Superconductivity and Magnetism in novel Fe-based superconductors

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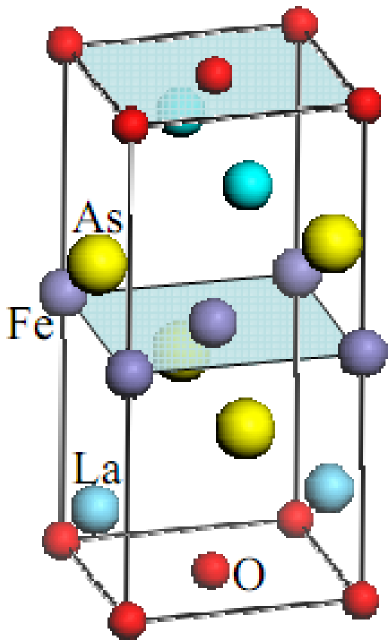
More a progress report than a talk

$Re(O_{1-x}F_x)FeAs$ Superconductors

Compound (powder & single crystals)	T_c	Reference
LaOFeP	~5 K	Y. Kamihara et al., J. Am. Chem. Soc.128, 10012 (2006)
LaNiOP	~3 K	T. Watanabe et al., Inorg. Chem. 46, 7719 (2007)
$La[O_{1-x}F^{-}_{x}]FeAs$ $La[O_{1-x}Ca^{2+}_{x}]FeAs$	26 K (x=0.05-0.12) 0 K	Y. Kamihara et al., J. Am. Chem. Soc.130, 3296 (2008)
$La[O_{1-x}F_x]NiAs$	3.8 K (x=0.1)2.75 K (x=0)	Z. Li et al., arXiv:0803.2572
$(La_{1-x}Sr_x)ONiAs$	3.7 K (x=0.1-0.2) 2.75 K (x=0)	L. Fang et al., arXiv:0803.3978
$(La_{1-x}Sr_x)OFeAs$	25 K (x=0.13)	H.-H. Wen et al., EPL 82, 17009 (2008)
$Ce[O_{1-x}F_x]FeAs$	41 K (x=0.2)	G.F. Chen et al., PRL 100, 247002 (2008)
$Pr[O_{1-x}F_x]FeAs$ $Nd[O_{1-x}F_x]FeAs$	52 K (x=0.11)	Z.-A. Ren et al., arXiv:0803.4283; Z.-A. Ren et al., EPL, 82 (2008)
$Gd[O_{1-x}F_x]FeAs$	36 K (x=0.17)	P. Cheng et al., Science China 51(6), (2008).
$Sm[O_{1-x}F_x]FeAs$	55 K (x=0.1-0.2)	Z.-A. Ren et al., Chin. Phys. Lett. 25, (2008); R.H. Liu et al., arXiv:0804.2105

Crystal Structure of ReFeAs($O_{1-x}F_x$)

Quasi-2D Fe-As layers divided by La with Fe forming a square lattice



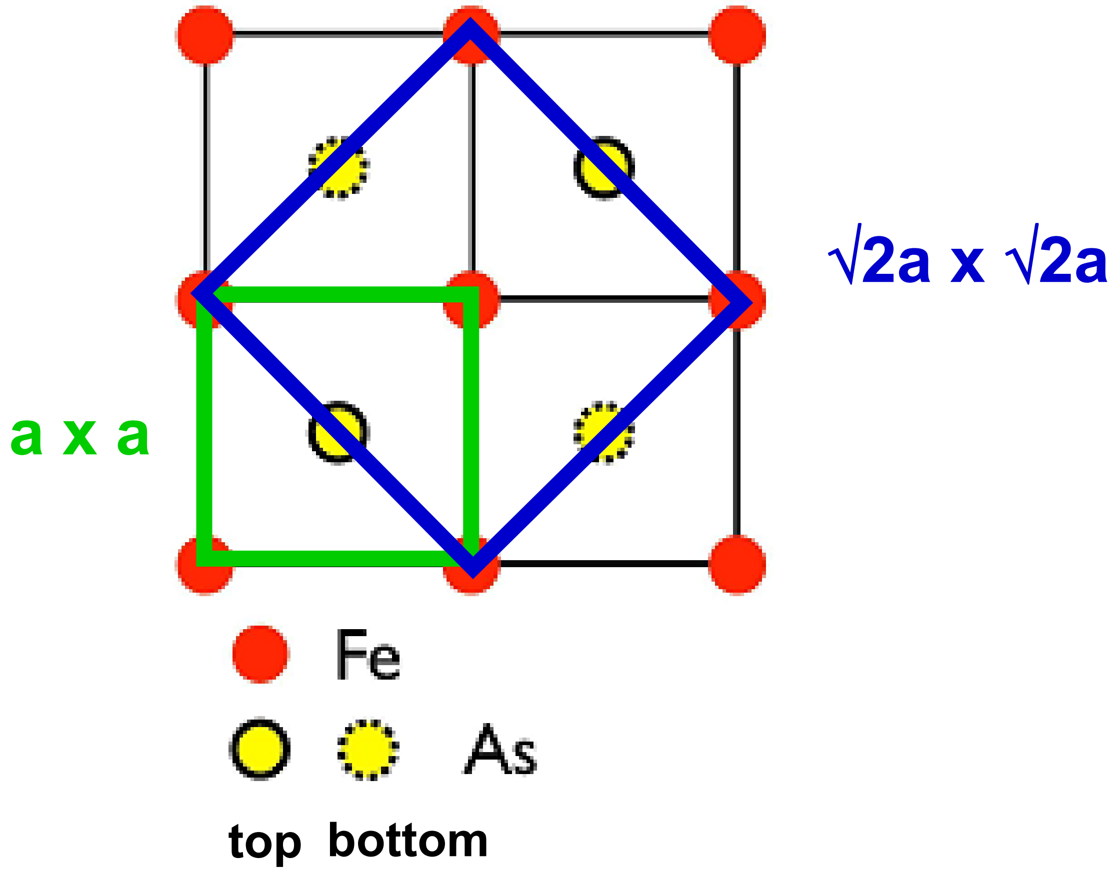
Tetragonal *P4/nmm* space group

The unit cell contains two molecules, and the chemical formula is represented by (La_2O_2)(Fe_2 As_2)

	a (Å)	c (Å)
SmOFeAs	3.940	8.496
NdOFeAs	3.965	8.575
PrOFeAs	3.985	8.595
CeOFeAs	3.996	8.648
LaOFeAs	4.038	8.753

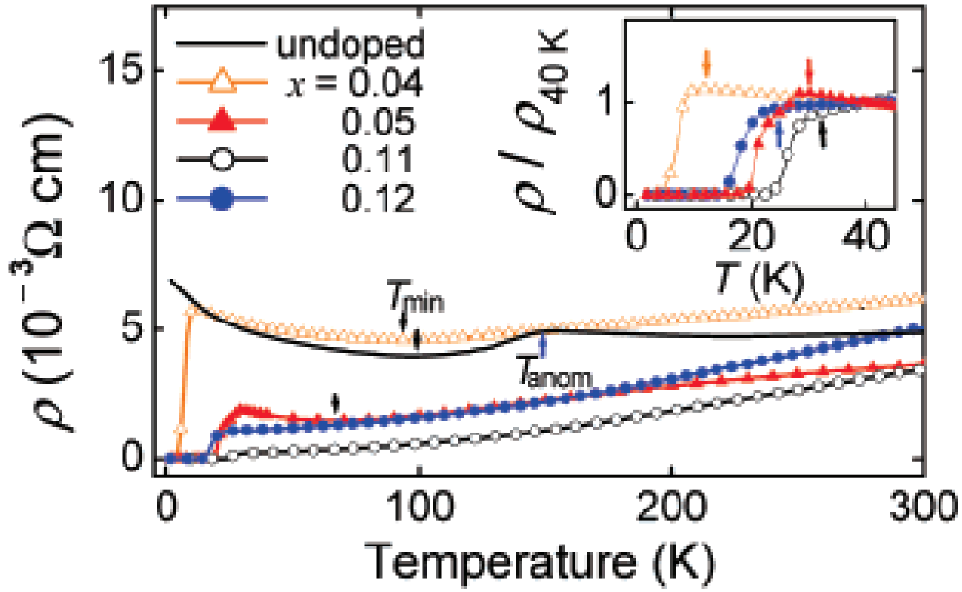
Y. Kamihara et al., J. Am. Chem. Soc. 130, 3296 (2008)

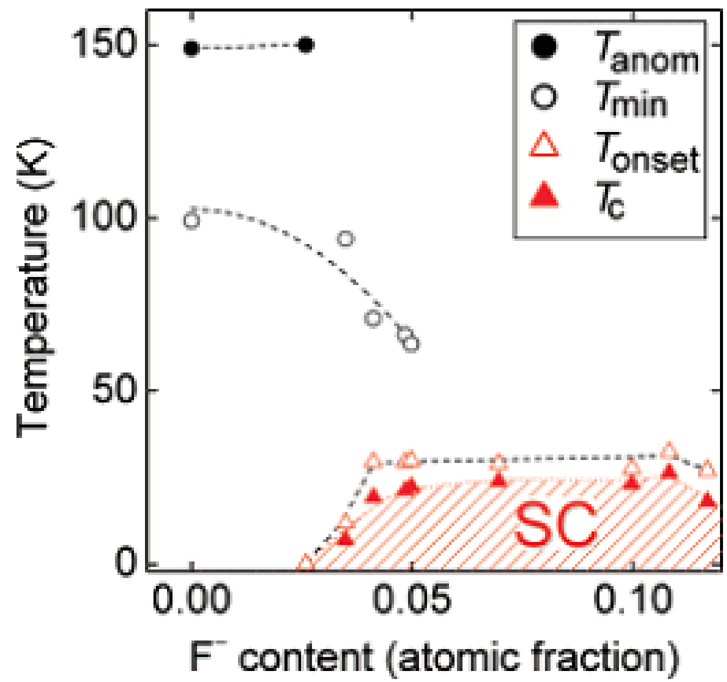
Fe-layered structure and elementary unit cell



Phase diagram: n-doped ($La^{3+}[O^{2-}{}_{1-x}F^{1-}{}_{x}]$) +($Fe^{2+}As^{3-}$)

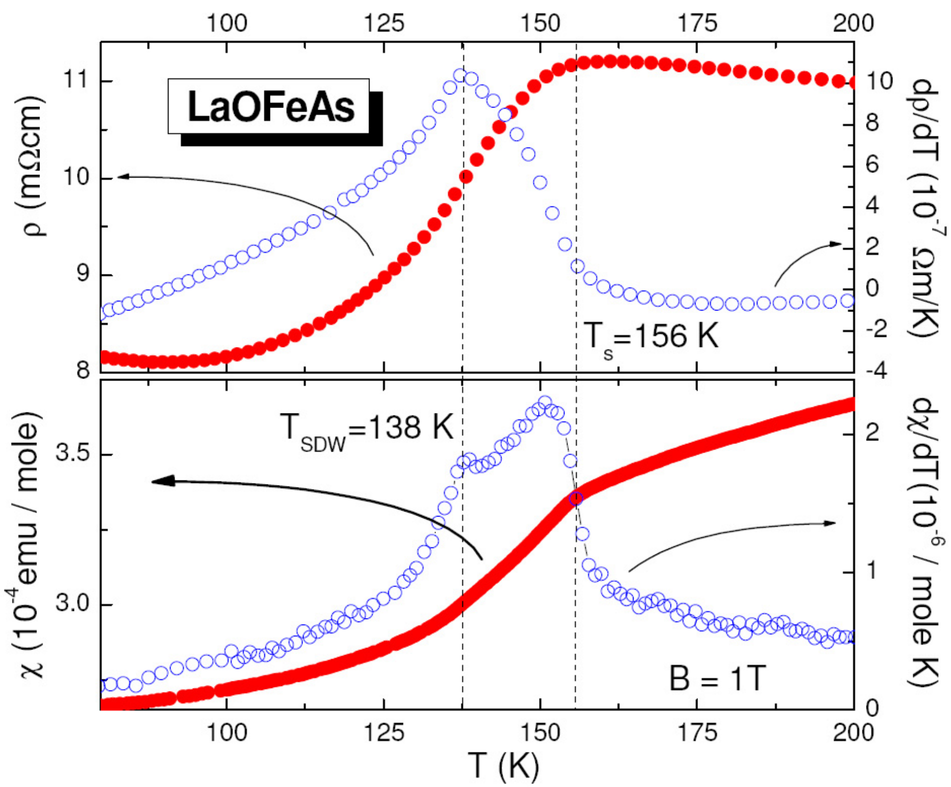
Y. Kamihara et al., J. Am. Chem. Soc. 130, 3296 (2008)

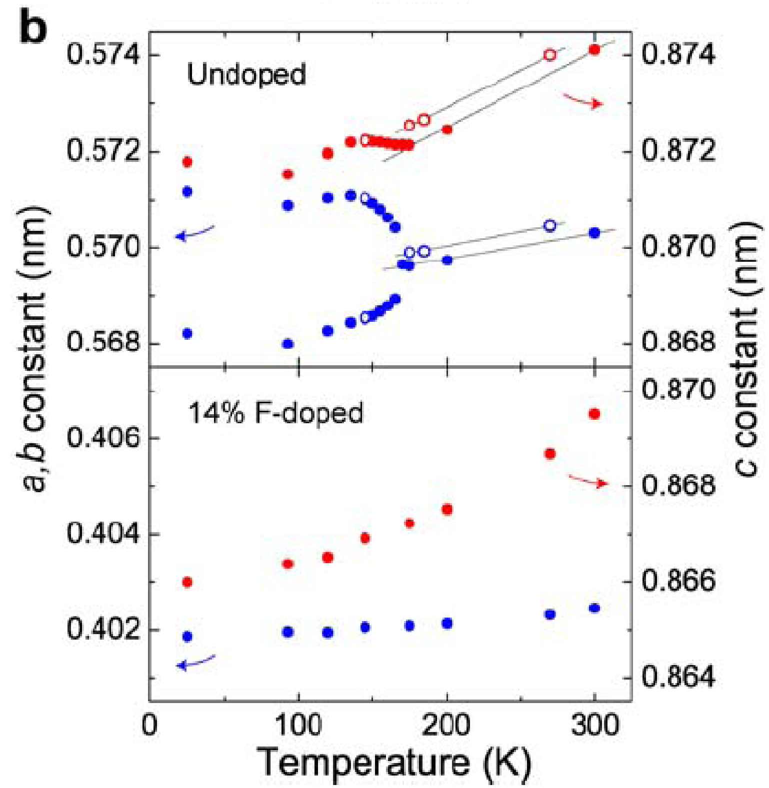




Similar phase diagrams in other **ReFeAs($O_{1-x}F_x$)**

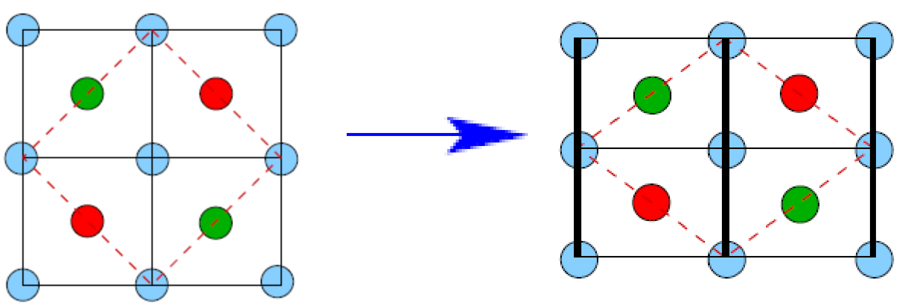
Phase diagram: two phase transitions at x=0





H.-H. Klauss et al., arXiv:0805.0264

T. Nomura et al., arXiv:0804.3569



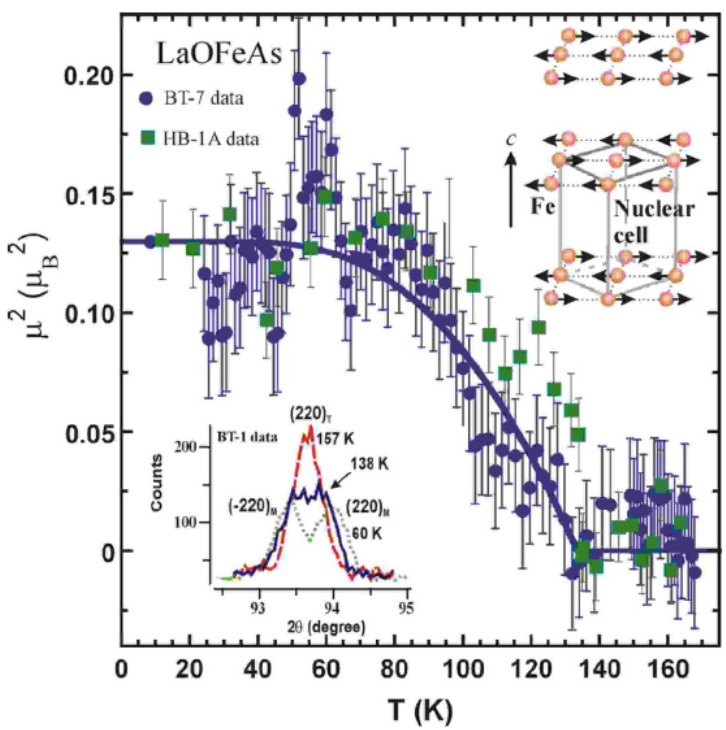
1) structural phase transition at 150K
2) no Curie-Weiss behavior above T_{struc}

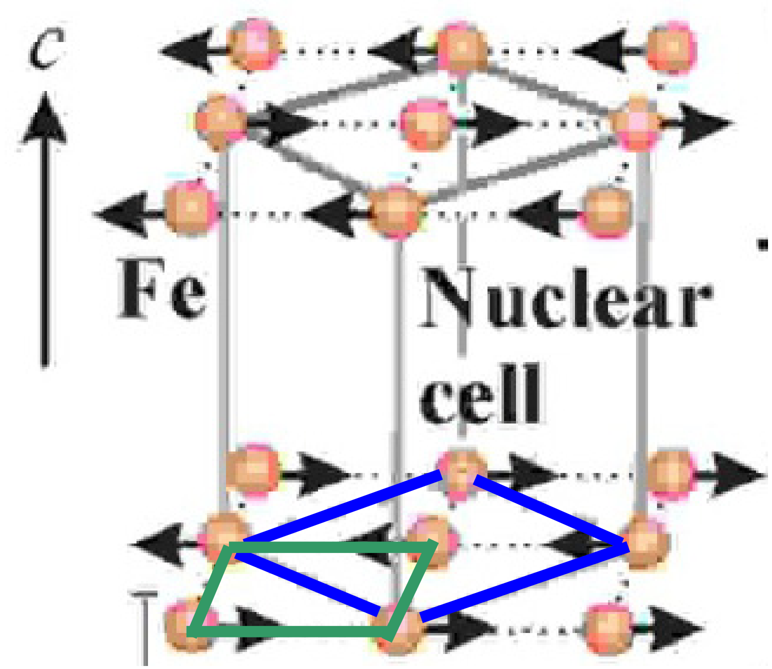
Magnetic structure below T_N

Neutron scattering: C. de la Cruz et al., Nature 453, 899 (2008)
μSR: H.-H. Klauss et al., arXiv:0805.0264

1) **SDW order with Q=(π,π) for √2a x √2a or Q'=(π,0) for a x a**

2) **magnetic moments ~ 0.3 μ_B**



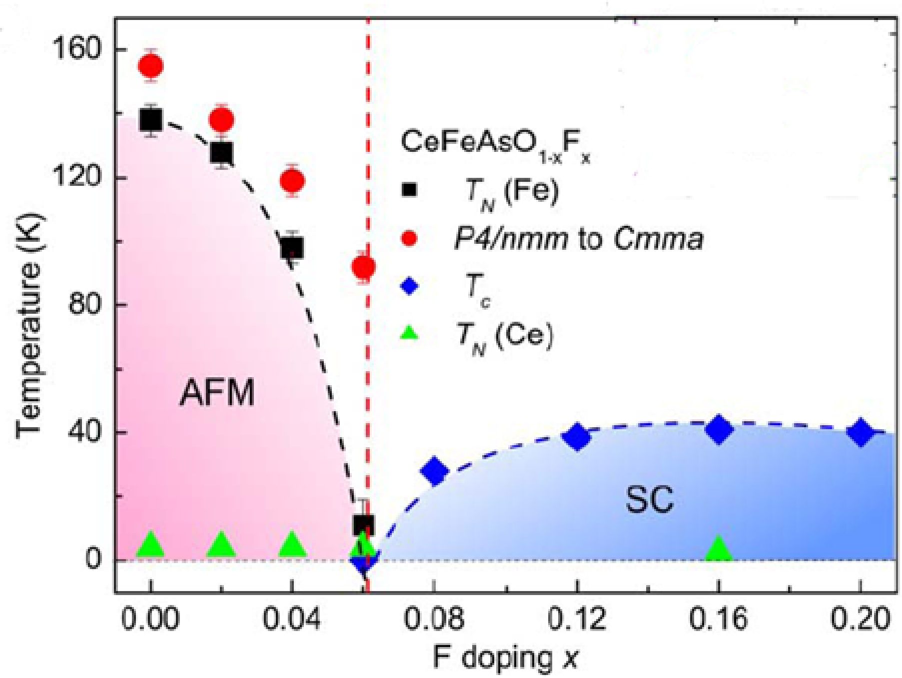


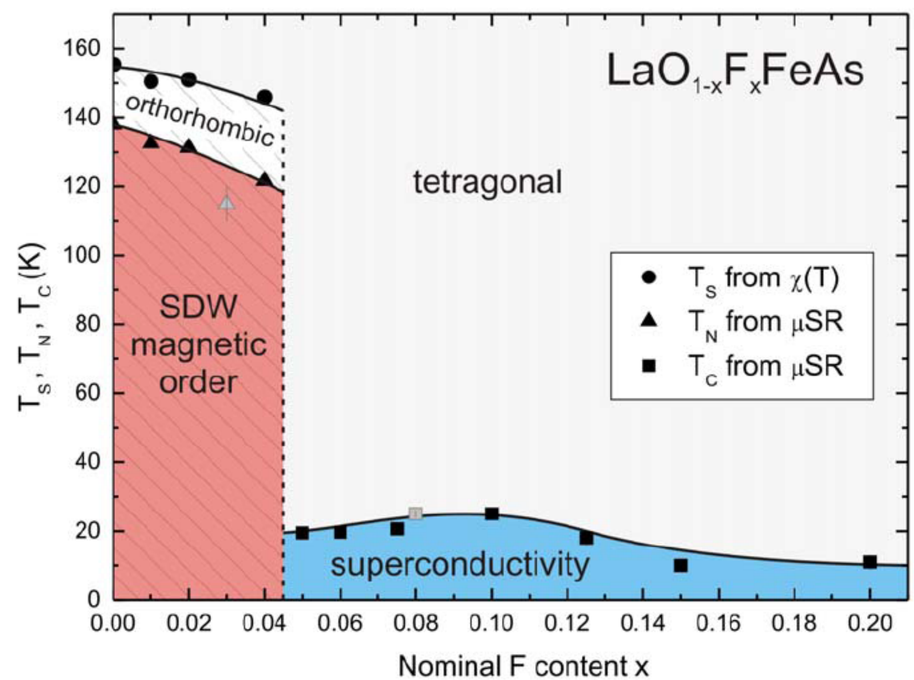
$CeFeAs(O_{1-x}F_x) \Rightarrow 0.8\mu_B$ Neutron scattering: J. Zhao et al., arXiv:0806.2528

Magnetism as a function of doping

$CeFeAs(O_{1-x}F_x)$

J. Zhao et al., arXiv:0806.2528





S. Margadonna et al., arXiv:0806.3962

Results for $LaFeAs(O_{1-x}F_x)$:

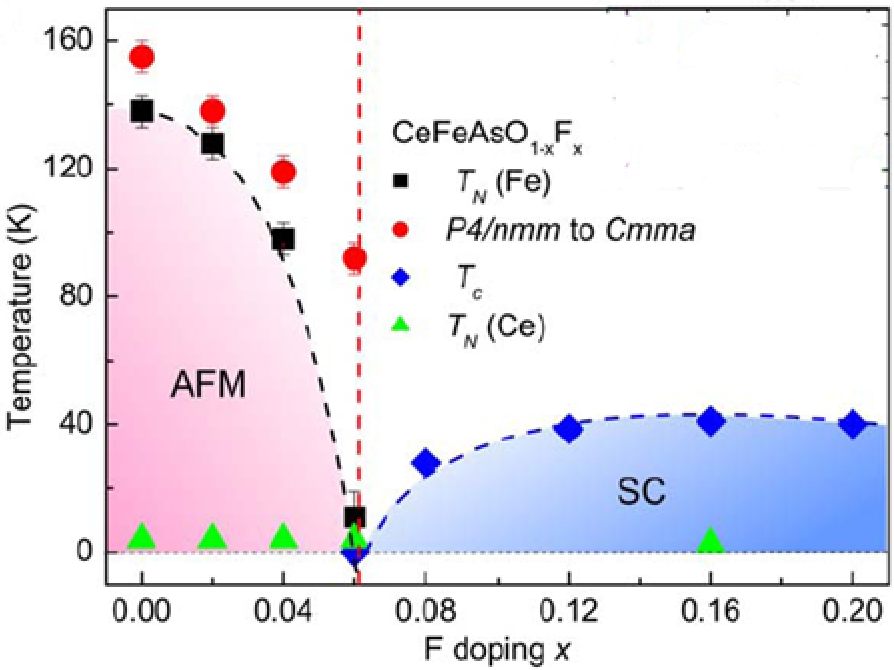
1) Magnetism and structural transition are closely bound together

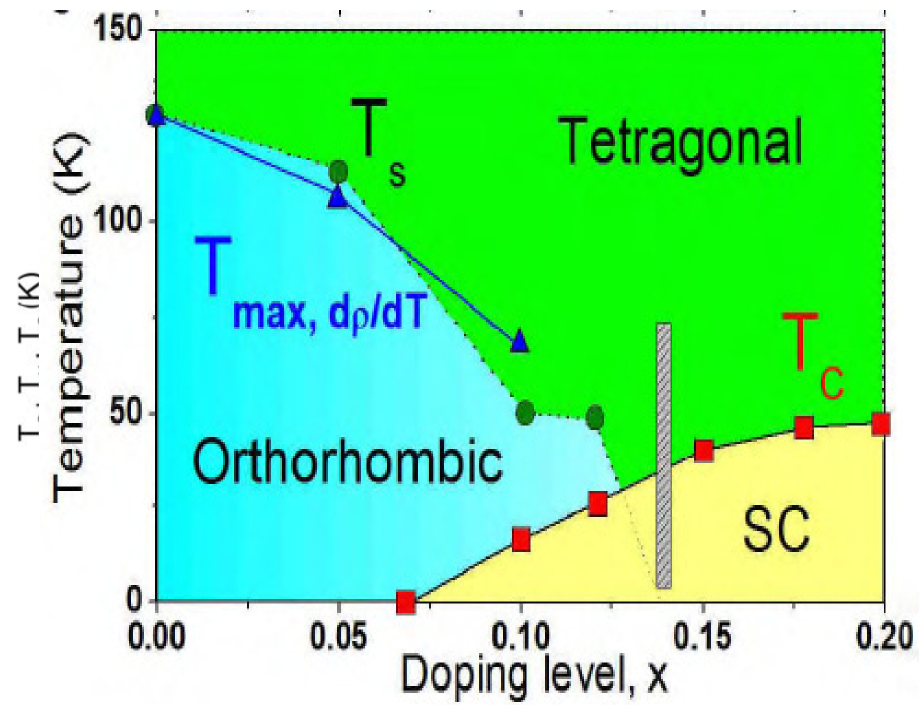
2) Antiferromagnetism and superconductivity do not coexist

Magnetism as a function of doping

$CeFeAs(O_{1-x}F_x)$

J. Zhao et al., arXiv:0806.2528





S. Margadonna et al., arXiv:0806.3962

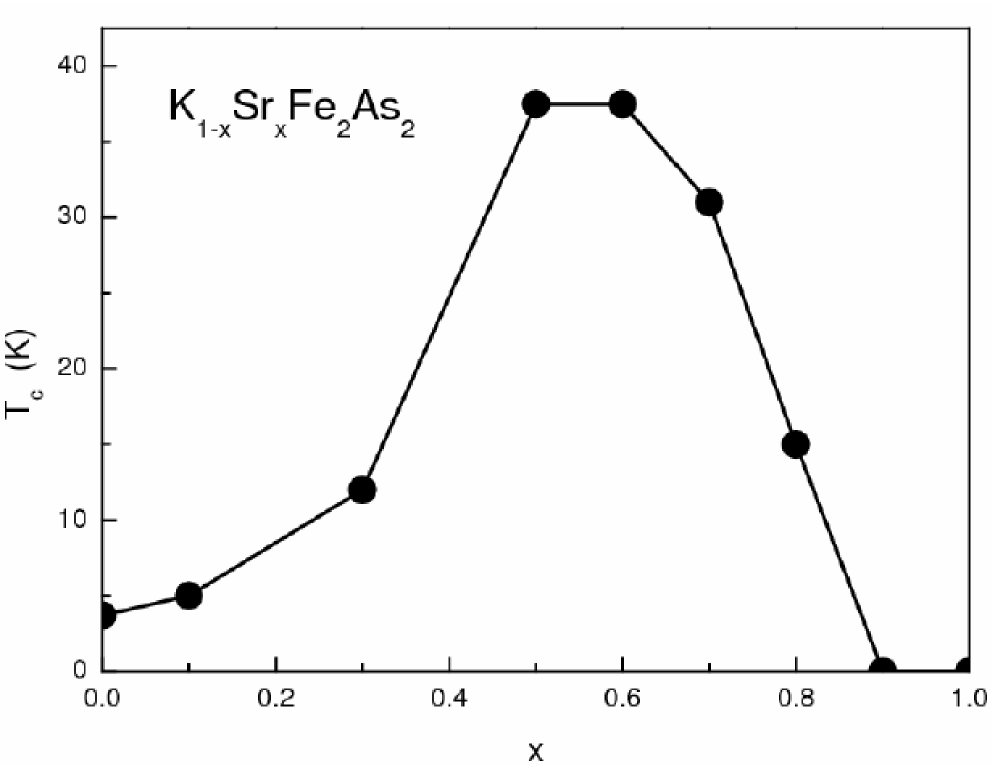
Results for $LaFeAs(O_{1-x}F_x)$;

1) Magnetism and structural transition are closely bound together

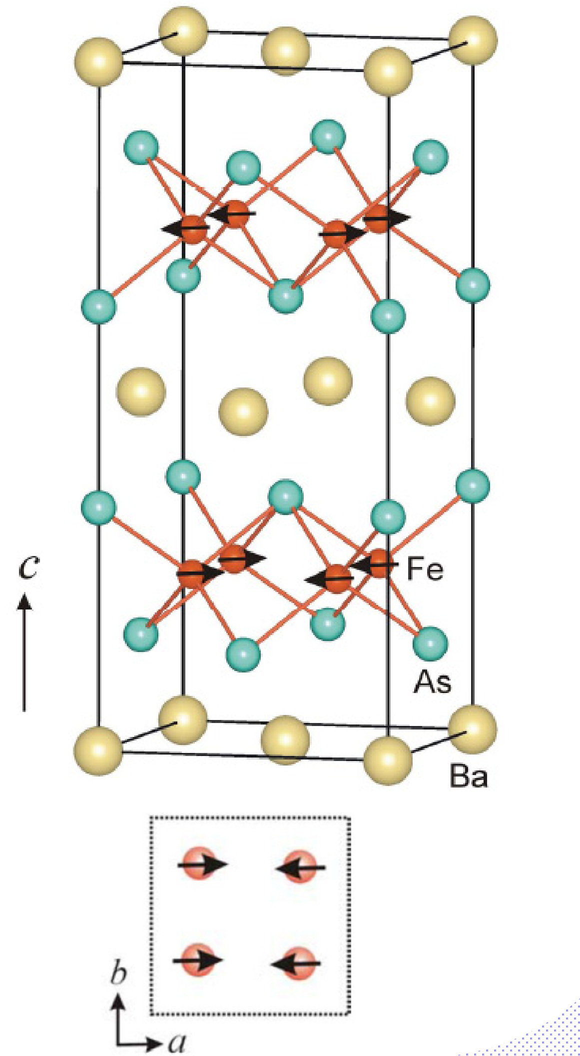
2) Antiferromagnetism and superconductivity do not coexist

Phase diagram: h-doped $K_{1-x}A_xFe_2As_2$ with A = Sr,Ba
$(Sr_{1-x}^{2+}K^+_x)$ $+(Fe^{2+}As^{3-})_2$

M. Rotter et al., arXiv:0805.4630 (2008); G.F. Chen et al., arXiv:0806.1209 (2008);
K. Sasmal et al., arXiv:0806.1301 (2008); G. Wu et al., arXiv:0806.1459 (2008).



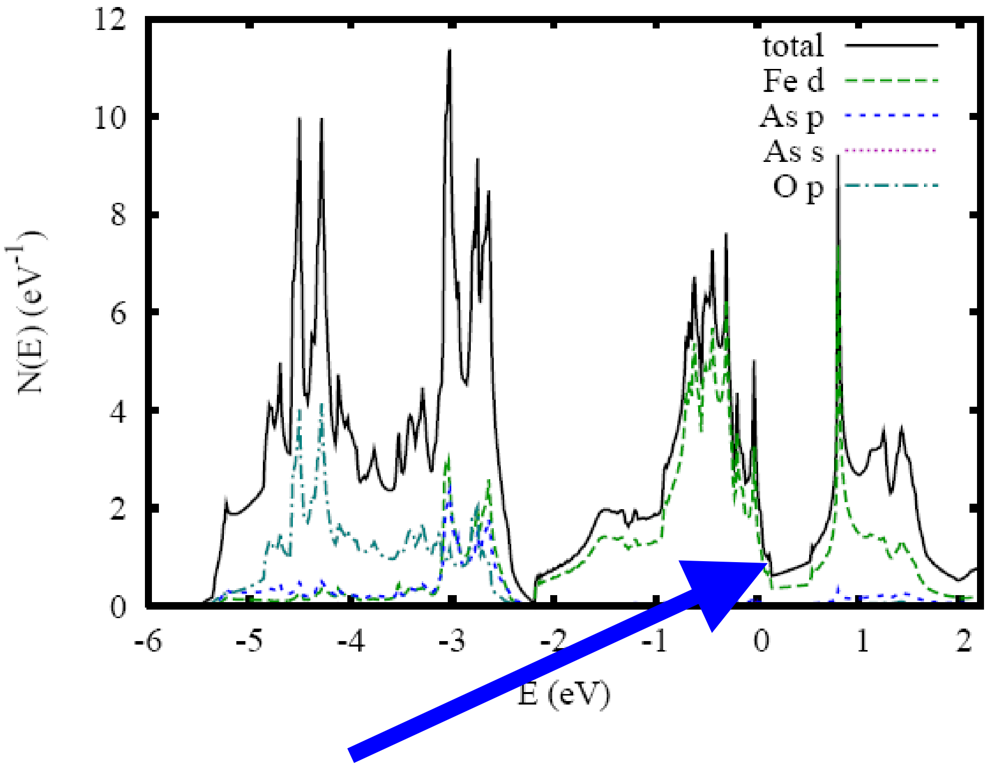
magnetic transition T_{SDW}=205K



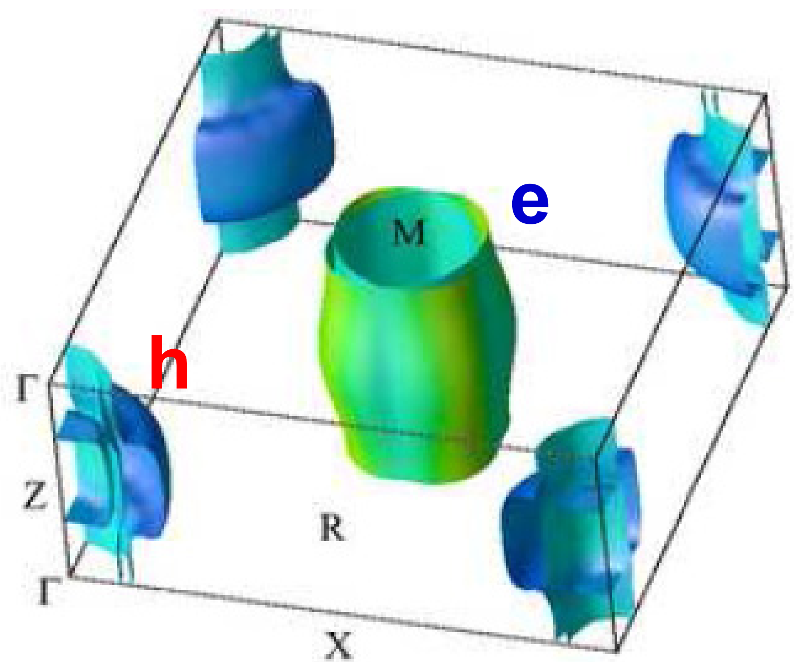
1) crystal structure is the same as $CeCu_2Si_2$
2) maximum T_c = 38K (two FeAs layers per unit cell)
3) structural and magnetic transition occur at the same temperature
4) FM along b direction, AFM along a direction (b<a)

Q. Huang et al., arXiv:0806.2776 (2008)

Electronic structure: LAPW LDA



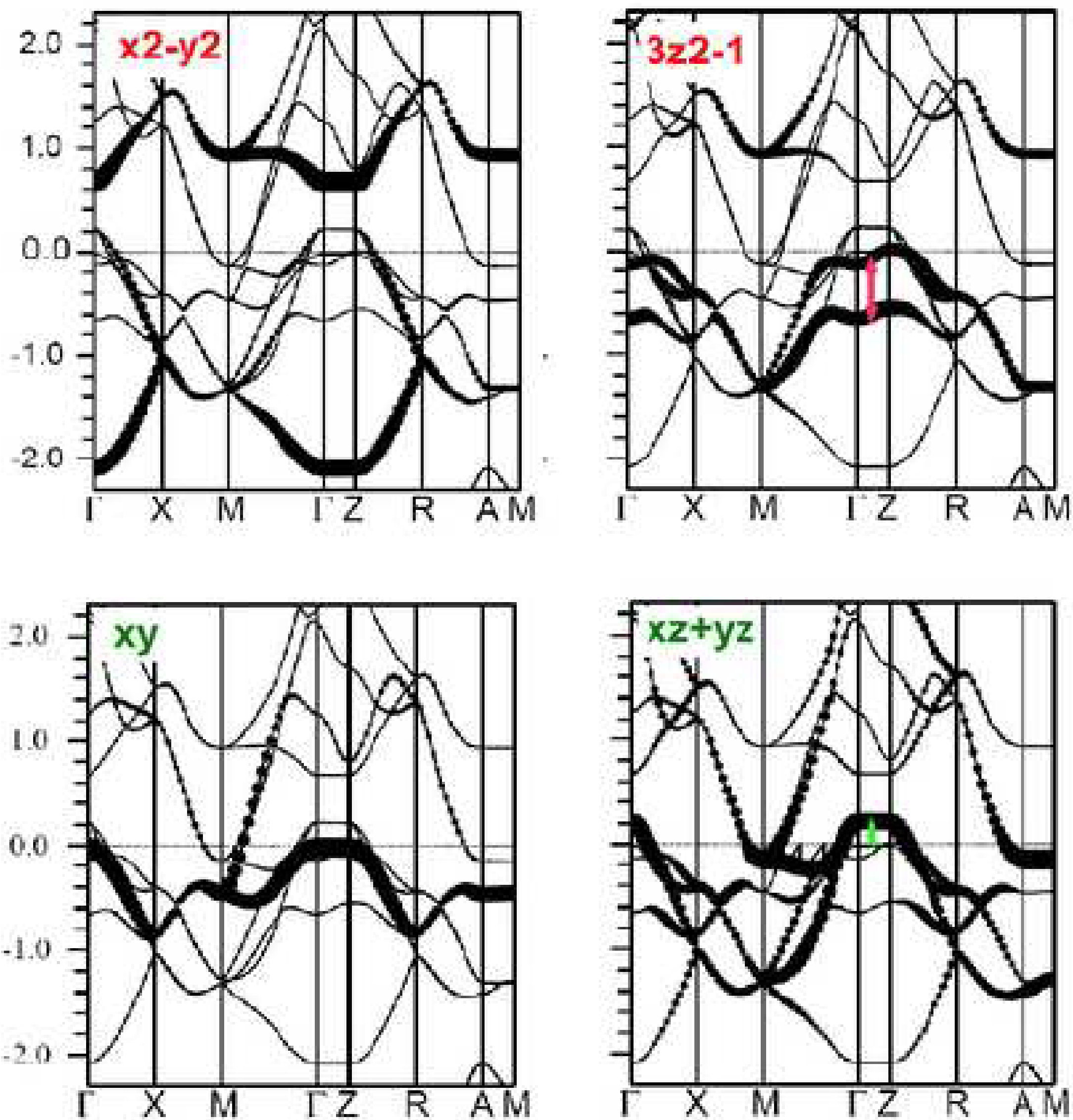
S. Lebegue, PRB 75, 035110 (2007);
D.J. Singh, and M.-H. Du, PRL 100, 237003 (2008);
I.I. Mazin et al., arXiv:0803.2740



Fe^{2+} $3d^6$-states

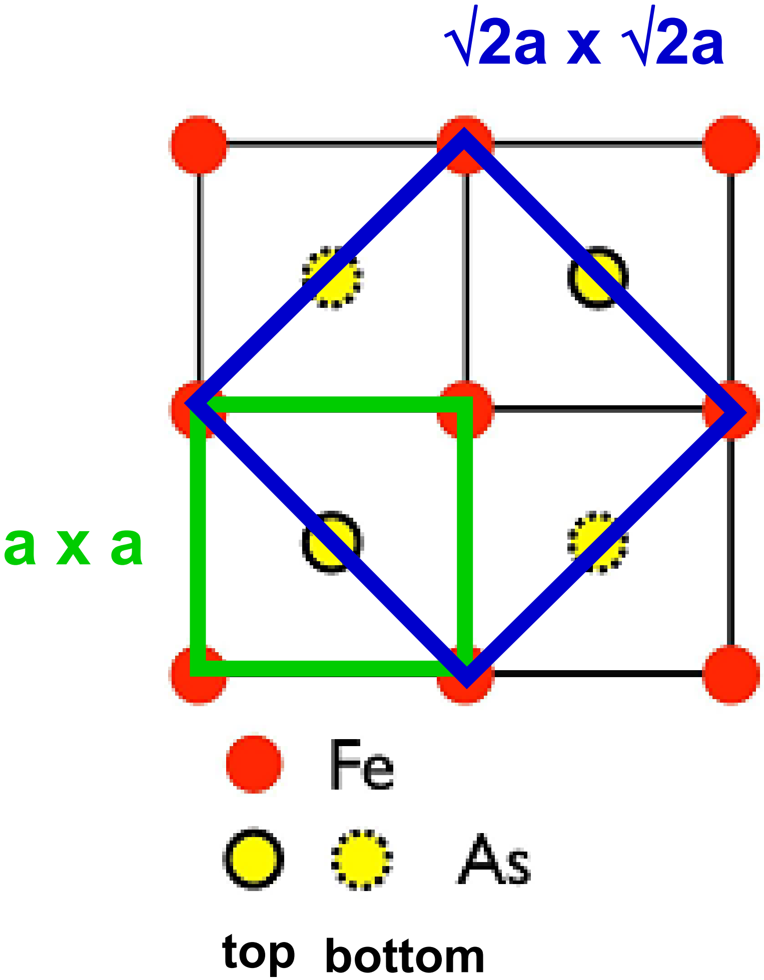
Weak CEF splitting: all 5(10) orbitals are crossing the Fermi level

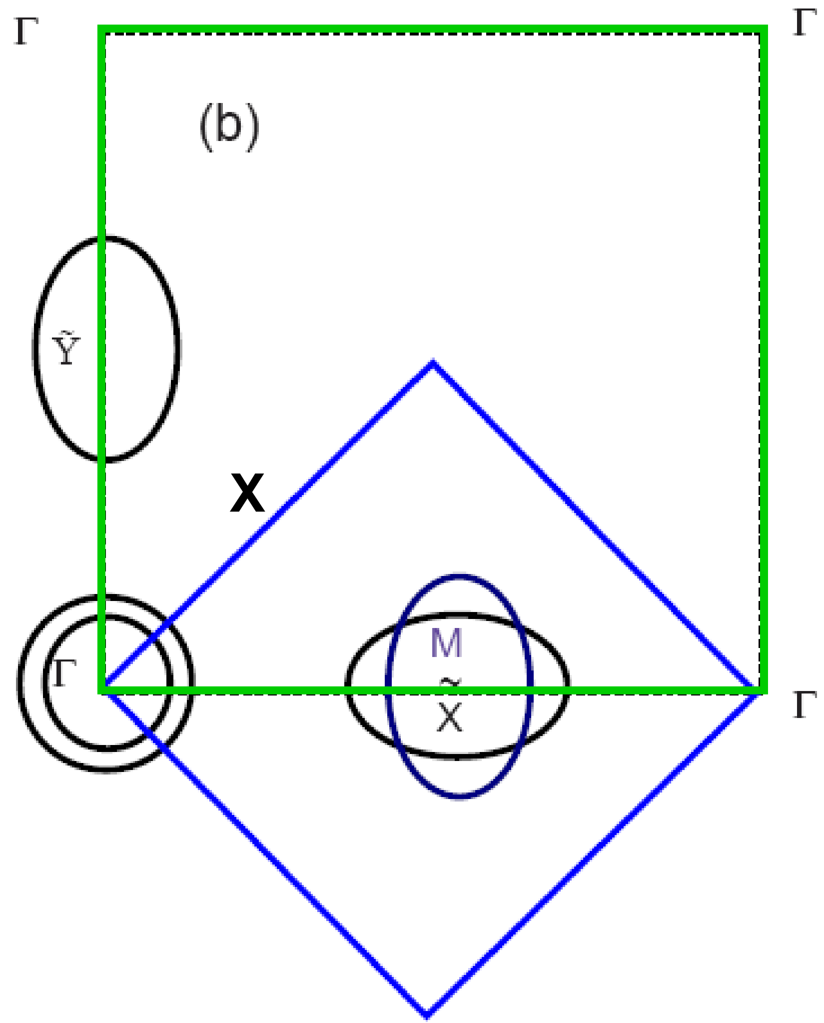
Electronic Structure: Bands close to Fermi Level



L. Boeri, O.V. Dolgov, and A.A. Golubov, PRL 101, 026403 (2008)

Electronic Structure: FS folding





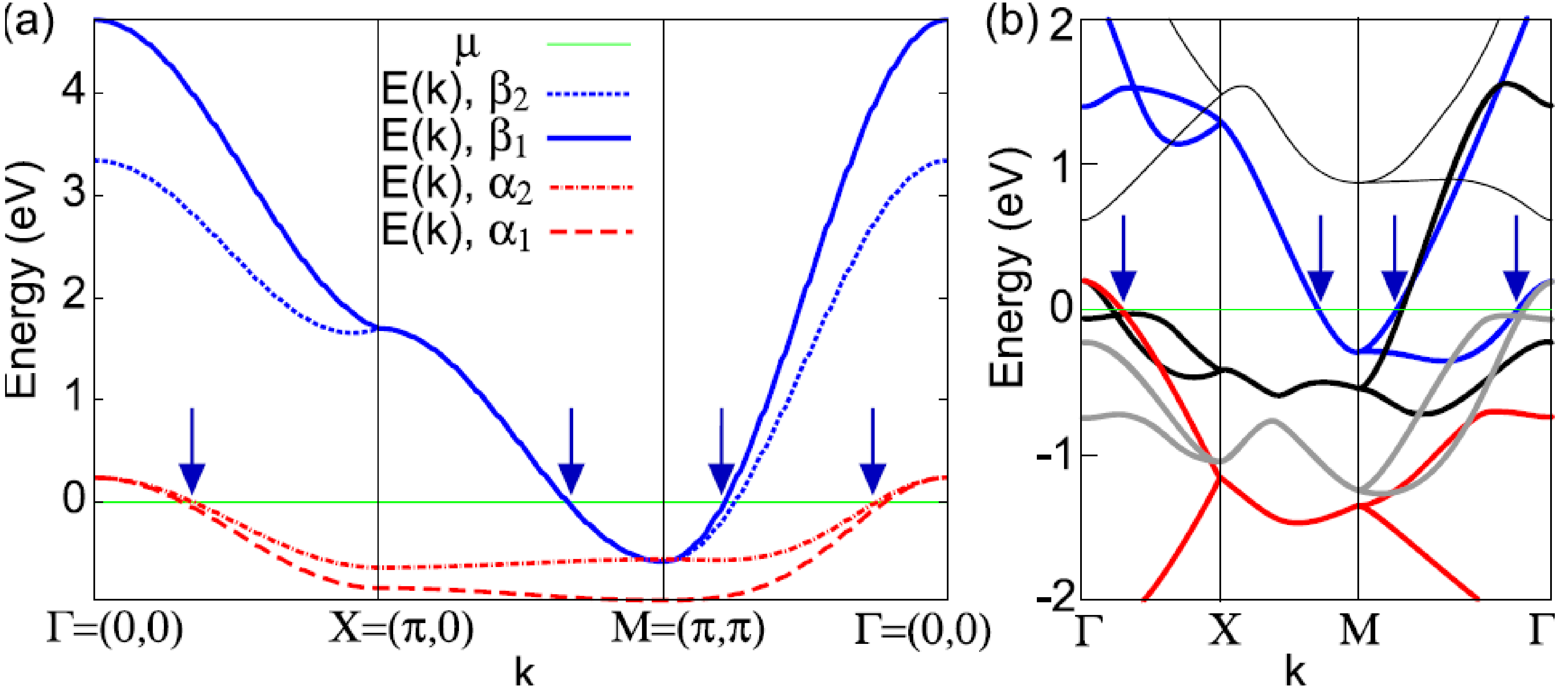
I.I. Mazin et al., arXiv:0803.2740v3

Effective low-energy model

1) based on the two (xz,yz) orbitals plus hybridiztion between them
S. Raghu et al., arXiv:0804.1113 (PRB 77 (R), (2008))

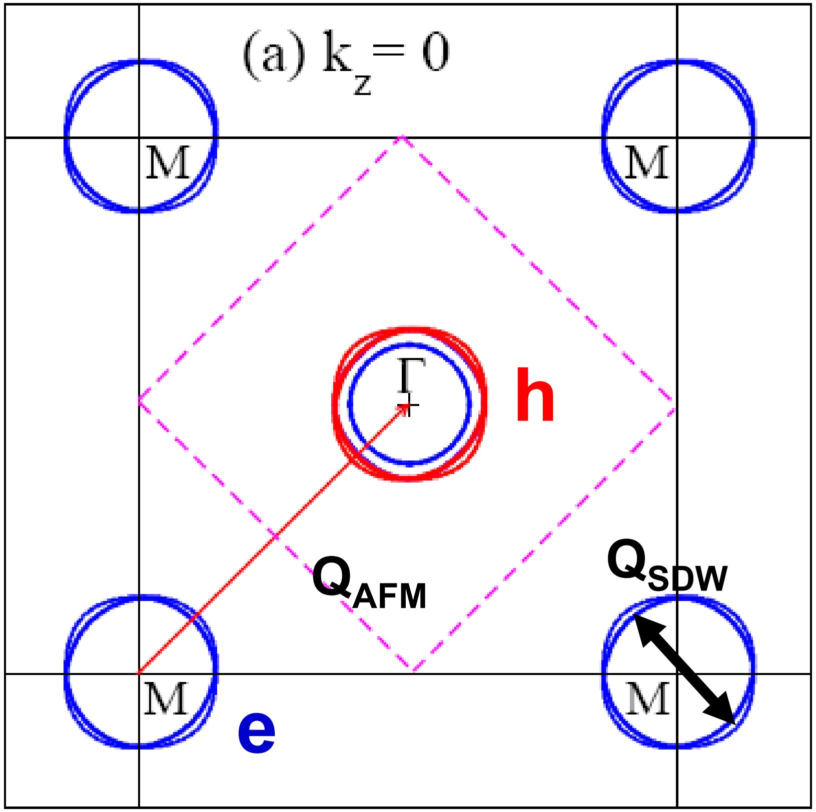
2) 5-bands tight-binding: K. Kuroki et al., arxiv:0803.3325

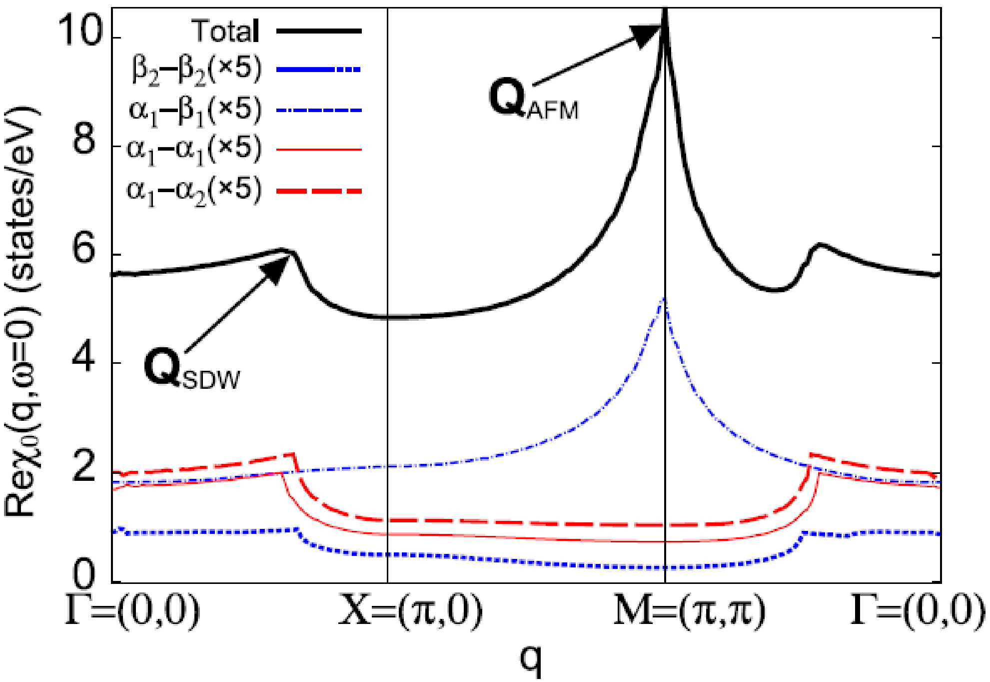
3) matrix elements equal unity: four-bands model



M. Korshunov and I. Eremin arXiv:0804.1793

Magnetic excitations: nearly perfect nesting at x=0





1) nearly perfect nesting, agrees with LDA [J. Dong et al., EPL 83, 27006 (2008).]

M. Korshunov and I. Eremin arXiv:0804.1793

Itinerant magnetism at AFM wave vector: RPA

$$\hat{\chi}_{RPA}(\mathbf{q}, i\omega_m) = [\mathbf{I} - \mathbf{\Gamma}\hat{\chi}_0(\mathbf{q}, i\omega_m)]^{-1}\,\hat{\chi}_0(\mathbf{q}, i\omega_m)$$

$$\mathbf{\Gamma} = \begin{bmatrix} U & J/2 & J/2 & J/2 \\ J/2 & U & J/2 & J/2 \\ J/2 & J/2 & U & J/2 \\ J/2 & J/2 & J/2 & U \end{bmatrix}$$

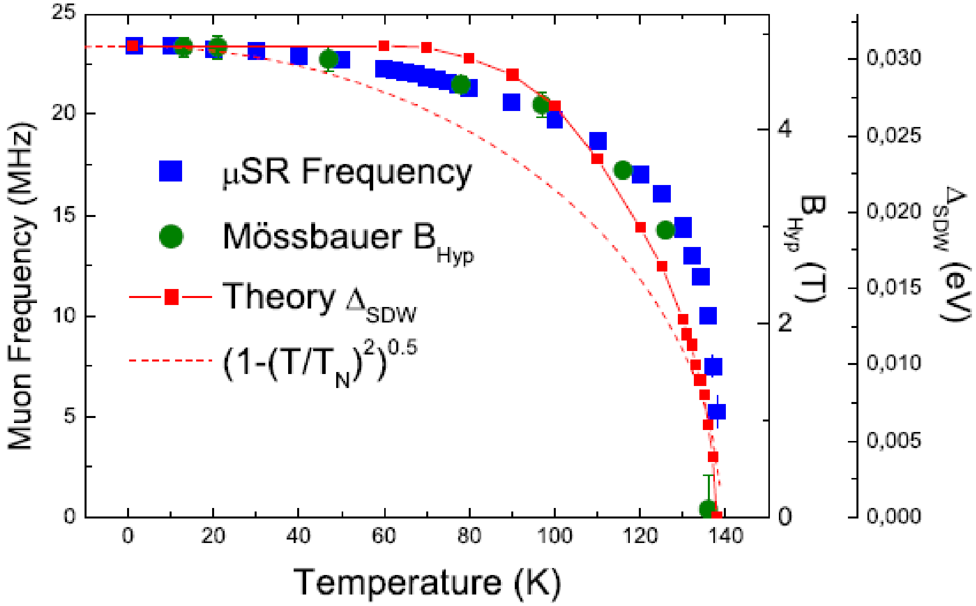
Magnetic instability at Q_{AFM}

$\det|\mathbf{I}-\Gamma\chi_0|=0$

U=0.26eV
J=U/5

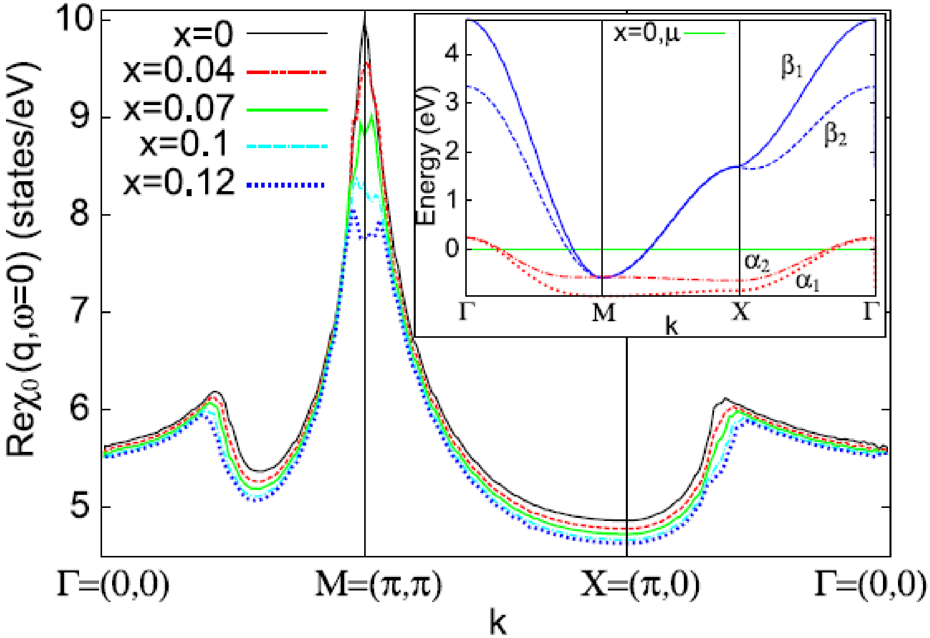
$\mu=0.32\ \mu_B$

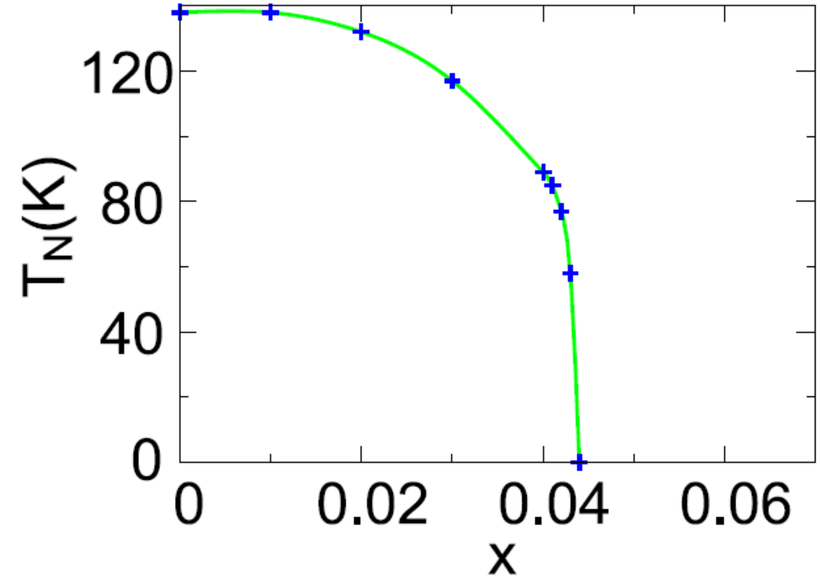
$\mu^2=0.1\ (\mu_B)^2$



H.-H. Klauss et al., arXiv:0805.0264

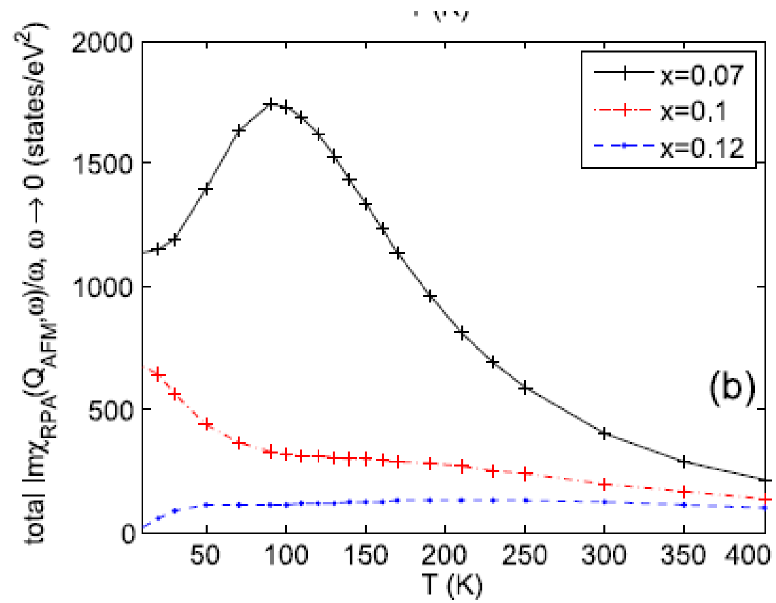
Itinerant magnetism: doping dependence





Instead of nesting → 'hot' spots

magnetic instability decreases

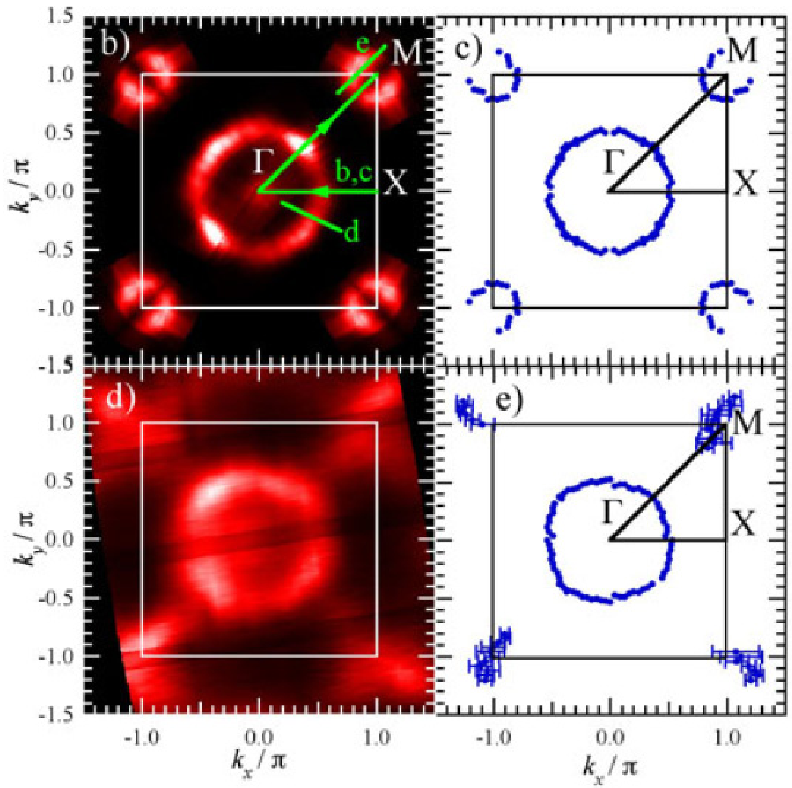


M. Korshunov and I. Eremin, Europhys. Lett.,

ARPES Fermi surfaces

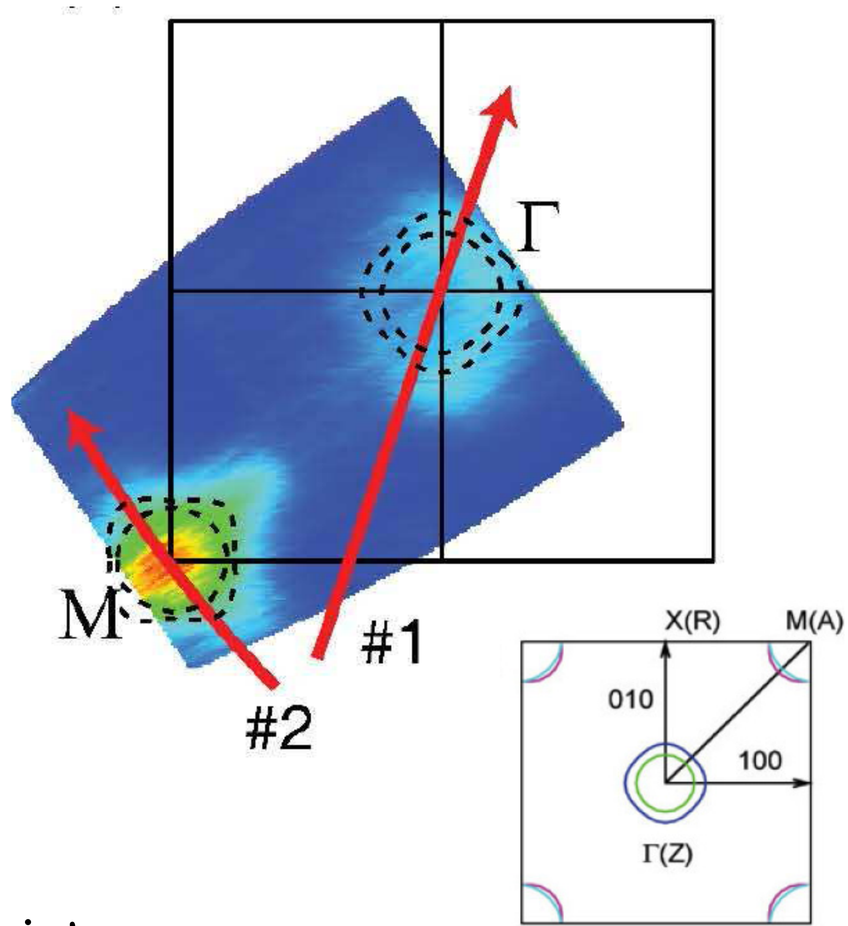
NdFeAs($O_{1-x}F_x$) (x=0.1 before cleavage)

C. Liu et al., arXiv:0806.2147v3



$BaFe_2As_2$

L.X. Yang et al., arXiv:0806.2627v1



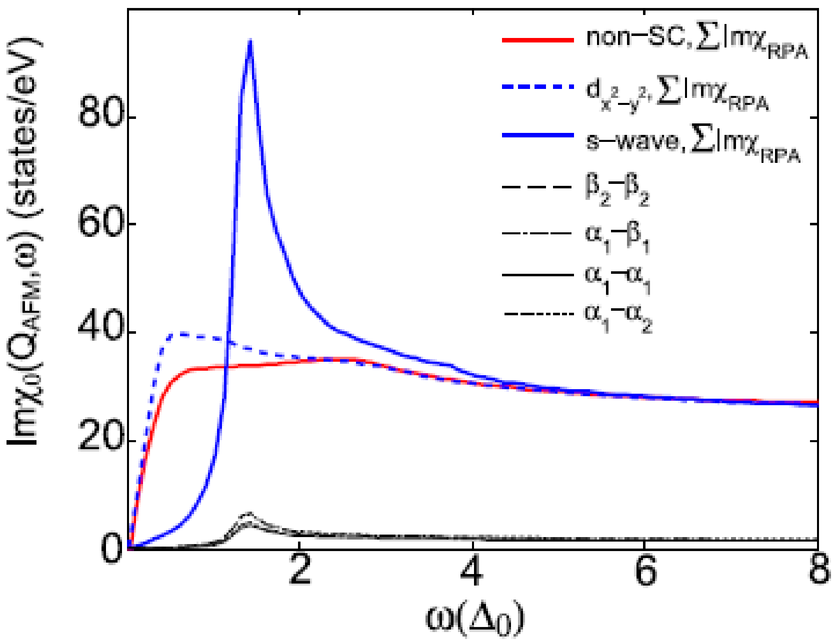
Both electron and hole pockets do exist

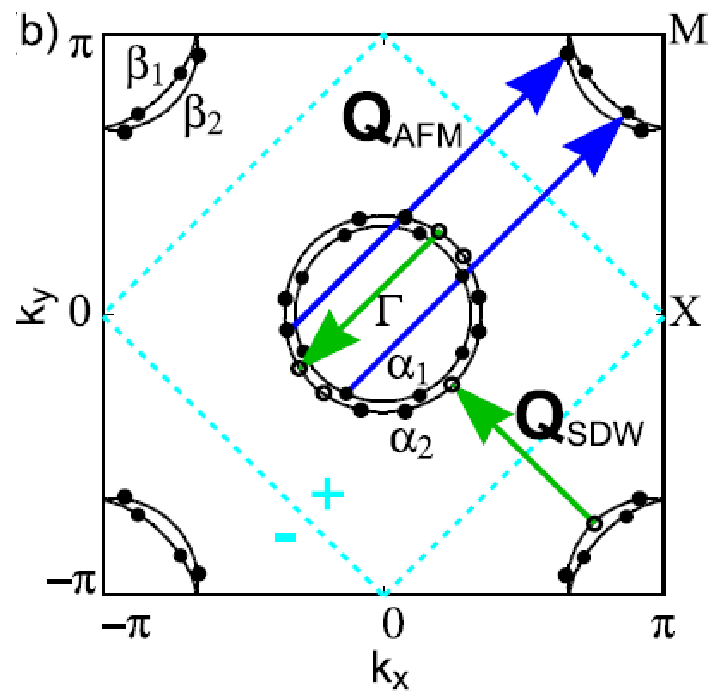
There is a Fermi surface even at zero doping

Non-phononic mechanism of superconductivity

interband AFM fluctuations enhancing interband Cooper-pair scattering: extended s-wave

$$\Delta_{\mathbf{k}} = \frac{\Delta_0}{2}\left(\cos k_x + \cos k_y\right)$$



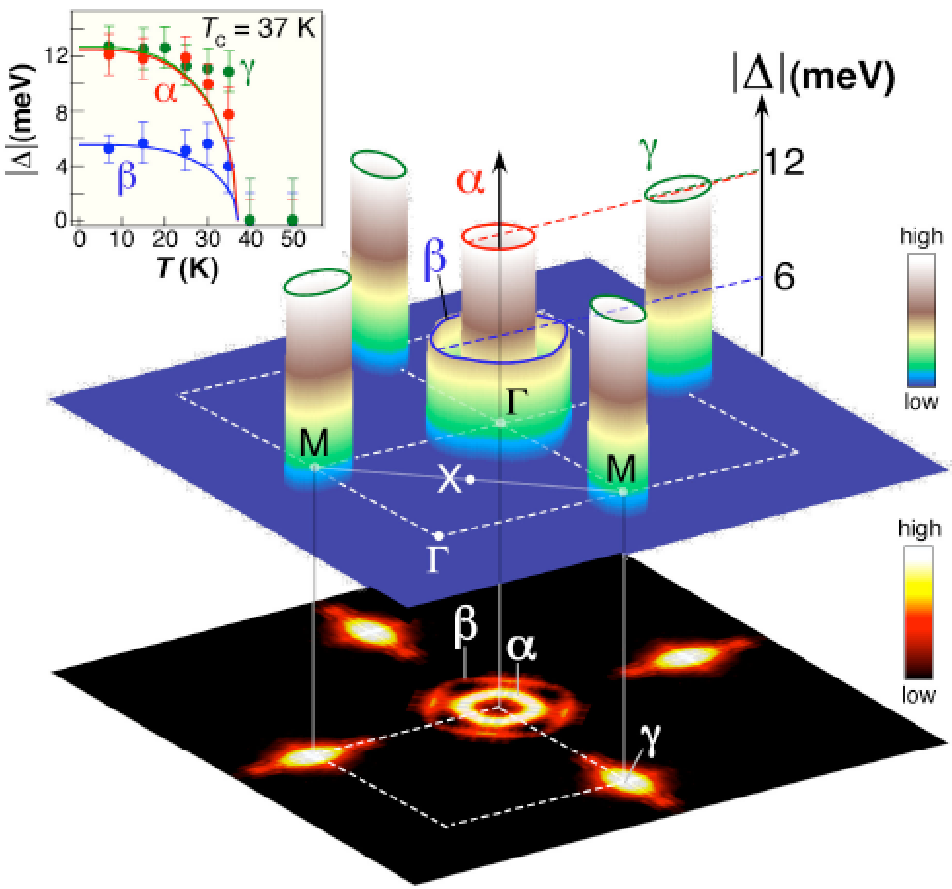


I.I. Mazin et al., arXiv:0803.2740;
K. Kuroki et al., arXiv:0803.3325;
M. Korshunov and I. Eremin, arXiv:0804.1793

1) isotropic gap in thermodynamics (no nodes at the Fermi surface – at least in simple picture)
2) no Hebel-Slichter peak in $1/T_1$, resonance peak in INS

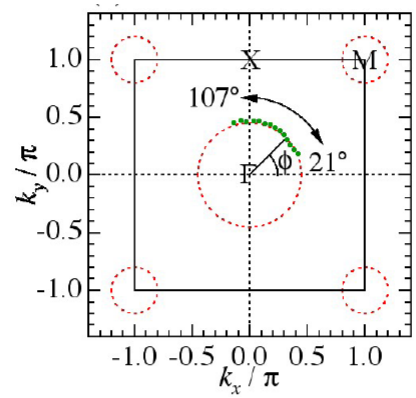
Symmetry of the superconducting gap

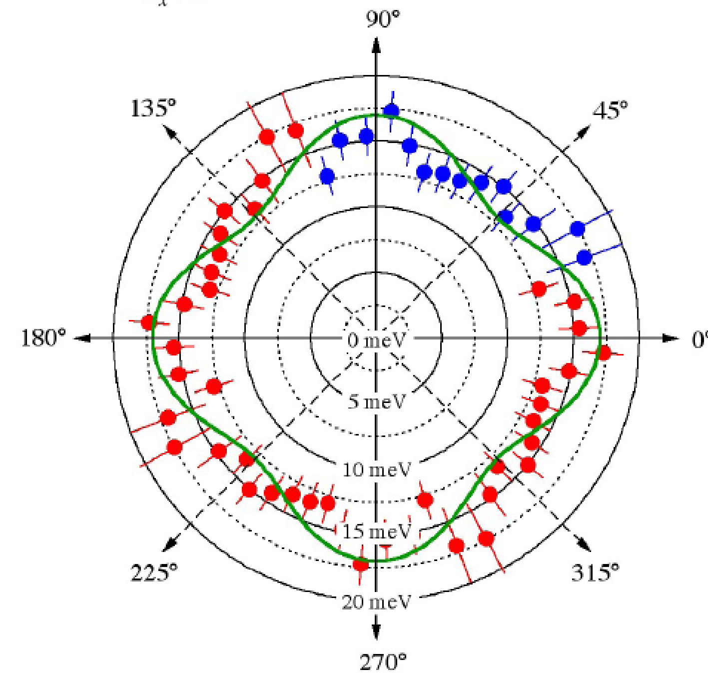
1) nearly isotropic gap in ARPES



$Ba_{0.6}K_{0.4}Fe_2As_2$

H. Ding et al., arXiv:0807.0419



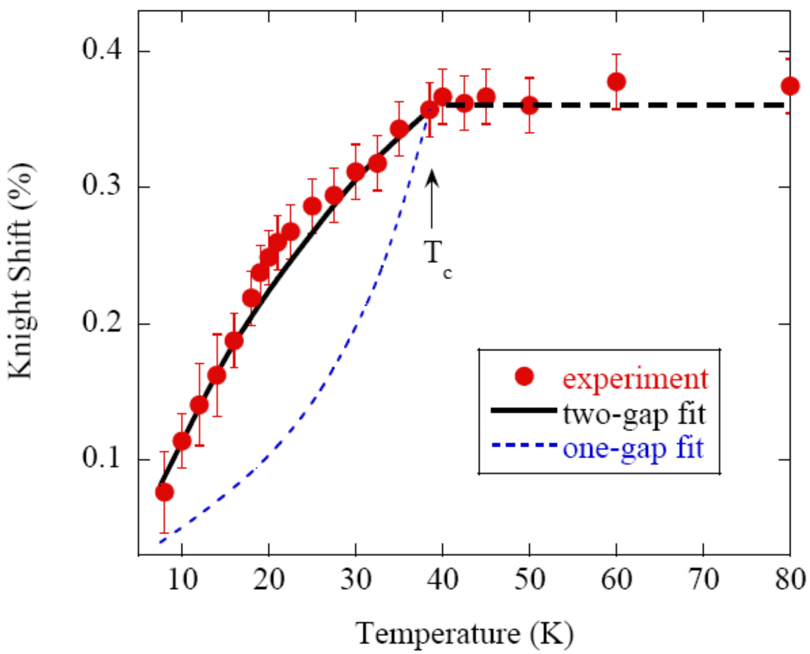


$NdFeAsO_{1-x}F_x$

T. Kondo et al., arXiv:0807.0815

Exp. situation: NMR data

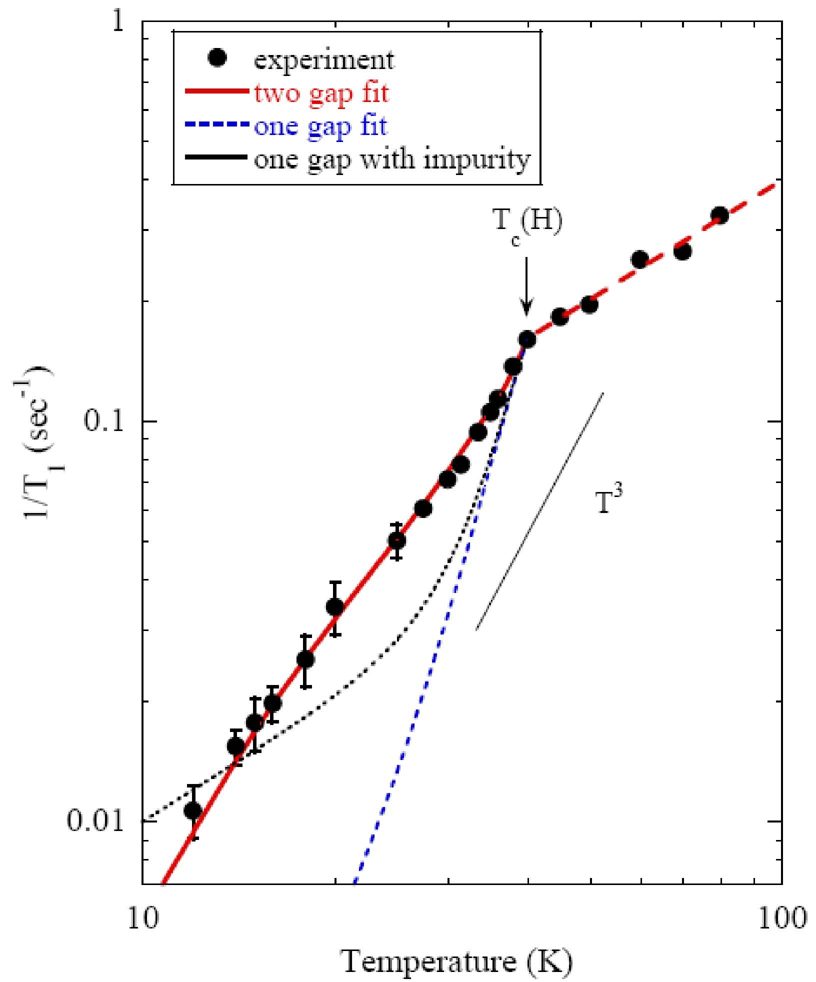
$PrFeAs(O_{1-x}F_x)$ (x=0.11)



K. Matano et al., arXiv:0806.0249

$LaFeAs(O_{1-x}F_x)$ (x=0.11)

Y. Nakai et al., JPSJ **77** (2008) 073701

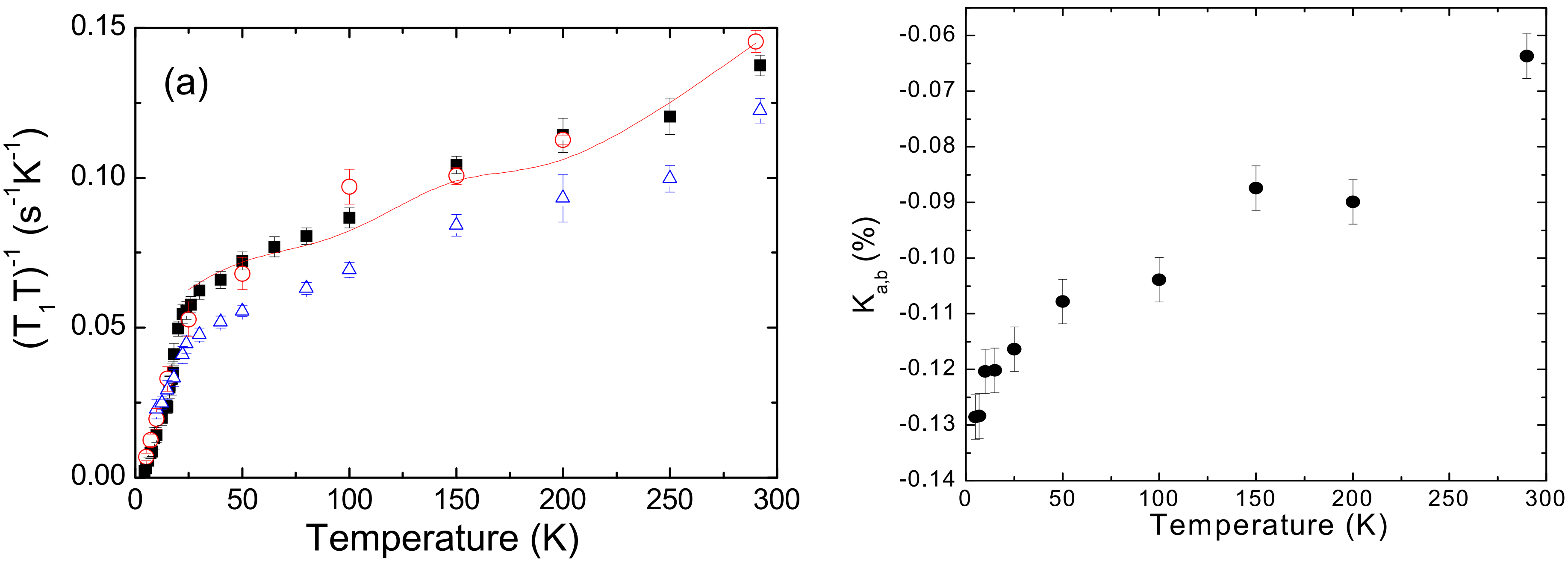


nodal lines at the Fermi surface (not expected in the extended s-wave gap), multiple gaps

further studies are necessary

(conflict with pen. depth, tunneling and μSR – isotropic gap)

Exp. situation: NMR data



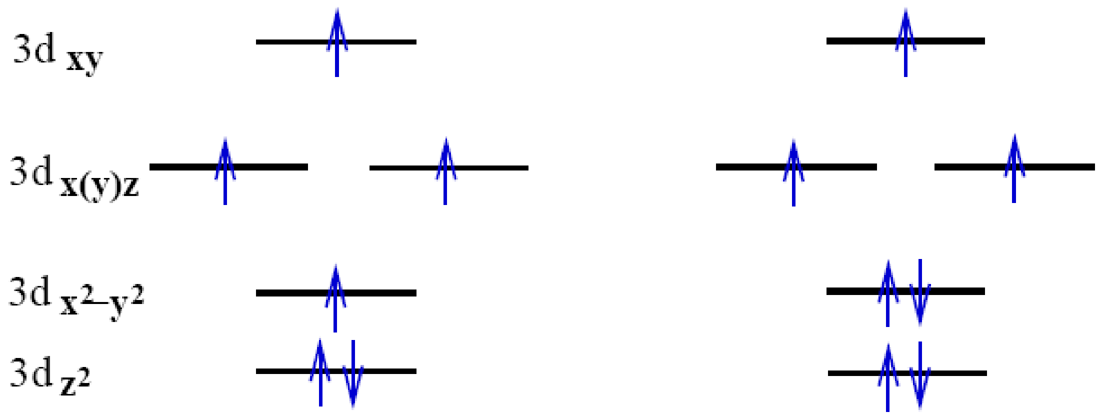
Spin lattice relaxation in the normal state:

- Korringa behavior: $K_{ab}^2/\alpha\kappa$, κ = Korringa constant typical for metals
- no signatures of spin fluctuations (in the As NMR!!!), Pseudogap

H. Grafe et al., cond-mat/0805.2595

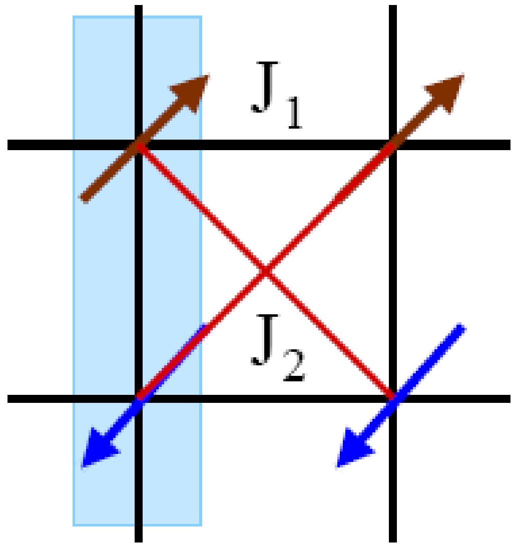
Possible effect of frustrations

Q. Si and E. Abrahams, arXiv:08.04.2480v1; C. Fang et al., arXiv: 0804.3843v1; T. Yildirim arXiv0804.2252; F. Ma, arXiv:0804.3370v3

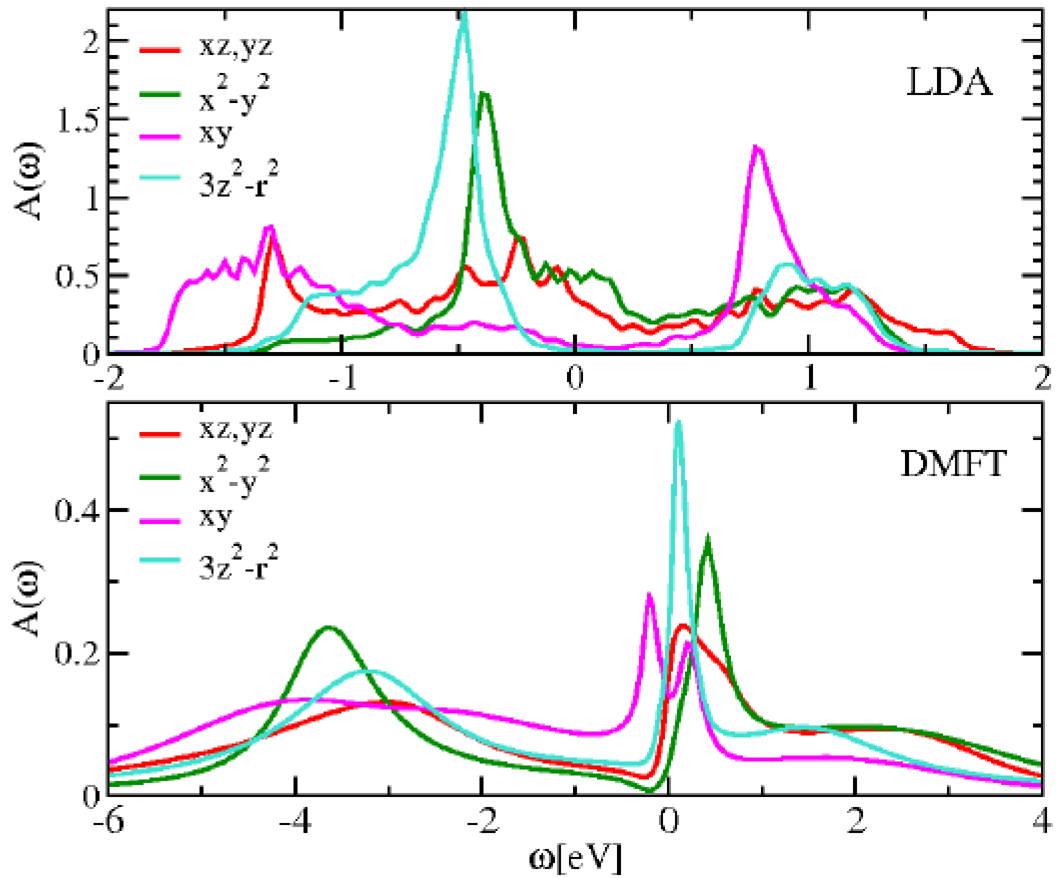


Undoped S=2 Electron doping S=3/2

$J_1 \sim J_2$



Electronic correlation effects



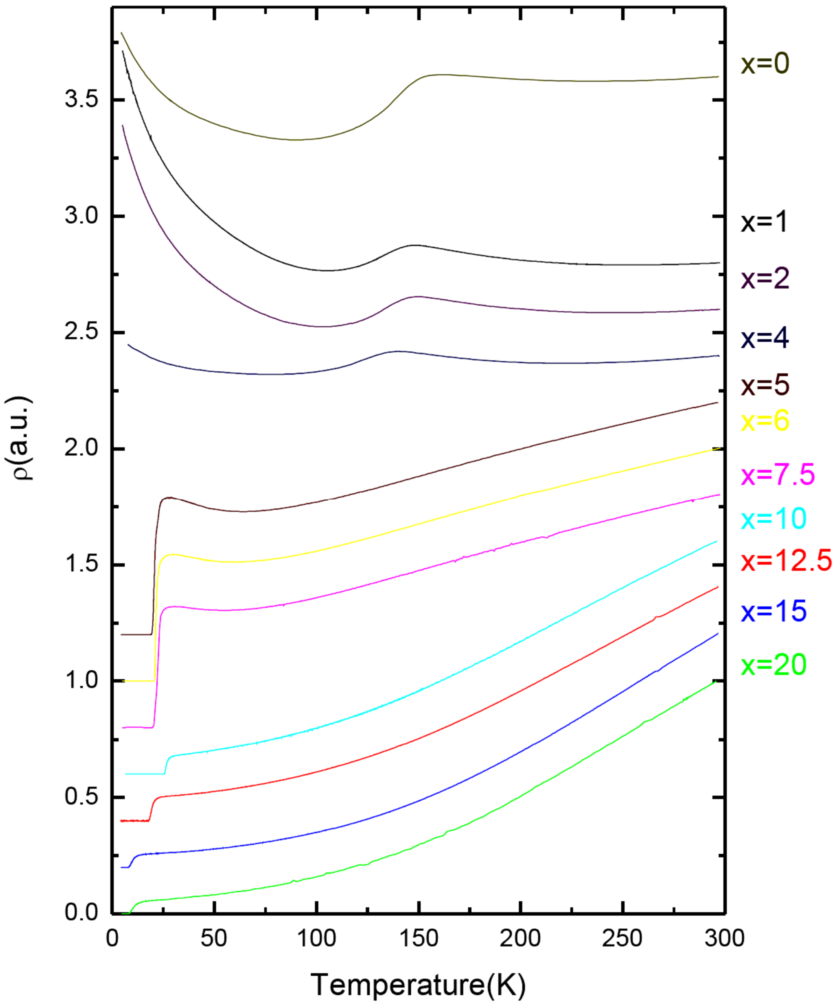
1) correlations are moderate ⇒ no Mott transition U~1eV
2) situation changes for significant J_H ~ 0.7 eV⇒ orbital selective Mott transition

K. Haule, J.H. Shim, and G. Kotliar, Phys. Rev. Lett. 100, 226402 (2008); K. Haule, G. Kotliar, arXiv:0805.0722

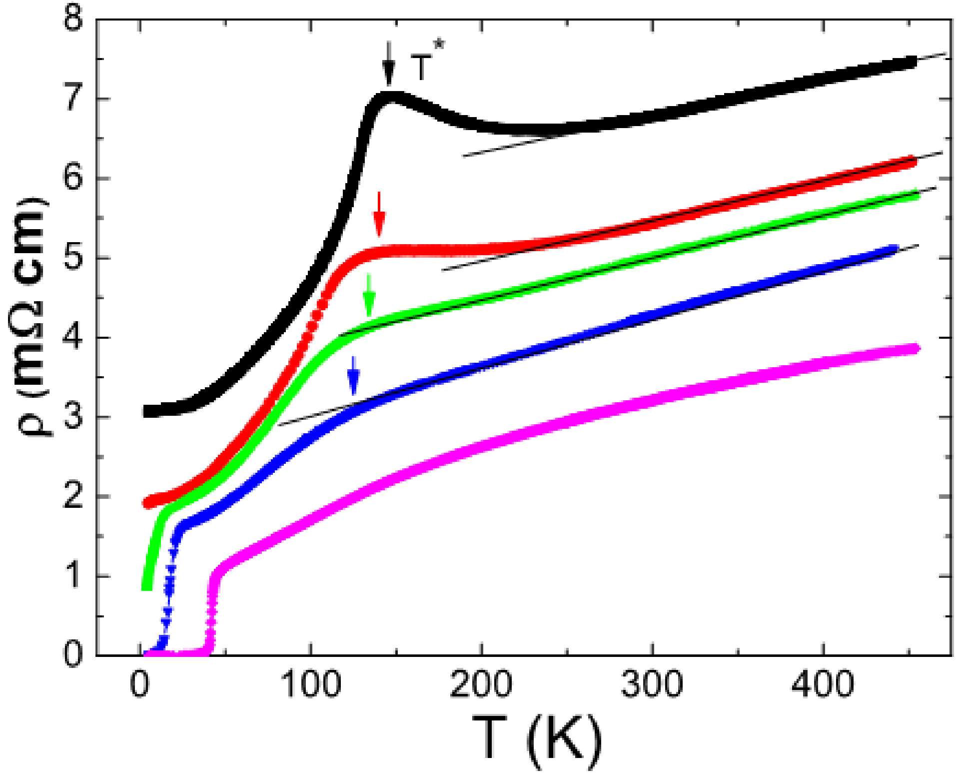
Effect of the magnetic rare-earth substitution

$LaFeAs(O_{1-x}F_x)$

B. Buechner et al., unpublished



$SmFeAs(O_{1-x}F_x)$

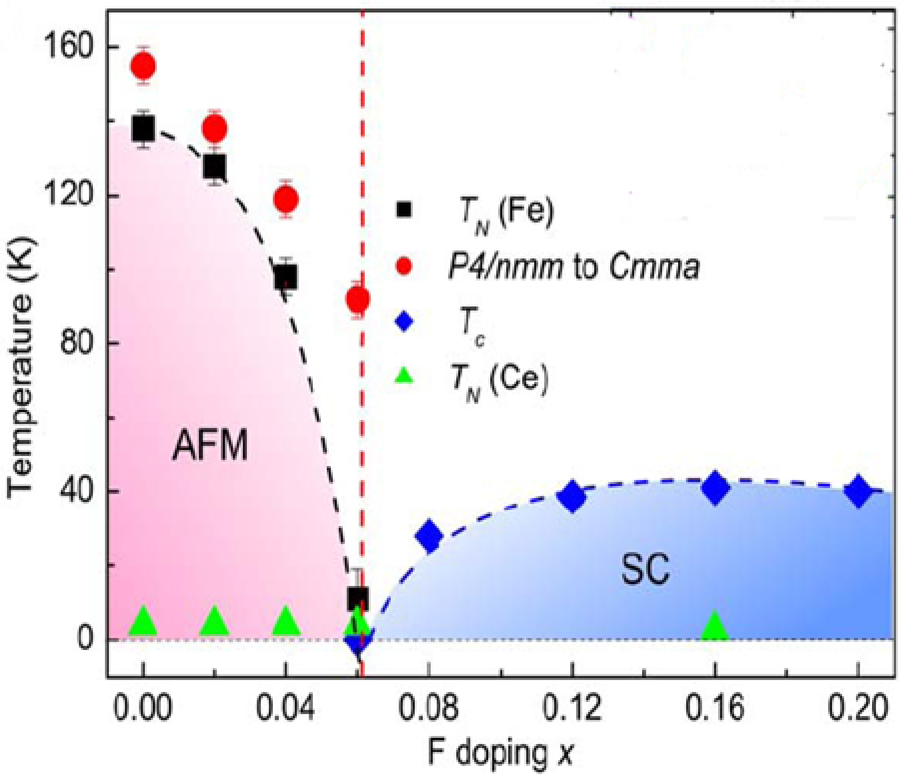


Resistivity does not $\sim T^2$ for large x

Resistivity $\sim T^2$ at x> 0.12

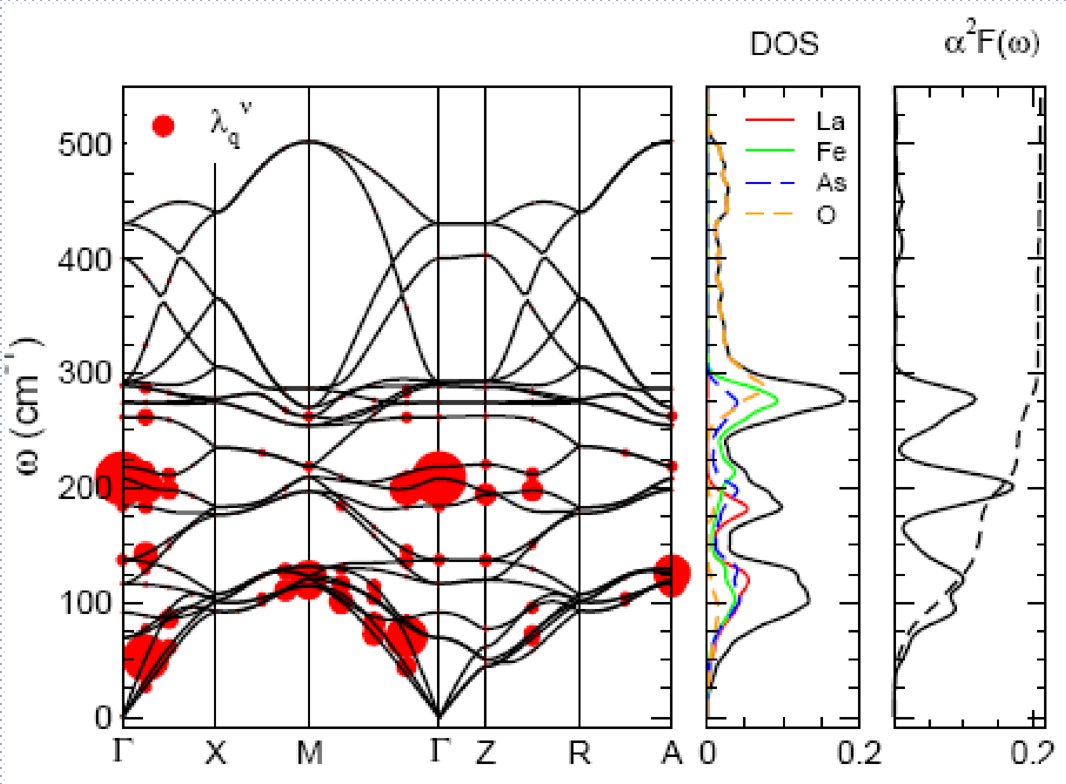
L. Pourovskii et al., arXiv:0807.1037

ReFeAs($O_{1-x}F_x$) and $K_{1-x}A_xFe_2As_2$ superconductors: present questions



1) Origin of the structural transition
2) Interrelation of structural transition and magnetism
3) frustrations effects?
4) orbital effects
5) symmetry of superconducting gap (extended s-wave)
6) relevance of spin fluctuations above T_c
7) influence of the magnetic rare-earth elements
8) effect of electronic correlations
9) …

Standard electron-phonon interaction



L. Boeri, O.V. Dolgov, and A.A. Golubov, arXiv:0803.2703;
D.J. Singh and M.-H. Du, arXiv:0803.0429

$$\lambda = 0.21$$

For Al λ=0.44

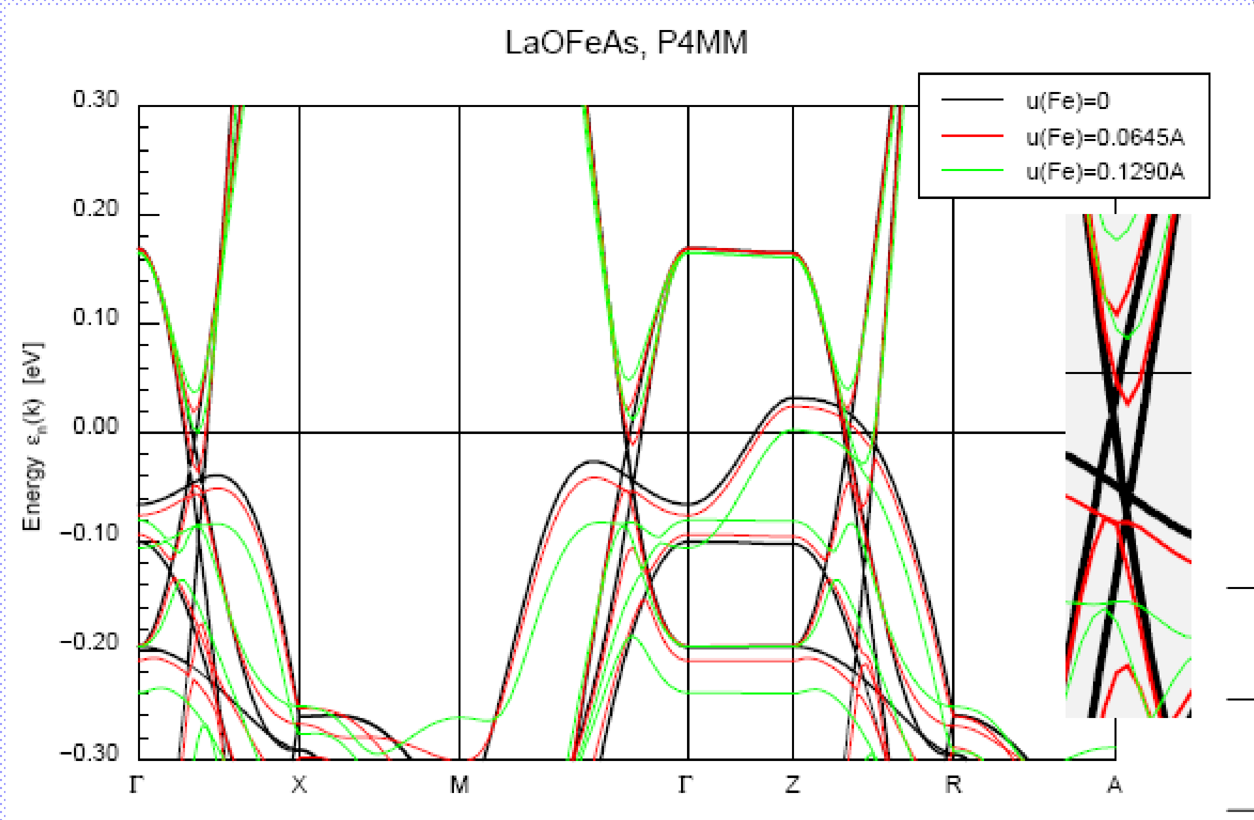
$$\alpha^2 F(\omega) = \frac{1}{N(0)} \sum_{nm\mathbf{k}} \delta(\varepsilon_{n\mathbf{k}})\delta(\varepsilon_{m\mathbf{k+q}}) \times \times \sum_{\nu\mathbf{q}} |g_{\nu,\, n\mathbf{k},\, m(\mathbf{k+q})}|^2 \delta(\omega - \omega_{\nu\mathbf{q}});$$

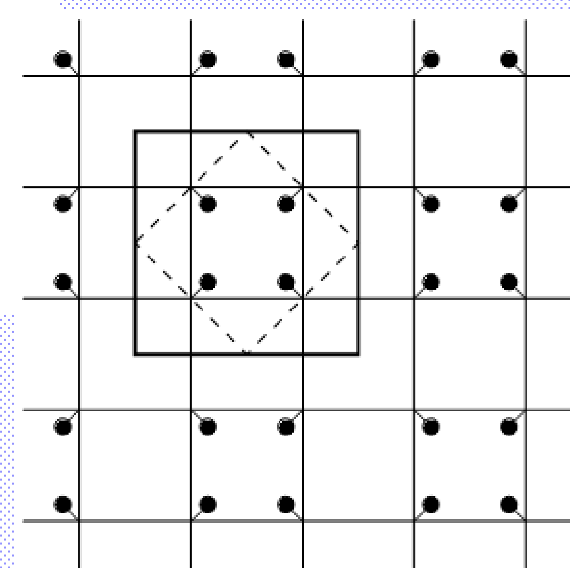
$$\lambda(\omega) = 2\int_0^{\omega} d\Omega \alpha^2 F(\Omega)/\Omega$$

Not sufficient to explain SC

El-ph interaction enhanced due to nesting

H. Eschrig, arXiv:0804.0186v2





DOS as a function of **Fe** breathing phonon mode displacement