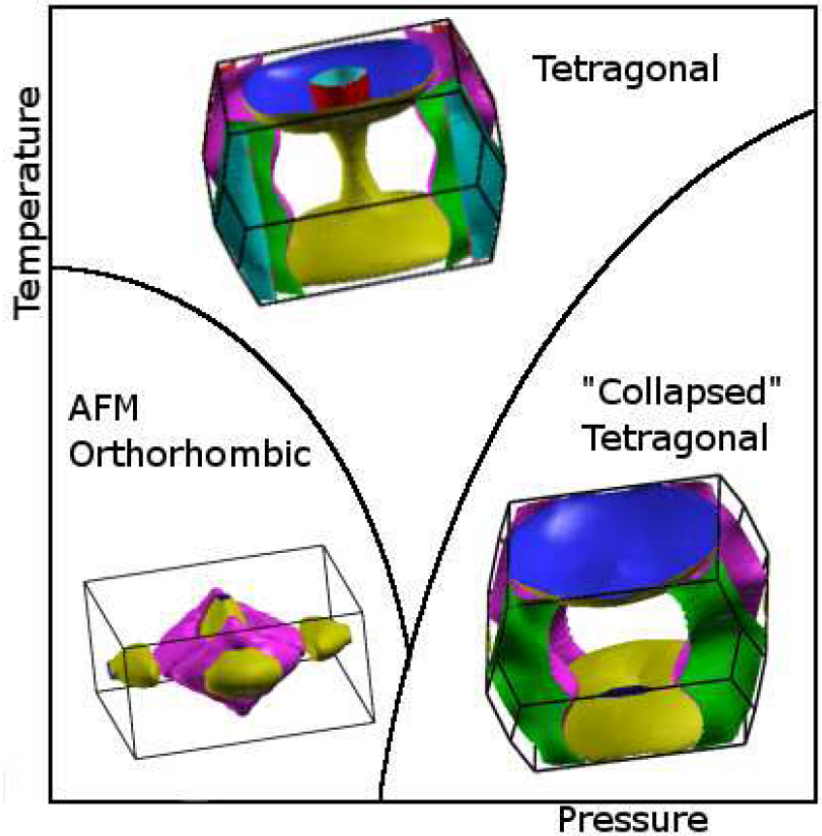
c/a=2.65

Small spacer between Fe layers enhances P-P bonding.

Journal of Alloys and Compounds 262–263 (1997) 516–520

Effect of applied pressure in pcnitides





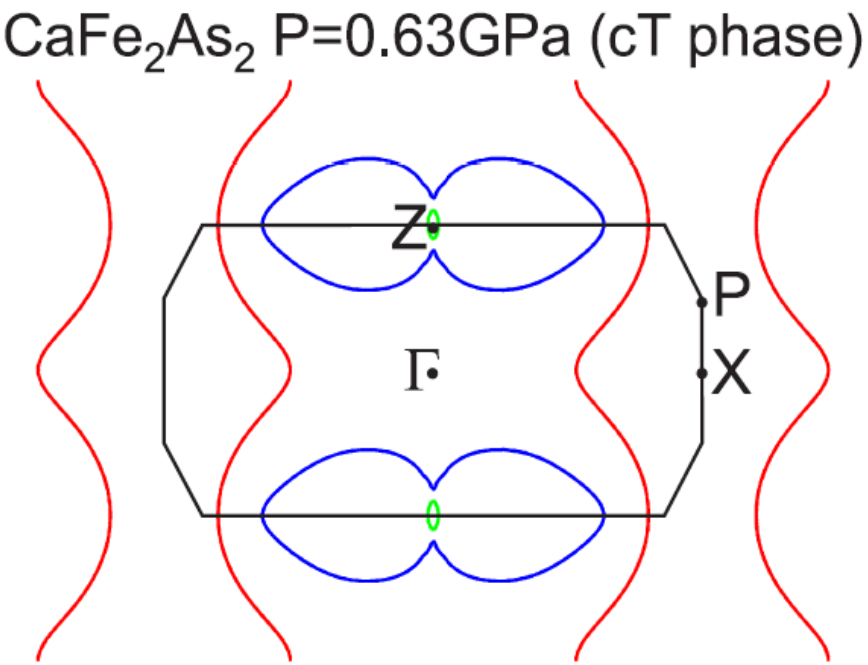
$CaFe_2A_2$ under pressure has a transition to a non-magnetic collapsed tetragonal (cT) state; ~ 10% decrease in the *c*-axis and a ~2% increase in the *a*-axis; ***c/a*=3** in the tetragonal phase to ***c/a*=2.65** in the cT phase;

•Superconductivity present under non-hydrostatic conditions (uniaxial pressure);

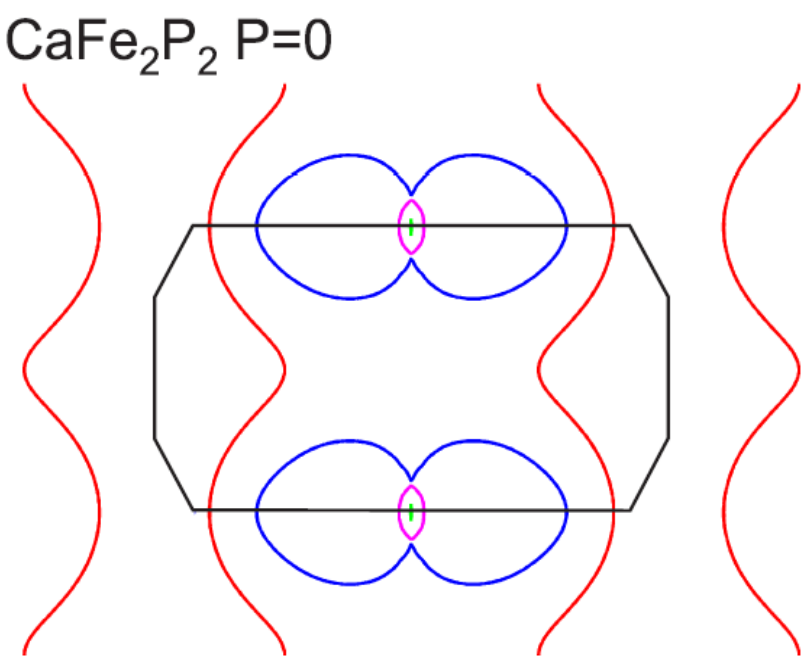
A.I. Goldman *et al.,* Phys. Rev. B 79, 024513 (2009)

D. A. Tompsett, G. G. Lonzarich,arxiv:0902.4859 (2009)

Effect of chemical pressure: small c/a ratio



c/a=2.65



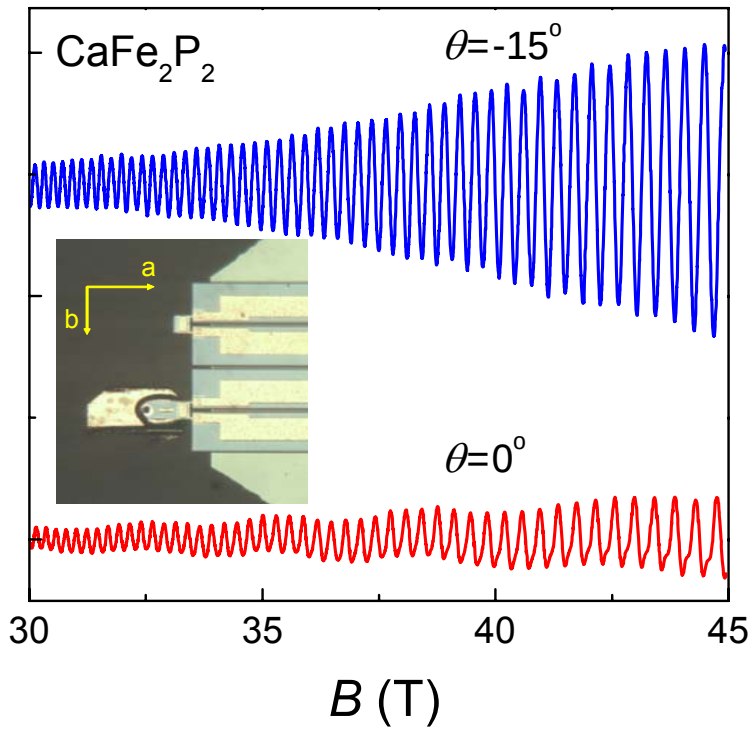
c/a=2.59

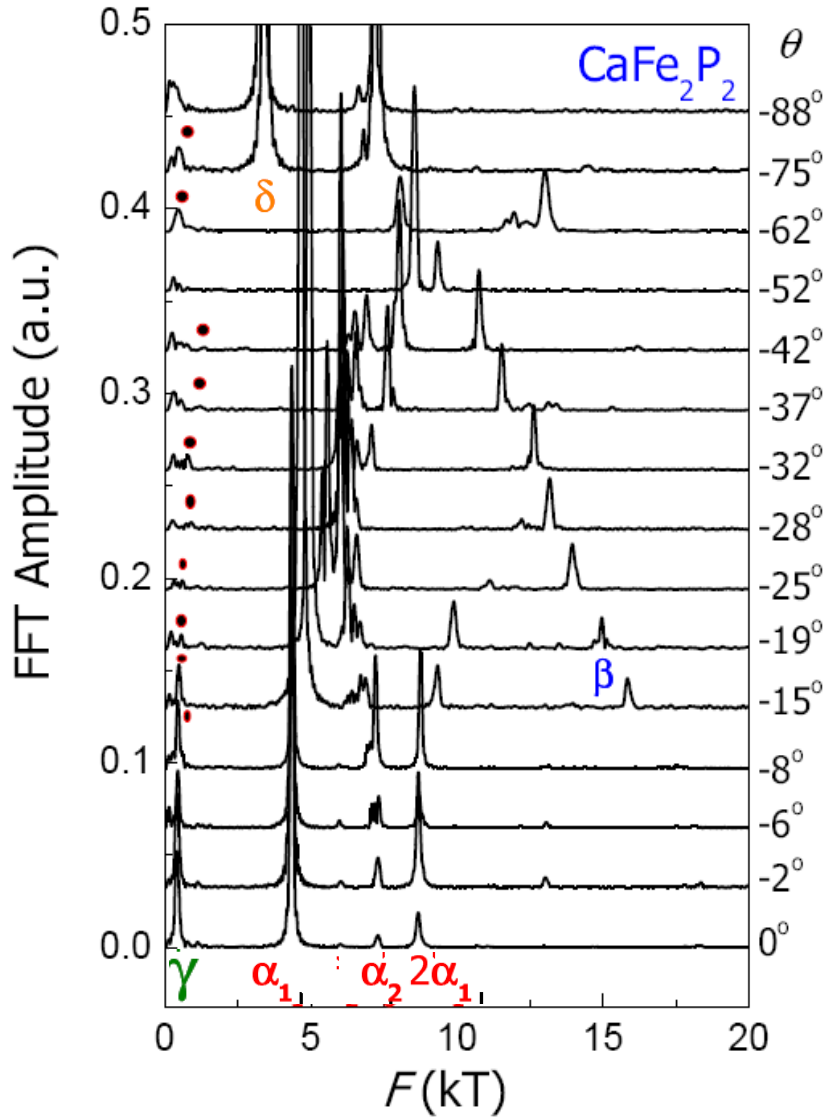
Band structure calculations predict:

- $CaFe_2P_2$ is a close structural analogue of the collapsed tetragonal non-magnetic phase of $CaFe_2As_2$ and shows a similar Fermi surface;
- single electron and hole sheets highly three-dimensional in character ;

A.I. Coldea *et al.*, PRL, 103, 026404 (2009)

Quantum oscillations in $CaFe_2P_2$

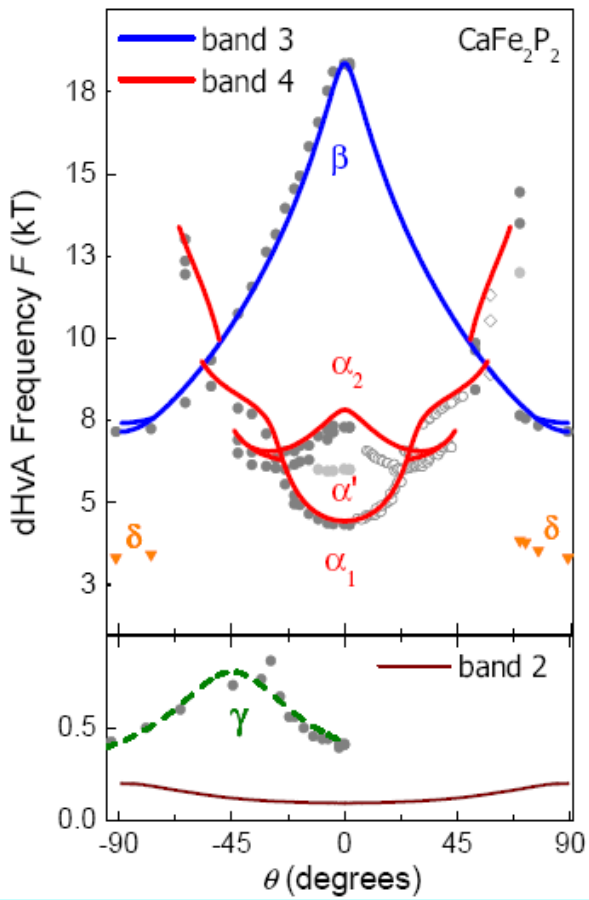


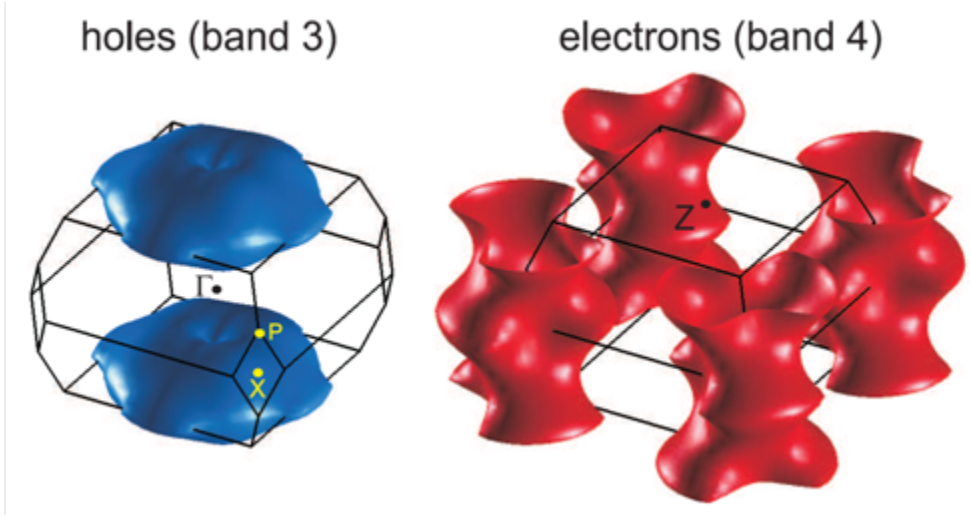


- torque measurements in 45 T at 0.4 K;
- series of different frequencies corresponding to various extremal areas on the Fermi surface;

A.I. Coldea *et al.*, PRL, 103, 026404 (2009)

Quantum oscillations in $CaFe_2P_2$





	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)

- good agreement between the band structure calculations and experimental data; no band shifts required.
- identical mass enhancement on both electron and hole pockets ~1.5;
- topological change of the Fermi surface;.

A.I. Coldea *et al.*, PRL, 103, 026404 (2009)

The strength of electronic correlations

		Mass enhancement: $1+\lambda$	λ
SC	LaFePO	m^*/m_b~2. 2 inner electron pocket 2.54 outer electron pocket	1.2 1.54
	$BaFe_2(As_{1-x}P_x)_2$	m^*/m_b~ 3 for electron pockets	~2
Non SC	$CaFe_2P_2$	m^*/m_b~1.5 electron/hole pockets	0.5
	$BaFe_2P_2$	m^*/m_b~1.5 electron pockets	0.5

$$m^*/m_b=(1+\lambda_{el\text{-}ph})(1+\lambda_{el\text{-}el}) \sim 1+\lambda_{el\text{-}ph}+\lambda_{el\text{-}el}$$

electron-phonon coupling

$\lambda^{th}_{el\text{-}ph}$~0.25 for Fe-pnictides

electron-electron interactions (nesting, spin fluctuations)

$\lambda_{el\text{-}el}$ ~ 0.5 – 1.5

- **Magneto-elastic coupling**
- large **pnictide polarizability**:

Kulic et al., arXiv:0904.3512

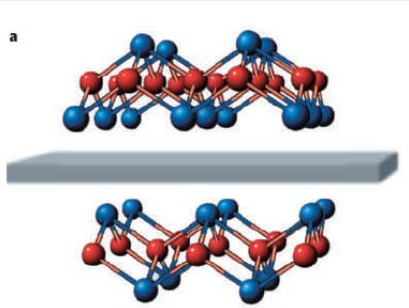
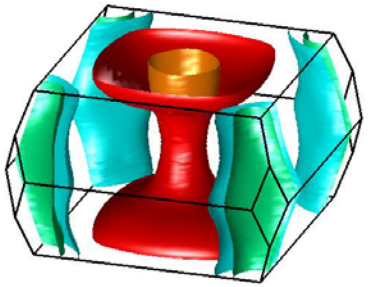
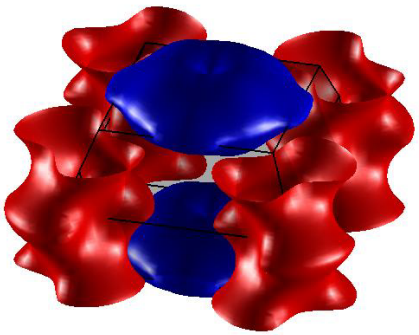
L. Boeri, Physica C **469**, 628 (2009)

Summary

•Fermi surface of 122 compounds extremely sensitive to **structural** effects (*c/a* ratio –uniaxial pressure ?).

•**For small spacer layer or large *d* orbitals** Fermi surface topology is strongly modified (in particular for the hole bands);

•**Anisotropic scattering**: hole pockets affected much more by impurity scattering as compared to the electron pockets; **orbitals**?

•**Shrinking of the Fermi surface** as compared with the band structure calculations –**electronic correlations**;

• Enhanced effective masses and increased FS nesting in LaFePO and $BaFe_2(P_{1-x}As_x)$ **– strength of electronic correlations;**