Electronic structure of iron-based superconductors

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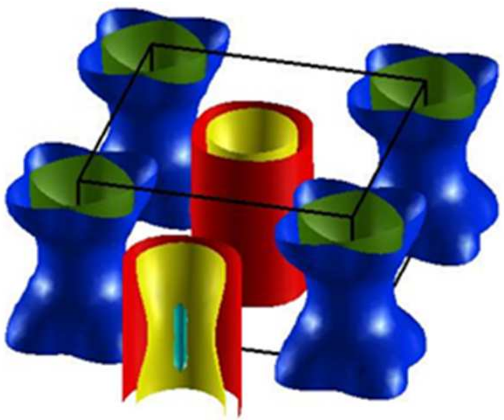
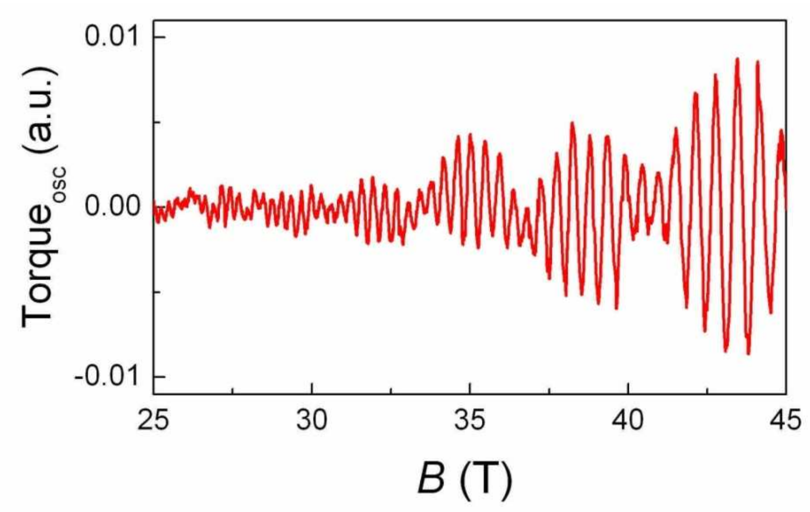
Oxford Physics

EPSRC Pioneering research and skills





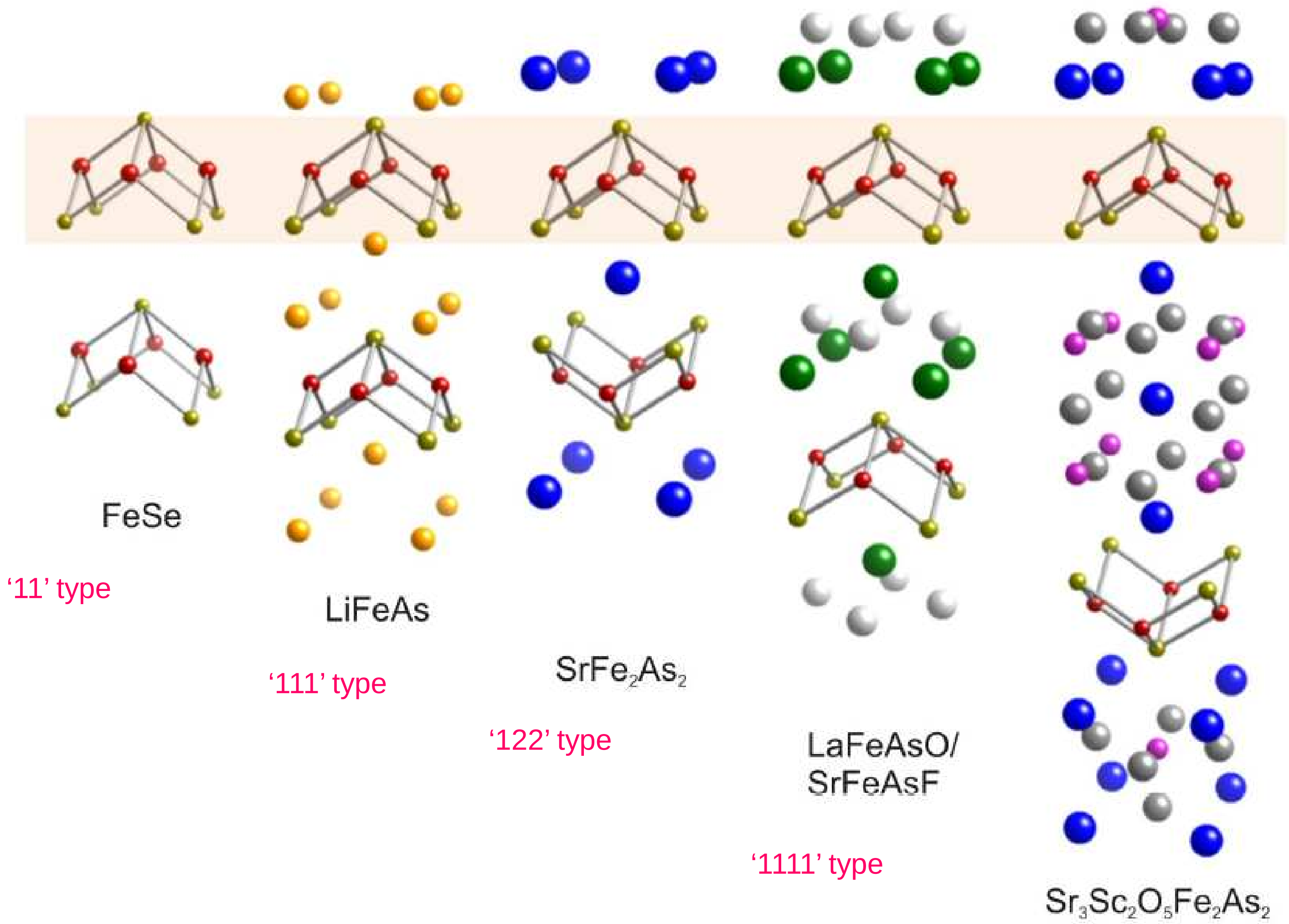
KITP, 30 September 2014

I. Fermi surface shrinking and the effects of electronic correlations

II. Electronic structure of bulk FeSe from ARPES and quantum oscillations

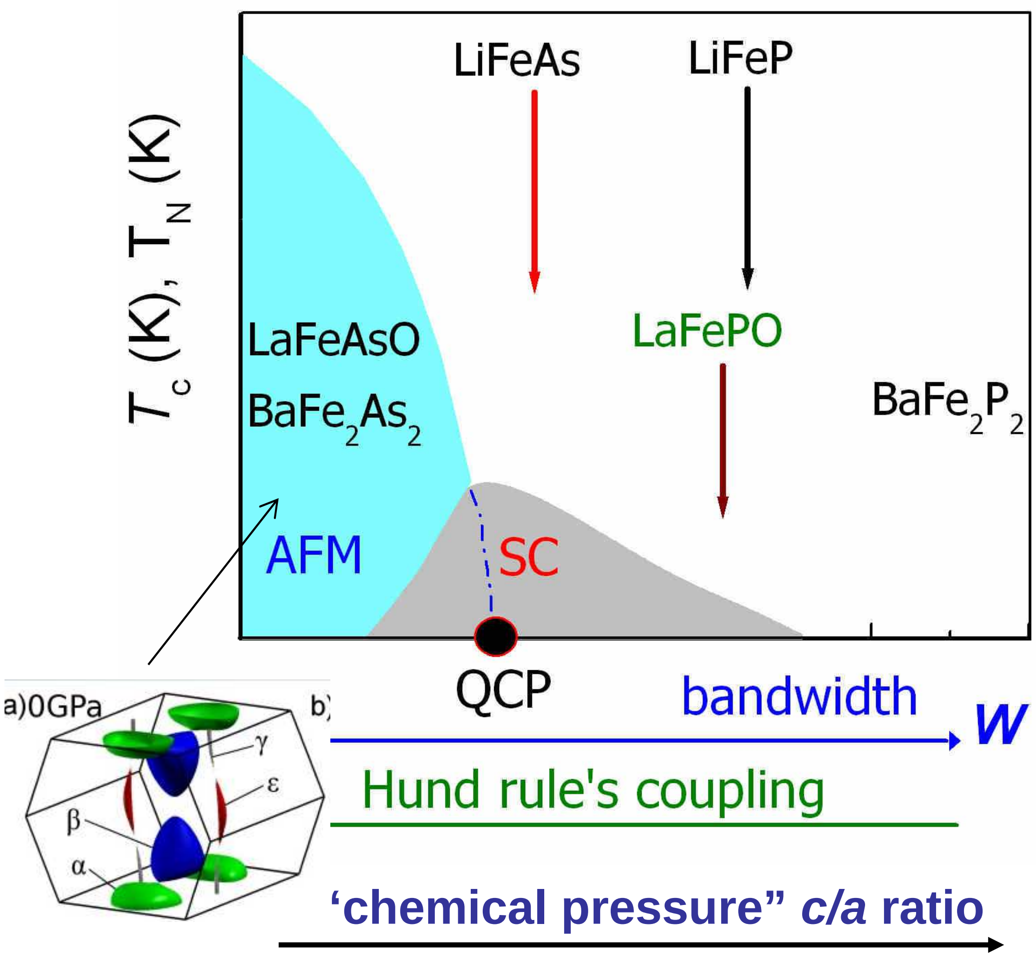
Classes of Fe-based superconductors

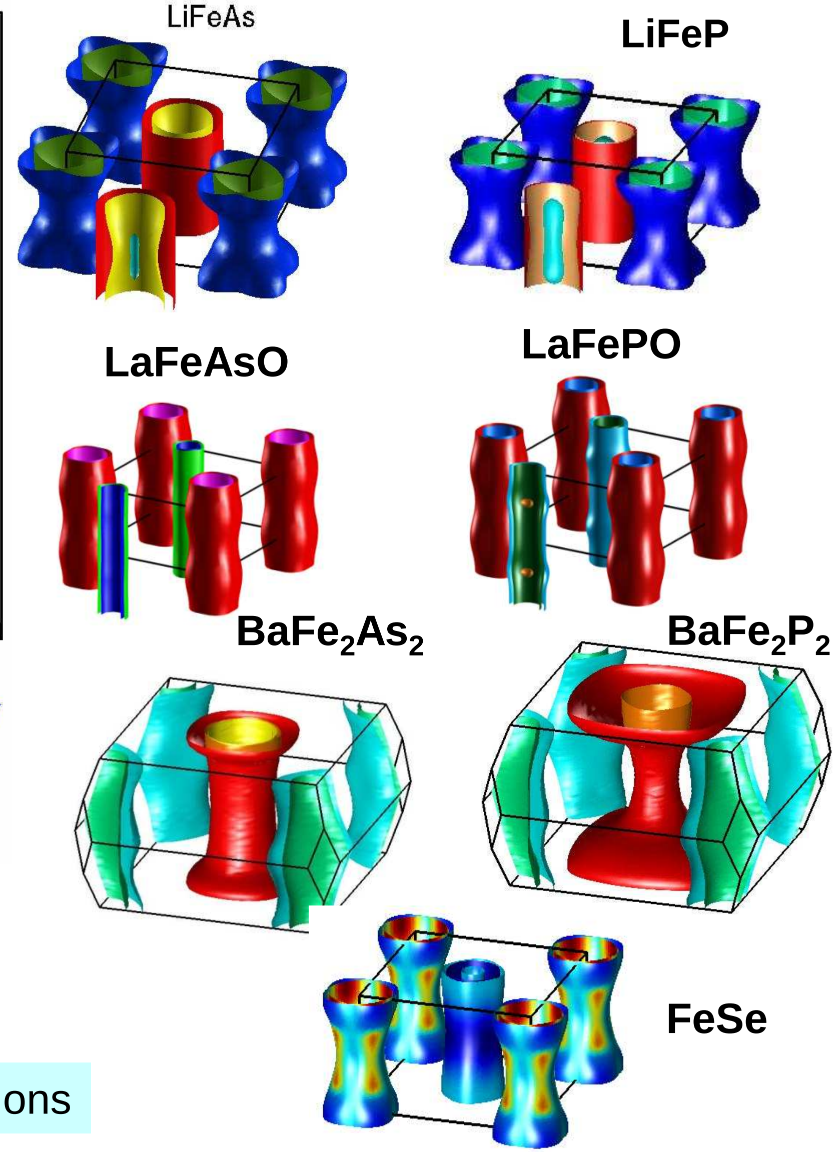
Tc~27 K | *Tc*~18 K | *Tc* ~ 38 K | *Tc* ~ 55 K | *Tc* ~ 37 K



The common features: robust Fe/(Pn=As,P) layers where Fe atoms are tetragonally coordinated by pnictide or chalcogenide atoms.

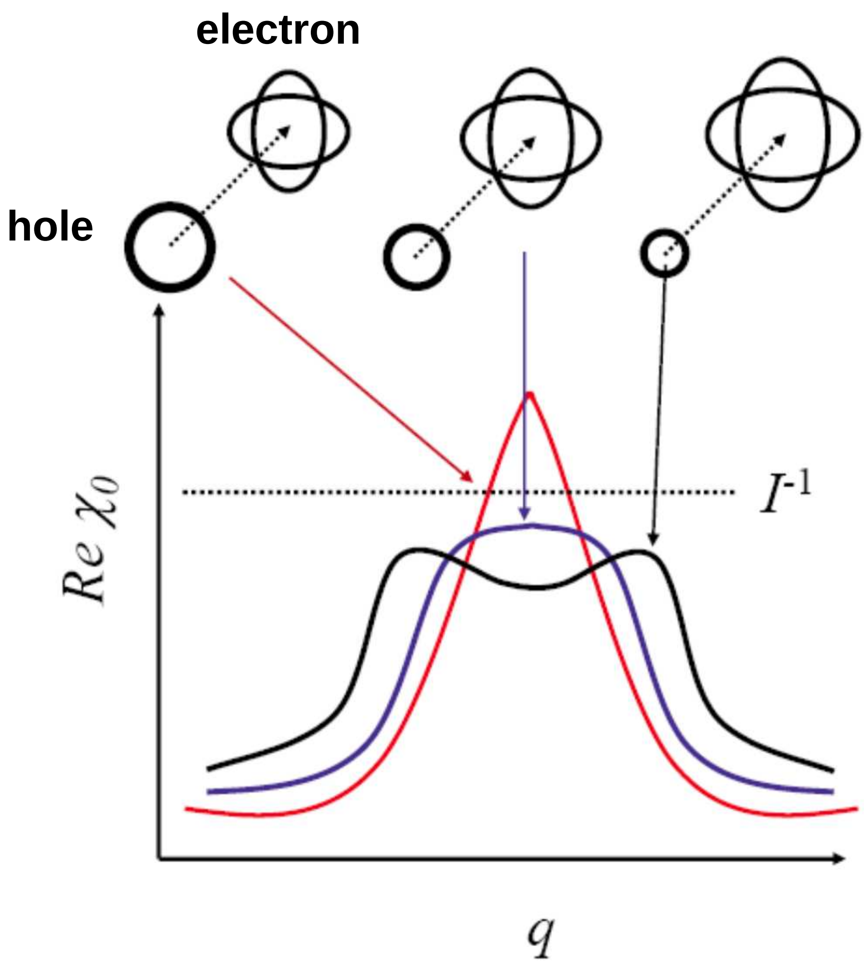
Generic phase diagram of isoelectronic pnictides

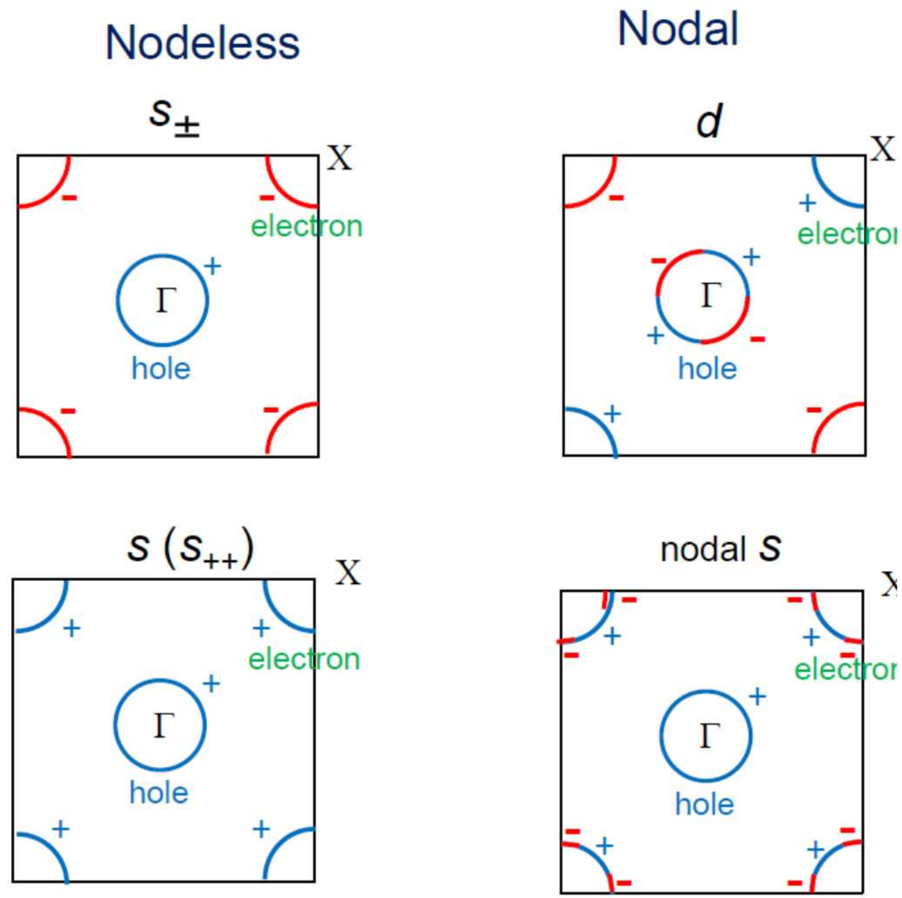




5 bands (orbitals), magnetism, structural distortions

Fermi surface nesting and gap symmetry





Superconductivity develops when the nesting / magnetism is destroyed.

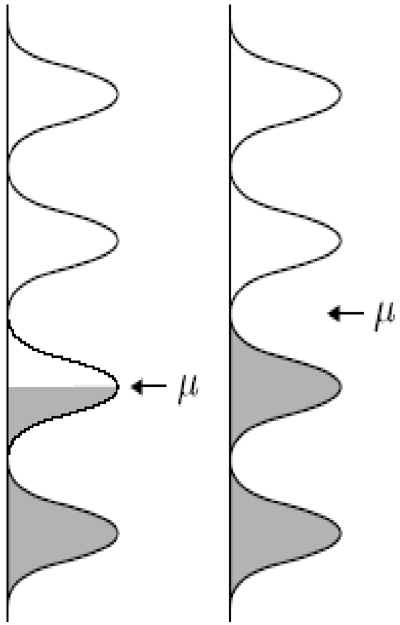
D. Singh

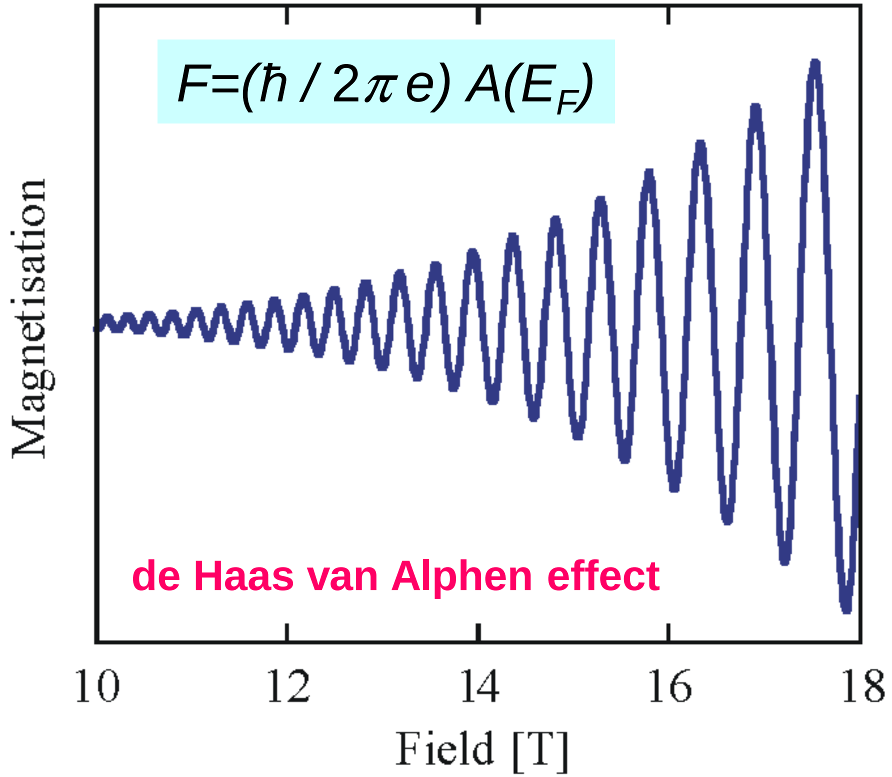
Different possible scenarios for nodal and nodeless superconductivity depend on orbital character.

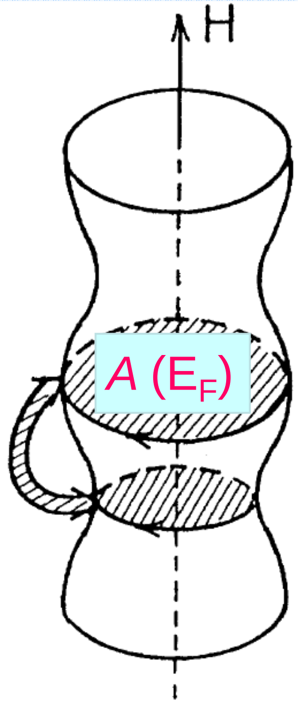
P. J. Hirschfeld et al, Rep. Prog. Phys. 74, 124508 (2011)

Quantum oscillations map out the Fermi surface

- oscillations of the density of states in magnetic field;







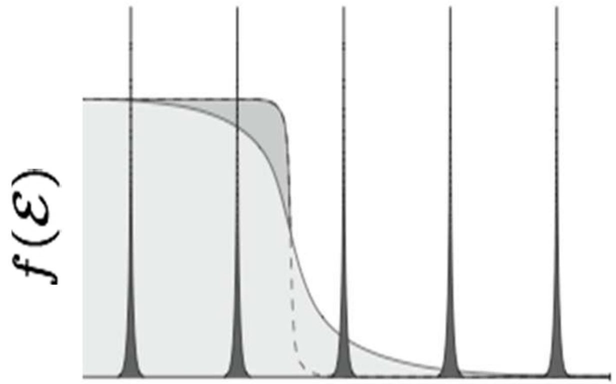
- **'k-space microscopy': 0.1% IBZ; 3D map of the Fermi surface;**
- **bulk probe; no sensitive to surface effects like ARPES;**

$$\tilde{M} \propto \sum_{\text{extremal } A_F} \frac{F B^{\frac{1}{2}}}{m^* \left| \frac{\partial^2 A_F}{\partial k_z^2} \right|^{\frac{1}{2}}} \sum_{p=1}^{\infty} R_T R_D R_S \, p^{-\frac{3}{2}} \sin\left(2\pi p \left(\frac{F}{B} - \gamma\right) \pm \frac{\pi}{4}\right)$$

Lifshitz-Kosevich formalism (LK formula)

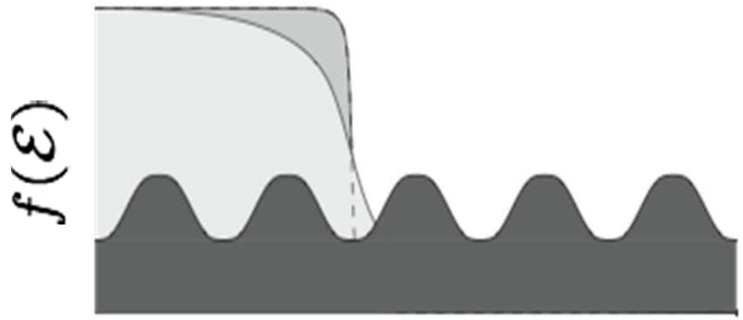
Shoenberg, *Magnetic oscillations in metals*, (1984)

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



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

$$R_D = \exp\left(-\frac{\pi m_b}{eB\tau}\right)$$

Superconducting state –random vortex lattice

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

Spin-splitting of the Fermi surface

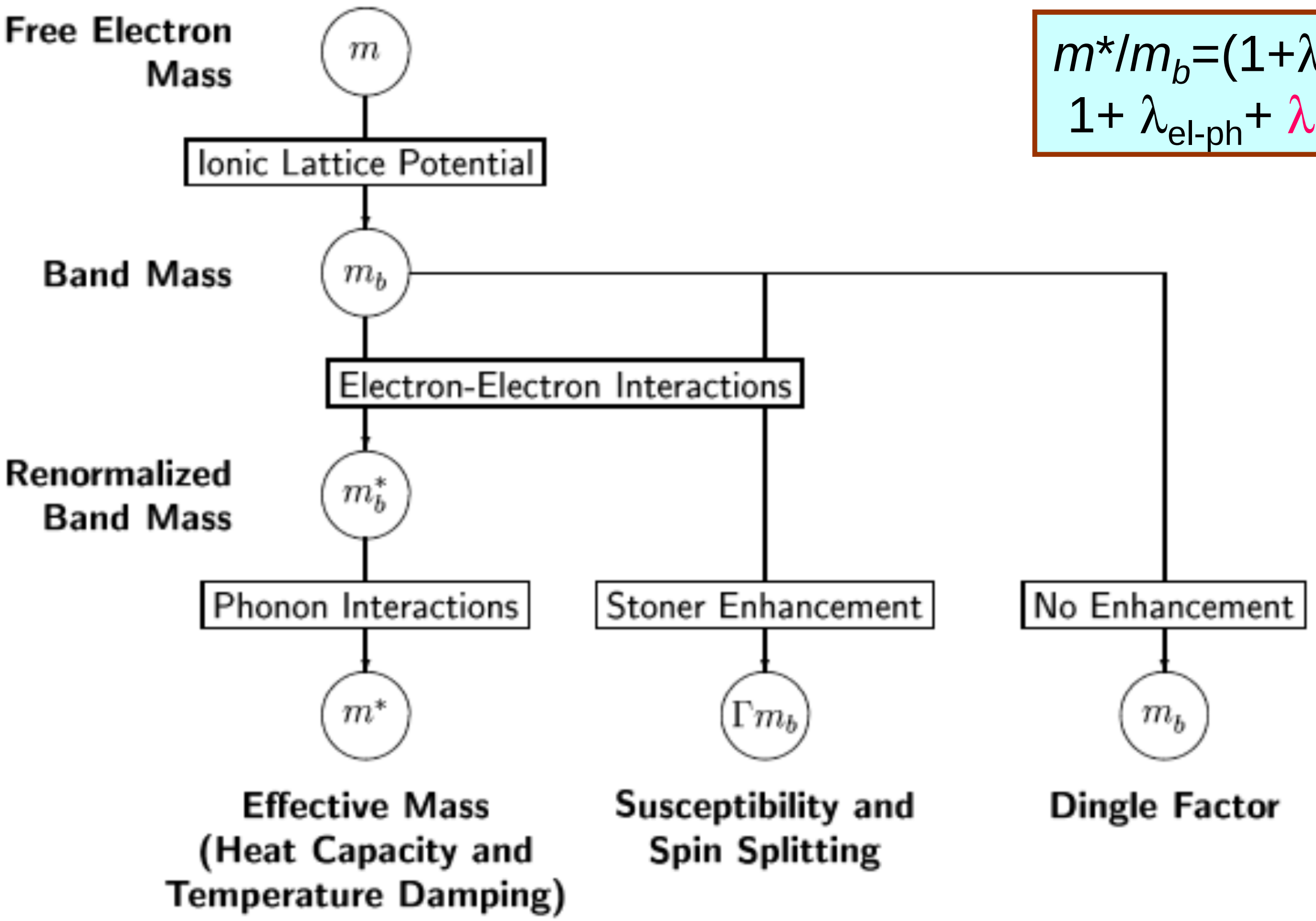
$$R_S = \cos\left(\frac{\pi g m_S}{2m_e}\right)$$

• extracted parameters: orbitally averaged quasiparticle effective mass ***m**(band renormalization near the Fermi energy),**

•scattering times ~τ, spin-splitting factor ***g****

Lifshitz-Kosevich formalism.
The effect of electronic correlations

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



$$C = \frac{m^* k_F k_B^2 T}{3\hbar^2} \qquad \chi_P = \frac{\Gamma m_b\, g^2 k_F\, \mu_0 \mu_B^2}{4\pi^2\hbar^2}$$

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

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

C Bergemann, PhD Thesis

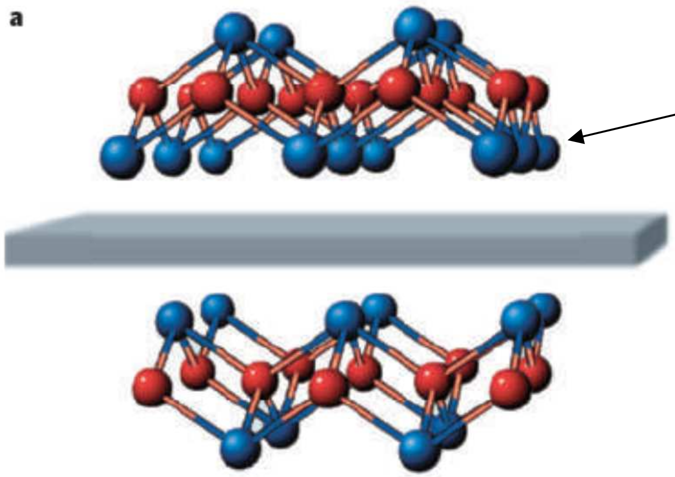
ADVANCES IN PHYSICS, 1996, VOL. 45, NO. 6, 471–503

Quantum oscillations in iron pnictides

-**Clean samples**: mean free path > 150 Å

- **End member compounds: (Ba/Sr/Ca)Fe_2As_2, (Ba/Sr/Ca)Fe_2P_2, KFe_2As_2, etc**

- twinning of samples is detrimental for the observation of quantum oscillations;



Disorder induced only outside the Fe plane **$BaFe_2(As,P)_2$**

$$\hbar\omega_c > k_B T,\ \omega_c \tau >> 1$$

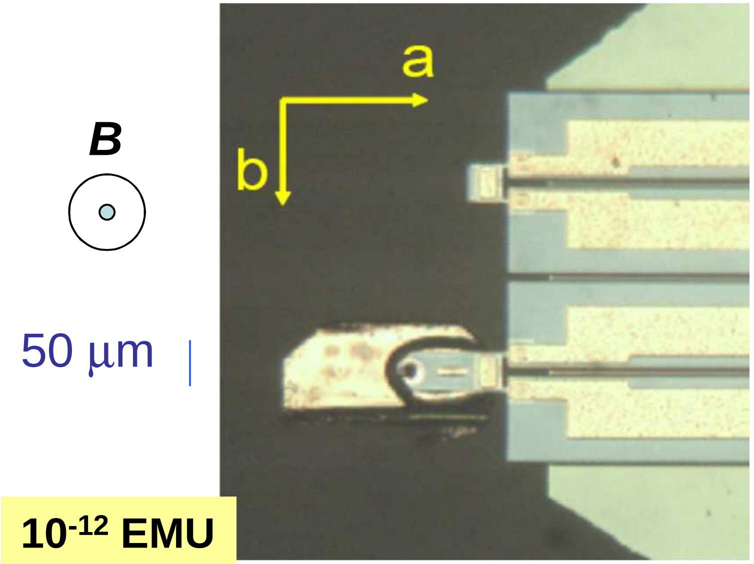
$$R_D = \exp(-\pi k_F / eB\ell)$$

-**Doped samples:** Co-doped or K-doped $BaFe_2As_2$; large upper critical fields > 60T and large randomness in the distribution of ions on the Fe sites;

-**Lighter masses** and **smaller frequencies** usually are easier to be observed than heavier masses and large frequencies;

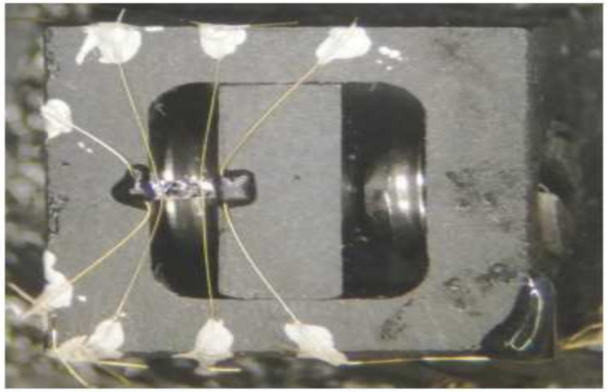
Measurement techniques of quantum oscillations

AFM piezocantilevers micron-size crystals



Capacitive levers mm-size crystals (Sebastian)

Transport measurements to de-twin crystals (Terashima)



BaFe2As2

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

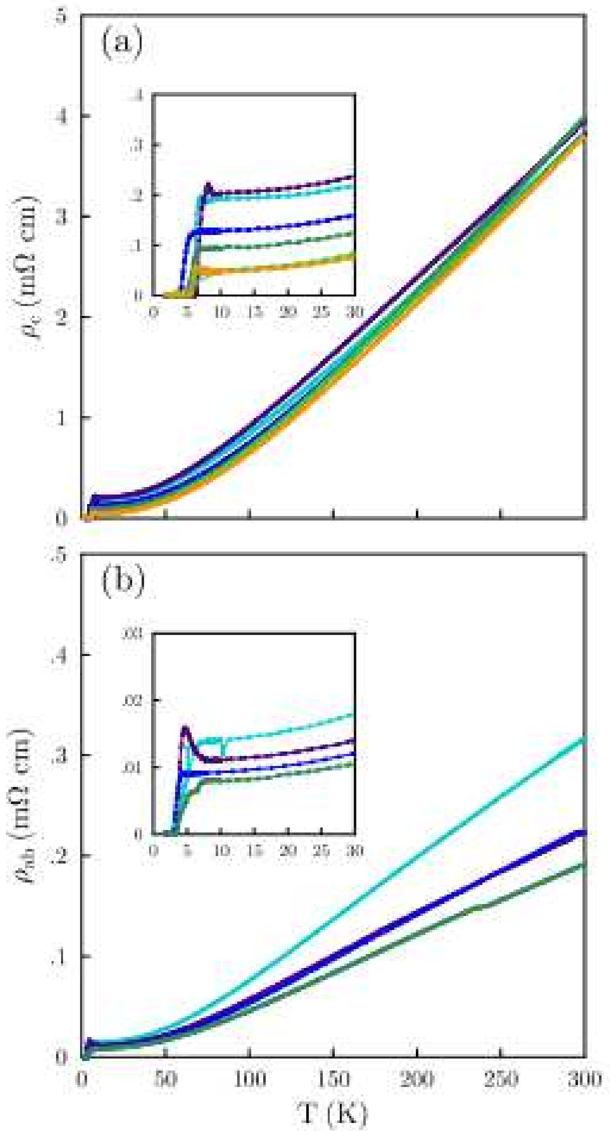
$$\tau = \mu_0(M_a H_c - M_c H_a)$$

$$\tau = \sum_{\text{orbits}} \frac{\partial F}{\partial \theta} \frac{V e^{5/2}}{\hbar^{1/2}\pi^2 m_e} \frac{B^{3/2}}{\left(2\pi \frac{\partial^2 A}{\partial k_\parallel^2}\right)^{1/2}} R_T R_D R_S \sin\left(\frac{2\pi F}{B} + \phi\right)$$

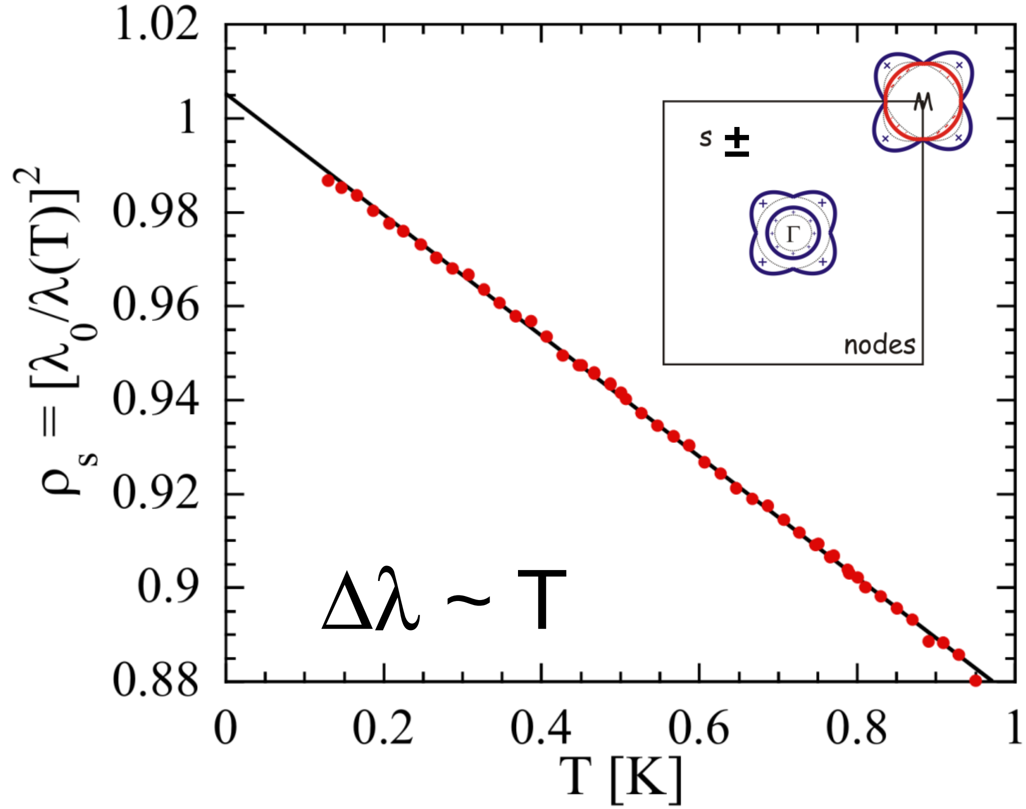
Low temperatures (0.3 K < T < 4 K), **high magnetic fields** (0 < B < 55 T)
rotation in field ($-90^0 < \theta < 90^0$);

I. Fermi surface shrinking and the effects of electronic correlations - LaFePO

Superconducting order parameter with line nodes in LaFePO



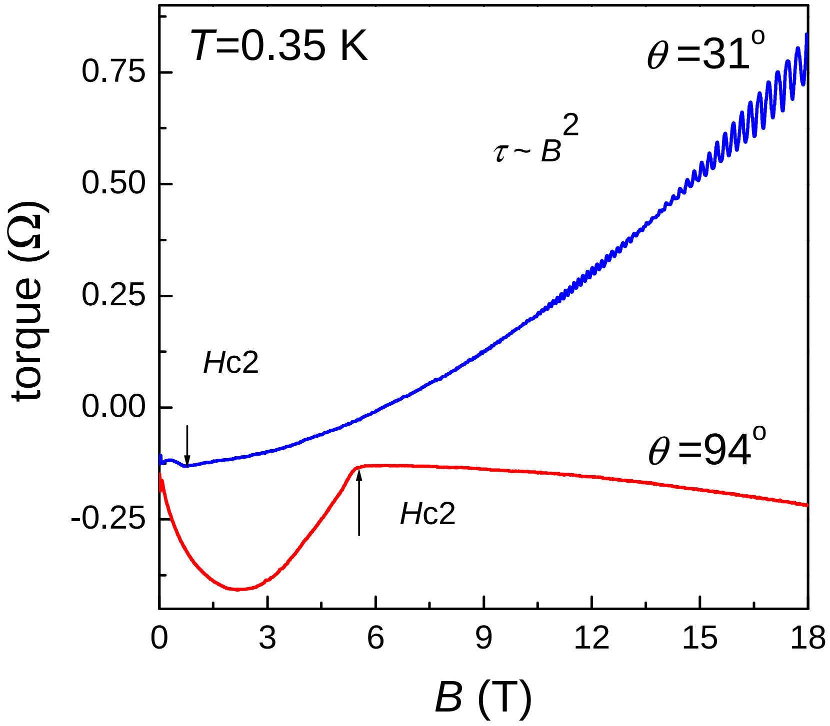
J. Analytis et al., arXiv:0810.5368



- Clean superconductor with no structural transition.Superfluid density show linear dependence down to 100 mK suggesting the presence of **nodes** in the symmetry of the superconducting gap;

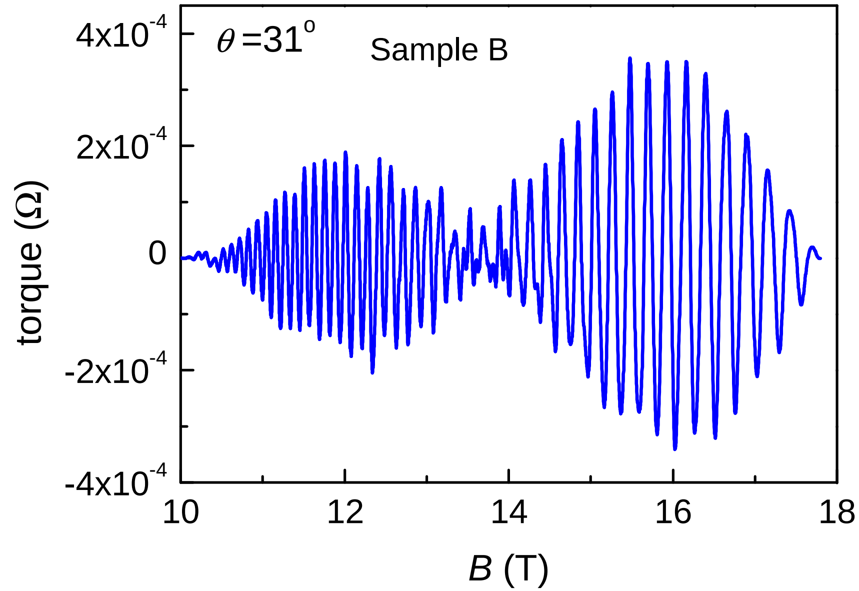
J. Fletcher, *et. al.*, PRL **102**, 147001 (2009)

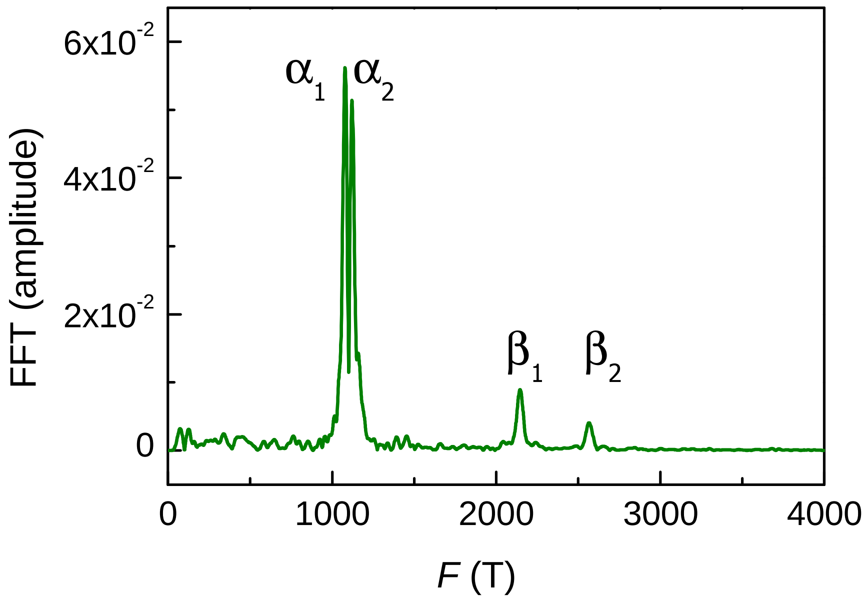
de Haas-van Alphen effect in LaFePO



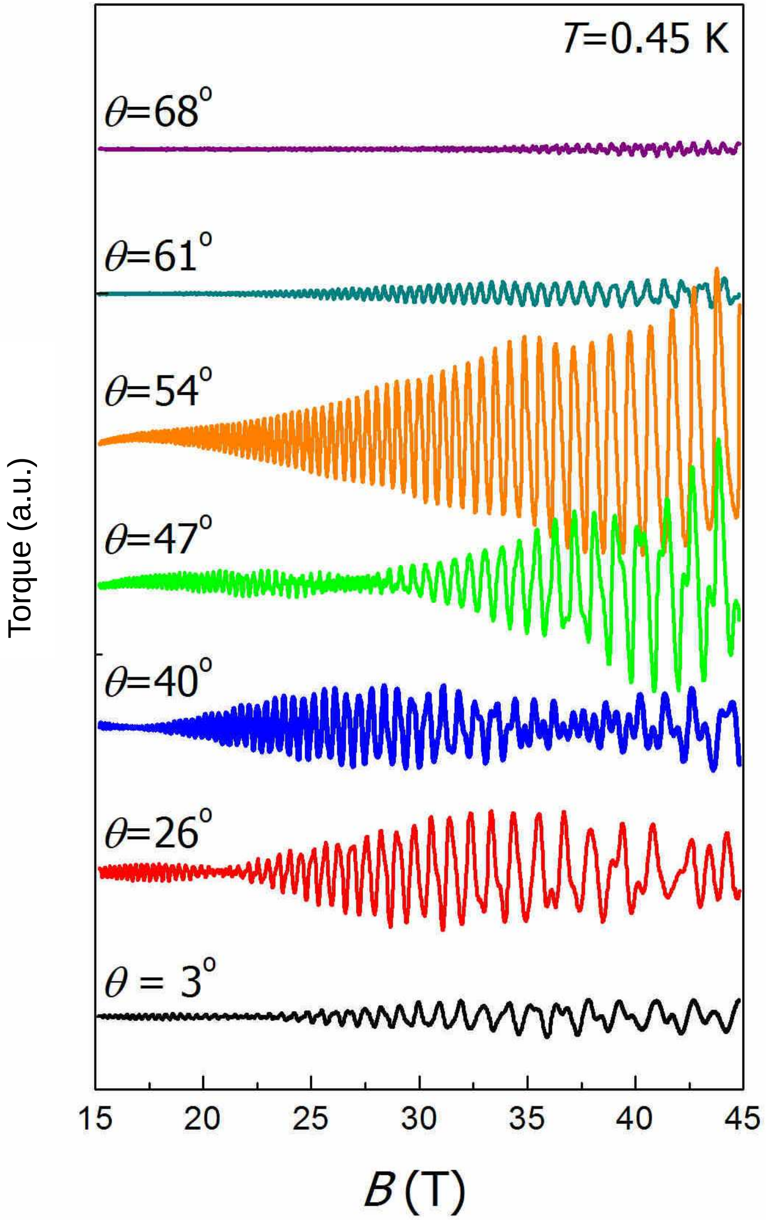
- high B: normal state; oscillations periodic in inverse field, de Haas-van Alphen effect.
- $\tau \sim B2$ –characteristic to a paramagnet;
- a simple corrugation of the Fermi cylinder leads to a beat pattern in the magnetization.

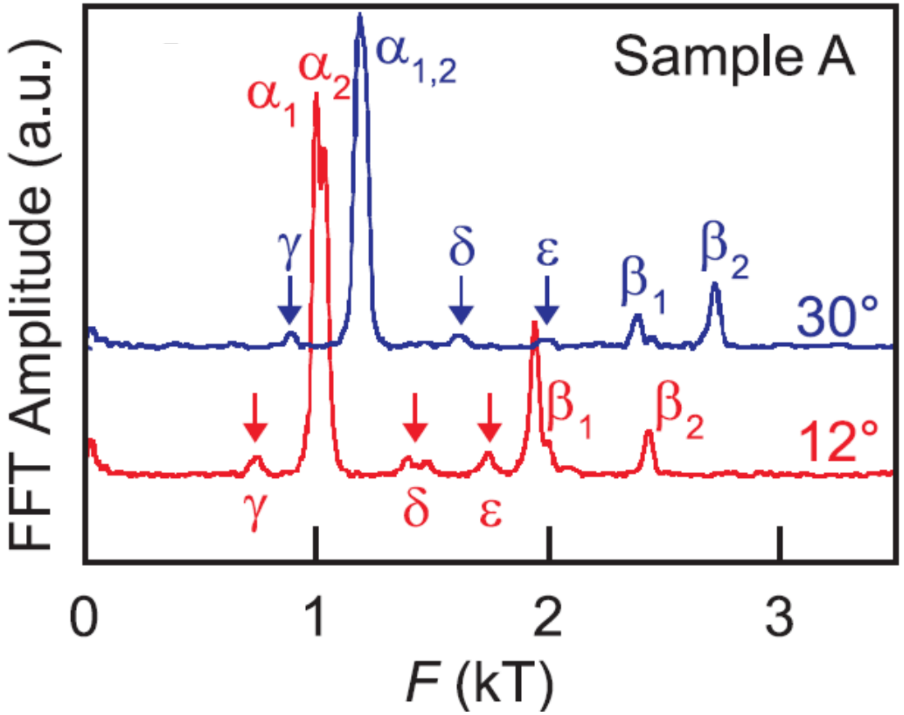
A.I. Coldea *et al.*, PRL, 101,216402 (2008)





de Haas-van Alphen effect in LaFePO



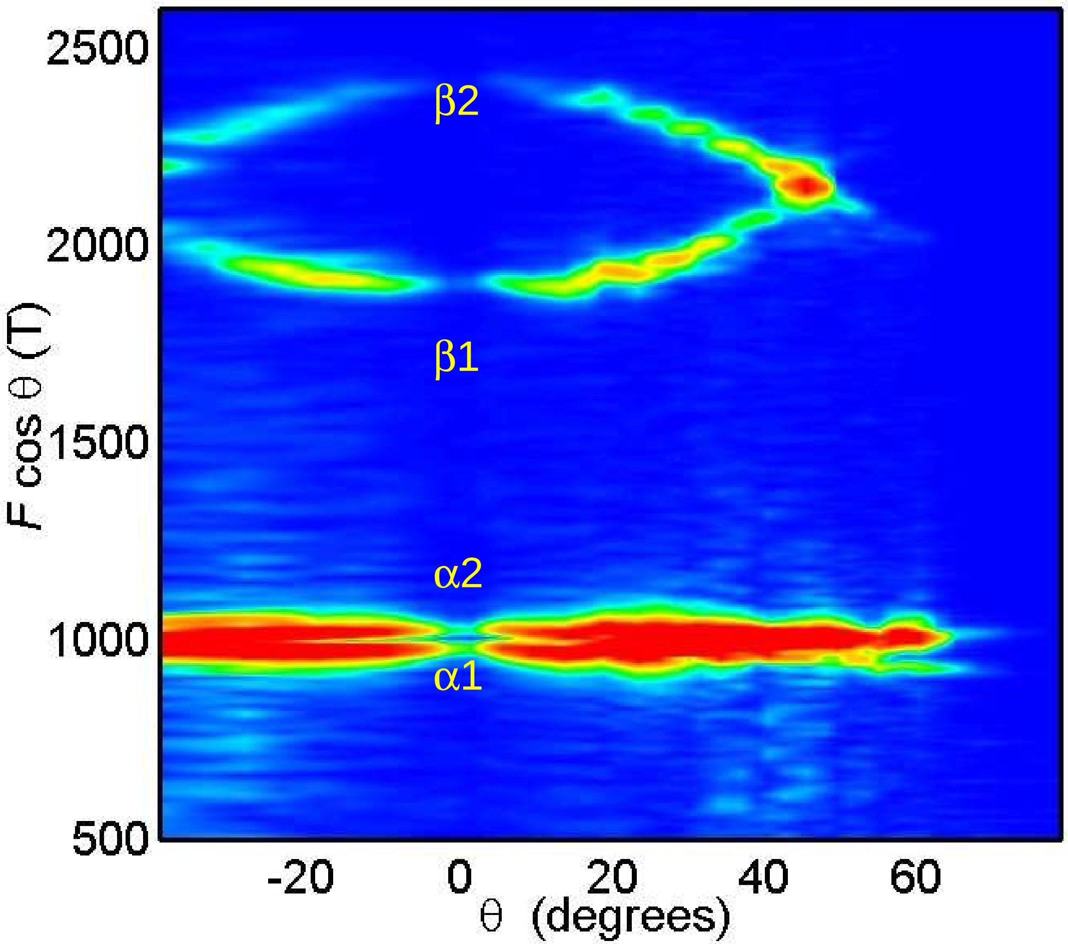


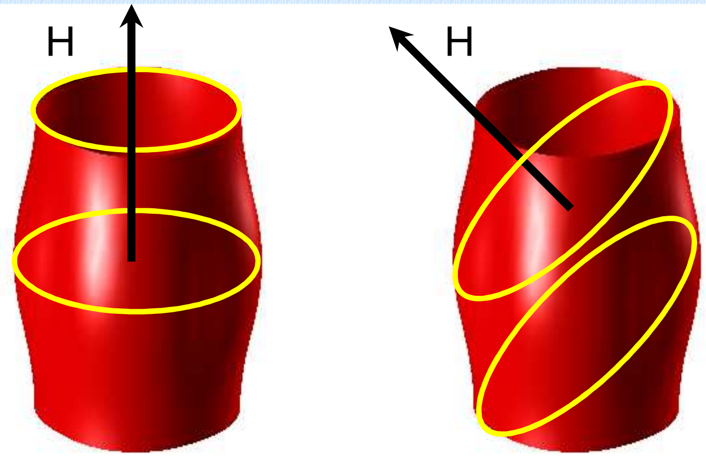
$$F = (\hbar / 2\pi e)\, A(E_F)$$

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





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

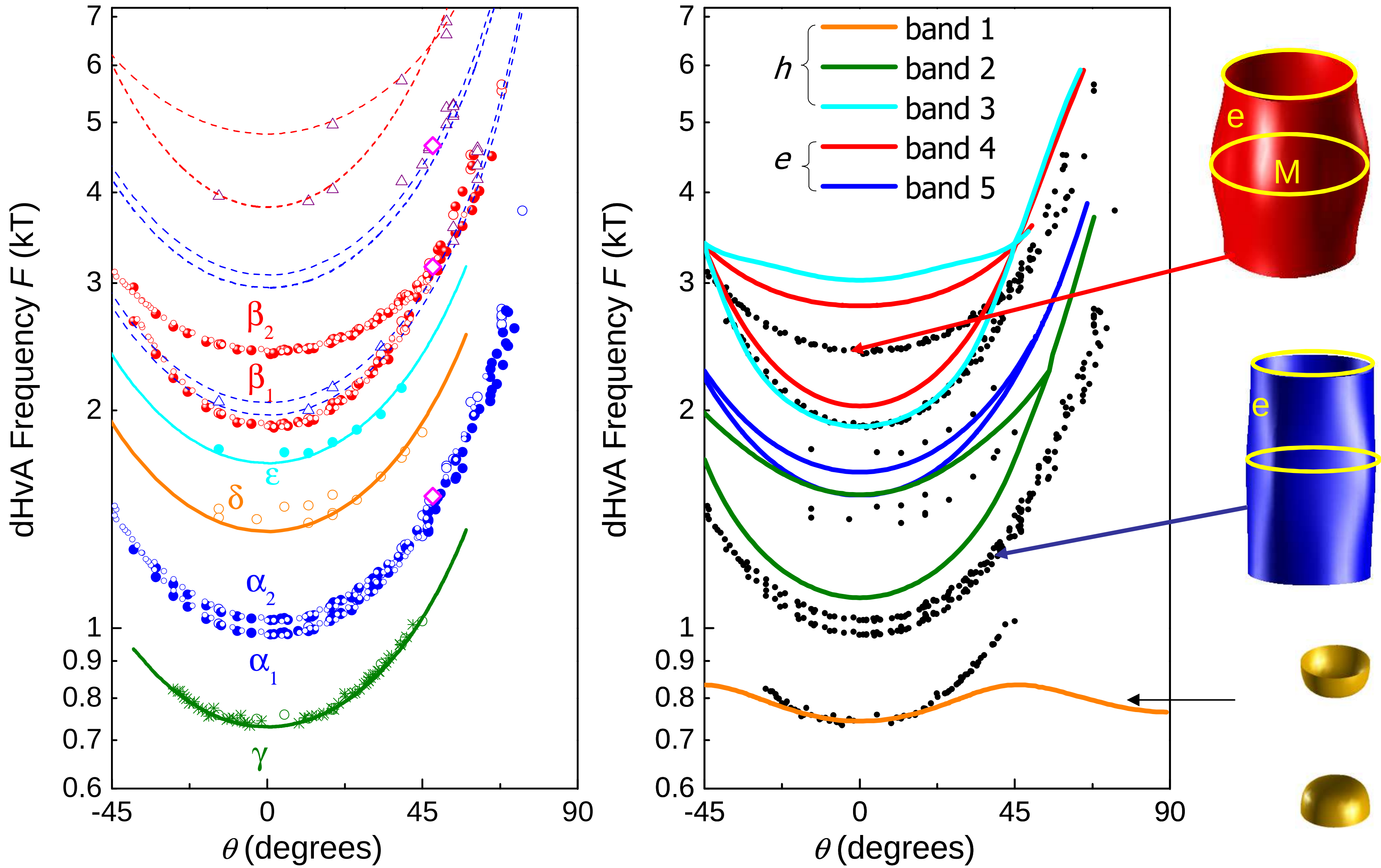
At Yamaji angles all Fermi surface cross sections have equal areas; their magnetization contributions interfere constructively=peak effect.

F(*θ*)=*F*(*0*) / cos*θ*
Quasi-two dimensional cylinder;

Δ*F*α/*F*α ~ 4%;
Δ*F*β/*Fβ* ~23 %;

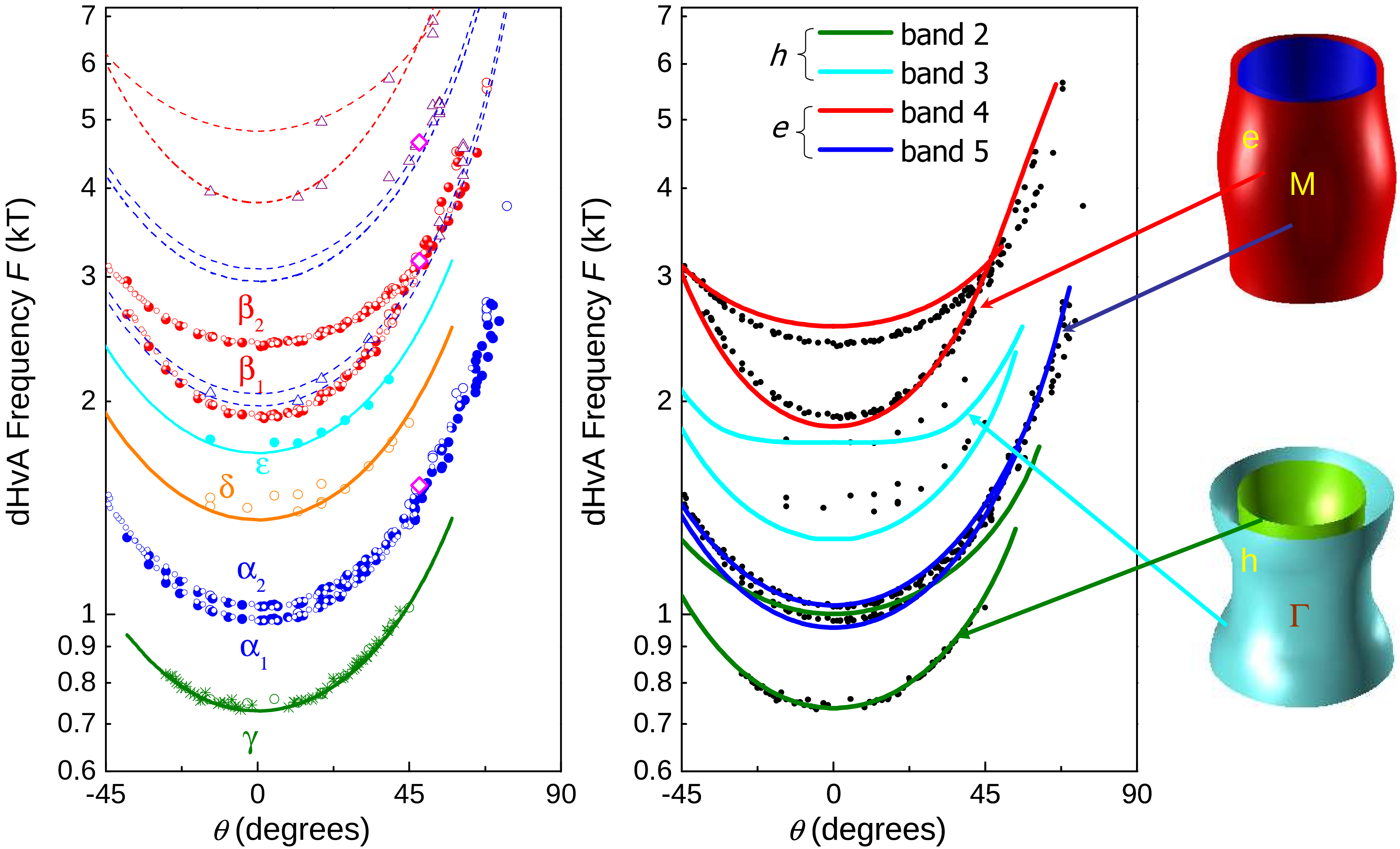
K. Yamaji, J. Phys. Soc. Jpn. 58, 1520 (1989)

dHvA data versus band structure calculations



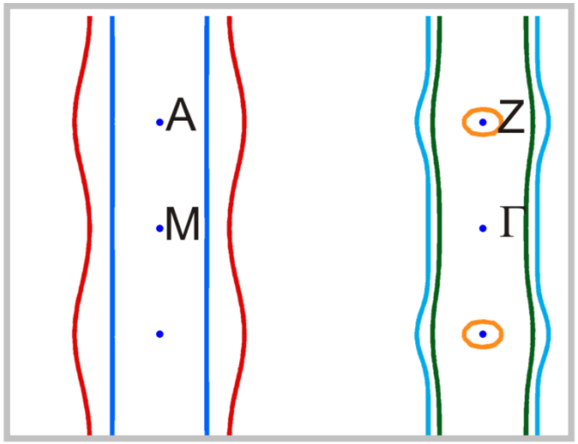
- electronic branches show similar dispersion to the experimental α and β pockets;
- no experimental branch matches the weak dispersion due to the 3D hole pocket;

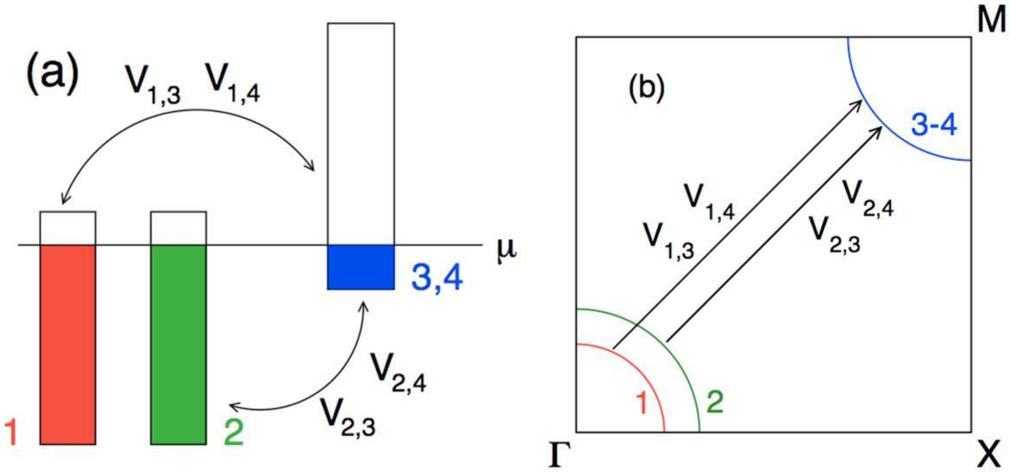
Band shifting and charge balance

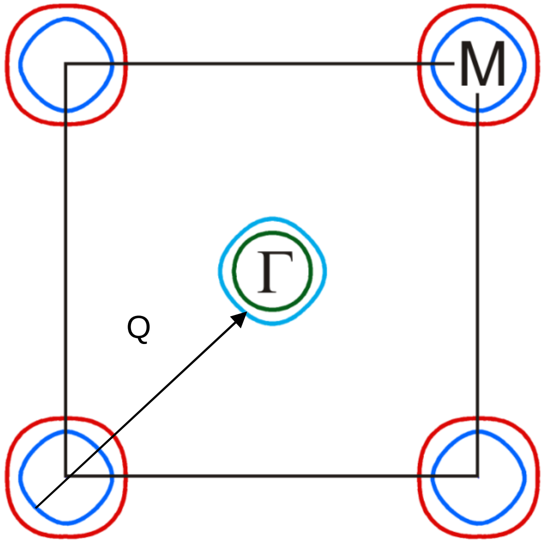


Electron bands shifted by ΔE=+85 meV (band 5), +30 meV (band 4); hole bands all shifted by ΔE=-53 meV; Charge imbalance ~0.034 el/fu; ~1.7% oxygen deficiency in LaFePO.

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);

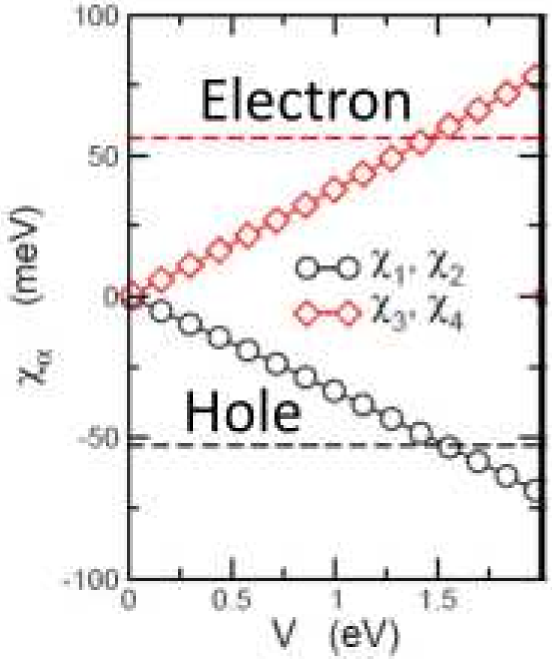
L. Ortenzi *et al.*, PRL 103, 046404 (2009).

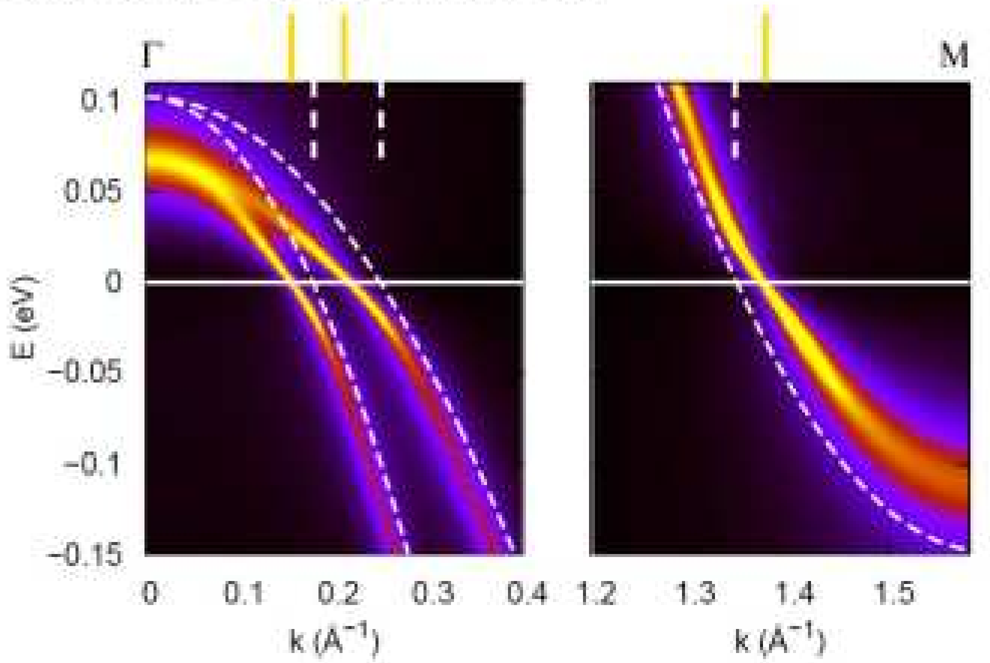
Shrinking of the Fermi surface in LaFePO

Shifts proportional to interband coupling V

Larger coupling → shrinks FS, increases mass, increases T_c

L. Ortenzi, E. Cappelluti, L. Benfatto, L. Pietronero (PRL 09)





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

Shrinking of the Fermi surface pockets

TABLE I. Summary of spin-density wave fluctuation driven superconducting pairing, Pomeranchuk instability, and charge current-density wave.

	Dual processes	Two ways of decoupling	Implication	Cuprate	Iron pnictide
SDW/SC	$Vc^{\dagger}_{\mathbf{k+Q}s}c^{\dagger}_{-\mathbf{k+Q}s'}c_{\mathbf{k}s'}c_{-\mathbf{k}s}$ $V>0$	$-V\vec{S}_{\mathbf{k}}\vec{S}_{-\mathbf{k}}$ or $V\Delta^{\dagger}_{\mathbf{k+Q}}\Delta_{\mathbf{k}}$ $\Delta^{\dagger}_{\mathbf{k}}=c^{\dagger}_{\mathbf{k}s}c^{\dagger}_{-\mathbf{k}s'}$ $\vec{S}_{\mathbf{k}}=\sum_{ss'} c^{\dagger}_{\mathbf{k+Q}s}\vec{\sigma}_{ss'}c_{\mathbf{k}s'}$	$\langle\Delta_{\mathbf{k}}\rangle\langle\Delta_{\mathbf{k+Q}}\rangle<0$ (*)	$\mathbf{Q}=(\pi,\pi)$, both $\cos k_x+\cos k_y$ and $\cos k_x-\cos k_y$ satisfy (*) FS determines $\cos k_x-\cos k_y$	$\mathbf{Q}=(\pi,0)/(0,\pi)$, both $\cos k_x \cos k_y$ and $\sin k_x \sin k_y$ satisfy (*) FS determines $\cos k_x \cos k_y$
SDW/PI	$Vc^{\dagger}_{\mathbf{k+Q}s}c^{\dagger}_{\mathbf{k}s'}c_{\mathbf{k}s'}c_{\mathbf{k+Q}s}$ $V>0$	$-V\vec{S}_{\mathbf{k}}\vec{S}_{\mathbf{k+Q}}$ or $Vn_{\mathbf{k+Q}}n_{\mathbf{k}}$ $n_{\mathbf{k}}=\sum_{s} c^{\dagger}_{\mathbf{k}s}c_{\mathbf{k}s}$ $\vec{S}_{\mathbf{k}}=\sum_{ss'} c^{\dagger}_{\mathbf{k+Q}s}\vec{\sigma}_{ss'}c_{\mathbf{k}s'}$	$\delta n_{\mathbf{k}}\delta n_{\mathbf{k+Q}}<0$	C_{4v} breaking FS distortion See Fig. 11(c)	Shrinking of all pockets. See Figs. 5(c) and 5(d)
SDW/CDW	$Vc^{\dagger}_{\mathbf{k+Q}s}c^{\dagger}_{\mathbf{k+Q}s'}c_{\mathbf{k}s'}c_{\mathbf{k}s}$ $V>0$	$-V\vec{S}_{\mathbf{k}}\vec{S}_{\mathbf{k}}$ or $Vd_{\mathbf{k}}d_{\mathbf{k}}$ $d_{\mathbf{k}}=\sum_{s} c^{\dagger}_{\mathbf{k+Q}s}c_{\mathbf{k}s}$ $\vec{S}_{\mathbf{k}}=\sum_{ss'} c^{\dagger}_{\mathbf{k+Q}s}\vec{\sigma}_{ss'}c_{\mathbf{k}s'}$	$\langle d_{\mathbf{k}}\rangle$=imaginary (orbital current)	DDW See Fig. 11(d)	$(\pi,0)/(0,\pi)$ Orbital-current order See Fig. 8

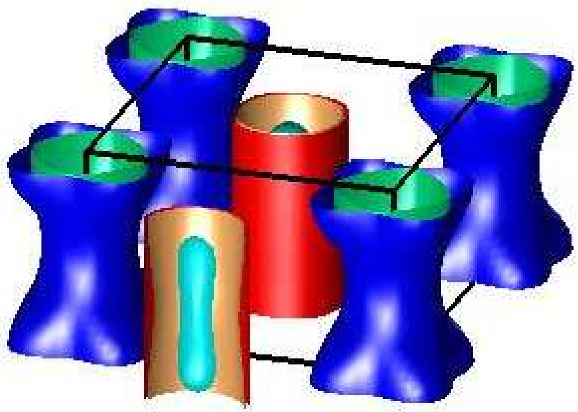
SDW/ Pomerachuk instability in the iron pnictide tends to shrink both the electron and hole pockets. Antiferromagnetically driven electronic correlations.

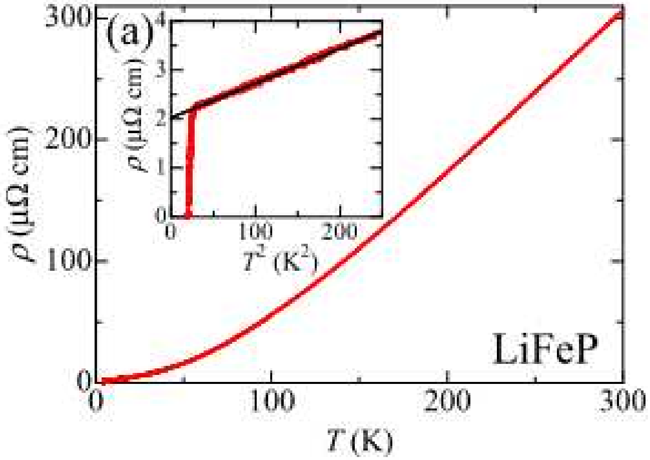
Hui Zhai, *et al.*, Physical Review B, 80, 064517 (2009)

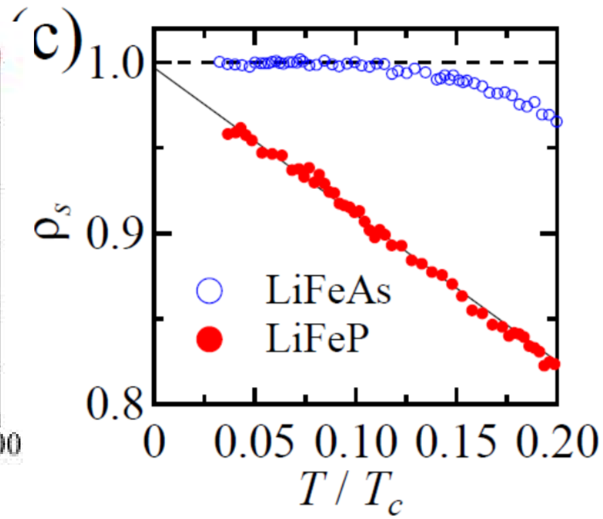
I. Fermi surface shrinking and the effects of electronic correlations – LiFeP and LiFeAs

Quantum oscillations in the superconducting LiFeP and LiFeAs

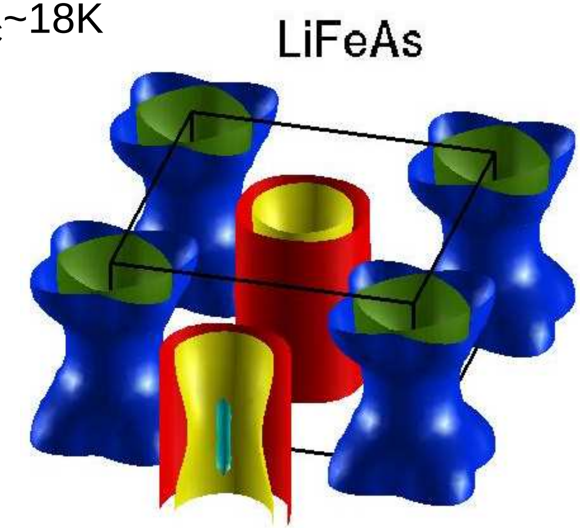
LiFeP nodal superconductor T_C~4K

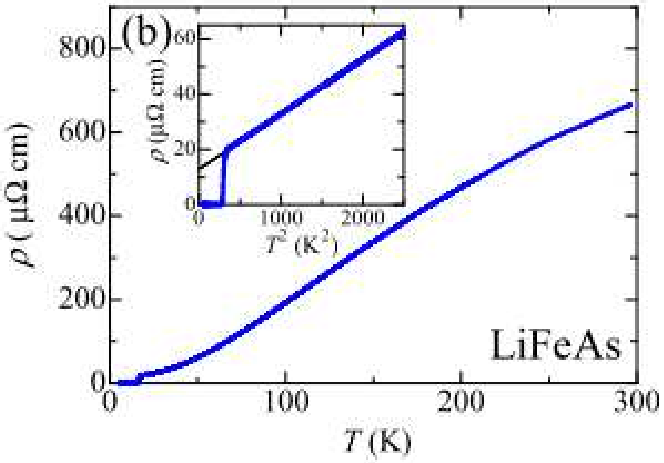


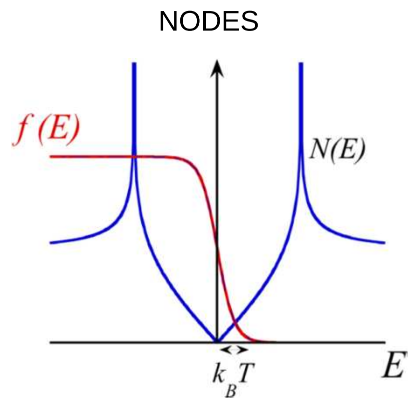




LiFeAs nodeless superconductor
T_C~18K

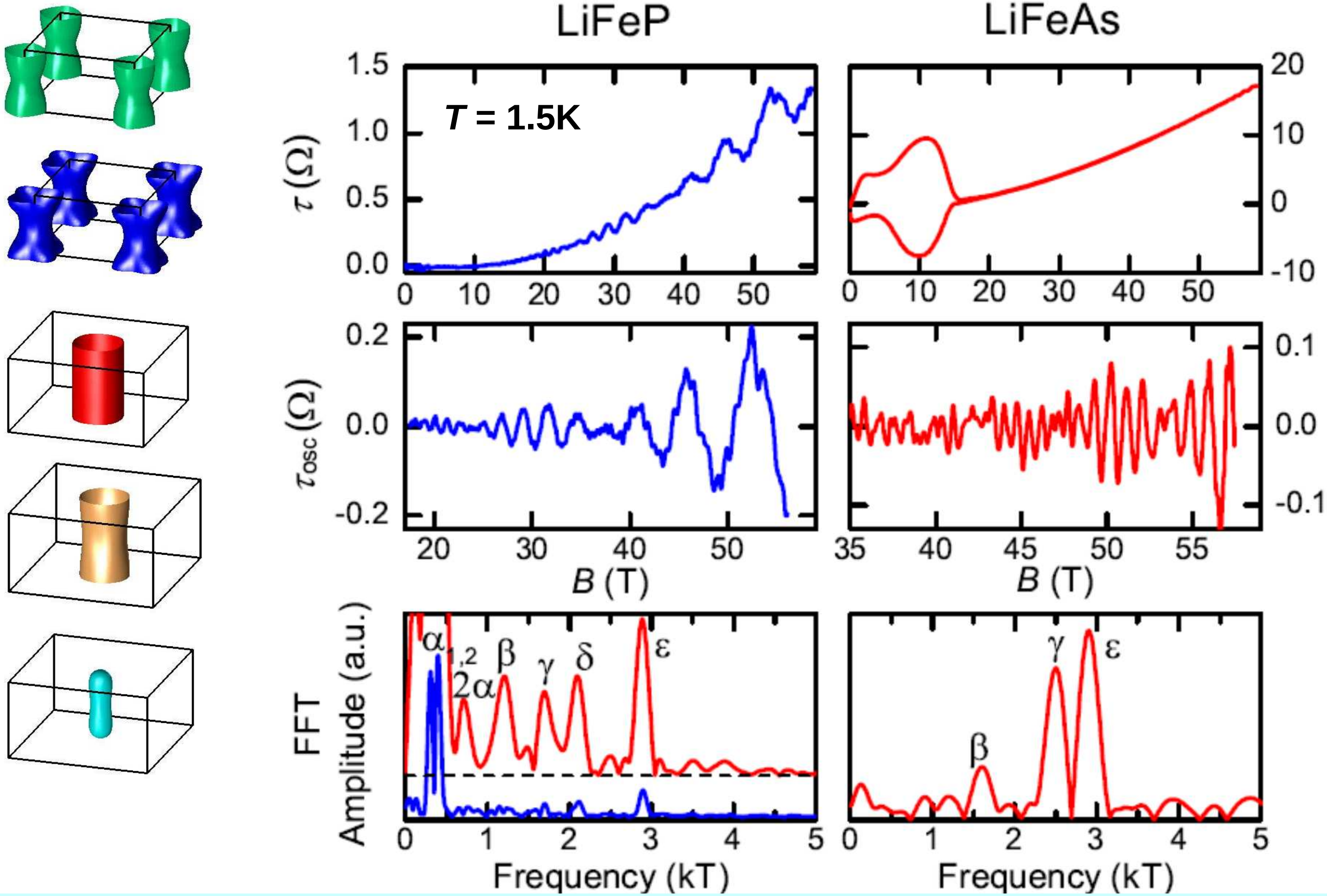






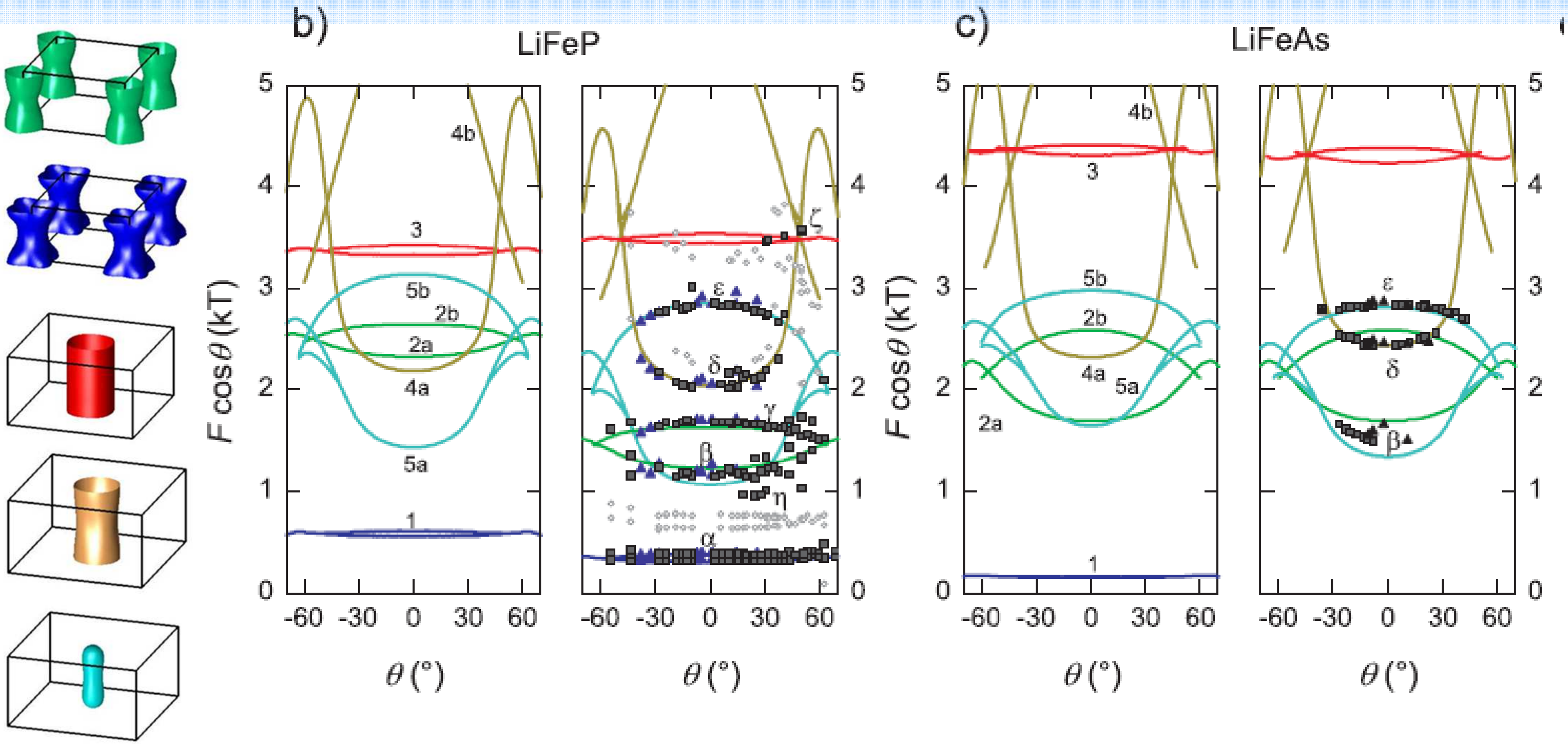
S. Kasahara et al., Phys. Rev. B 85, 060503(R) (2012)
K. Hashimoto et al., Phys. Rev. Lett. 108, 047003

Quantum oscillations in LiFeAs and LiFeP



Torque shows quantum oscillations in LiFeP and LiFeAs above H_{c2}. There are 5 different frequencies for LiFeP and 3 different frequencies observed for LiFeAs.

Quantum oscillations in LiFeAs and LiFeP



For LiFeP, small shifts of the band energies: +20 meV and +45 meV for band 4 and 5 (electron) and −65, −80, 18 meV for bands 1, 2 and 3 (hole) bring the observations and calculations into almost perfect agreement. These shifts shrink both the electron and hole FSs and likely originate from many body corrections to the DFT bandstructure.

C. Putzke, A.I. Coldea *et al.*, Phys. Rev. Lett. **108**, 047002 (2012)

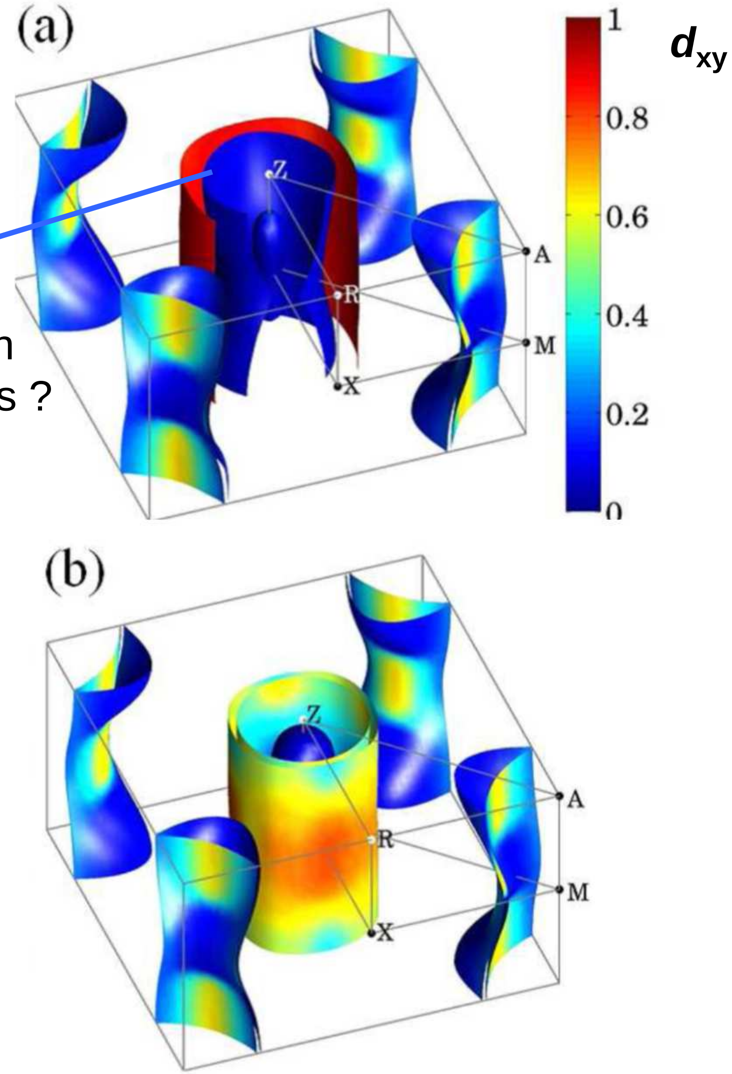
Fermi surface parameters in LiFeAs and LiFeP

LiFeP DFT calc.			Experiment			
Orbit	$F(T)$	m_b	Orbit	$F(T)$	m^*	$\frac{m^*}{m_b}-1$
1_a	557	−0.44	α_1	316(2)	1.1(1)	1.5(3)
1_b	607	−0.39	α_2	380(2)	1.0(1)	1.6(3)
2_a	2325	−1.7	$\beta^\dagger$	2040(10)†	4.4(1)†	0.6(2)†
2_b	2645	−1.6	γ	1670(10)	2.7(2)	0.7(1)
3_a	3328	−1.8	$\zeta^\dagger$	5550(10)†	7.7(2)†	2.1(5)†
3_b	3428	−1.6	$\zeta^\dagger$	5550(10)†	7.7(2)†	2.1(5)†
4_a	2183	+0.92	δ	2040(20)	2.2(1)	1.4(2)
4_b	6014	+1.8				
5_a	1430	+1.1	$\beta^\sharp$	1160(10)	3.6(2)$^\sharp$	2.3(2)$^\sharp$
5_b	3142	+0.83	ε	2840(10)	2.2(2)	1.6(3)

Location of nodes ?

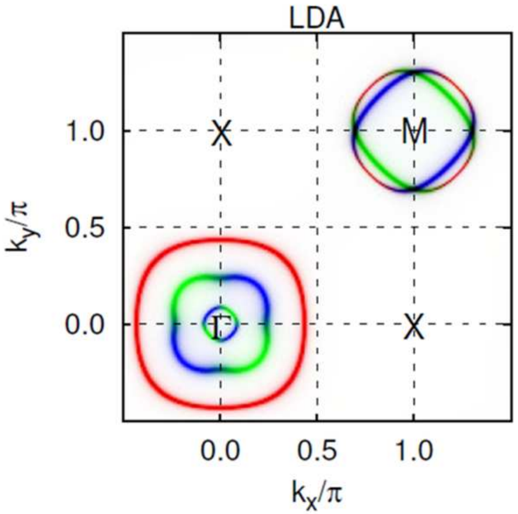
LiFeAs DFT calc.			Experiment			
Orbit	$F(T)$	m_b	Orbit	$F(T)$	m^*	$\frac{m^*}{m_b}-1$
1_a	130	−0.31				
1_b	149	−0.23				
2_a	1585	−2.11				
2_b	2529	−1.50				
3_a	4402	−2.11				
3_b	4550	−2.12				
4_a	2359	+1.22	δ	2400(25)	5.2(4)	3.3(3)
4_b	6237	+2.34				
5_a	1584	+1.54	$\beta^\sharp$	1590(10)	6.0(4)$^\sharp$	2.9(3)$^\sharp$
5_b	2942	+1.02	ε	2800(40)	5.2(4)	4.1(4)

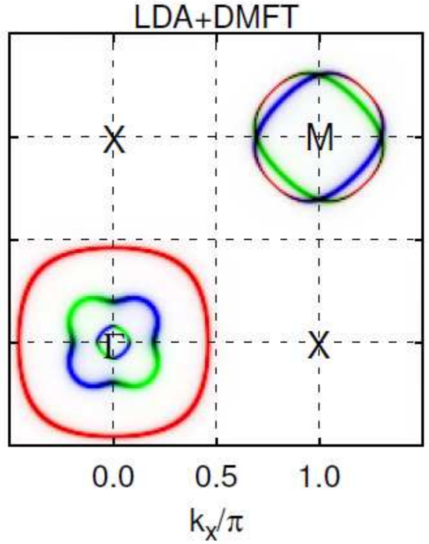
PRL **108**, 047002 (2012)

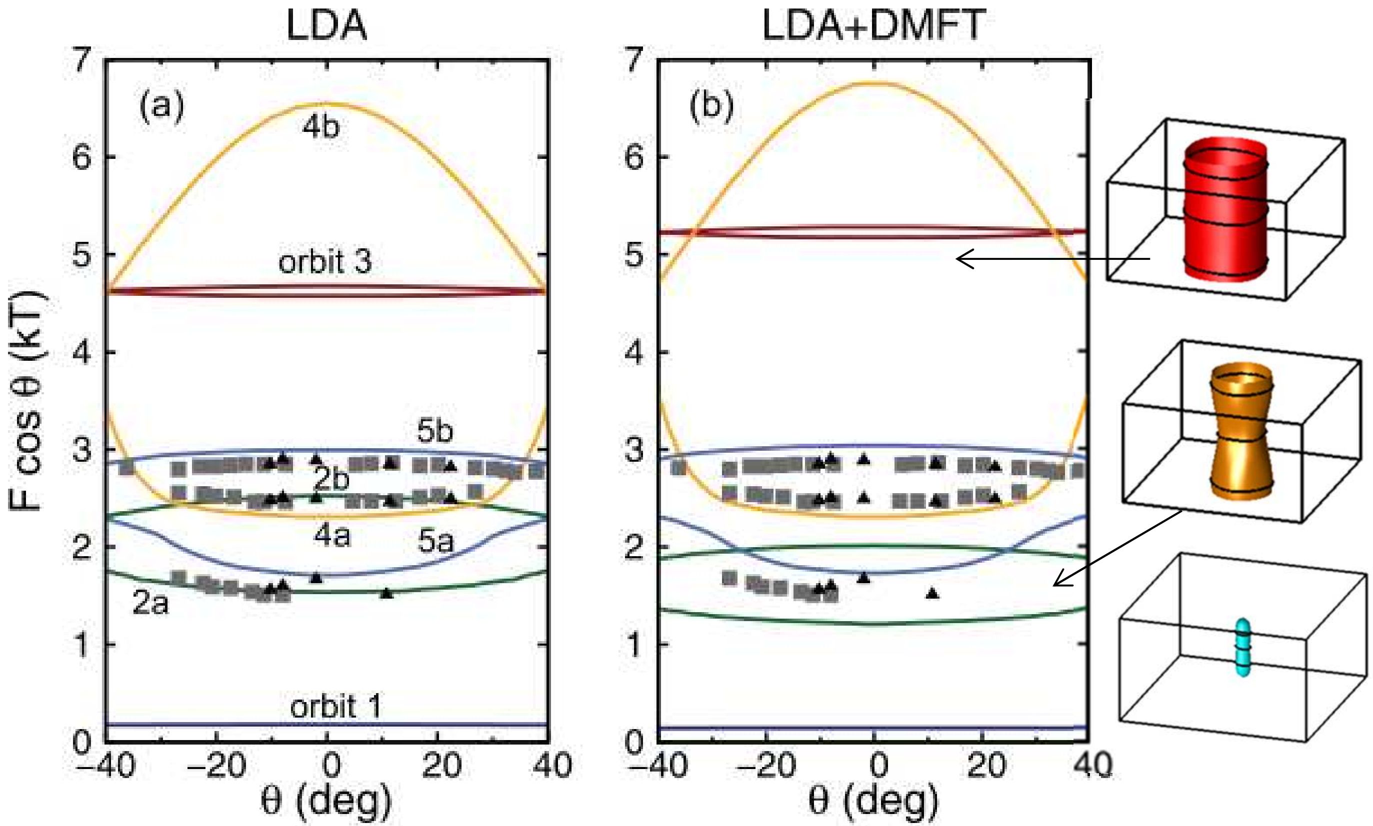


K. Hashimoto *et al.*, arXiv:1107.4505 (2011)

Effect of electronic correlations in LiFeAs







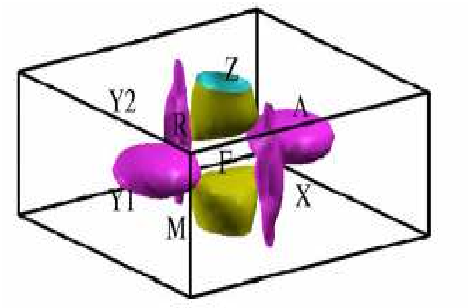
The effect of correlations on the Fermi surface manifests itself mainly in a shrinking of the middle hole pocket, and, in order to preserve the electron count, an increase of the outer hole pocket size.

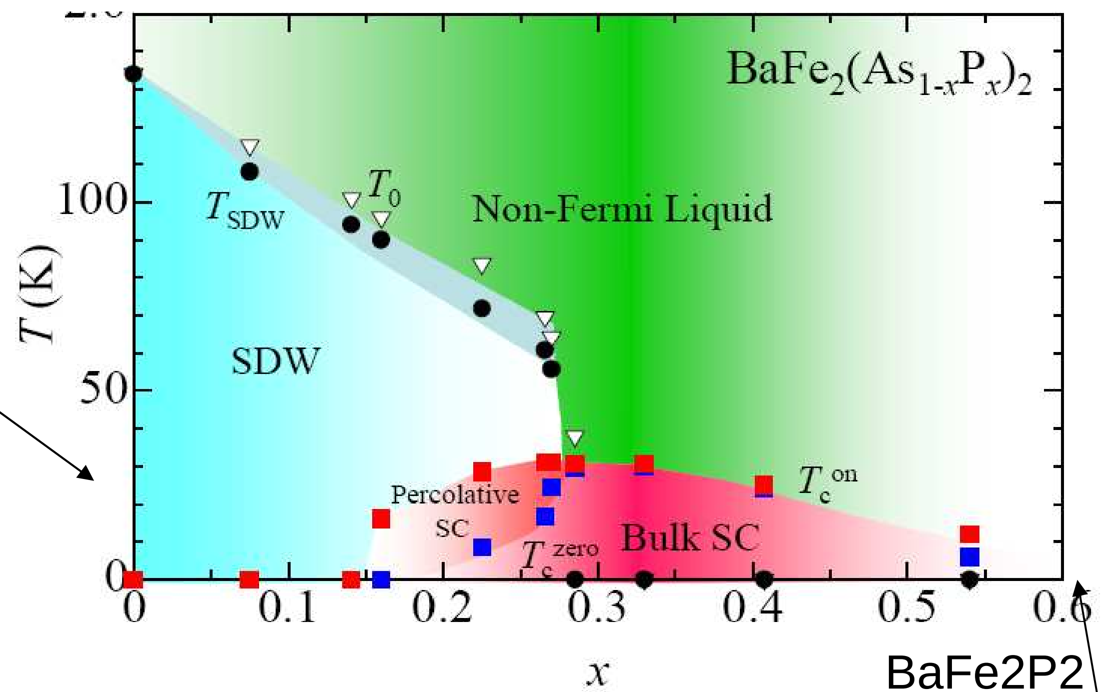
Ferber et al., Phys. Rev. B 85, 094505 (2012)

I. Fermi surface shrinking and the effects of electronic correlations – BaFe2(As,P)

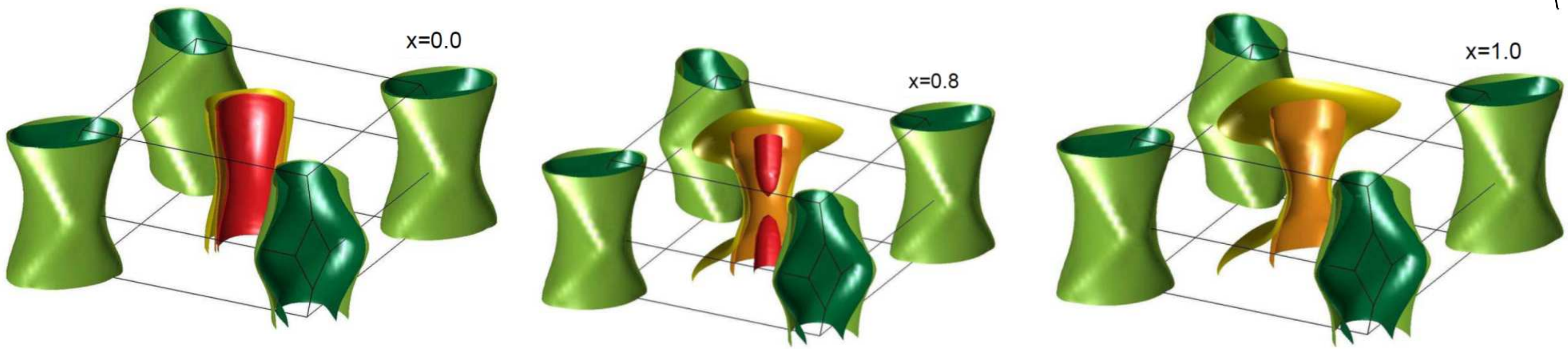
Effect of chemical pressure: P/As substitution

BaFe2As2 (low T)





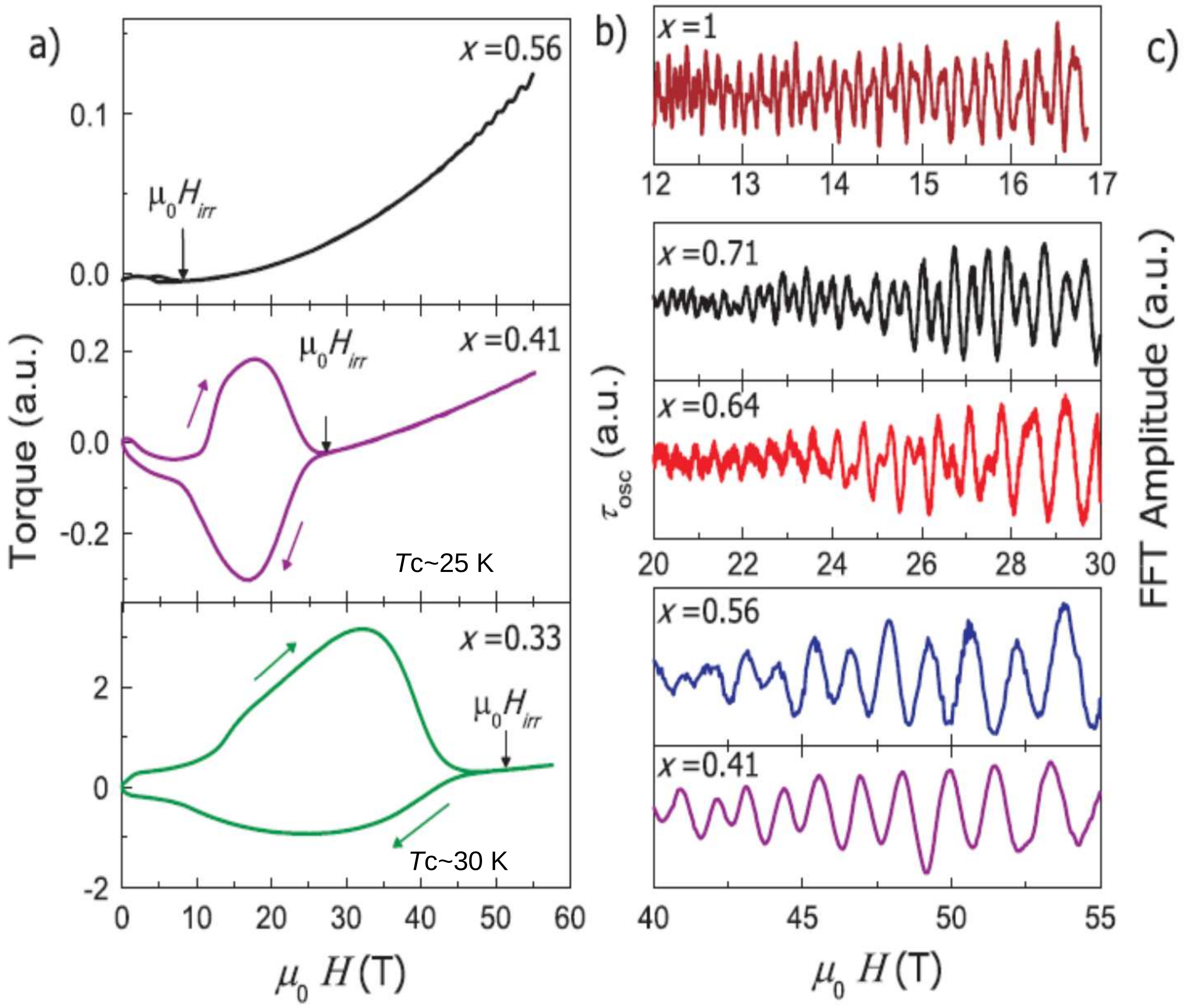
BaFe2P2



W. Xie, PRB 79, 115128 (2009)

S. Kasahara et al. , PRB 81, 134422 (2010)

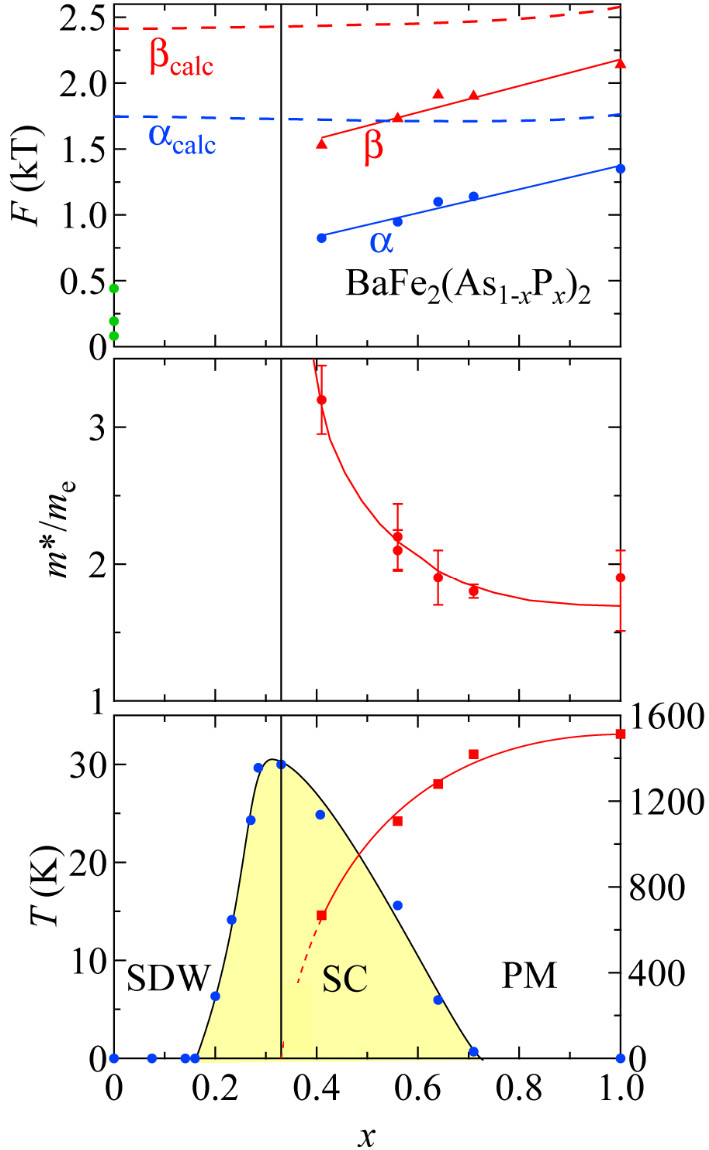
Evolution of Fermi surface in $BaFe_2(As_{1-x}P_x)_2$



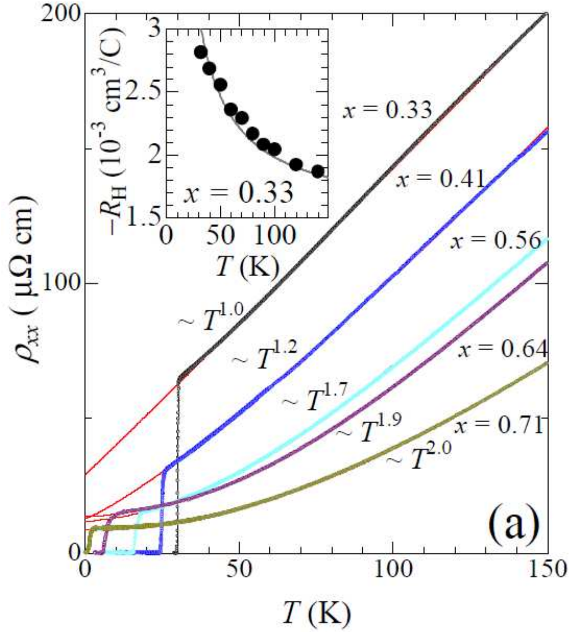
oscillations observed for materials with *T*c = 0 – 25 K; *T*max=30 K for *x* = 0.33;

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

Spin fluctuations in BaFe2(As1-xPx)2

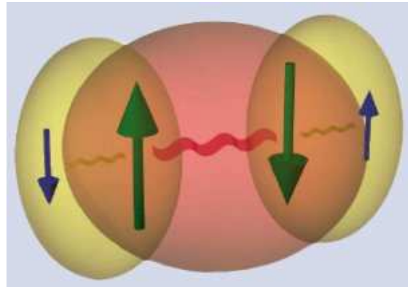


H. Shishido *et al., AIC,* PRL 104, 057008 (2010)

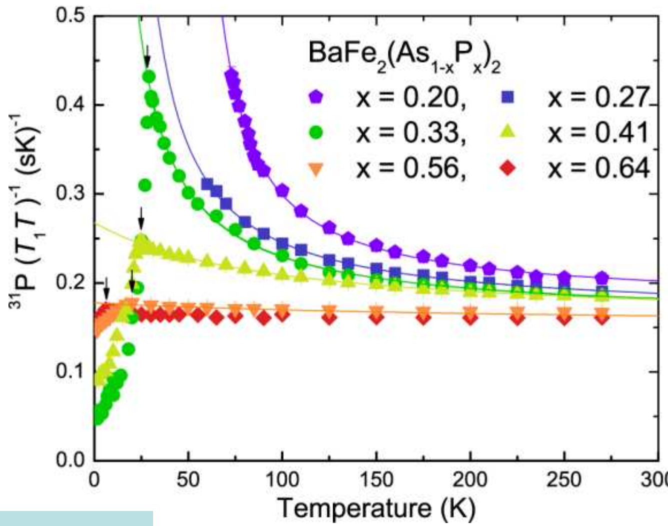


$\rho = \rho_0 + AT^\alpha$

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



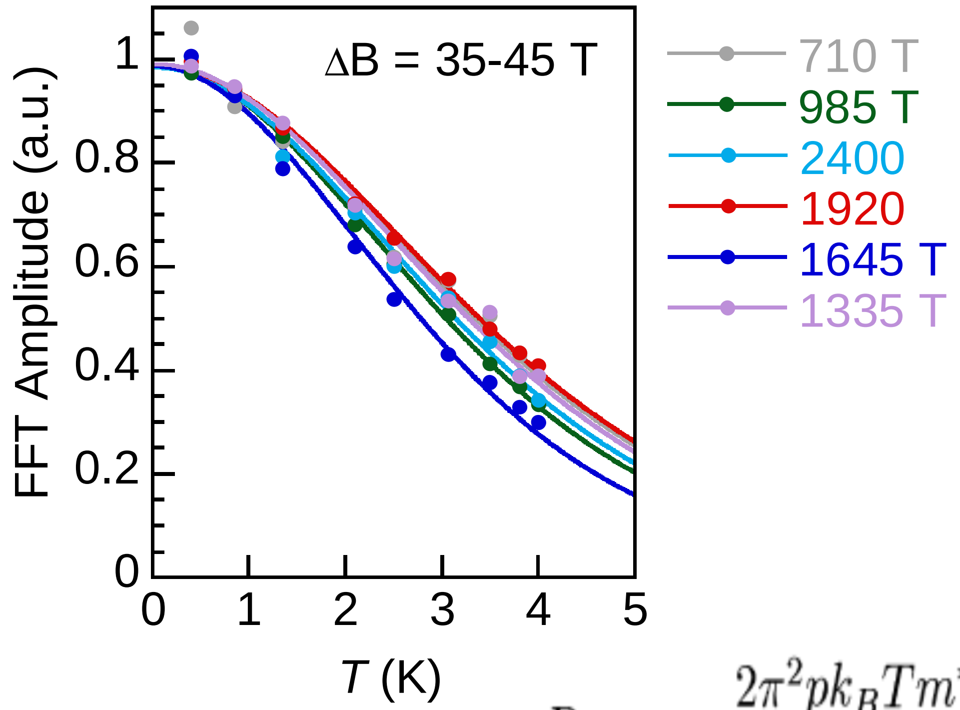
Antiferromagnetic spin fluctuations close to QCP

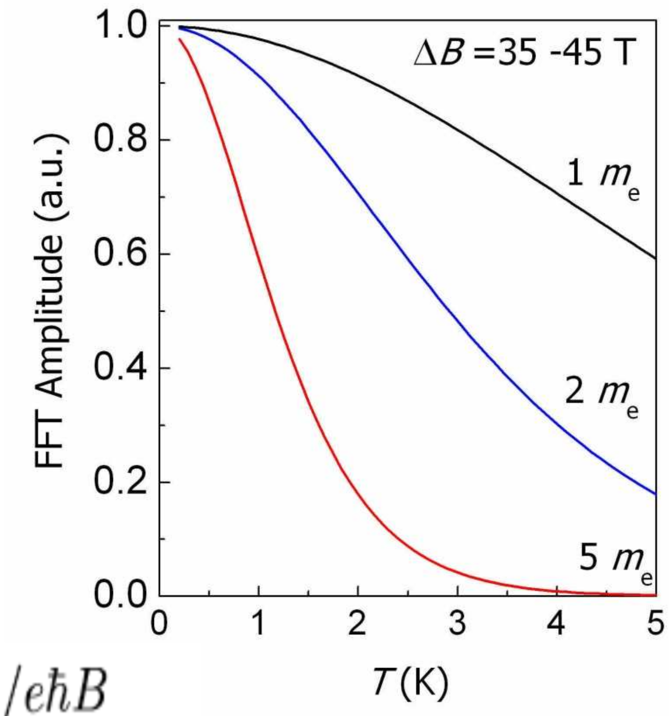


$1/T_1T \sim 1/(T+\theta)$

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

Moderate mass enhancement in LaFePO





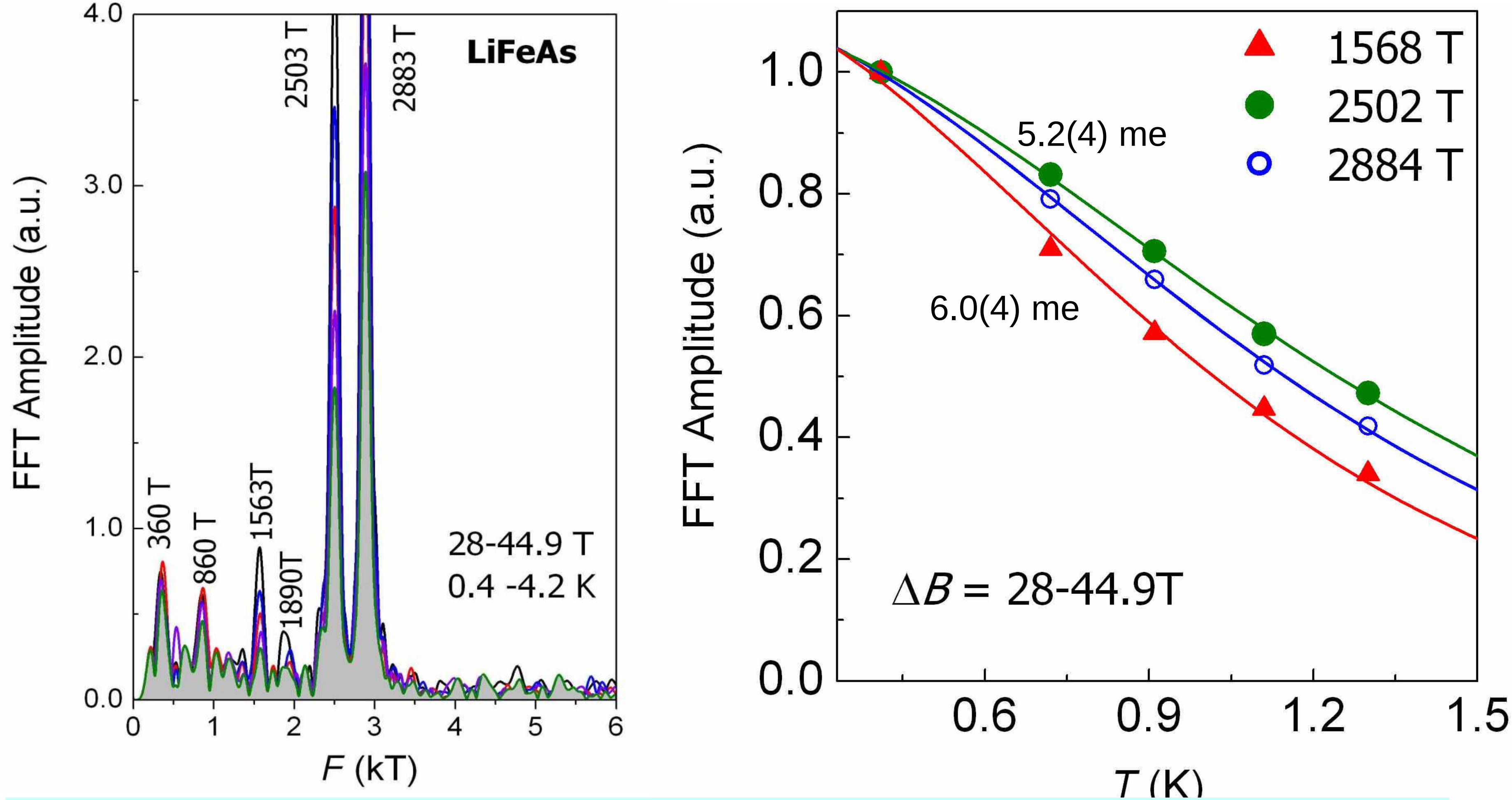
$$R_T = \frac{2\pi^2 p k_B T m^*/e\hbar B}{\sinh\left(2\pi^2 p k_B T m^*/e\hbar B\right)}$$

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

(el-el + el-ph)

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

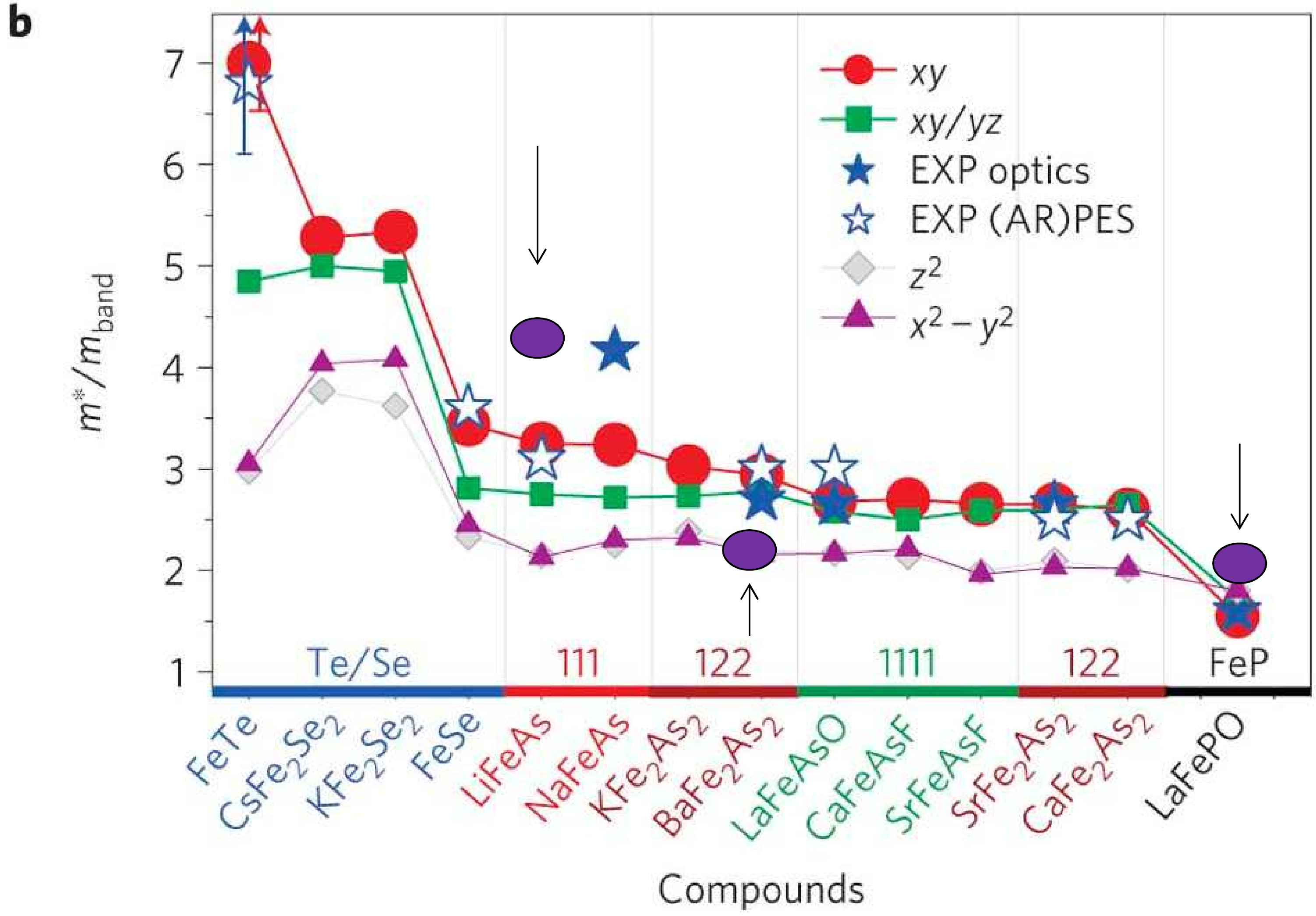
Heavier quasiparticles in LiFeAs



Heavy effective masses in LiFeAs for the electron bands as compared to other iron pnictides; band masses 1-1.5 me and electron-phonon coupling ~0.25;

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

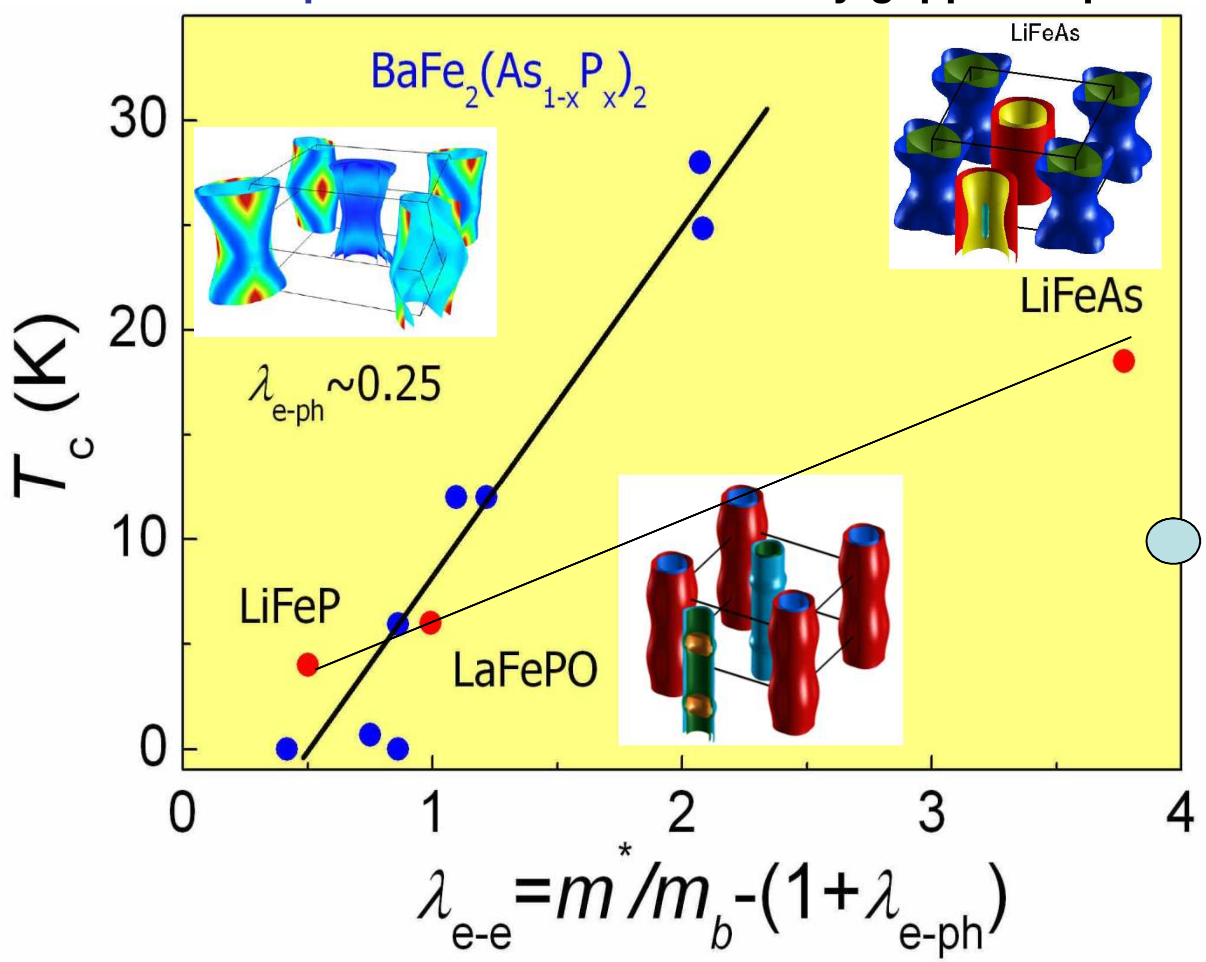
Correlations in iron pnictides



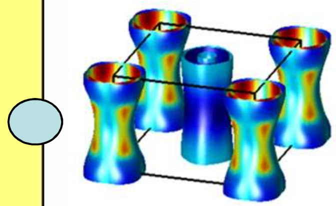
Nature Materials, 10, 932–935, (2011)

The strength of electronic correlations. Electronic bands in clean superconductors

Nodal superconductors **Fully gapped superconductor**



FeSe



PRL **108**, 047002 (2012)**;** PRL **101**, 216402 (08); PRL **104**, 057008 (2010);

Summary of quantum oscillation in iron-based superconductors

- Quantum oscillations in iron pnictides are in broad agreement with band structure.

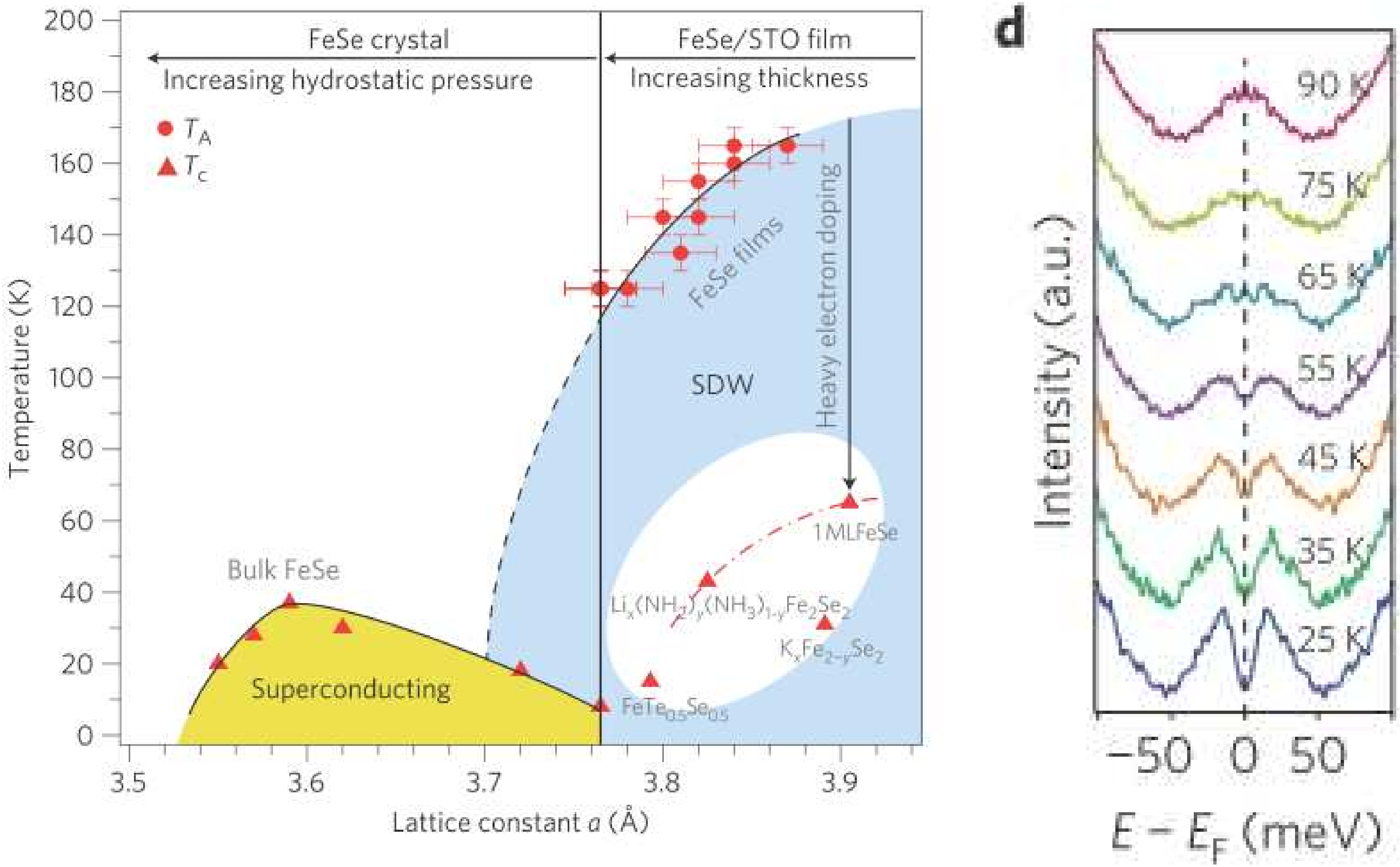
- Fermi surface shrinking for superconducting compounds as compared with band structure calculations; local correlations or partially from long-range spin fluctuations?

- Mass enhancement in the clean and nodal superconductors correlates with the increase in *T*c for isoelectronic system like $BaFe_2(P_{1-x}As_x)_2$ and LiFeAs and LiFeP; electronic correlations are important (quantum critical point ?).

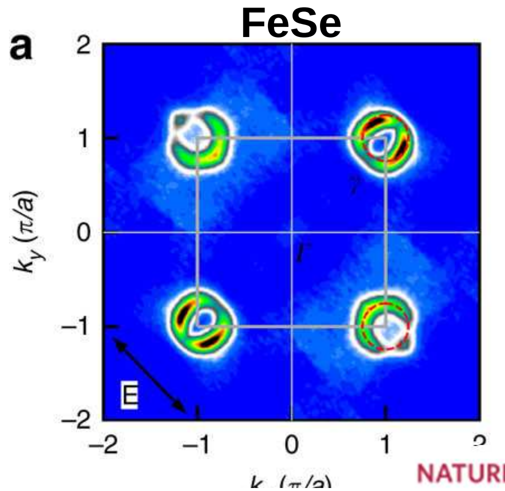
PRL **101**, 216402 (08); PRL**103**, 026404 (09), PRL**103**, 076401 (2009) ; PRL **104**, 057008 (2010);

Electronic structure of bulk FeSe from ARPES and quantum oscillations

Unusual high *Tc* in a mono-layer of FeSe



ARPES and pressure effects



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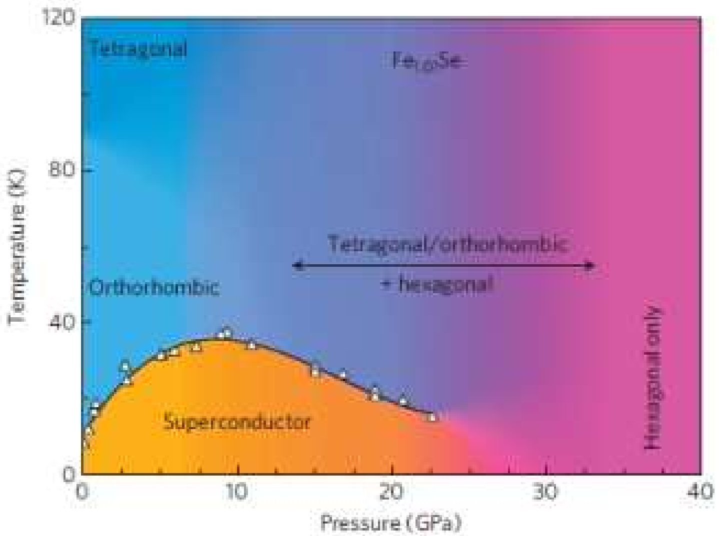
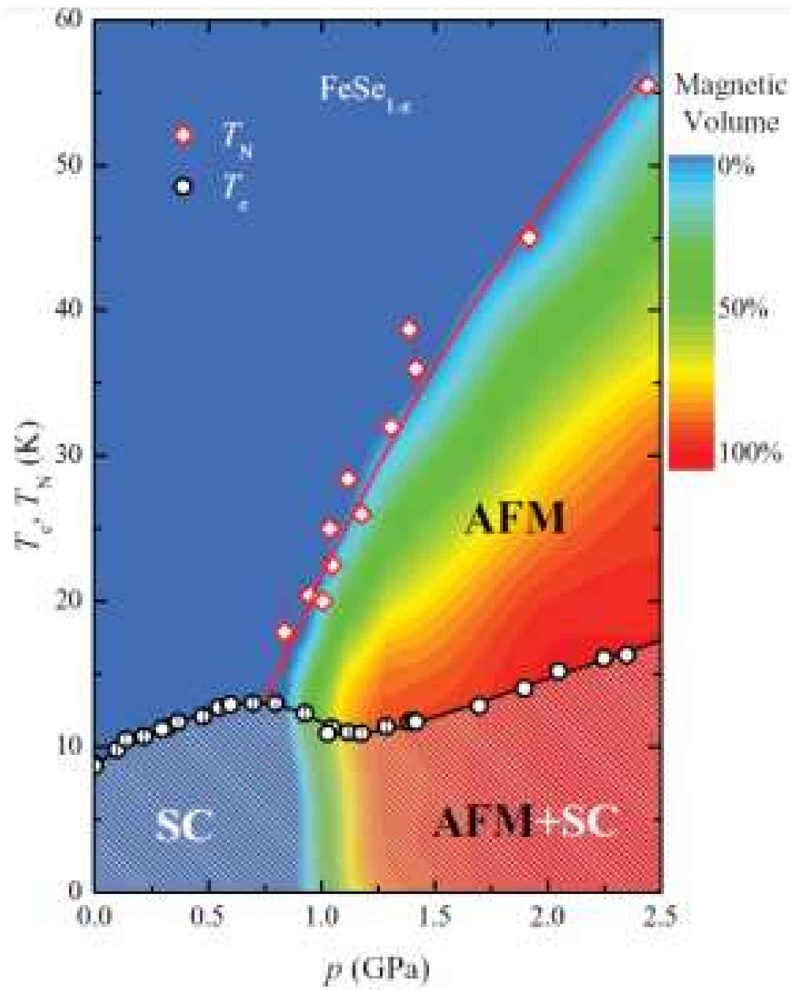
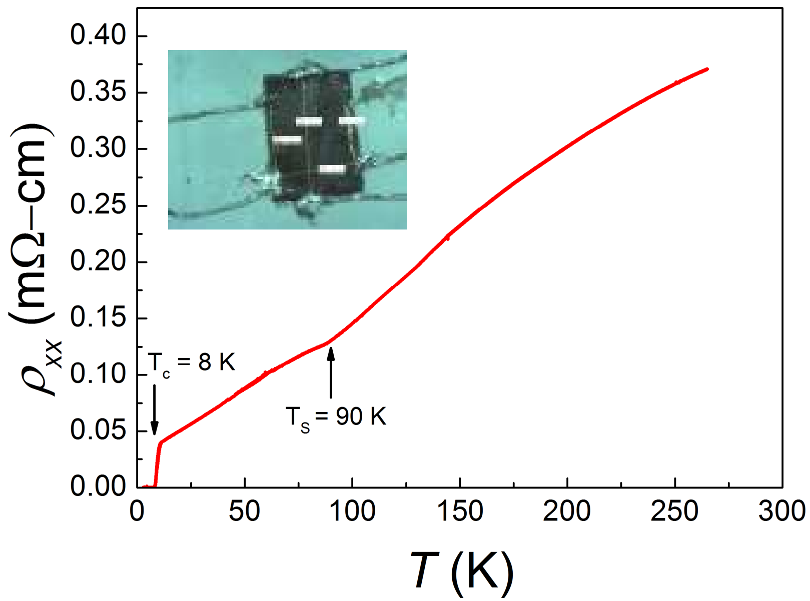


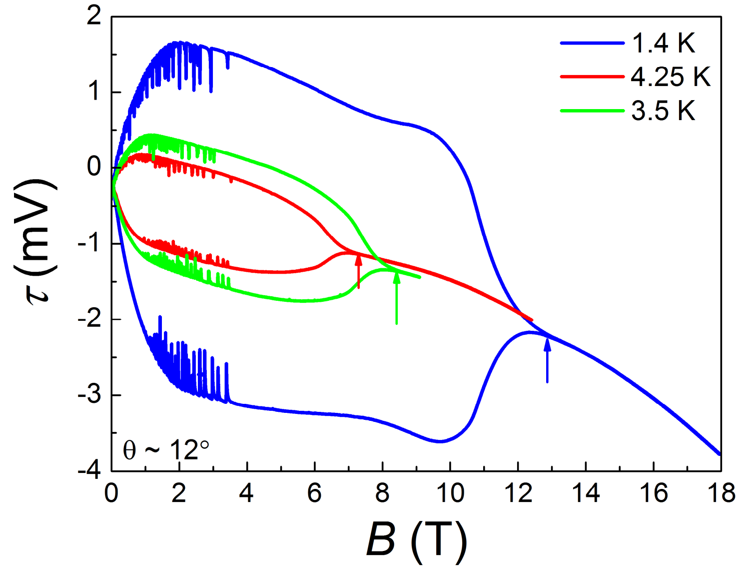
Medvedev et al 2010

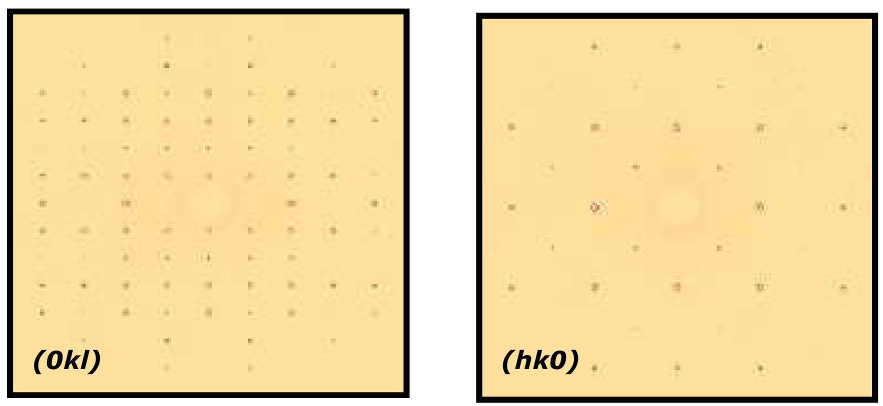


Bendele et al 2012:
magnetic state at low pressure

Superconductivity and structural transition in FeSe







M. Watson et al., Oxford (2014)